LIQUID CRYSTAL DIFRACTIVE OPTICAL ELEMENTS:
APPLICATIONS AND LIMITATIONS

A dissertation submitted
to Kent State University in partial
fulfillment of the requirements for the
degree of Doctor of Philosophy

by

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June 2005
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ACKNOWLEDGEMENTS

This work is dedicated to my wife Ming Cen and my family. Without their support, it would be impossible for me to finish.

I especially would like to express my appreciation for my advisor Dr. Phil Bos. He’s knowledge and passion in science always inspired me and had been a strong motivation for me to exploit new knowledge. Without him, I would not be able to finish this work. I would also like to thank Dr John West, Dr Peter Palffy-Muhoray, Dr Denke Yang, for the guidance and advice during the time I spend in their labs; and Dr Oleg Lavrentovich, Dr L.-C. Chen, Dr Sergij Shiyanovskii, Dr Antal Jakli, Eugene Gartland and all CPIP faculty members who passed on precious knowledge to me. I would like to thank the committee members to participate for my defense and share their valuable insights.

I would also like to express my appreciation for Vassili Sergen, Mike Fisch, Bin Wang, James Anderson, John Ruth, Merrill Groom, Doug Bryant, Ivan Smalyukh, Chenhui Wang, Wenyi Cao etc. who have helped me kindly in numerous cases during my research and all LCI staff and CPIP students for all their help during this work.

I would also like to appreciate DARPA THOR, STAB project and NASA space communication project for funding this research.
Chapter 1

Introduction

1.1 Introduction to the liquid crystal material

The liquid crystal material is a fascinating material discovered first by Reinitzer\(^1\) in 1888 and Lehmann\(^2\) in 1890. Its unique properties and physics attracted scientific interest in a variety of field since then. However, it is not until the demonstration of the first practical liquid crystal electro-optic device in 1968\(^3\), that liquid crystal related research becomes explosive and heavily perused. It the race of discovering new applications, a most widely spread technology and fastest growing industry of liquid crystal displays become a reality. Nowadays, liquid crystal technology has a broad influence in many areas of science and engineering including information display, optical science and engineering, material science, medicine and biology, astronomy, telecommunication, chemistry etc. Yet many new areas, such as photonic liquid crystal, nano-liquid crystal, liquid crystal in biology and medicine, liquid crystal for optical metrology and instrumentation etc. are still awaiting discovery.

One of the reasons that liquid crystal materials have many unique properties is related to the geometry of the liquid crystal molecule. It can be elongated, disk-like or banana shape etc., that breaks the symmetry in space. It also has the tendency of pointing along a common direction to minimize the free energy in the system. This preferred direction of alignment is called the liquid crystal director \( \hat{n} \) and is an average of the alignment direction of liquid crystal molecule in space. The physical properties of liquid
crystal material along the director orientation direction and perpendicular direction is very different. This leads to many unique properties such as dielectric anisotropy, birefringence, ferroelectricity, flexoelectricity, nonlinear effect etc \(^4\).

1.2 Liquid crystal diffractive optical element

The combination of responding to external field and having optical anisotropy makes liquid crystal material very attractive for electro-optical application. One of the most important applications of such electro-optical modulation device is the liquid crystal flat panel display. We will not go into details about liquid crystal display, for more information, a very good introduction to the liquid crystal displays can be found in Ref \(^5\).

Another important application is phase modulation of light for optical computing, laser beam shaping, laser beam steering, high resolution aberration control, optical tweezers, digital holography, active interferometer etc. Such a device is very similar to a conventional liquid crystal display in a sense both pixelized device is required and each individual pixel can be controlled independently. Such a device that can modulate the phase of the light spatially is called a Liquid Crystal (LC) Spatial Light Modulator (SLM). However, there are some important difference between a liquid crystal display and a SLM. First, a typical liquid crystal display uses Twist Nematic (TN) mode or Super Twist Nematic (STN) mode to achieve amplitude modulation of light. Although the main purpose of such device is for amplitude modulation, the phase of light passing through each pixel is coupled with the amplitude modulation. For some applications like digital holography, such coupling is not desirable. In a LC SLM, an Electronic Controlled Birefringence (ECB) mode is used. Such device only modulates the phase of light
without changing the intensity of light. Second, for many applications, the pixel size of a LC SLM is desired to be close to the wavelength of light and diffraction effect is utilized to achieve different purpose. This is different in a liquid crystal display where diffraction effect is not desirable in most cases. Third, the inter-pixel gap between adjacent pixels in a liquid crystal display is relatively large. The filling factor of the usable aperture is normally on the order of 50%~70%. For a LC SLM, this low filling factor will cause strong diffraction loss, and should be reduced as much as possible. Otherwise, the performance of a LC SLM will be very poor. Fourth, for phase modulation of light, large Optical Path Difference (OPD) change is required. For example, if a device is operating at MWIR region, the OPD change of the device needs to be several micrometer to achieve one wave of phase retardation. However, many applications required tens and hundreds of waves of phase retardation, such as wide angle beam steering, aberration correction in large optics etc. This will require the cell thickness of the liquid crystal device to be impractically large. To address this issues in monochromatic scheme, the phase modulation depth of a LC SLM is limited to one wave, and any required phase modulation is generated with a modulo $2\pi$ version of the desired phase modulation. So the device becomes a programmable Diffractive Optical Element (DOE) or programmable diffractive phase plate $^6$.

Such a programmable DOE have many applications in aerospace, defense, communication, optical instrumentation, optical metrology etc. because of its low cost, easy to manufacture, high resolution, accurate phase modulation, low power consumption etc.
1.3 Applications of liquid crystal diffractive optical element

One of the most important applications of LC DOE is for long distance free space laser communication. In both the laser transmitter and receiver, an active beam control device is required to control the beam pointing, target tracking, beam shaping, as well as aberration control for large primary optics. In a conventional system, the beam pointing is achieved by mechanically rotate a telescope mounted on a gimble system; the focusing and defocusing is achieved by mechanically adjust the position of lens; and wavefront control is achieved by deform the surface shape of a deformable mirror with actuators behind such deformable mirror. Such a mechanical system involves very complicated mechanical motions, which make the total system very heavy, bulky, expensive and consumes lots of power. The inertia, stability, accuracy, and speed of such a system is of serious concern. There are many desirable capabilities for example, multiple beam control, high-resolution aberration correction, random access beam pointing etc. that a mechanical system could not offer. However, a 1-D LC DOE with line shape electrodes, which is normally called Optical Phased Array (OPA)\textsuperscript{7,8} can address these issues by modulating the laser beam with a calculated phase plate, to simultaneously achieve wide angle beam steering, very fine beam steering, dynamic focusing of the beam, multiple beam control in a non-mechanical fashion. It can be inertia free, inexpensive, light-weight, small size, low power consumption etc. It also enables many new concepts such as combined Radio Frequency/Electro-Optical antenna\textsuperscript{9}, and Phased Array of Phased Array\textsuperscript{9,10}. This made a liquid crystal diffractive optical element very attractive for this application.
In a long distance laser communication transmitter/receiver, the aperture of the primary mirror needs to be very large to maintain a small beam divergence. However, a diffraction limited meter scale telescope is too heavy and expensive for a laser communication system. People proposed to use a membrane type material to make a large telescope\textsuperscript{11}. However, such membrane type of mirror can introduce severe aberration to the optical system. A LC SLM can be used to correct for such aberration introduced by the primary optical element and thus restoring the performance of the telescope. Similar applications that use a liquid crystal device to correct for aberration in retina imaging system\textsuperscript{12}, bio imaging system\textsuperscript{13} etc has great potential to extend the current capability of adaptive optics system.

The same LC SLM can be used for opto-electronic reconstruction of digitally recorded hologram for 3-D display system\textsuperscript{14}. In principle, a digital camera is used to record the hologram like in a conventional holography recording system. Then the captured digital holography can be subsequently transferred to the SLM. An illumination source will illuminate the LC SLM and reconstruct the virtual image of the recorded object. For this application, the LC SLM is replacing the conventional holographic film to the 3-D image reconstruction. Since the LC SLM is electronically addressable, such a system can display 3-D movie instead of a static 3-D image.

Utilizing similar concepts, if a laser is phase modulated with a pre-calculated phase plate, and focused subsequently. One could design the modulation pattern to generate any random intensity distribution at the focus, because the intensity distribution at the focus of a thin lens is approximately the spatial Fourier transform of the phase
distribution on the LC SLM plane. One can use a LC SLM to generate laser trap or laser tweezer to trap small particles that are normally hard to manipulate.

Another application is a variable period LC binary grating for wide angle beam steering and grating interferometer. In this case, the LC device is addressed by line shape electrodes with line spacing close to or smaller than the wavelength of light. By controlling the voltage applied to each line shape electrodes, the periodicity of the resulting LC binary grating can be changed. For monochromatic light, the laser beam can be diffracted to different angles. If the device is used in white light operation such as in a hyperspectral remote sensing system, changing the periodicity of the grating can change the sensitive wavelength of grating interferometer, thus tune the interested spectral for imaging purpose. For wide angle beam steering application, this LC binary grating may have higher efficiency than a LC blazed grating discussed in later chapters.

1.4 Computer simulation in studying LC DOE and optical system

For the above mentioned LC DOEs and their applications, it is very important to understand the performance of the device and how to optimize the system performance. In this work, extensive simulation and modeling is performed to study the physics behind each system as well as the limitation of each approach. However, the author is not focused on the modeling algorithm but using such tools to study LC binary grating, blazed grating, fringing electric field in high resolution LC DOEs and their optical properties. In this work, the main simulation software used is OPASIMU 2.0 software package, which contains of two major parts. The first part is a 3-D LC director simulation package based on modified LC3D equilibrium director calculation core routine written
by James E. Anderson. The LC director configuration, LC DOE phase profile is all modeled with this core routine. The second part is the Finite Difference Time Domain (FDTD) simulation package written by Bin Wang. The wave optics simulation of light propagation in a LC DOE is calculated by this FDTD simulation. Another software that are used to do ray tracing and diffractive beam propagation is the CODE V optical system design software. Aberration correction in large aperture telescope using LC DOE is studied with this software.

These simulations provided many insights that otherwise would not be possible regarding the design and performance issues of LC DOE, and it a very important part of this work.

1.4 The structure of the dissertation

A total of six chapters are included in this work. The first chapter is the introduction that illustrates the background and focus of the work.

Chapter Two includes a brief introduction and review of the simulation software used in this work. This includes the basic principles of 3-D director simulation software, the detailed arrangements of the director simulation, the basic principles of the FDTD simulation, the computation grid and the absorbing boundary of the FDTD simulation, the detailed arrangements of the FDTD simulation and experimental verification of the accuracy of this whole simulation software package. The CODE V ray tracing software is a commercially available software, we will not describe too much of the details regarding the ray tracing algorithm. So this part will be introduced in Chapter Five for consistency.
Chapter Three will describe the main performance limitation of the LC blazed grating for laser beam steering. Fringing electric field in a high resolution LC DOE is studied in full detail. Potential ways to alleviate the fringing field effect to achieve wide angle beam steering at high efficiency is discussed.

Chapter Four will focus on using LC SLM to achieve high resolution aberration control in large aperture optics. This includes the characterization of response and uniformity of a LC SLM, the measurement of aberration in optical system with interferometry technique, and the performance valuation of our Liquid Crystal On Silicon (LCOS) SLM for beam steering and aberration control in large telescope. CODE V ray tracing study to understand the performance limitation of correction for very large aberration in high numerical aperture telescope system is discussed.

Chapter Five will focus on LC binary gratings for wide angle beam steering and the study of LC SLM for digital holography. Fringing electric field problem in a LC binary grating will be discussed, and an discovery of a highly non-symmetrical diffraction behavior of a wide angle variable period LC binary grating will be introduced.
Chapter 2

Modeling of Liquid Crystal Diffractive Optical Element

2.1 Introduction to 3-D director simulation

To simulate the LC DOE device, the first step is to determine the equilibrium LC director configuration, thus obtain the phase profile of the LC DOE. The overall approach is to express the free energy in the system, and by minimizing the total free energy in the system, the equilibrium LC director configuration can be obtained. There are two methods to represent the elastic energy in the system, one is the vector method $^{19,20,21}$ and the other one is the Q tensor method $^{22,23}$. A comparison of these two methods is discussed in Ref $^{24}$

For the first method, the contribution to the free energy of the liquid crystal ‘director’ $\hat{n}$ is considered, which is the average orientation of the LC molecules in a small domain. According to continuum theory developed by Oseen $^{25}$, Zocher $^{26}$ and Frank $^{27}$, when the system is free of point defects or line defects (like the liquid crystal diffractive optical elements we use in this work), the LC director varies slowly and smoothly in space. The deformation to the LC director can be described by a continuous director field disregarding the details of the structure on the molecular scale. The free energy density associated with such distortion to the director field can be expressed as Frank-Oseen free energy density.

$$ f_d = \frac{1}{2} K_{11} (\nabla \cdot \hat{n})^2 + \frac{1}{2} K_{22} (\hat{n} \cdot \nabla \times \hat{n} + q_0)^2 + \frac{1}{2} K_{33} (\hat{n} \times \nabla \times \hat{n})^2 \quad (2.1) $$
Here $f_d$ is the Frank-Oseen free energy density, $K_{11}, K_{22},$ and $K_{33}$ are the splay, twist and bend elastic constants. $\hat{n}$ is the unit vector director of liquid crystal. $q_0$ is the intrinsic chiral wave number for cholesteric liquid crystal materials. It specifies the equilibrium twisting power of the helical structure and is the related to the intrinsic pitch $P_0$ of cholesteric LC material as $q_0=2\pi/P_0^{28}$.

When an external electric field $\vec{E}_0$ is present in an ideal dielectric media, the induced dipole is $\vec{P}$. The electric free energy density $f_e$ can be written in terms of the electric displacement, $\vec{D}$, as in Equ. 2.2:

$$f_e = -\frac{1}{2} \vec{p} : \vec{E}_0 = -\frac{1}{2} \left( \vec{p}_\parallel : \vec{E}_0 + \vec{p}_\perp : \vec{E}_0 \right)$$

$$= -\frac{1}{2} \vec{E}_0 (\vec{p}_\parallel \cos \theta + \vec{p}_\perp \sin \theta)$$

$$= -\frac{1}{2} \vec{E}_0 E_0 (\chi_\parallel \cos^2 \theta + \chi_\perp \sin^2 \theta)$$

$$= -\frac{1}{2} \vec{E}_0 E_0 (\epsilon_\parallel \cos^2 \theta + \epsilon_\perp \sin^2 \theta - 1)$$

$$= -\frac{1}{2} \vec{E}_0 E_0 (\epsilon_\parallel \cos^2 \theta + \epsilon_\perp \sin^2 \theta - 1)$$

$$= -\frac{1}{2} \vec{E}_0 E_0 (\epsilon_\parallel \cos^2 \theta + \epsilon_\perp \sin^2 \theta - 1)$$

$$= -\frac{1}{2} \vec{E}_0 E_0 (\epsilon_\parallel \cos^2 \theta + \epsilon_\perp \sin^2 \theta - 1)$$

$$= -\frac{1}{2} \vec{E}_0 D + \frac{1}{2} \vec{E}_0 E_0$$

Here, $\theta$ is the angle between the electric field and the liquid crystal director, $\chi$ is the susceptibility, $\overline{\epsilon}$ is the average dielectric constant of the liquid crystal. $\parallel$ and $\perp$ denote the component parallel or perpendicular to the liquid crystal director. We now have two cases: fixed charge and fixed potential. For fixed charge, the displacement
doesn’t change, so $\bar{D} = \bar{D}_0$. We therefore rewrite $f_e$ completely in terms of the displacement, as in Equ. 2.3:

$$f_e|_q = -\frac{1}{2} E_0 D_0 + \frac{1}{2} E_0 E e_0$$

(2.3)

Note that the first term is not affected by the director orientation and will not contribute a torque; therefore it can be dropped:

$$f_e|_q = +\frac{1}{2} E_0 E e_0 = +\frac{1}{2} D_0 \cdot E \quad \text{or} \quad f_e|_q = +\frac{1}{2} \bar{D} \cdot \bar{E}$$

(2.4)

For the constant voltage case, we consider the second term in Equ(). If we consider the contribution of this term to the total free energy, $F_e = \int f_e dv$, we find

$$\frac{1}{2} E_0 e_0 \int Edl = \frac{1}{2} E_0 e_0 V$$

so this term is also a constant which can be dropped. In this case,

$$f_e|_V = -\frac{1}{2} \bar{D} \cdot \bar{E}$$

(2.5)

For various historical reasons, the constant charge case ($+\frac{1}{2} \bar{D} \cdot \bar{E}$) is called the “Helmholtz” free energy, and the constant potential case ($-\frac{1}{2} \bar{D} \cdot \bar{E}$) is called the “Gibbs” free energy. In our method, we will minimize the free energy with respect to $n_x$, $n_y$, and $n_z$ for a fixed voltage $V$. We will separately find the value of $V(x,y,z)$ that satisfied $\nabla \cdot \bar{D} = 0$. In this approach, it is appropriate to use the electric free energy expression for constant voltage.
Combine the elastic free energy and electric free energy in the system, the total free energy in the system is expressed in Equ. 2.6,

$$F = \int f_g dv = \int \left( \frac{1}{2} K_{11} (\nabla \cdot \hat{n})^2 + \frac{1}{2} K_{22} (\hat{n} \cdot \nabla \times \hat{n} + q_0)^2 + \frac{1}{2} K_{33} (\hat{n} \times \nabla \times \hat{n})^2 - \frac{1}{2} (\hat{D} \cdot \hat{E}) \right) dv \quad (2.6)$$

Here F is the total free energy, $f_g$ is the total free energy density, $D(x,y,z)$ is the electric field displacement and $E(x,y,z)$ is the electric field, the sign of the electric free energy depends on whether it is a constant voltage case or constant charge case. For our modeling, we always consider a constant voltage case so the sign is “-”. We can see the minimum total free energy state may not correspond to a uniform director alignment, but depends on the electric field distribution.

This method does not taking into account the free energy associated with local order parameter change, when the director field has strong distortion close the defect core. It is impossible to model the transition between two topologically indistinct director configurations $^{25,26}$.

For the second method, the Q tensor method, the free energy is expressed in a Q tensor representation, as in Equ. 2.7, where not only the liquid crystal director is taking into consideration, but also the order parameter S. A detailed description of this method is shown in Ref$^{27}$.

$$Q_{jk} = \frac{S}{2} (3n_j n_k - \delta_{jk}) \quad (2.7)$$
This method is very suitable for modeling of the director configuration and energy around the defect core where the director field has strong variations and the local order parameter may vary. It is possible to model the transition between two topologically distinct states because the Q tensor always incorporates the multiplication of two directors $\hat{n}$. This means the sign of the director is always cancelled out even when finite differences for the spatial derivatives are considered. The temperature dependence of the free energy is fully taking into account because the change of the order parameter as function of the temperature is considered. Unlike in the first case, the temperature dependence of the free energy is only reflected in the temperature dependence of elastic constants (elastic constant is a function of order parameter). In principle, the Q tensor method will give very accurate results regarding a 2D or 3D direction configuration, but it takes a much finer grid resolution and longer computation time.

Comparing the two methods, the vector method is mathematically simpler, computationally faster and requires fewer grid points to obtain accurate results. For the liquid crystal diffractive optical element we are interested in, the system does not have any temperature gradient across the device, and the normal operation of the device is at temperature far way from the clearing temperature $T_{c}$ of the liquid crystal material. In this case, the contribution of the order parameter to the free energy of the system is several orders larger than that of the liquid crystal director, and it can be treated as a large constant, which does not have any spatial variation with respect to the electric field. In another word, it will not influence our calculation results for the system we are interested in. Also, there are no defects in any of the liquid crystal diffractive optical element for
our interest, nor is there any transition between topologically inequivalent states during operation. Thus, the vector method is a better choice for studying the system we are interested in.

2.2 Review of modeling algorithm

To obtain the equilibrium director configuration with vector method, one needs to minimize the total free energy as in Equ. 2.6 and find out the director configuration that corresponds to the minimum total free energy state. Following Berreman’s derivation\(^{27}\), solving the minimization problem in Equ. 2.6, is mathematically equivalent to solve the Euler-Lagrange equation in Equ. 2.8 (following derivation of D.W. Berreman\(^{27}\)), with proper boundary condition. (This is an analogy to solving an one dimensional scalar minimization problem by considering the derivative of the function is zero, but only in this case, we are talking about multi-dimensional vector problem.)

\[
-\left[f_g\right]_{n_i} = 0 \quad \text{i=x, y, z} \quad (2.8)
\]

Where

\[
\left[f_g\right]_{n_i} = \frac{\partial f_g}{\partial n_i} - \sum_{j=x, y, z} \frac{d}{dj} \left[ \frac{\partial f_g}{\partial (\frac{dn_i}{dj})} \right] \quad (2.9)
\]
To solve Eqn. 2.8, we use a time relaxation method, where we add a Rayleigh dissipation function (Goldstein) which value is zero at equilibrium state to both side of the Eqn. 2.8.

\[-[f_g]_{n_i} + \frac{\partial F_d}{\partial \dot{n}_i} = 0 \quad \text{i=x, y, z} \tag{2.10}\]

Where the dot denotes differentiation with respect to time. The Rayleigh dissipation function takes the form of

\[F_d = \frac{1}{2} \gamma_1 \left(\dot{n}_x^2 + \dot{n}_y^2 + \dot{n}_z^2\right) \tag{2.11}\]

where \(\gamma_1\) is the rotational viscosity. Combine Eqn. 2.10 and Eqn. 2.11, and work out the differentiation with respect to time, we get

\[\frac{\partial F_d}{\partial \dot{n}_i} = -[f_g]_{n_i}\]

\[\Leftrightarrow \frac{\partial}{\partial \dot{n}_i} \left[\frac{1}{2} \gamma_1 \dot{n}_i^2\right] = -[f_g]_{n_i} \tag{2.12}\]

\[\Leftrightarrow \gamma_1 \frac{\partial n_i}{\partial t} = -[f_g]_{n_i}\]

If we discretize the left size with finite difference, then Eqn. 2.12 hold true when the time step \(\Delta t \to 0\).
\[
\gamma_1 \frac{n_i^{t+1} - n_i^t}{\Delta t} = -\left[ f_g \right]_{n_i} \tag{2.13}
\]

Rewrite the equation in a different way, we can obtain the updating rule for time relaxation of the director configuration in the computation grid.

\[
n_i^{t+1} \bigg|_{\text{BeforeNorm}} = n_i^t - \frac{\Delta t}{\gamma_1} \left[ f_g \right]_{n_i}, \quad i = x, y, z \tag{2.14}
\]

Here \( n_i^{t+1} \bigg|_{\text{BeforeNorm}} \) is the \( i \)th component of the director at time step \( t+1 \) before normalized, and \( n_i^t \) is the \( i \)th component of the director at time step \( t \), \( \Delta t \) is the time interval, \( \gamma_1 \) is the rotational viscosity of liquid crystal material, \( \left[ f_g \right]_{n_i} \) is the functional derivative of the free energy.

The boundary condition associated with the problem is fully described in Ref.\textsuperscript{17}, such will not be illustrated here.

Another constraint needs to apply is that a unit length of the director needs to be maintained during the time relaxation, where \( |\hat{n}| = 1 \) \textsuperscript{24,25}, this constraint is achieved in the program by renormalizing the director after each relaxation step as in Equ. 2.15

\[
n_i^{t+1} = \frac{n_i^{t+1} \bigg|_{\text{BeforeNorm}}}{\sqrt{(n_x^{t+1} \bigg|_{\text{BeforeNorm}})^2 + (n_y^{t+1} \bigg|_{\text{BeforeNorm}})^2 + (n_z^{t+1} \bigg|_{\text{BeforeNorm}})^2}} \tag{2.15}
\]

However, this means we are not directly solving the exact Euler-Lagrange equation. Under condition that the time step \( \Delta t \) is infinitesimally small, this method is
accurate and the accuracy of this method has been verified by numerous studies by many researchers.

To obtain the functional derivative in Equ. 2.14, one needs to determine the electric field distribution across the computation grid. Because the liquid crystal materials have an anisotropic dielectric constant, the electric field distribution in a LC cell depends on the LC director configuration. The electric field distribution in the LC cell is obtained by discretizing and numerically solving the Laplace’s equation in (2.16)

$$\nabla \cdot \vec{D} = 0$$  

(2.16)

Here $\vec{D}$ is the electric field displacement. For more details regarding the detailed numerical implementation, please see Ref\textsuperscript{17}.

The dielectric tensor the liquid crystal material can be written as:

$$\varepsilon(x,y,z) = \begin{bmatrix} \varepsilon_{xx}(x,y,z) & \varepsilon_{xy}(x,y,z) & \varepsilon_{xz}(x,y,z) \\ \varepsilon_{yx}(x,y,z) & \varepsilon_{yy}(x,y,z) & \varepsilon_{yz}(x,y,z) \\ \varepsilon_{zx}(x,y,z) & \varepsilon_{zy}(x,y,z) & \varepsilon_{zz}(x,y,z) \end{bmatrix}$$  

(2.17)

For a uniaxial nematic media we are interested in, the dielectric tensor is just:

$$\varepsilon_{xx} = \varepsilon_{\perp} + (\varepsilon_{||} - \varepsilon_{\perp}) \cos^2 \theta \cos^2 \phi = \varepsilon_{\perp} + \Delta \varepsilon n_x^2$$

$$\varepsilon_{xy} = \varepsilon_{yx} = (\varepsilon_{||} - \varepsilon_{\perp}) \cos^2 \theta \sin \phi \cos \phi = \Delta \varepsilon n_y$$

$$\varepsilon_{xz} = \varepsilon_{zx} = (\varepsilon_{||} - \varepsilon_{\perp}) \sin \theta \cos \theta \cos \phi = \Delta \varepsilon n_z$$

$$\varepsilon_{yy} = \varepsilon_{\perp} + (\varepsilon_{||} - \varepsilon_{\perp}) \cos^2 \theta \sin^2 \phi = \varepsilon_{\perp} + \Delta \varepsilon n_y^2$$

$$\varepsilon_{yz} = \varepsilon_{zy} = (\varepsilon_{||} - \varepsilon_{\perp}) \sin \theta \cos \theta \sin \phi = \Delta \varepsilon n_z$$

$$\varepsilon_{zz} = \varepsilon_{\perp} + (\varepsilon_{||} - \varepsilon_{\perp}) \sin^2 \theta = \varepsilon_{\perp} + \Delta \varepsilon n_z^2$$  

(2.18)
Here $\varepsilon_{||}$ is the dielectric constant along the long axis of the liquid crystal director and $\varepsilon_{\perp}$ is the dielectric constant along the short axis of the liquid crystal director. $(\theta, \phi)$ is the polar angle and the azimuthal angle of the liquid crystal director.

The electric field in the spatially varying dielectric media is:

$$E(x, y, z) = \begin{pmatrix} \frac{\partial V(x, y, z)}{\partial x}, & \frac{\partial V(x, y, z)}{\partial y}, & \frac{\partial V(x, y, z)}{\partial z} \end{pmatrix}$$  \hspace{1cm} (2.19)$$

To solve Equ. 2.16, we can discretize the equation as shown in Appendix A in the “Voltage.mws” maple script. Once the voltage distribution in the computation grid is determined, the electric free energy can be computed as in the attachment in Appendix A “Feni.mws”.

The functional derivatives of the elastic free energy can be computed to obtain the updated director configuration as in Equ. 2.14 and 2.15. The detailed derivation and discretization in very complicated due to the fact we need to solve a particle differential equation in 3-D space with full vector representation. The details of the implementation is shown in Appendix A “vectorenergy.mws”, where the derivation, discretization and some sample codes are all shown. The full numerical implementation of the 3-D director modeling is also shown in Appendix E.
2.3 Implementation example in 2-D case

As an example of our simulation, Fig. 1 shows the simulated director configuration of a LC Optical Phased Array (OPA) with eight level stair like blazed grating configuration. The eight electrode corresponds to the eight level is arranged in the computation grid in a way that the first electrode is split in half, the first half is at the beginning of the grid and the second half is placed at the end of the grid. Periodical boundary condition is used to terminate the computational grid along X axis. Along Y axis, the computational grid has five layer. From the top to the bottom, each layer is glass substrace, alignment layer, liquid crystal layer, alignment layer and glass substrace again. The Indium Tin Oxide (ITO) transparent conductor is located in the alignment layer which is 100 nm thick and a dielectric constant of $\varepsilon = 4.5\varepsilon_0$. the interface of the liquid crystal layer and glass substrace.

A liquid crystal material with elastic constant $K_{11} = 14.1 \times 10^{-12}$ N, $K_{22} = 7.1 \times 10^{-12}$ N, $K_{33} = 19.1 \times 10^{-12}$ N, dielectric constant $\varepsilon_\parallel = 12.1$, $\varepsilon_\perp = 4.1$, refractive index $n_\parallel = 1.5035$, $n_\perp = 1.6742$ is used. The cell thickness of the LC OPA is $d = 4.0$ µm. The geometry of the electrode is defined as the pixel spacing is 19.4 µm with a gap between electrodes of 0.4 µm. The top and bottom substrate is assumed to have anti-parallel rubbing with a pretilt angle of 3°. The device is then an Electronic Controlled Birefringence (ECB) device with director within XZ plane.

If we integrate the optical path length of the extra-ordinary light along the cell thickness direction (Fig. 1), the phase profile of such LC DOE can be obtained as shown in Fig. 2. From the phase profile of the DOE, the performance of the device can be
estimated. In later chapters, we will discuss more details of the relationship between the configuration of the LC OPA and the performance of the device. The electric field distribution within the LC OPA can also be obtained. This is shown in Fig. 3 as the isopotential lines in a LC OPA.
Fig. 1: Director configuration of an ECB LC OPA in an eight level stair like blazed grating configuration. (Operation wavelength of the device is 632.8 nm) $K_{11}=14.1\times 10^{-12}$ N, $K_{22}=7.1\times 10^{-12}$ N, $K_{33}=19.1\times 10^{-12}$ N, $\varepsilon_\parallel=12.1$, $\varepsilon_\perp=4.1$, $n_o=1.5035$, $n_e=1.6742$. Cell thickness $d=4.0 \mu$m, pixel spacing $=19.4 \mu$m, gap between electrode$=0.4 \mu$m, pretilt$=3^\circ$. 
Fig. 2: The corresponding phase profile of the director configuration as in Fig. 1. The straight line in the figure is the ideal phase profile of an eight level stair like blazed grating; the smooth line is the simulated phase profile of the LC OPA. (Operation wavelength of the device is 632.8 nm)
Fig. 3: The electric field distribution in the LC OPA as in Fig. 1. The lines are the isopotential lines in the LC OPA with a voltage difference of 0.1v for each adjacent line. (Operation wavelength of the device is 632.8 nm)
2.5 Review of the Finite Difference Time Domain simulation algorithm and detailed implementation examples

2.5.1 Introduction to the Finite Difference Time Domain (FDTD) simulation

Optical simulation of polarized light propagation in birefringence media is usually achieved by matrix-type methods based on the stratified-medium approach, such as 2x2 Jones method 29, Extended Jones’ matrix 30 and Berreman 4x4 method 31. However, these methods are not applicable to study the diffractive properties of LC structures with spatially inhomogeneous materials and complicated dielectric distribution in 3-D space. More general methods for solving the electromagnetic wave propagation in inhomogeneous birefringent media has to be engaged for our purpose. An excellent candidate is the Finite-Difference Time Domain method (FDTD) introduced by Yee 32.

The FDTD method is a direct numerical solution to Maxwell equations. By direct discretization of both the spatial and temporal derivatives of the complex vector fields, and the Maxwell equation is solved in a time relaxation fashion. Since no other assumptions or simplifications are made in this method, it can accommodate multidimensional inhomogeneity of the dielectric tensor, it is capable of very accurately modeling of many optical systems with complicated media that has feature size compatible with the wavelength of light. Diffraction effect in this case is non-neglectable. It is one of the most robust and accurate wave optics simulation methods that has been used to study a wide variety of problem’s like microwave antenna system, fast semiconductor chip design, photonic circuits. This includes several studies of liquid crystal system using FDTD method 33, 34, 35, 36, 37, 38. The FDTD algorithm used in this
work is a 2-D TE\textsubscript{z} mode FDTD simulation based on the Allen Taflove’s book\textsuperscript{39}. Some derivation and algorithm has been reviewed in Appendix A.

As an example of the FDTD simulation for light propagation in a LC OPA, a reflective LC OPA with 24 pixels is considered. The pixel spacing of the LC OPA is 19.4 µm, and an eight electrode/reset configuration is considered. The light source is located at 2 µm below the LC OPA. An input Guassian beam is turned on at t=0 time and when the first wave the light reaches the metal mirror on top of the LC OPA, the light source is turned off. The light is reflected by the metal mirror on the device and is reflected back to the light source. The near field electric field distribution E\textsubscript{z} at final time step is shown in Fig. 4. In this example, the input plane wave has bee steered to a steering angle of 4.07 mrad with about 87% of efficiency.

The near field phase and intensity of the light is collected and the far field diffraction pattern is calculated. The details regarding the method used in the near field to far field transformation is discussed in Appendix A. The calculated far field diffraction pattern is shown in Fig. 5.
Fig. 4: Near field electric field intensity distribution at final time step ($t=6.59 \times 10^{-14}$ s) of a Gaussian beam propagated through a reflective liquid crystal blazed grating as in Fig. 1. $\lambda=632.8$ nm, grid spacing $\Delta x=\Delta y=1/20 \lambda$, $\Delta t=\Delta x/2c$, $c$ is the speed of light. Input beam with $1/e^2$ diameter=$140 \mu$m.
Fig. 5: Far field diffraction peak simulated by near field to far field transformation. The upper figure is the magnified view of the 1\textsuperscript{st} order diffraction peak. (\(\lambda=632.8\) nm)
2.6 Accuracy of the LC director simulation and FDTD simulation for simulating LC DOE

It is always important to know the accuracy of the simulation software before more analyze work has been carried out. Both of these software packages have gone through scrutiny by our group members and have been tested to be accurate for numerous times for different cases. However, when simulating a LC DOE’s where the pixel size of the device is close to the wavelength of light, the accuracy of the simulation software hasn’t been compared with experimental results due to the difficulty in fabricating a test device to verify the accuracy. In this section, we will show a comparison of simulation results with experimental results and results from an empirical model to verify the accuracy of the simulation. These results have been published, and please see Ref 40 for more details.

In this comparison, a LCOS device made by Hana Microdisplay Technology Inc. is used in the experiment. The liquid crystal material and the LCOS device specification is given in Table 1. For more information regarding the performance of the device, please see Ref 41, 42. A stair like blazed phase profile similar to what is shown in Fig. 2 is written on the device to steer a laser beam to 0~12 mrad range. The diffraction efficiency of such a blazed grating is measured for each steering angle. The detailed experimental process is quite complicated and we will discuss more in Chapter 4.
Table 1: Specification of the test LC DOE based on ECB LCOS device

<table>
<thead>
<tr>
<th>Manufacture:</th>
<th>Hana Microdisplay Technology Inc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid Crystal Material</td>
<td></td>
</tr>
<tr>
<td>$K_{11}$</td>
<td>$14.1 \times 10^{-12}$ N</td>
</tr>
<tr>
<td>$K_{22}$</td>
<td>$7.1 \times 10^{-12}$ N</td>
</tr>
<tr>
<td>$K_{33}$</td>
<td>$19.1 \times 10^{-12}$</td>
</tr>
<tr>
<td>$\epsilon_{\parallel}$</td>
<td>12.1</td>
</tr>
<tr>
<td>$\epsilon_{\perp}$</td>
<td>4.1</td>
</tr>
<tr>
<td>$n_o$</td>
<td>1.5035</td>
</tr>
<tr>
<td>$n_e$</td>
<td>1.6742</td>
</tr>
<tr>
<td>Liquid Crystal Cell Type</td>
<td>Reflective Electric Controlled Birefringence (ECB)</td>
</tr>
<tr>
<td>Temporal bandwidth</td>
<td>50Hz</td>
</tr>
<tr>
<td>Cell Thickness</td>
<td>4 $\mu$m</td>
</tr>
<tr>
<td>Pixel Size</td>
<td>19.0 $\mu$m</td>
</tr>
<tr>
<td>Inter Pixel Gap</td>
<td>0.4$\mu$m</td>
</tr>
<tr>
<td>Resolution</td>
<td>1024*768</td>
</tr>
<tr>
<td>Aperture</td>
<td>20mm*15mm</td>
</tr>
<tr>
<td>Maximum Non-uniformity</td>
<td>23 nm</td>
</tr>
<tr>
<td>Maximum retardation value observed with the current LCOS driver</td>
<td>700 nm (measured at 632.8nm)</td>
</tr>
</tbody>
</table>

The simulation of the performance of such device is carried out. First, the LC direction configuration is performed. To determine the direction configuration, the voltage applied to each pixel of the device has to be calculated first.
Fig. 6: Electro-Optical response of the LCOS device and the voltage phase pair for each of the eight electrodes. (For $\lambda=632.8$ nm)
This is achieved by calculating the voltage vs. phase curve (or Electro-Optical response curve) of the device with a 1-D direction configuration simulation program. The simulated Electro-Optical curve in shown in the solid line in Fig. 6. Because the simulation program is only a 1-D program, the electrode along the width and length direction of the cell is assumed to be infinitely large, thus the fringing electric fields in the device is neglected. Since the size of the array element is relatively larger of close to 20 µm, the neglecting the fringing field effect is justified. (We will discuss more details related to the fringing electric field problem in Chapter 3.) The required voltage to produce an eight level stair like blazed grating phase profile can be obtain from the E-O response curve. Such voltage-phase pair determined this method is shown as the 8 data points in Fig. 6. The director configuration of such blazed grating is shown in Fig. 1 and the phase profile of the blazed grating is shown in Fig. 2. The obtained director configuration is input into the FDTD simulation program to simulate the near field propagation.

In the FDTD simulation program, the light source, LC OPA is placed in the main computational grid. To be noticed, since the test device we have been using is a reflective LCOS device, in the FDTD simulation, a layer of ideal metal reflector is placed on top of the LCOS device to simulate a reflective device. However, the difference between experiments and simulation is that in the simulation, a continuous mirror is used in the simulation instead of a segmented mirror. This is to isolate the effect of diffraction loss from the segmented mirror and that of liquid crystal phase profile. A single layer Anti-Reflection coating is also used to reduce the front surface reflection of the LC OPA. The
refractive index of the single layer AR coating is chosen to be \( n_{air} = \sqrt{n_{glass} n_{air}} \), where
\( n_{glass} = n_{e,LC} \) and the thickness of the AR coating is \( \lambda / (4n_{air}) \). A plane wave with Guassian intensity distribution is propagated through 24 electrodes with three resets. The light source is turned on from the beginning time step until the first wave reaches the metal mirror. For the rest of the time step, the light source remained off. The reason to take this approach is that the front surface of the LC OPA and the metal mirror located at the rear of the LC OPA will reflect laser beam. If the light source remained on all the time, the forward propagating light from the source and the backward propagating light reflected by the front surface of LC OPA and the metal mirror will be spatially overlapping with each other to make the analyze more difficult. The simulated electric field distribution in the FDTD main computation grid is shown in Fig. 4.

The collection of time averaged complex field distribution at near field is carefully chosen, so that the front surface reflection and the main reflection from the metal mirror are spatially separated. This way, the simulated diffraction efficiency pertains to a LC-OPA with no front surface reflection. The far field diffraction pattern can be obtained by near field to far field transformation as shown in Fig. 5. The percentage of energy goes into the -1 diffraction peak is 86.7% of total energy, and the peak intensity of the -1 diffraction order is 89.3%. The steering angle in this case is 4.075 mrad.

With similar method, we can simulate the case with different steering angles. The simulated phase profile and the far field diffraction pattern are shown in Fig. 7.
Fig. 7: Phase profile and corresponding far field of LC blazed grating. (a) (d) corresponds to steering angle =2.04 mrad, (b) (e) steering angle =8.16 mrad, (c) (f) steering angle =12.24 mrad. (For $\lambda$=632.8 nm)
Several parameters can be used to compare the diffraction pattern of the simulation results with experimental results. This includes the diffraction pattern, diffraction efficiency, diffraction angle etc. Both the simulation and experimental results show very similar pattern that one main diffraction peak is shifted from zero position and all high order diffraction peaks are small. For the steering that corresponds to eight level stair like blazed phase profile, an analytical expression of an ideal blazed grating that maximizes the energy of the 1st diffraction order is given by

\[ \eta = \left( \frac{\sin(\pi / q)}{\pi / q} \right)^2 \]  

(2.20)

Here \( q \) is the number of steps for every reset. However, the blazed phase profile formed by a liquid crystal OPA is not an ideal one. The liquid crystal director orientation changes continuously in space that causes a fly-back region to form. Such fly-back region diffracts light to undesirable diffraction order and is the main factor for the efficiency loss. A simple model assumes that any light passes through this region is totally lost can be derived by adding a correction factor to Equ. 2.20 as proposed by McManamon and et al.; and in this case, the approximation for DE is

\[ \eta_{total} = \left( \frac{\sin(\pi / q)}{\pi / q} \right)^2 \left( 1 - \frac{\Lambda_F}{\Lambda} \right)^2 \]  

(2.21)

Here \( \Lambda_F \) is the width of the fly-back region and \( \Lambda \) is the total length of one period of the grating. To evaluate the diffraction efficiency, the width of the fly-back region is unknown yet. With our computer simulation of the phase profile of a LC OPA,
as shown in Fig. 2, the width of such fly-back region can be estimated by choosing the criteria to define the width of the fly-back region. Such criteria are that whenever the difference between the simulated value and the desired value is greater than 1/10 wave, the region is defined as the fly-back region. Following the criteria, the width of the fly-back region can be estimated to be about 5 µm. With this simple model, the diffraction efficiency of a LC OPA can be estimated.

For the steering corresponding to eight level stair like blazed grating, the simulated, measured and theoretical steering angle is 4.076 mrad, 4.071 mrad and 4.075 mrad respectively; the diffraction efficiency is 89.1%, 84.6% and 89.3% respectively. These results show excellent agreement with each other.

Another comparison is carried out for the diffraction efficiency of steering laser to different angles with different blazed grating configuration. The diffraction efficiency as a function of steering angle is shown in Fig. 8. The simulated results agree excellently with the simple model and the maximum difference between these two results are less than 0.3%. However, the experimentally measured diffraction efficiency is about 5% lower than the prediction by the simple model and the FDTD simulation. This is because in the diffraction efficiency simulation and the simple model, the diffraction efficiency is calculated for an aberration free system. However, in the experiment, additional correction of 18.7 waves of aberration is needed to remove the aberration introduced by the silicon backplane of the LCOS device\(^{47}\), which causes loss of efficiency. Air turbulence and electronic noise on the LCOS device can also contribute to the 5% diffraction efficiency loss.
Fig. 8: The comparison of diffraction efficiency of LC OPA as function of steering angle between experimental results, FDTD simulation and simple model. (For $\lambda=632.8$ nm)
2.6 Conclusion

With the above consideration, excellent agreement between simulation results, experimental results and empirical model has been shown. The accuracy of the director simulation and FDTD simulation is very high. The limitation factor that prevents us from getting better agreement between FDTD simulation is the accuracy of the experiments, which contains many factors that are not considered in the FDTD simulation.

The liquid crystal director simulation and the Finite Difference Time Domain (FDTD) optical simulation can be a powerful tool to study the LC OPA. The full 3-D director simulation software used in this article takes into account of the electric field distribution between electrodes, thus can accurately determine the phase profile of the LC OPA for feature size smaller than the wavelength of light. The diffraction of light through the phase reset region is taken into account by Finite Difference Time Domain simulation. Thus, the simulation method used in this article is extendable to cases where the electrode size of the LC OPA is close to wavelength of light and the fringing electric field between neighboring electrodes becomes the dominating factor of the diffraction efficiency of the LC OPA.
3.1 Introduction

One very important application of a LC DOE is for long distance free space laser communication. In order to direct the laser signal to the desired target, a laser communication system needs to have a transmitter/receiver that can perform beam pointing, target acquiring, target tracking and many other beam control functions. In a conventional system, the beam pointing is achieved by mechanically rotating a telescope mounted on a gimble system; the focusing and defocusing is achieved by mechanically adjust the position of the lens; and the wavefront control is achieved by deform the surface shape of a deformable mirror with actuators behind such deformable mirror. A mechanical beam direct system evolves very complicated mechanical motions, which make the total system very heavy, bulky, expensive and power consuming. The inertia, stability, accuracy, and speed of such a system are of serious concern.

On the other hand, a LC DOE can be an Electro-Optical programmable phased array antenna that can provide many active beam control functions such as high accuracy wide angle beam steering, dynamic focusing, simultaneous multiple beam control and high resolution wavefront control with no mechanical movements. This substantially reduces the size, weight and profile of the system, while provide excellent long term stability. In comparison, an active beam control system based on liquid crystal device can be fast, inexpensive, and more dependable. There are many desirable capabilities for
example, multiple beam control, high-resolution aberration correction, random access beam pointing etc. that a mechanical system could not offer. This made a liquid crystal tunable diffractive optical element very attractive for this application.

A simple case of LC DOE is a 1-D tunable grating with line shape electrodes. The main application of such device is for fine angle laser beam steering and beam pointing. Such a device is also called Liquid Crystal Optical Phased Array (LC OPA)\(^8,9\). It evolves a liquid crystal device with parallel rubbed surfaces and independently addressable line shape electrodes. By applying control voltage to each electrode of the LC OPA, a stair like blazed phase profile can be generated with modulo-2\(\pi\) resets, the device act like a blazed grating that can steer laser radiation in the plane perpendicular to the electrode direction. However, the steering angle range of the current available LC OPA is limited to less than 2° with acceptable diffraction efficiency\(^43\). As pointed out in Ref\(^{44,45,46}\), this limitation is mainly imposed by the fringing electric field in a high resolution LC OPA. In many systems, steering angle of at least 10° is required. To achieve such large steering angle, cascading of multiple LC OPA is necessary. Even in this case, the loss of efficiency is still serious because of large number of elements evolved.

A LC OPA can be combined with other type of device to achieve continuous wide angle beam steering. A little review of those approaches could help us to understand in more depth of the advantage and disadvantage of the LC OPA. So far the most mature wide angle steering system is the rotating Risley prism approach\(^47\). However, this approach is still a mechanical system. An non-mechanical wide angle beam steering
approach is the Digitial Beam Deflector (DBD) approach. This type of device consists of two elements for each steering stage. The first element is a polarization rotation device such as a TN device, this device is to switch the incoming polarization of light to orthogonal direction. The second element is a passive birefringence prism, for example a Wollaston polarizing prism. Depends on the polarization of incident of light, the incident beam can be deflected to different angles. This type of beam steering device could provide relatively large angle with excellent efficiency. The main draw back to this approach is the steering angle is limited to only two different angles. If a large number of steering angle is required, many stage of the DBD is required which increased the total length of the system.

Another approach developed by Caltech is a surface relief grating made by electron beam etching of PMMA. Liquid crystal material is sandwiched between such substrate with surface relief blazed grating and a cover glass. When no electric field is applied to LC, the effective refractive index of the LC is different from PMMA, such laser is diffracted to large angle; when electric field is present, the refractive index of LC decreases and becomes the same as the PMMA, thus no steering occurs. Up to 13.5° of beam steering has been demonstrated, however, the efficiency of such a system is still very low, because of the phase mismatch between the neighboring blazed element. The steering angle of this device is also limited to two different angles.

Photo-Thermal-Refractive (PTR) glass developed by CREOL is another approach to achieve large angle beam steering. Volume holographic Bragg grating is written on the PTR glass. The layer normal of the Bragg grating tilted with respect to the
surface normal of the glass. When an incident laser satisfied the Bragg reflection condition, the laser beam will be reflected by the Bragg grating thus deflecting the laser beam to large angle if the incident light satisfy the Bragg condition. This glass is then an amplifier which can amplify the incident angle of a laser beam to large output. 20°-40° degree of steering can be easily achieved with excellent efficiency. However, this device itself is a passive device itself and still needs LC OPA to deflect the laser beam to angles that satisfy Bragg condition, and this process is called Zone select. The final efficiency of such a system is still very lower of on the order of 20% efficiency due to the large number of LC OPAs used to for zone select and fine steering after the wide angle steering.

We can see that all the above mentioned non-mechanical wide angle beam steering approaches can only steer laser beam to discrete wide angles. A LC OPA is critical to fill in the gap between the discrete angles as a fine steering stage. The total performance of the complete system strongly depends on the performance of the LC OPA. Since a complete beam steering system that can provide both wide angle steering and continuous scanning of the beam has many layers of structures, it would be very advantageous to have a wide angle LC OPA to reduce the number of element in the system and achieve higher efficiency. In this chapter, our main objective is to study the physics behind the limiting factor of a wide angle LC OPA, and to provide wide angle LC OPA design with optimized structure.
3.2 Ideal 1-D Liquid Crystal Optical Phased Array

What is the fundamental physical limitation to the angular performance of a single stage LC OPA is the first question to the overall picture of the LC OPA design. The answer to that question determines the potential of the LC DOE in laser beam steering application, and it will influence the overall structure the lasercom beam steering system.

To study the maximum deflection angle that can be achieved with a LC OPA, we first consider a LC OPA with an ideal LC director configuration, where the pixilation effect and the inter-electrode coupling effect is neglected. From geometrical optics considerations, the ideal phase profile that gives the highest diffraction efficiency is when the phase delay is a linear function with respect to position, as in Equ. 3.1. The desirable LC director configuration is described in Equ. 3.3. In this case, we assume the grating period of the ideal LC blazed grating is $L$, and the angle $\theta$ is the tilting angle of the LC director, which is defined as the angle between the surface normal of the LC cell and the LC director.

\[
n_{\text{eff}}(x) = \Delta n \frac{x}{L} + n_o
\]  

(3.1)

\[
n_{\text{eff}}(x) = \frac{n_o n_e}{\sqrt{n_o^2 \sin^2 \theta + n_e^2 \cos^2 \theta}}
\]  

(3.2)

\[
N_x^2(x) = \left( \frac{\frac{2}{L} \frac{2}{n_o} \frac{2}{n_e} - n_e^2}{\left(\frac{L - x}{n_o} + xn_e\right)^2} \right) \frac{1}{n_o^2 - n_e^2}
\]  

(3.3)
The diffraction efficiency of such an ideal LC OPA can be simulated with Finite Difference Time Domain (FDTD) simulation like before. The relationship between diffraction efficiency and diffraction angle as calculated by the FDTD modeling is shown in Fig. 9. If we define an efficiency-angle metric to describe the angular performance of the LC OPA, for example, if the efficiency loss that can be tolerant in the system is 50%, then the diffraction angle that have 50% DE is defined as the 50% efficiency steering angle, then for a wide angle LC OPA with 1st order reset that operates at 1550 nm wavelength (shown in Fig. 9), the 70.7% efficiency steering angle is about 31.5°, and the 50% efficiency steering angle is 40.5°. We can see, with an ideal LC director configuration, the diffraction angle of the LC OPA can be very large at high efficiency.
Fig. 9: Diffraction efficiency as function of steering angle for an ideal LC OPA working at 1550 nm wavelength.
3.3 The basic configuration of a real 1-D LC OPA and the fringing electric fields

In a real LC OPA, to produce a desirable director configuration for a wide angle LC OPA, a very important factor we need to consider is the electric field distribution. Generally, the electric field in a LC OPA device is desired to be normal to the surface of the LC cell, as in the case when the electrode of the LC OPA is an infinitely large one. However, this is not possible for a wide angle LC OPA, where the electrode width is very large compared with the thickness of the LC cell. In this case, the electric field at the edge of the electrode is not perpendicular to the surface but has some tangential component. Such tangential components of the electric field are generally referred to as the “fringing electric fields”.

The fringing electric fields issue in a LC device has been studied as early as 1970's, and is well know to the LC display community. More recent research addressed high spatial resolution devices for optical application. Fringing field issues in a binary LC blazed grating is studied by Ref. A more systematic work regarding the cell thickness dependence of fringing field effect in LC blazed grating is given by. However, the optical simulation used in this work is not a wave optics simulation but based on Fast Fourier Transformation (FFT) approximation. Only the liquid crystal cell thickness variation is systematically studied.

If we define a width/height ratio $\tau_E$, which is the ratio between the electrode width and the cell thickness, such width/height ratio of the LC OPA is an indicator of how strong the fringing field effect will be regarding the overall performance.
Here $\tau_E$ is the width/height ratio, and $w$ is the width of one electrode and $d$ is the LC cell thickness. A comparison of the electric field distribution between a high resolution LC OPA (small $w$ value) and a low resolution LC OPA (large $w$ value) is shown in Fig. 10. (The rubbing direction is perpendicular to the electrode direction.) The iso-potential line in a LC OPA with 10.5 $\mu$m pixel spacing is shown in case a; and iso-potential line in a LC OPA with 1.5 $\mu$m pixel spacing is shown in case b. The voltage profile in the case (a) is relatively well defined. However in the case (b), the iso-potential line extends to the pixel with zero volts; in a substantial portion of the pixel region, the electric field is pointing to direction not perpendicular to the normal direction of the cell surface because of the tangential component of electric field.

There are two possible configurations of 1-D LC OPA, as shown in Fig. 11. The two configurations have different behavior due to the fringing electric field effect. The first one is for the rubbing direction parallel to the electrodes, and the second one is for the rubbing direction perpendicular to the electrodes. The coordinate system used here is defined so that the thickness direction for the LC OPA is the Z axis, and the line shaped electrodes are along Y axis. For either one of these structure, an in plane Electronic Controlled Birefringence (ECB) director configuration is desired. Any out of plane director component will lead to a complicated polarization effect of the laser beam.
Fig. 10: Iso-potential line in ECB LC OPA for cell thickness $d=2 \, \mu m$. $dv=0.1v$ for adjacent iso-potential lines. (a) Top figure. Electrode width=10 \, \mu m, gap between electrode=0.5 \, \mu m. (b) bottom figure. Electrode width=1 \, \mu m, gap =0.5 \, \mu m.
Fig. 11: Basic configuration of ECB LC OPA with 1-D line shape electrodes. (a) Rubbing direction perpendicular to the electrode direction. (b) Rubbing direction parallel to the electrode direction.
Since the LC director tend to align to the direction of the electric field. The two configuration of the 1-D LC OPA may have quite different director configuraton, which may strongly influence the performance of the LC OPA. For the first case in Fig. 11, the fringing electric field is in the rubbing plane. The LC director in the LC OPA as shown in Fig. 12 (a). No out of rubbing plane director component is present in the system. Bend and splay director configuraiton is the dominant structure in most cases, except for when a defect is formed in a high resolution device. When an incident field polarized along the rubbing direction propagates through such a LC OPA, the polarization of light preserves while light propagates through the device. In Fig. 13(a), such effect is shown with a Finite Different Time Domain (FDTD) calculation that can simulation both the TE and TM mode of light propagation in a complex LC structure.

However, for the second case in Fig. 11, the fringing electric field is perpedicular to the rubbing plane. In this case, due to the director fluctuation or other imperfection in the LC OPA, the LC director will be aligned along the electric field direction, thus have strong out of rubbing plane component. This is shown in Fig. 12 (b). Twist structure is the dominant director configuration. In this case, the nominal elastic constant of LC material is the twist elastic constant, which can be much smaller than the splay and the bend elastic constant. The magnitude of the polarization effect depends on the pixel spacing of the LC OPA. When the pixel spacing is large, for example the previous Liquid Crystal On Silicon device with pixel spacing 19.4 µm \(^{47}\), the polarization induced by the out of plane twist director configuration is measured to be less than 1%. However, for the OPA with pixel spacing 1.5 µm, significant out of the YZ plane twist configuration is
present. When incident light polarized along the rubbing direction propagates through the
device, the linear polarized light becomes elliptically polarized at the output aperture of
the device. This effect is shown in Fig. 13(b). For a LC OPA, such polarization effect is
not desirable, since it may lower the diffraction efficiency of the device.
Fig. 12: Director configuration of an ECB LC OPA in an eight level stair like blazed grating configuration. $n_e=1.85$, $n_o=1.50$. Cell thickness $d=2.5 \, \mu m$, pixel spacing $=1.5 \, \mu m$, gap between electrode=$0.5 \, \mu m$, pretilt=$3^\circ$. (a) Upper figure. Rubbing direction perpendicular to the electrode direction. (b) Bottom figure. Rubbing direction parallel to the electrode direction. (For $\lambda=1550 \, nm$)
Fig. 13: FDTD simulation of light propagation in a transmissive LC OPA. (a) The rubbing direction is perpendicular to the electrode direction. (b) The rubbing direction is parallel to the electrode direction. ($\lambda=1550$ nm)
3.4 Wide angle 1-D LC OPA with rubbing direction perpendicular to the electrodes

3.4.1 Possible defect formation and the stability of the ECB structure

For the 1-D LC OPA with rubbing direction perpendicular to electrode, the fringing fields between electrodes are in the same plane of LC director: the XZ plane. The mechanism for this can be explained by considering Fig. 12 (a). The director configuration in the case (a), if no voltage was applied to any of the electrodes, would be nearly horizontal aligned except for a slight rotation in a clockwise direction that is due to the surface pretilt of the director. When the voltages that provide the shown director configuration are applied, the strongest fringing fields are on either side of the first full electrode on the right side because it has a much higher voltage applied to it than those on either side of it. This fringing field causes the director to rotate with a counter clockwise sense on the right side of the electrode and clockwise along the left side, preventing the director over the top of the electrode from tipping upwards in a uniform manner and trapping a “tilt wall” over the electrode. In liquid crystal materials, the elastic constant for a twist deformation is much lower than that for a bend configuration, so the elastic energy in this “tilt wall” can be reduced by the director twisting out of the plane of the figure as shown. This twisting of the director field causes a polarization effect of light that was incident on the OPA with its polarization axis in the plane of the figure, and lowers the device efficiency. However, if the pretilt angle of the surface alignment is high enough, it can overwhelm the effect of the fringing field on the right side of the high voltage electrode to rotate in the counterclockwise direction, and therefore prevent the formation of the “tilt wall” and its possible change to a twisted structure.
In order to estimate the minimum pretilt angle required to prevent an out of plane component of the director field, we modeled a system with the condition specified in Fig. 12. However, in the computer modeling method we use, meta-stable LC director configurations can cause the modeling software to give a false result for the equilibrium director configuration. To prevent this, the initial director configuration in the LC bulk is set to have an initial out of the XZ plane component, that we called perturbation angle. This is the angle between the projection of director on the XY plane and the X axis. We vary the perturbation angle from 0° to 3° uniformly across the thickness direction of the cell, except at the boundary where the director was fixed along the X direction. If the in plane director configuration of the LC OPA has lower energy than the out of plane twist structure, the director in the LC bulk will rotate back into the XZ plane, otherwise, the director will twist out of the XZ plane to form a twist structure. In Table 2, we shown the out of plane twist structure at the equilibrium state for example device considered in Fig. 12. When the pretilt angle of the LC OPA is 0° and the initial perturbation is 1°, a twist structure is present. The director configuration in this case is shown in Fig. 12 (b). It is clear that for pretilt angle less than 1°, the out of plane twist structure is more likely to form, and for pretilt higher than 3°, such twist structure can be prevented. One thing to be noted is that the stability condition of 3° pretilt is a function of the electrode spacing, the cell gap and the voltage applied to the LC OPA. When the electrode spacing of the LC OPA is low, a 1° pretilt may be enough to prevent the out of plane twist, but for high spatial resolution the LC OPA, and the larger the difference of the voltage is applied to a
neighboring electrodes of the LC OPA, a higher pretilt is required to prevent out of plane twist structure.

Table 2: The stability of ECB structure in high resolution LC OPA as function of pretilt angle

<table>
<thead>
<tr>
<th>Pretilt Angle</th>
<th>Initial out of XZ plane azimuthal angle (perturbation angle)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0°</td>
</tr>
<tr>
<td>0°</td>
<td>N</td>
</tr>
<tr>
<td>1°</td>
<td>N</td>
</tr>
<tr>
<td>3°</td>
<td>N</td>
</tr>
</tbody>
</table>

N: The final equilibrium director configuration has no significant out of XZ plane twist component

Y: The final equilibrium director configuration has significant out of XZ plane twist component
Fig. 14: Equilibrium director configuration that contains out of XZ plane twist director configuration in a high resolution LC OPA with eight electrode blazed grating configuration. The initial perturbation of out of plane twist azimuthal angle is 1°.
3.4.2 Effect of fringing electric field on the phase profile

For 1-D LC OPA with rubbing direction perpendicular to the electrode, since no polarization effect is involved, the device is simply an electronically tunable diffractive grating. The steering angle of this 1-D LC OPA is determined by the slope of the phase profile produced by the LC OPA. The diffraction efficiency of the device depends mainly on how accurate the phase profile of the device is, as oppose to an ideal blazed grating. The sharpness of the phase jump at the reset is determined by a combination of the elastic force in the LC bulk and the electric field distribution. For the first part, the elastic force in LC material is related to the material property and the director configuration. The larger the splay, twist and bend elastic constant $k_{11}$, $k_{22}$ and $k_{33}$, the larger the elastic force is stored in the LC bulk for the same director configuration. It is reasonable to think that if the elastic constant becomes smaller, it will be easier to deform the LC director to achieve the desired phase profile. However, through our study, we find things are not that simple because of the fringing electric fields in the LC OPA.

As an example of the fringing field effect’s influence on the performance of the LC OPA, a LC OPA designed to steer 1550 nm laser beam to 7.4° has been simulated. The design parameters are: the pretilt angle is chosen to be 3° to prevent possible twist structure formation; the driving voltage is limited to be 0-5V, which is enough to harvest 95% of retardation that a LC OPA can produce in most of the cases. The cell thickness of the LC OPA is $d=6$ µm. An eight electrode per reset configuration 1550 nm wavelength is considered with pixel spacing of 1.5 µm. The steering angle of the LC OPA in this case is 7.42°. The driving voltage for each pixel of LC OPA is obtained by the phase vs
voltage relationship as in Fig. 6. For each pixel, the driving voltage is not optimized to give the best performance, but are from the simple curve obtained by neglecting the fringing electric field induced inter-pixel coupling. Then the 2-D director simulation is carried out to obtain the director configuration and the phase profile as shown in Fig. 15 (a). The phase profile of such a device strongly deviated from the desired phase profile due to the fringing electric field induced inter-pixel coupling. Far field diffraction pattern obtained by FDTD simulation is shown in Fig. 15 (b). If we define the diffraction efficiency (DE) to be the peak intensity of the -1 diffraction order versus the peak intensity of the non-steered beam. Then the DE is only 26.3% in this case.

For this configuration, although the pixel spacing is small enough to achieve wide angle beam steering, the wide angle performance of such a LC OPA is still very poor. The 70.7% efficiency angle is limited to 1.85°, and the 50% efficiency angle is 4.36°. In order to determine what configuration of the LC OPA will have high efficiency at large diffraction angle, different design parameters that will influence the DE of the LC OPA is studied. We will discuss these parameters such as the cell thickness, birefringence of the LC material, pixel spacing, voltage profile, gap between electrodes, pretilt angle, elastic constant, optical axis one by one to achieve the best wide angle performance.
Fig. 15: Simulated phase profile and far field diffraction pattern of a reflective LC OPA. The segmented horizontal lines in (a) Top figure. The desired phase profile of a stair like blazed grating. (b) Bottom figure. The far field diffraction pattern of the blazed grating. The continuous line is the simulated phase profile. Here $\lambda=1550$ nm, $K_{11}=14.1 \times 10^{-12}$ N, $K_{22}=7.1 \times 10^{-12}$ N, $K_{33}=19.1 \times 10^{-12}$ N, $\varepsilon_\parallel=12.1$, $\varepsilon_\perp=4.1$, $n_e=1.7100$, $n_o=1.5076$. pixel spacing $=1.5 \mu$m, gap between electrode $=0.5 \mu$m, cell thickness $d=6.0 \mu$m and pretilt $=3^\circ$. 
3.4.3 Effect of pixel spacing, cell thickness and LC material birefringence

First of all, the DE depends strongly on the spatial resolution of the LC OPA. As shown in Fig. 16, if the pixel spacing of the LC OPA is reduced, while all other parameters remain the same, the phase modulation depth becomes smaller and the corresponding steering angle increases. When different birefringence of liquid crystal material used for the LC OPA, different cell thickness of the LC OPA can be used while keeping the total birefringence similar.

Table 3: Diffraction efficiency as function of pixel spacing of LC OPA. Here eight electrode LC OPA is considered. \(\lambda=1550\ \text{nm} \ K_{11}=14.1\times 10^{-12}\ \text{N}, K_{22}=7.1\times 10^{-12}\ \text{N}, K_{33}=19.1\times 10^{-12}\ \text{N}, \varepsilon_{||}=12.1, \varepsilon_{\perp}=4.1, n_o=1.50, n_e=n_o+\Delta n, \) pixel spacing =1.5~19.4 \(\mu\text{m}, \) gap between electrode=0.5 \(\mu\text{m}, \) cell thickness \(d=2.5, 3.0\) and \(6.0\ \mu\text{m}, \) pretilt=3°.

<table>
<thead>
<tr>
<th>Pixel Spacing</th>
<th>1.5 (\mu\text{m} )</th>
<th>2.5 (\mu\text{m} )</th>
<th>4.5 (\mu\text{m} )</th>
<th>7.5 (\mu\text{m} )</th>
<th>10.5 (\mu\text{m} )</th>
<th>19.4 (\mu\text{m} )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Steering angle</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MLC6080 (\Delta n=0.2024)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(d=6 \mu\text{m} )</td>
<td>-1 order 26.3% 49.4% 63.7% 74.8% 79.9% 86.9%</td>
<td>0 order 49.4% 16.9% 3.3% 0.9% 0.5% 0.2%</td>
<td>+1 order 18.7% 20.4% 8.7% 2.8% 1.2% 0.2%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\Delta n=0.35) (d=3 \mu\text{m} )</td>
<td>-1 order 47.6% 60.6% 70.8% 80.1% 83.5% 88.3%</td>
<td>0 order 11.2% 3.8% 3.3% 0.9% 0.7% 0.2%</td>
<td>+1 order 17.1% 7.4% 6.9% 0.7% 0.4% 0.5%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\Delta n=0.35) (d=2.5 \mu\text{m} )</td>
<td>-1 order 55.0% 69.7% 80.0% 84.0% 86.9% 91.0%</td>
<td>0 order 11.3% 3.9% 1.2% 0.2% 0.1% 0.1%</td>
<td>+1 order 15.5% 6.5% 1.6% 0.4% 0.2% 0.1%</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
In Fig. 17 and Table 3, the effect of the thickness, liquid crystal material birefringence and pixel spacing on the diffraction efficiency of the LC OPA is shown. The overall trend is that the DE decreases as the pixel spacing gets higher and higher. However, there is a critical value of pixel spacing. For different cell thickness, such critical value is different. For example, in the case where cell thickness d=6 µm, the critical value of the pixel spacing is around 8~10 µm; however in the case where cell thickness d=2.5 µm, the critical value of pixel spacing is around 4 µm. This critical value is related to the fringing field effect in a high resolution LC OPA, as indicated by the width/height ratio $\tau_E^\tau$. From the simulated curve, the critical value of the pixel spacing corresponds to when $\tau_E=0.5$~2. Since the phase modulation depth in Fig. 15 (a) shows reduced modulation depth of the LC OPA, it is natural to think that by increasing the cell thickness (increase the $\Delta n*d/\lambda$ at the same time) the phase modulation depth will increase. However, we find this is only true for a LC OPA with $\tau_E>>1$. For cases when $\tau_E<<1$, the phase modulation depth decreases as the cell thickness becomes larger, because fringing electric fields become a dominant factor in this case.

One way to describe the strength of the fringing electric field’s influence on the diffraction efficiency is described in Chapter 2, Equ. 2.30, where the loss of efficiency is related to the width of the fly-back region $\Lambda_f$. However, since the width of the fly-back region is also related to the cell thickness of the LC OPA, it is reasonable to construct an empirical expression as in Equ. (3.5) by assuming the width of the fly-back region is related to the cell thickness to a power of $\beta$:
Here $a$ is a constant related to the strength of the fringing electric field, $d$ is the thickness of the liquid crystal device and PS is the pixel spacing of the LC-SLM, which is used here as a normalizing factor to make the left side of the equation dimensionless. We can fit the diffraction efficiency data obtained by director simulation and FDTD simulation using an expression in Equ. 3.6.

$$\eta = \left(1 - \frac{\Lambda_r}{\Lambda}\right)^2 = \left(1 - a \left(\frac{d}{PS}\right)^\beta\right)^2$$

Here $\bar{N}$ is the average number of pixels for every wave of aberration, which value is 8 for eight electrode/reset scheme considered Fig. 17. The fitted line agrees excellently with the FDTD simulation data. The coefficient $a$ is found to be $a = 1.4$, and the value of $\beta$ is found to be 0.7 for all cases.
Fig. 16: Simulated phase profile of liquid crystal device with different electrode configuration. (for \( \lambda = 1550 \) nm) Liquid crystal material used is MLC 6080, with \( \Delta n = 0.20 \), \( d = 6 \) \( \mu \)m. Pixel spacing is (a) 19.4 \( \mu \)m (b) 10.5 \( \mu \)m (c) 7.5 \( \mu \)m (d) 4.5 \( \mu \)m (e) 2.5 \( \mu \)m (f) 1.5 \( \mu \)m
Fig. 17: (a) Top figure is the diffraction efficiency of LC OPA as function of spatial resolution. (b) Bottom figure is the corresponding diffraction efficiency of a LC OPA as function of steering angle. Here $\lambda=1550$ nm, $K_{11}=14.1 \times 10^{-12}$ N, $K_{22}=7.1 \times 10^{-12}$ N, $K_{33}=19.1 \times 10^{-12}$ N, $\varepsilon_{\parallel}=12.1$, $\varepsilon_{\perp}=4.1$, $n_o=1.50$, $n_e=n_o+\Delta n$, pixel spacing $=1.5$~$19.4$ µm, gap between electrode=0.5 µm, pretilt=3°.
A reflective LC OPA has substantial advantage in both reducing the fringing field effect and improving the switching speed for the wide angle LC OPA. We will consider a reflective LC OPA through later discussions in this article. The cell thickness of a LC OPA is determined by the operational wavelength of the LC OPA and the birefringence of the LC material available. Generally, the double pass retardation value $2\Delta n d/\lambda$ is desired to be larger than one to be able to achieve a modulo $2\pi$ version of the desired phase profile. Different combination of cell thickness and $\Delta n$ of the LC material that gives $2\Delta n d/\lambda$ value ranging from 0.86 to 2.61 is compared in Table 4. The highest DE corresponds to when cell thickness is 2.1 µm, which gives a $2\Delta n d/\lambda$ value of 0.95. The reason for this is that the total modulation depth only needs to be $1-1/8=0.875$ waves for an eight level blazed gratings. However, if we choose such a cell thickness, the DE will be lower for small steering angles, because the number of steps in the grating will increase. A trade off has to be made between high efficiency at large and small steering angles.

In any case, it is very important to reduce the cell thickness and improve the diffraction angle of a LC OPA. By using high birefringence LC material and very thin reflective cell, the performance of the LC OPA can be improved dramatically. For example, using $\Delta n=0.35$ material can allow a very thin LC OPA with cell thickness of 2.5 µm to be able to operate at 1550 nm wavelength. The diffraction efficiency of such LC OPA is much higher than the LC OPA with lower birefringence. As shown in Fig. 17, to achieve a 70.7% diffraction efficiency for a LC OPA with a $\Delta n=0.35$ LC material, the electrode spacing needs to be 2.6 µm, which corresponds to a diffraction angle of $4.2^\circ$. 
Similarly, to achieve 50% diffraction efficiency, the electrode spacing needs to be 1.5 µm, which corresponds to a diffraction angle of 8.7°. This means, a high birefringence LC material if very critical for high efficiency wide angle LC OPA.

Table 4: Diffraction efficiency as function of cell thickness. Here \( \lambda = 1550 \text{ nm} \), \( K_{11} = 14.1 \times 10^{-12} \text{ N} \), \( K_{22} = 7.1 \times 10^{-12} \text{ N} \), \( K_{33} = 19.1 \times 10^{-12} \text{ N} \), \( \varepsilon_\parallel = 12.1 \), \( \varepsilon_\perp = 4.1 \), \( n_o = 1.50 \), \( n_e = n_o + \Delta n \), pixel spacing = 1.5 µm, gap between electrode = 0.5 µm and pretilt = 3°.

<table>
<thead>
<tr>
<th>( \Delta n )</th>
<th>( d ) (µm)</th>
<th>( 2\Delta n \times \frac{d}{\lambda} )</th>
<th>DE</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.350</td>
<td>1.9</td>
<td>0.86</td>
<td>59.2%</td>
</tr>
<tr>
<td>0.350</td>
<td>2.1</td>
<td>0.95</td>
<td>60.0%</td>
</tr>
<tr>
<td>0.350</td>
<td>2.3</td>
<td>1.04</td>
<td>58.9%</td>
</tr>
<tr>
<td>0.350</td>
<td>2.5</td>
<td>1.13</td>
<td>55.0%</td>
</tr>
<tr>
<td>0.350</td>
<td>3.0</td>
<td>1.16</td>
<td>48.9%</td>
</tr>
<tr>
<td>0.350</td>
<td>3.0</td>
<td>1.35</td>
<td>47.6%</td>
</tr>
<tr>
<td>0.300</td>
<td>4.0</td>
<td>1.80</td>
<td>37.2%</td>
</tr>
<tr>
<td>0.2024</td>
<td>6.0</td>
<td>1.56</td>
<td>26.3%</td>
</tr>
<tr>
<td>0.2024</td>
<td>10</td>
<td>2.61</td>
<td>14.1%</td>
</tr>
</tbody>
</table>
3.4.3 Effect of the aperture ratio of the electrodes

Another factor related to the DE of a LC OPA is the influence of the gap between electrodes. For the LC OPA considered in this article, a continuous mirror as a common electrode is assumed to avoid possible diffraction loss from a segmented mirror. The patterned electrode is a transparent conductor, for example Indium Tin Oxide (ITO). To describe the efficiency factor associated with the patterned electrodes, we define the aperture ratio of the electrodes to be the ratio between the size of the electrode and the electrode spacing. If we assume the gap between electrodes is at least half micron wide (due to manufacturing consideration), as the spatial resolution of the LC OPA becomes higher, the aperture ratio of the LC OPA becomes smaller. The DE as function of the aperture ratio of the LC OPA is shown in Table 5 (no voltage optimization is carried out for this cases). We can see that for an electrode gap less than the cell thickness, the DE loss is almost independent of its exact value. However, for electrode gap larger than the half the cell thickness, the DE loss increases. In the this consideration, we use 0.5 μm gap between electrodes and the aperture ratio larger than 66.7% in our later consideration. In a LC device, a dielectric layer (usually a polyimide alignment layer) between the electrode and the LC material is often used as an alignment layer. Such layer could have effect on the fringing fields. Since most of the LC device manufacturer use very thin polyimide layer, we will not discuss the influence of the alignment layer thickness in this case. We assume a perfect non-conductive dielectric layer with thickness of 50 nm, and a dielectric constant of 4.5 as the alignment layer.
Table 5: Diffraction efficiency of LC OPA for different electrode configuration. Here \( \lambda = 1550 \text{ nm} \), \( K_{11} = 14.1 \times 10^{-12} \text{ N} \), \( K_{22} = 7.1 \times 10^{-12} \text{ N} \), \( K_{33} = 19.1 \times 10^{-12} \text{ N} \), \( \varepsilon_\parallel = 12.1 \), \( \varepsilon_\perp = 4.1 \), \( n_o = 1.50 \), \( n_e = 1.85 \), cell thickness \( d = 2.5 \mu\text{m} \) and pretilt=3°.

<table>
<thead>
<tr>
<th>Pixel spacing (( \mu\text{m} ))</th>
<th>Size of electrode (( \mu\text{m} ))</th>
<th>Size of gap between electrodes (( \mu\text{m} ))</th>
<th>Aperture ratio</th>
<th>DE</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.5</td>
<td>1.4</td>
<td>0.1</td>
<td>93.3%</td>
<td>56.0%</td>
</tr>
<tr>
<td>1.5</td>
<td>1.0</td>
<td>0.5</td>
<td>66.7%</td>
<td>55.0%</td>
</tr>
<tr>
<td>1.5</td>
<td>0.8</td>
<td>0.7</td>
<td>53.3%</td>
<td>54.6%</td>
</tr>
<tr>
<td>1.5</td>
<td>0.5</td>
<td>1.0</td>
<td>33.3%</td>
<td>52.5%</td>
</tr>
<tr>
<td>1.5</td>
<td>0.1</td>
<td>1.4</td>
<td>7.1%</td>
<td>43.4%</td>
</tr>
</tbody>
</table>
### 3.4.4 Influence of the elastic constant

The influence of the elastic constant on the DE also needs to be considered. The phase vs. voltage curve for different elastic constants are shown in Fig. 18. The larger the splay, twist and bend elastic constants ($k_{11}$, $k_{22}$ and $k_{33}$), the larger the elastic energy associated with a non-uniform director configuration. It is reasonable to think that if the elastic constants become smaller, it will be easier to deform the LC director to achieve the desired phase profile. However, through our study, we find this is not a significant factor related to the DE, because the dominating factor is the fringing electric field effect. As an example, The DE without voltage optimization improved only to 59.3% from 58.9% (as shown in Table 6), when the splay and bend elastic constants is reduced to 7.1×10^{-12} N.

Table 6: Diffraction efficiency of LC OPA with different elastic constant. Here $\lambda=1550$ nm, $\varepsilon_\parallel=12.1$, $\varepsilon_\perp=4.1$, $n_\parallel=1.50$, $n_\perp=1.85$, cell thickness $d=2.3$ µm, pixel spacing =1.5 µm, gap between electrode=0.5 µm and pretilt=3°.

<table>
<thead>
<tr>
<th>$K_{11}$ (10^{-12} N)</th>
<th>$K_{22}$ (10^{-12} N)</th>
<th>$K_{33}$ (10^{-12} N)</th>
<th>DE</th>
</tr>
</thead>
<tbody>
<tr>
<td>14.1</td>
<td>7.1</td>
<td>19.1</td>
<td>58.9%</td>
</tr>
<tr>
<td>7.1</td>
<td>7.1</td>
<td>7.1</td>
<td>59.3%</td>
</tr>
<tr>
<td>3</td>
<td>7.1</td>
<td>3</td>
<td>56.5%</td>
</tr>
<tr>
<td>1</td>
<td>7.1</td>
<td>1</td>
<td>49.6%</td>
</tr>
</tbody>
</table>
Fig. 18: Influence of elastic constant on the Electro-Optical response curve. ($\lambda=1550$ nm)
3.4.5 Influence of the pretilt angle

The main effect of the surface pretilt of the director is mainly related to the control of an fringing electric field induced “tilt wall”. Excluding this effect, the effect of the pretilt angle on the DE is small as shown in Fig. 19 and Table 7. Thus, we will use the 3° pretilt configuration in our following discussion.

Table 7: Diffraction efficiency of d=2.5 μm LC OPA for different pretilt angle. (∆τ=1550 nm)

<table>
<thead>
<tr>
<th>Pretilt angle (deg)</th>
<th>1°</th>
<th>3°</th>
<th>5°</th>
<th>10°</th>
</tr>
</thead>
<tbody>
<tr>
<td>DE</td>
<td>53.4%</td>
<td>55.0%</td>
<td>55.6%</td>
<td>56.2%</td>
</tr>
</tbody>
</table>
Fig. 19: Influence of pretilt on the phase vs. voltage curve. ($\lambda=1550$ nm)
3.4.6 Non-symmetrical behavior of the LC OPA

Another effect that has strong effect on the DE of the LC OPA is related to the symmetry of the LC OPA. If the LC OPA is programmed to steer to -1 and +1 diffraction order, the peak intensity or DE is different in these two cases. Two effects could contribute to the broken of symmetry in the LC OPA.

The first one has to do with the interaction of the surface director tilt orientation to the desired phase gradient direction. Due to this effect, the phase profile of the LC OPA corresponding to steering to -1 and +1 diffraction order is not exactly a mirror image of each other, as shown in Fig. 20. The DE for these two cases may be different.

The other effect that contributes to this non-symmetrical behavior is related to the tilting of optical axis in a LC OPA. For example, if we change the sign of the tilt angle every where in the cell, the phase gradient will stay the same, but the diffraction efficiency is not the same. This is caused by the direction of energy flow of light (poynting vector) in LC OPA breaks the symmetric in the system. This effect has been discussed by Chuck 45 for a transmissive LC OPA, where the difference between the DE in the +1 and -1 diffraction order can be as high as 5~10%. In the reflective LC OPA discussed in this section, since light passes through the LC layer twice and thus the difference of DE for steering to -1 order and +1 order are smaller as shown in Table 8.
Table 8: Diffraction efficiency for steering to -1 and +1 diffraction order. (For \( \lambda = 1550 \) nm)

<table>
<thead>
<tr>
<th></th>
<th>d=2.1( \mu )m</th>
<th>d=2.3( \mu )m</th>
<th>d=2.5( \mu )m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Forward voltage ramp to steer to -1 order</td>
<td>60.1%</td>
<td>58.9%</td>
<td>55.0%</td>
</tr>
<tr>
<td>Reverse voltage ramp to steer to +1 order</td>
<td>60.0%</td>
<td>61.0%</td>
<td>57.5%</td>
</tr>
</tbody>
</table>
Fig. 20: Comparison between forward phase ramp and reverse phase ramp of a blazed grating. ($\lambda=1550$ nm) (a) Forward phase ramp that steer beam to -1 diffraction order. (b) Reverse phase ramp that steer beam to +1 diffraction order.
3.4.7 Optimization the voltage control on LC OPA

From the above discussion, by using high birefringence LC material and very thin reflective cell (d=2.5 µm), the performance of the LC OPA improved greatly. The 70.7% efficiency steering angle is 4.2° and the 50% efficiency angle is 8.7°, almost twice of a d=6 µm LC OPA with 70.7% efficiency angle of 1.8° and 50% efficiency angle of 4.3°. However, the DE of such a LC OPA with d=2.5 µm is still not optimized. For steering angle of 7.42°, the DE is 55%. As shown in Fig. 21, the problem lies in the phase error caused by fringing fields induced strong inter-pixel coupling. We can see the phase under pixel number 1 and 2 is much smaller than the desired phase value. Also the phase slope of pixel number 2~8 is larger than the desired phase slope. One way to alleviate this phase error is to optimize the voltage profile on each of the eight pixels. Since no analytical solution is available to guide us for the proper adjustment of voltage on each pixel, a stochastic blind optimization process is used. In the practices, the simulated phase profile is compared with the ideal phase profile. If the phase at the center of a particular pixel is lower than the desired phase profile, the voltage applied to that pixel is adjusted higher; if the phase at the center of the pixel is higher than the desired one, the voltage is adjusted lower. Within several iterations, the phase value on each pixel is closer to the desired phase profile.
Fig. 21: Phase profile of the LC OPA before voltage optimization. The phase under pixel 1 and pixel 2 is much lower than desired value, and phase slope from pixel 3 to Pixel 8 is larger than desired phase slope. Here $\lambda=1550$ nm, $K_{11}=14.1 \times 10^{-12}$ N, $K_{22}=7.1 \times 10^{-12}$ N, $K_{33}=19.1 \times 10^{-12}$ N, $\varepsilon_\parallel=12.1$, $\varepsilon_\perp=4.1$, $n_o=1.50$, $n_e=1.85$, $d=2.5\mu m$, pixel spacing $=1.5 \mu m$, gap between electrode$=0.5 \mu m$, pretilt$=3^\circ$. 
The voltage introduced on each of the electrode for every iteration of our process is listed in Table 9. If we call the difference between the optimized voltage on each pixel in iteration 5 and the original voltage profile on iteration 1 the “bias voltage”. The shape of the bias voltage is of high interest for optimizing the wide angle performance of LC OPA. As shown in Fig. 22, the horizontal axis is the normalized position of each pixel, where the first pixel is defined to be in normalized position 0 and the last pixel is in normalized position 1. We can see in order to optimize the voltage profile, the first pixel has to have a large negative bias voltage, the second pixel has to have a medium positive bias and the last pixel has a large positive bias. The eight discrete bias voltages can be fit very well by a 7th order polynomial. It can also be relatively well represented by an 8th order polynomial. Other order of polynomial fails to give a good fit to the data.

Experimentally, it is difficulty to directly image and measure the phase profile of a high resolution LC OPA with pixel spacing of 1.5 µm to an acceptable accuracy. The knowledge of the shape of the bias voltage is very meaningful that an experimental blind optimization process can be performed. For example, the eight coefficient of 7th order polynomial can be the independent parameter automatically varied by a computer program. For each parameter set, the peak intensity is recorded. The highest DE at far field for particular set of the eight parameters can be obtained as the optimized bias voltage profile. Such bias voltage can be pre-calibrated to obtain higher efficiency for the LC OPA for different steering angle. Such optimization has been carried out experimentally by Scott et al. 49 in a slightly different way, big improvement is reported which illustrated the value of the optimization process.
Table 9: Optimization process of voltage on each electrode

<table>
<thead>
<tr>
<th>Iteration Number</th>
<th>Voltage on each electrode (v)</th>
<th>Electrode Number</th>
<th>DE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>1</td>
<td>1.184</td>
<td>1.577</td>
<td>1.754</td>
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<tr>
<td>2</td>
<td>0.000</td>
<td>1.877</td>
<td>1.954</td>
</tr>
<tr>
<td>3</td>
<td>0.00</td>
<td>1.901</td>
<td>1.963</td>
</tr>
<tr>
<td>4</td>
<td>0.200</td>
<td>2.118</td>
<td>1.792</td>
</tr>
<tr>
<td>5</td>
<td>0.130</td>
<td>2.092</td>
<td>1.792</td>
</tr>
</tbody>
</table>
Fig. 22: Bias voltage to correct for fringing field induced phase error in high resolution LC OPA. Discrete data points are from the optimization process from simulation. The continuous line is the 7th order polynomial fit of the data points. The coefficients for the 7th order polynomial are: $p_1 = 1192.8$, $p_2 = -4439.6$, $p_3 = 6700.6$, $p_4 = -5237.3$, $p_5 = 2236.8$, $p_6 = -500.83$, $p_7 = 49.621$, $p_8 = -1.05$. 
Fig. 23: Optimized phase profile and far field diffraction pattern of a wide angle LC OPA. Simulation parameter used here is: $\lambda=1550$ nm, $K_{11}=14.1 \times 10^{-12}$ N, $K_{22}=7.1 \times 10^{-12}$ N, $K_{33}=19.1 \times 10^{-12}$ N, $\varepsilon_{\parallel}=12.1$, $\varepsilon_{\perp}=4.1$, $n_e=1.85$, $n_o=1.50$. Cell thickness $d=2.3$ μm, electrode width $W=1$ μm, gap between electrode $=0.5$ μm. (a) Optimized phase profile by adjusting voltage profile on the 8 electrodes. (b) Corresponding far field diffraction pattern
The phase profile of the wide angle LC OPA after optimization and the corresponding far field diffraction pattern is shown in Fig. 23. The DE of the wide angle LC OPA after such optimization is 72.7%. The optimization process improved the DE of the LC OPA by 18%. This is clearly seen in Fig. 24, of the DE of a wide angle LC OPA as a function of cell thickness before and after voltage optimization. For a LC OPA with cell thickness larger than 4 µm, the improvement of the DE can be as large as 30%, or a factor of 2 as compared with the DE before voltage optimization. With thinner cell, because the fringing field effect is less strong, the DE improvement is less apparent. However, even for a d= 2.5 µm LC OPA, the DE improved by 17.7% after voltage optimization. The calculated diffraction efficiency as a function of cell thickness can be fit according to Equ. 36. For cases where no voltage optimization process is carried out, the coefficient $a$ is 1.4. However, for cases where voltage optimization is carried out, the coefficient $a$ is 0.8. $\beta$ is 0.7 for all cases.

A comparison between the diffraction efficiency as a function of steering angle (and corresponding pixel spacing) for different wide angle LC OPA is shown in Fig. 25. For the optimized design, the 70.7% efficiency angle is 7.7° and the 50% efficiency angle is 14.4°, which is more than tripled the value of the LC OPA with d=6 µm.
Fig. 24: Comparison of diffraction efficiency as function of cell thickness without voltage optimization and with optimization. Simulation parameter used here is: $\lambda=1550$ nm, $K_{11}=14.1 \times 10^{-12}$ N, $K_{22}=7.1 \times 10^{-12}$ N, $K_{33}=19.1 \times 10^{-12}$ N, $\varepsilon_{\parallel}=12.1$, $\varepsilon_{\perp}=4.1$, $n_e=1.85$, $n_o=1.50$, pixel spacing $=1.5$ µm, gap between electrode $=0.5$ µm and pretilt=$3^\circ$. 

![Diffraction Efficiency Graph](image-url)
Fig. 25: Comparison of diffraction efficiency as function of (a) Pixels Spacing (top figure) (b) steering angle (bottom figure) for LC OPA with voltage optimization and without optimization. Simulation parameter used here is: $\lambda=1550$ nm, $K_{11}=14.1 \times 10^{-12}$ N, $K_{22}=7.1 \times 10^{-12}$ N, $K_{33}=19.1 \times 10^{-12}$ N, $\varepsilon_{\parallel}=12.1$, $\varepsilon_{\perp}=4.1$, $n_e=1.85$, $n_o=1.50$, pixel spacing =1.5 $\mu$m, gap between electrode =0.5 $\mu$m and pretilt=$3^\circ$. 
3.4.8 1-D LC OPA with pinned electrodes

From the above discussion, it is clear that even after the optimization of the liquid crystal cell design, liquid crystal material and the control voltage, the diffraction efficiency and angle of the LC OPA is still very low. This limits the potential of the LC OPA for a broad range of application where the diffraction angle of the tunable diffractive optical elements needs to larger than 10°. Although the optimization process can alleviate the fringing electric field effect’s influence on the diffraction efficiency of the LC OPA to some extent, it cannot substantially defeat the fundamental mechanism of the fringing electric field. A method that can defeat the mechanism of the fringing electric field would be precious to enable tunable diffractive optical element’s application in wide angle beam steering, electronic holography, optical tweezers, optical pattern recognition.

Is there any solution to this problem? If we look carefully at the phase profile the LC OPA as shown in Fig. 23(a), it is clear that a serious reduction in the phase modulation depth of the LC OPA comes from the lowest voltage electrode. The fringing electric fields induced strong inter-pixel coupling, so the LC director in this region sees a much higher voltage than the desired one. If we can somehow fix the director configuration of the LC material within this region, and prevent the higher than desired voltage to reorient the liquid crystal director, we can prevent the reduction in the phase modulation profile. Or, in another word, defeat the fringing electric field’s influence on the diffraction efficiency of the LC OPA.
This is achievable by adding a small percent (5~10%) of reactive monomer and photo-initiator into the liquid crystal material, and expose the regions that correspond to the low voltage pixels on the LC OPA to UV exposure. Such process of making a LC OPA with polymer wall in certain position is shown in Fig. 27. Only the photo-initiator under this region will produce reactive free radicals under UV exposure, which will cause the polymerization process to happen in these localized regions. As the photo-polymerization process goes on, reactive monomers and photo-initiator in this region will be consumed by the polymerization process, reactive monomers and photo-initiator in the neighbouring region will diffuse into this region to fuel further polymerization process. After the polymerization process completes, a polymer network wall will form within these regions with UV exposure. The polymer chains in these regions will be crosslinked, and the liquid crystal director in this region will be fixed by the polymer chains. In this case, even if there are higher voltage than desired due to the fringing electric field, the liquid crystal director cannot resonate to such field due to the very high elastic energy required to deform the polymer network. Such that the phase profile of the LC OPA under selective pixels is preserved by the polymerization process. We call this approach a pinned electrode LC OPA approach.
Fig. 26: The comparison of the phase profile and director configuration of a transmissive LC OPA with and without pinned electrode. Here $\lambda=1550$ nm, $K_{11}=14.1 \times 10^{-12}$ N, $K_{22}=7.1 \times 10^{-12}$ N, $K_{33}=19.1 \times 10^{-12}$ N, $\varepsilon_\parallel=12.1$, $\varepsilon_\perp=4.1$, $n_e=1.7100$, $n_0=1.5076$. pixel spacing =0.6 µm, gap between electrode=0.4 µm, cell thickness $d=7.5$ µm and pretilt=3°.

(a) (b) LC OPA without pinned electrode. (c) (d) LC OPA with pinned electrode
The practical issue regarding forming such a polymer wall is related to the ratio of the height of the wall and the width of the wall. Consider a LC OPA for 1550 nm, the height of the wall needs to be about 7−10 µm for a transmissive LC OPA or 4−6 µm for a reflective LC OPA. However, for wide angle LC OPA that can deflect beam to larger than 10°, the width of electrode is usually less than 1.5 µm. In this case, the height/width ratio of the wall is larger than 1. One possible solution is to add inhibitor to the liquid crystal and monomer mixture before photo-polymerization. This helps to prevent premature polymerization to happen in the non-pinned electrode region, and to get a more well defined polymer network wall in the pinned electrode region.
Fig. 27: Method of producing polymer wall in a LC OPA
The advantage of the pinned electrode LC OPA is apparent. As shown in Fig. 26, the above mentioned pinned electrode LC OPA approach can be studied by liquid crystal director simulation. In case a and b, a conventional LC OPA with no pinned electrode is shown. The diffraction efficiency for this case is 34.3% for 7.4° diffraction angle. In case c and d, a LC OPA with pinned electrode is shown. The shadowed region is the polymer network region and the orientation of the LC director is fixed. On the high voltage electrode side, the phase modulation depth is still not perfect. However, higher voltage can be applied to this electrode to improve the phase modulation depth, as long as no twist defect will form in the device and the director will remain in the rubbing plane. With this approach, the phase modulation depth of the LC OPA can be substantially improved. The diffraction efficiency increases by more than two fold to 82.8% for the same diffraction angle. As we can see from Table 10, even for a transmissive LC OPA (a transmissive LC OPA normally have lower diffraction efficiency than a reflective LC OPA), the 70.7% diffraction angle improved substantially over no pinned electrode approach.

Table 10: Comparison of different wide angle LC OPA (λ=1550 nm)

<table>
<thead>
<tr>
<th></th>
<th>Off the shelf LC material</th>
<th>High Δn LC</th>
<th>High Δn LC+ voltage optimization</th>
<th>Pinned Electrodes</th>
<th>Ideal LC OPA</th>
</tr>
</thead>
<tbody>
<tr>
<td>70.7% efficiency angle</td>
<td>1.8°*</td>
<td>4.4°*</td>
<td>7.7°*</td>
<td>17°+</td>
<td>32°+</td>
</tr>
</tbody>
</table>

* Reflective LC OPA, + Transmissive LC OPA
However, in the above comparison, one may argue that the cell thickness of the two LC OPAs are not optimized to their best performance. We consider only the case where the thickness of both is the nominal thickness of $d^*$, where $\Delta n d^* = \lambda$, where $\Delta n$ is the birefringence of the liquid crystal cell, and $\lambda$ is the operation wavelength. As we previously reported, the highest efficiency configuration of the LC OPA with no pinned electrode corresponds to when the thickness of the LC OPA $d$, is slightly smaller than the nominal thickness of the cell $d'$. And in the case of the pinned electrode LC OPA, the highest efficiency configuration corresponds to when the cell thickness of the LC OPA $d$, is slightly larger than the nominal thickness of the LC OPA $d'$. To make a fair comparison, we consider a transmissive LC OPA where the nominal cell thickness of the LC OPA is $d$=6µm. The material birefringence of the liquid crystal material is $\Delta n$ =0.25, and the pixel spacing is fixed to be 1µm and the number of steps in each blaze ranges from q=4~60, so the diffraction angle ranges from 22.8° to1.48°. Different thickness of each LC OPA is considered for 5µm, 6 µm and 7µm to optimize the performance. The maximum diffraction efficiency corresponds to each case is obtained by numerical modeling that optimize the voltage applied to each electrode. The results are shown in Fig. 28. Even considering the variation in the cell thickness, the pinned electrode LC OPA still has substantially higher efficiency. Especially at angle of larger than 20°, the efficiency of the pinned electrode LC OPA can be 4~8 times higher than the conventional LC OPA. This approach may enable a wide variety of application of tunable diffractive optical element that are conventionally not achievable.
Fig. 28: The comparison of maximum diffraction angle for LC OPA with and without pinned electrode ($\lambda = 1550$ nm)
However, there is also complications associated with this approach. In a conventional LC OPA, the deflection of laser beam to different angle is achieved by changing the period of the blazed grating. With the pinned electrode approach, the liquid crystal director configuration is fixed periodically, which means the period of the grating is fixed. If an arbitrary diffraction angle is desired, there will be phase mismatch at the phase jumps. An additional phasing LC OPA with electrode width equal to the grating period of the pinned electrode LC OPA will be required to match the phase of each blaze.
3.5 Wide angle 1-D LC OPA with rubbing direction parallel to the electrodes

3.5.1 Polarization effect in a LC OPA with rubbing direction parallel to the electrodes

In the case where the rubbing direction is parallel to the line shape electrode of the 1-D LC OPA as shown in Fig. 11 (b), the rubbing direction of the LC OPA is in the YZ plane. The fringing electric field could reorient the director to out of rubbing plane direction (See Fig. 12 (b)), thus strong polarization effect could happen. If an incident light $E_y$ is polarized along the rubbing direction of the LCOS SLM, as light propagates through the device, the output light contains both polarization, as shown in Fig. 13 (b). The polarization effect is very strong when the pixel spacing is much smaller than the cell thickness of the device. For example, the case we considers in Fig. 12 (b) and Fig. 13 (b) is such a worst case.

We can use Extended Jones calculation to try to model the polarization effect in such LC OPA, for example, a LC OPA with eight pixel/blaze is considered, the thickness of the device is $d=6\mu m$, with LC material MLC6080 being used, the electrode width is $8\mu m$ and the gap between electrodes is $0.5\mu m$. Light polarized along the rubbing direction (p-polarized input light) is considered. From the Extended Jones calculation, we can see there are two none zero polarized output light, due to the polarization effect. The phase of the output light after passing through the device is shown in Fig. 29. In case (a), the output p-polarized light with polarization along the rubbing direction is shown. The phase profile for p-polarized light is a stair like blazed grating. However in case (b), the phase for the output s-polarized light is shown. This polarization of light is the depolarized part of the light and the phase profile is not a very good phase grating.
Fig. 29: Phase of the light passing through a LC OPA with rubbing parallel to the electrodes. ($\lambda=1550$ nm) (Input light has only p-polarization, the output light contains both polarization). (a) Output p-polarization (polarization along the rubbing direction). (b) Output s-polarization (polarization perpendicular to the rubbing direction). Eight pixel/blaze, $d=6\mu$m, MLC6080, electrode width =8\mu$m, gap between electrodes =0.5\mu$m.
Fig. 30: Intensity of the light ($\lambda=1550$ nm) passing through a LC OPA with rubbing parallel to the electrodes (Input light has only p-polarization, the output light contains both polarization). (a) Output p-polarization (b) Output s-polarization.
In Fig. 30, the intensity of the light for both polarization is shown. It is clear that serious polarization only happens at regions close to the phase resets where the out of rubbing plane director component is present. In the other inter-pixel regions, only small amount of polarization is also observed.

If we use a more accurate method, the FDTD simulation to study the light propagation in such complex structure. In Fig. 31, light propagation in such a reflective LC OPA is shown. The field distribution is much more complex than a transmissive LC OPA as shown before because we considered a worst case with very strong polarization effect. The phase of light and intensity distribution is not very similar to what Extended Jones calculated. This is especially true for cases where the pixel spacing of the LC OPA is close to the wavelength of light. Most importantly, the wavefront of the light passing through the device is not very well matched from one blaze to another. This is due to the fact the twist structure of the LC OPA lowered the total phase modulation of the device.

Due to the fact the twist structure changed the phase profile of the LC OPA, the phase reset on such LC OPA is no longer one wave for 1550 nm light. Strong zero order diffraction peak is present for p-polarized output light, as shown in Fig. 32(b).
Fig. 31: FDTD simulation of light ($\lambda=1550$ nm) propagation in a reflective LC OPA with very strong polarization effect (Input light is p-polarized or along Y axis). (a) Near field of the output s-polarization light. (b) Near field of the output p-polarization light.
Fig. 32: Far field diffraction pattern of the two output polarization of light ($\lambda=1550$ nm) for a LC OPA with very strong polarization effect. (a) Output s-polarization light. (b) Output p-polarization.
3.5.2 Diffraction efficiency of an 1-D LC OPA with rubbing direction parallel to the electrodes

To compare the diffraction of the 1-D LCOS SLM with rubbing direction parallel to the electrode and perpendicular to the electrode, the diffraction efficiency of the two cases of 1-D LCOS SLM (With no voltage optimization) is plotted as a function of the pixel spacing in Fig. 33. The diffraction efficiency for a 1-D LCOS SLM with parallel rubbing is about 5%~15% lower than the case of perpendicular rubbing. There are two reasons associated with such drop in the diffraction efficiency. The first one the parallel rubbing case has polarization effect associated with the LCOS SLM structure. For example, in Fig. 34, the polarization ratio of the LCOS SLM with parallel rubbing is shown. Another possible effect is that due to the out of plane structure of LC director, the phase profile of the LCOS SLM is not accurate any more. Relatively smaller phase modulation depth is observed, which lower the diffraction efficiency further more.

Like previous case, voltage optimization can be carried out for 1-D LCOS SLM. The diffraction efficiency for 1-D LCOS SLM with both parallel and perpendicular rubbing improved substantially. The voltage optimization improvement is more substantial for LCOS SLM with small pixel spacing. The results are shown in Fig. 35.
Fig. 33: The comparison of diffraction efficiency for 1-D LCOS SLM with rubbing direction perpendicular to electrodes and parallel to electrodes (no voltage optimization, $\lambda=1550$ nm).
Fig. 34: Comparison of polarization ratio for 1-D LCOS SLM with rubbing direction parallel to electrodes (no voltage optimization, $\lambda=1550$ nm).
Fig. 35: The comparison of diffraction efficiency for 1-D LCOS SLM with rubbing direction perpendicular to electrodes and parallel to electrodes (with voltage optimization, $\lambda=1550$ nm).
3.6 Optical defect formation and diffraction efficiency for a 2-D LC OPA

A 2-D LC OPA is a pixilated liquid crystal device that can generate a random phase modulation profile within a clear aperture. It is sometimes referred to as a Spatial Light Modulator (SLM), for example, a 1024 × 768 resolution Liquid Crystal on Silicon (LCOS) device discussed in Chapter 4. The efficiency of such device highly depends on the phase pattern generated on such device. However, it is possible to estimate the reasonable range of the diffraction efficiency of a 2-D LCOS SLM, for a particular phase modulation pattern. The two extreme cases of 1-D LC OPA as in Fig. 33, discussed in the previous section, gives the upper and lower value of the range of the diffraction efficiency for a 2-D LCOS SLM. However, some efficiency estimation assumes there will be no “twist wall” formation in such device.

However, the fringing electric field between pixel may cause liquid crystal director to have out of rubbing plane components, which depolarized the input light. The “twist wall” in a 2-D LCOS with 3×3 array of pixels is shown in Fig. 36, where the device is observed under a crossed polarizer. (the electrode size is 2 μm and the inter-pixel gap is 0.4 μm. The cell thickness of the LCOS SLM is 4 μm. ) Within these two regions, the director configuration of the “twist wall” is shown in Fig. 37, where the LC director follows the direction of the electric field. The director component of $n_y$ and $n_z$ is plotted across the XZ plane.
Fig. 36: Polarization effect in 2-D LCOS SLM with small pixel spacing. $\lambda=1550$ nm) (a) Voltage applied to the center pixel is 1.2v; the voltage applied to all other pixel is 2.35v. (b) Voltage applied to the center pixel is 0v; the voltage applied to all other pixel is 5v.
The voltage difference between the neighbouring pixels has strong influence on the formation of the “twist wall”. For example, if the voltage applied to the central pixel in Fig. 36 is $V_1$ and the voltage applied to the other eight pixels are $V_2$. When $V_1=1.2\, \text{v}$ and $V_2=2.35\, \text{v}$, the voltage difference between the neighboring electrode is small, no defect is observed and the polarization effect is small. However, when $V_1=0\, \text{v}$ and $V_2=5\, \text{v}$, a “Twist wall” on both side of the center pixel is observed, the polarization effect is strong. A summery of the influence of voltage difference between the neighboring pixel on the polarization effect of a 2-D LCOS SLM is shown in Table 11.

**Table 11: Polarization effect in 2-D LC SLM**

<table>
<thead>
<tr>
<th>Case</th>
<th>Pixel size (µm)</th>
<th>Gap size (µm)</th>
<th>Voltage $V_1$ (v)</th>
<th>Voltage $V_2$ (v)</th>
<th>Trapped tilted wall observed</th>
<th>Average light leakage through center pixel</th>
</tr>
</thead>
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<tr>
<td>1</td>
<td>16</td>
<td>1.6</td>
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</tr>
<tr>
<td>2</td>
<td>8</td>
<td>0.8</td>
<td>0</td>
<td>5</td>
<td>Yes</td>
<td>17.0%</td>
</tr>
<tr>
<td>3</td>
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<td>5</td>
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</tr>
<tr>
<td>4</td>
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<td>0.4</td>
<td>0</td>
<td>5</td>
<td>Yes</td>
<td>13.5%</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>0.4</td>
<td>1.25</td>
<td>2.3</td>
<td>No</td>
<td>1.07%</td>
</tr>
<tr>
<td>6</td>
<td>1</td>
<td>0.4</td>
<td>1.25</td>
<td>2.3</td>
<td>No</td>
<td>0.2%</td>
</tr>
</tbody>
</table>

The formation of the trapped wall also depends on the pixel size of the LCOS SLM. When the pixel size is larger than 8 µm, the “Twist wall” is pushed to the edge of the active area, and the influence of such wall is very small. For example, this is shown in the polarization effect in a 16 µm LCOS SLM in Fig. 38. However, for a pixel size of smaller than 8 µm, the trapped wall is in the active area of the pixel and will have influence on the efficiency.
Fig. 37: LC director component of ny and nz in the XZ plane. (a) Voltage applied to the center pixel is 1.2v; the voltage applied to all other pixel is 2.35v. (b) Voltage applied to the center pixel is 0v; the voltage applied to all other pixel is 5v.
Fig. 38: Polarization effect in a LCOS SLM with large pixel spacing of 16.5 µm.
3.7 Conclusion

Fundamental physics behind different possible configuration of 1-D and 2-D LC OPA is studied by numerical modeling, which shows a LC OPA with ideal director configuration can deflect light to over 40.5° with an efficiency of 50%. The basic idea of a LC OPA is promising, however, the major limitation of the diffraction efficiency for a real LC OPA is the fringing electric field effect. The influence of such effect in different configuration of 1-D and 2-D LC OPA is studied by accurate modeling the 3-D LC director configuration and Finite Difference Time Domain (FDTD) simulation. Many possible methods to alleviate the fringing electric field effect, or to defeat its mechanism is proposed. Optimization the design of a wide angle LC OPA, form the material selection, voltage optimization, device configuration etc can substantially improve the performance of the LC OPA. A variety of application can benefit from such study. Possible defeat formation mechanism in high resolution LC OPA is also studied.
Chapter 4

Liquid Crystal Spatial Light Modulator for advanced wavefront control

4.1 Introduction

In Chapter 3, we have discussed the performance limitation of the LC OPA, which is a tunable diffractive optical element with 1-D array element. In this chapter, a tunable diffractive optical element with 2-D array element (often referred to as LC Spatial Light Modulator (SLM)) and its application in free space laser communication will be discussed. We place our main focus in aberration correction of large aperture telescope using such element. However, many other applications can benefit from a high resolution 2-D tunable diffractive optical element too. We try to address the basic properties of such LC DOE that are applicable to all applications such as the Electro-Optical response, the optical quality of such device, the diffraction efficiency and the polarization effect etc.

A LC SLM can be used to correct for large aberration in an optical system by spatially introducing a programmable phase delay to the optical beam. This is beneficial for an optical system designer because although minimizing the aberration in the optical system is always an optical designer’s primary goal, in some circumstances, to keep the aberration of the optical element within tolerance will make the whole system too chunky, expensive, or complicated for practical considerations. One good example is in the space deployable large optics, where extremely light weighted large aperture telescope is required to maintain a small beam divergence for the long distance free space laser
communication. Ideally, the primary optical element of the laser communication transmitter can be a reflective surface made of a membrane type of material coated with highly reflective coating. This allows the large optical element to be extremely lightweight, folderable, and inflectable for convenience of deployment of such a large aperture telescope in space. However, the vibration, thermal expansion, mechanical stress and manufacturing imperfection can seriously reduce the surface accuracy of the primary mirror, thus introduce large aberration to the telescope. 

There are several types of wavefront correction devices that potentially have the ability to address this issue, for example the deformable mirror, Microelectromechanical systems (MEMS) etc. The LCOS SLM is very suitable for active correction of aberration introduced by the primary optical element of the laser communication transmitter because the advantage of a liquid crystal based device lies in its low cost, high resolution, low profile, lightweight and its capability of handling medium to high laser power at low power consumption. Active laser beam control such as random-access beam pointing, multipole beam control, dynamic focus/defocus of laser beam as well as agile beam steering can be achieved simultaneously by programming the desired wavefront to the laser beam. A free space laser communication transmitter based on above concept can greatly reduce the tolerance requirement of the large expensive optics and improve the capability of the system as well.
4.2 Performance of the Liquid Crystal Spatial Light Modulator

4.2.1 Electro-Optical response of the LC SLM

For all phase modulation applications of LC SLM, it is very important to accurately modulate the phase of light to achieve excellent optical quality. However, the manufacturing process of a liquid crystal device may give rise to many issues. For example, the thickness of the liquid crystal layer may not be exactly the same across the clear aperture of the device, so the response of the LC SLM has some spatial non-uniformity. For different LC SLM device, the liquid crystal layer thickness is not exactly the same, so the response of the device has to be calibrated one by one. An imaging system that can measure the response of the LC SLM spatially is very helpful in accurately calibrating the LC SLM. As shown in Fig. 39, such a system consists of several major parts. The first one is the laser source and the beam expansion system to deliver the required beam waist. The second part is a Soleil-Babinet compensator (an adjustable birefringence retarder) and the sample LC SLM to measure place in between crossed polarizer. The polarizer and analyzer in the system is at 45° and -45° with respect to horizontal direction; the fast axis of the Soleil-Babinet compensator and the LC SLM is at 0° and 90° respectively. The third part of the system is a computer controlled digital camera and the frame grabber to record the transmitted intensity of beam through the crossed polarizer.
Fig. 39: A 2-D birefringence imaging system that can measure the Electro-Optical response of the LC SLM
There is a simple algorithm to measure the retardation of a birefringent material with such system, based on the principle that when the total retardation in between the crossed polarizer is zero, the transmission of the crossed polarizer is at minimum. However, when the LC SLM has non-zero birefringence, one can adjust the Soleil-Babinet variable retarder so the total retardation on the Soleil-Babinet compensator is of the same magnitude as the LC SLM but of opposite sign. In this case, minimum transmission is observed at the CCD camera and the retardation value of the LC SLM is obtained.

However, such simple algorithm didn’t work very efficient for a sample with large non-uniformity, because it is impossible to adjust the variable retarder to minimize the transmission for all position across the clear aperture of the LC SLM. A more robust algorithm is similar to a five step phase shifting interferometer fringe analyze algorithm \(^{61}\), while introducing a phase retardation of 0, π/2, π, 3π/2, 2π on the Soleil-Babinet compensator, seven frame of images of the transmitted intensity image is recorded by the CCD camera. The intensity for each frame of image can be expressed in Equ. 4.1 for a birefringent sample placed between crossed polarizer with optical axis along 45° of the polarizer.

\[
I(x, y) = \cos^2 \left( \frac{\tau(x, y)}{2} \right) = \frac{1}{2} + \frac{1}{2} \cos(\tau(x, y)) \tag{4.1}
\]

Here \(\Gamma(x,y)\) is the total retardation of the sample in between the cross polarizer. Since in our setup, two birefringence sample is present, the first is the Soleil-Babinet compensator, the second one is the LC SLM. In this case, the total transmission can be expressed as:
\[ I(x, y) = I_o(x, y) + \frac{1}{2} I_1(x, y) \cos(\tau_{\text{LCSLM}}(x, y) + \tau_{\text{SB}}(x, y)) \] (4.2)

Here \( I_o(x, y) \) is the background intensity, \( I_1(x, y) \) is some constant term, \( \tau_{\text{LCSLM}} \) is the retardation on the LC SLM, and \( \tau_{\text{SB}} \) is the retardation on the Soleil-Babinet compensator.

When the retardation introduced on the Soleil-Babinet compensator is from 0 to 2\( \pi \), Equation 4.2 can be a series of Equations

\[
\begin{align*}
I_1(x, y) &= I_o(x, y) + I_1(x, y) \cos(\tau_{\text{LCSLM}}(x, y)) & \tau_{\text{SB}} &= 0 \\
I_2(x, y) &= I_o(x, y) - I_1(x, y) \sin(\tau_{\text{LCSLM}}(x, y)) & \tau_{\text{SB}} &= \frac{\pi}{2} \\
I_3(x, y) &= I_o(x, y) - I_1(x, y) \cos(\tau_{\text{LCSLM}}(x, y)) & \tau_{\text{SB}} &= \pi \\
I_4(x, y) &= I_o(x, y) + I_1(x, y) \sin(\tau_{\text{LCSLM}}(x, y)) & \tau_{\text{SB}} &= \frac{3\pi}{2} \\
I_5(x, y) &= I_o(x, y) + I_1(x, y) \cos(\tau_{\text{LCSLM}}(x, y)) & \tau_{\text{SB}} &= 2\pi
\end{align*}
\] (4.3)

With these five equations, the retardation value of the sample can be obtained as:

\[
\tau_{\text{LCSLM}}(x, y) = \tan^{-1}\left( \frac{2(I_4(x, y) - I_2(x, y))}{2I_3(x, y) - I_1(x, y) - I_5(x, y)} \right) \] (4.4)
Fig. 40: 2-D birefringence map across the active area of LC SLM at zero voltage applied to the LC SLM.
According to Ref.\textsuperscript{67}, in order to obtain accurate retardation value, a five step phase shifting algorithm is the minimum requirement. More accurate algorithm that has more phase shifting steps can be used such as seven steps phase shifting algorithm and thirteen steps phase shifting algorithm etc. is used in our system. The accuracy of such seven steps algorithm is estimated to be higher than $\lambda/100$ \textsuperscript{67}. With such 2-D birefringence measurement system, for each driving voltage on LC SLM, the 2-D birefringence map can be obtained as shown in Fig. 40. An array of 100×100 points across the device is shown in the measurement. The retardation value is slightly different on different parts of the device due to non-uniformity in cell gap, rubbing etc. Different voltage can be applied to the LC SLM, and the 2-D birefringence map is measured with similar procedure. Because the test device we use here is a LC SLM based on Liquid Crystal On Silicon (LCOS) device. The driver we used a display driver, where instead of directly specify the voltage needs to apply to each pixel of the LCOS device, a grayscale level of 0–255 is applied. Such grayscale range corresponds to a voltage range of 1.3v~3.5v. Depending on the Gamma correction and display setting used in the control computer, the voltage range may vary slightly. For different grayscale (or voltage) applied to the LCOS device, the maximum peak to valley non-uniformity is not the same. In Fig. 41, such dependence of non-uniformity as function of grayscale is shown. For the middle range between grayscale 120~180, the non-uniformity is apparently higher than other parts. The reason is that at low grayscale, the tilt of LC director in the bulk is small, so the non-uniformity is comparable to that of zero voltage stage. At high grayscale, because the LC director is aligned close to perpendicular to surface, LC close to the surface layer
contribute mostly to the retardation variation. In this case, the effective refractive index is close to ordinary extraordinary refractive index $n_o$ of LC material, so the difference between the two is very small compared with zero voltage stage. In this case, even for the same mount of orientation variation in LC director, the non-uniformity will be smaller than zero voltage stage. For grayscale in the middle range, since the LC director orientation is most sensitive to applied voltage, and the difference between effective extraordinary refractive index and ordinary refractive index is still large, the cumulative retardation non-uniformity is more susceptible to non-uniformity for example voltage non-uniformity, cell gap non-uniformity etc.

Another observation is that some less than 1% de-polarization is observed in the middle grayscale range, where out of plane director component is most apparent. This is partially due to the fact that LC director twist configuration is formed in the cell because of fringe field effect from adjacent activated pixels, which also explains why the maximum non-uniformity is the largest in the middle voltage range. Nevertheless, the device is very uniform as the maximum retardation non-uniformity across the LCOS device is very small of less than $\lambda/12$ peak to valley at 632.8 nm for any given grayscale.

We plot the retardation of the LCOS for each voltage as a function of the grayscale applied to the device. Such retardation versus grayscale curve is then the Electro-Optical curve for each position on the LCOS device. Another manual measurement which measures only the central part of the device is also carried out as in the first algorithm. The two algorithm agrees with each other perfectly and the results is shown in Fig. 42.
Fig. 41: Non-uniformity of LCOS device for different grayscale: The maximum peak to valve birefringence difference as function of the grayscale.
Fig. 42: Electro-optical response of the LCOS device for different measurement results.
M1, M2: Precision mirror

F1: Neutral density filter    P: Polarizer    R: $1/2\lambda$ retarder

L1: Precision objective M-20X    F2: Pinhole    L2: Lens NT45-418

M3: Piezo mirror with LVPZT nano positioning system

BS: Nonpolarizing beam splitter plate    L3: Imaging lens

Fig. 43: Phase shifting interferometer setup
4.2.2 Interferometer measurement of aberration introduced by LCOS backplane

To perform aberration correction for optical element or system, it is important to be able to measure the aberration with an accuracy of at least a fraction of wavelength. Several techniques can be used such as a wavefront sensor based on microlens array, curvature sensor, phase contrast method etc. However, these methods have drawbacks that they are relatively indirect and the spatial resolution of the measurement is low. They are not very suitable for cases where high order aberration is present in the system. A conventional method in measuring aberration is by interferometric method. This method can sample the wavefront at a very high resolution, which is ideal for our application where high spatial frequency aberration can be corrected with a high resolution LCOS device.

In our setup, a Michelson interferometer is used to measure the aberration introduced by optical component. Since such method is well know, we will not go in to details in discussion the measurement system, any basic optics book has discussion regarding different types of interferometer and their characteristics. The system setup is shown in Fig. 43. Interferograms are taken for each phase shifting steps and recorded by the CCD camera. A seven step 60° shift algorithm has been used to reconstruct the phase profile as in Ref. 67. Phase unwrapping is performed to take out the discontinuity of phase profile and the obtained wavfront map is filtered with 4×4 Wiener adaptive noise removal filter to reduce high frequency noise of the phase profile.
Fig. 44: One frame of interferogram captured by the CCD camera for beam reflected from LCOS. ($\lambda$=632.8 nm) (a) Non-compensated beam with aberration present. (b) Compensated beam with aberration removed. (c) Compensated beam with aberration removed and linear tip-tilt added to the phase ramp on LCOS to steer beam to 0.6 mrad.
Fig. 45: Measured wavefront aberration introduced by the surface deformation of the LCOS backplane.
Table 12: Zernike mode of the transmitted wavefront aberration introduced by surface deformation of silicon backplane of the LCOS device. Here we use Fringe Zernike polynomials developed by University of Arizona, which is a subset of standard Zernike polynomial with the terms of the Zernike mode arranged in a different order.

<table>
<thead>
<tr>
<th>Zernike term</th>
<th>Order</th>
<th>waves</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Piston</td>
<td>0</td>
<td>4.5913</td>
</tr>
<tr>
<td>2 Tilt</td>
<td>1</td>
<td>-0.0267</td>
</tr>
<tr>
<td>3 Tilt</td>
<td>1</td>
<td>0.2328</td>
</tr>
<tr>
<td>4 Focus</td>
<td>1</td>
<td>4.4795</td>
</tr>
<tr>
<td>5 Astig.</td>
<td>2</td>
<td>-2.9831</td>
</tr>
<tr>
<td>6 Astig.</td>
<td>2</td>
<td>0.1839</td>
</tr>
<tr>
<td>7 Coma</td>
<td>2</td>
<td>-0.4421</td>
</tr>
<tr>
<td>8 Coma</td>
<td>2</td>
<td>0.0257</td>
</tr>
<tr>
<td>9 Spherical</td>
<td>2</td>
<td>-0.0573</td>
</tr>
<tr>
<td>10 Astig.</td>
<td>3</td>
<td>-0.0204</td>
</tr>
<tr>
<td>11 Astig.</td>
<td>3</td>
<td>-0.0679</td>
</tr>
<tr>
<td>12</td>
<td>3</td>
<td>0.0442</td>
</tr>
<tr>
<td>13</td>
<td>3</td>
<td>-0.0103</td>
</tr>
<tr>
<td>14 Coma</td>
<td>3</td>
<td>-0.0097</td>
</tr>
<tr>
<td>15 Coma</td>
<td>3</td>
<td>-0.0105</td>
</tr>
<tr>
<td>16 Astig.</td>
<td>3</td>
<td>-0.0378</td>
</tr>
</tbody>
</table>
In Fig. 44, one frame of interferogram is shown for the transmitted wavefront aberration introduced by the surface deformation of the LCOS device. The LCOS backplane is made of thin layer of silicon substrate and it is very easy to deform in the manufacturing process. For this particular device, the wavefront aberration introduced is 18.7 peak-valley waves at 632.8 nm, or 3.97 waves r.m.s. Some other devices have about 1~2 waves of aberration have been observed. The measured aberration map is shown in Fig. 45. When such aberration is decomposed into Fringe Zernike polynomial components as shown in Table 11, the dominant Zernike terms are the primary defocus and the primary Astigmatism along X axis.

4.2.3 Wavefront correction for aberration introduced by LCOS backplane

By combining the Electro-Optical curve of the LCOS device and the measured wavefront map, a conjugate compensation image is generated and displayed on the LCOS device. Since the effective stroke length of the device is 1 wave, the modulo-2π version of the conjugate image is used as shown in Fig. 46. In the previous chapter, we have discussed the influence of the phase reset to the diffraction efficiency. Since a LCOS with $1024 \times 768$ resolution is used in the experiments, 18 waves of aberration will not introduce serious loss of efficiency to the system. However, such diffraction effect could influence the subsequent wavefront measurement by introducing some noise at the reset pattern. Because light diffracted from the resets does not satisfy the requirement for our phase shifting algorithm.
Fig. 46: Correction phase ramp introduced on LCOS SLM to compensate for the wavefront aberration introduced by the surface deformation of the silicon backplane.
Fig. 47: Measured residual aberration after second step of wavefront compensation.
When the wavefront correction is turned on, the residual wavefront after a first compensation is measured again and the residual wavefront map is shown in Fig. 47. The peak is around 0.6 waves P-V. Such wavefront compensation is far from ideal due to the complexity of the wavefront evolved. The residual wavefront is added to the original wavefront and a second compensation image is generated the same way. After the second compensation, the residual wavefront is measured as 0.11 waves (P-V) and 0.032 waves RMS at 632.8 nm. One frame of the interferogram after wavefront correction is shown in Fig. 44(b). From the near field wavefront quality point of view, diffraction limited aberration correction is realized after the second compensation. However, a very week ring like structure is observed in residual wavefront map. This is due to the 1.4% front surface reflection as well as small diffraction from the reset region. Such noise is very small and can be neglected for our discussion.

4.2.4 Beam steering after aberration correction

After the compensation for the surface shape of the LCOS backplane, additional tip and tilt is added to the phase map to further steer the laser beam. The new phase plate serves as a dual purpose: correction of surface deformation due to the silicon backplane and steering the laser beam. Fig. 44(c) is shown the interferogram when an additional tip-tilt is added to the wavefront. We can see very good parallel fringes are present in the system which corresponds to only tip-tilt to the wavefront.

An important parameter regarding the performance of the LC OPA is the quality of beam transmitted through the device. This is studied by first focusing the beam reflected
from the LCOS with a 3-inch clear aperture small numerical aperture lens (effective focal length=1170 mm) and measuring the far field beam profile at the focus of the lens. This method of measuring the far field can spatially separate high spatial frequency component due to diffraction from resets. Thus, more faithful representation of the beam profile at infinity far field can be obtained. The intensity profile at focus is recorded with both CCD camera and beam profiler from Photo-Inc. With the absence of the LCOS in the optical system, the far field beam waist was 1.11\times \text{diffraction limited beam waist}. (The diffraction limited beam waist is 89.6 \mu m) Thus, the optical system is close to aberration free.

It is been observed that once the LC OPA is programmed to have complicated diffraction pattern on, air turbulence in the lab environment has strong effect on the measured peak intensity at the far field. The measured peak intensity value can vary up to 10\% depends on the lab environment. In light of this effect, the best observed peak intensity during 1 minute of recording time is considered as the measured peak intensity, to exclude the influence of the air turbulence. This is justified because the air turbulence will only lower the measured peak intensity but not increase the measured value.

In order to measure the strehl ratio of the beam after wavefront compensation, several loses that could reduce the peak intensity of the compensated beam has to be considered. This includes: 1. The diffraction loss due to the segmented mirror on LCOS can be about 1-0.96^2 =8\% of total optical power for coherent light. (The 96\% is the filling factor of the LCOS panel.) 2. An 8\sim 12\% absorption or scattering loss of aluminum mirror, which is not coated with dielectric enhancement layer. These loses are intrinsic to the
device and has nothing to do with the wavefront compensation. In experiments, the reflectivity of LCOS is measured to be 80%. When the laser is reflected by the LCOS device, only the optical power goes in zero order diffraction peak is collected. However, in this case, the 20% loss of power will not include the loss due to front surface reflection. Although the front cover glass of LCOS is coated with broadband AR in visible region, about 1.4% loss is observed for the front surface reflection for 632.8 nm. Since the front surface reflection is spatially overlapping with the main reflection beam from the LCOS device, both contributions will be recorded by the detector.

In Fig. 48, the far field point spread function captured by the CCD camera is shown. The Fig. 48 (a) shows the case when a uniform grayscale is put on the LCOS and the aberration introduced by the silicon backplane is not removed. At the presence of the strong aberration, the beam at the nominal focus has very low peak intensity but large spot size. In Fig. 48 (b), the modulo $2\pi$ version of the compensation phase plate is introduced to the LCOS. The subsequent far field peak is sharp and the $1/e^2$ beam waist is about 1.2x diffraction limited beam waist. In Fig. 48 (c), additional tip-tilt is added to the compensation phase plate and to further steer the beam by 4.07 mrad. The cross section of the laser beam as in Fig. 48 (b) (c) is shown in Fig. 41. The peak (a) in Fig. 49 is for the laser beam reflected from a mirror with the peak intensity reduced by 80% to take into account the reflectivity loss of the LCOS. The peak (b) is the beam after wavefront compensation. The strehl ratio of peak (b) using peak (a) as reference is 0.82. The peak (c) is the cross section of beam after wavefront compensation and steering. The strehl ratio of peak (c) using peak (b) as reference is 0.846.
Fig. 48: Far field point spread function measured at the focus of a low numerical aperture lens. (a) Wavefront compensation turned off (b) Wavefront compensation on. (c) Wavefront compensation + maximum steered beam.
Fig. 49: Far field beam profile. (a) Aberration free laser beam with intensity reduced by 80% to take into account the reflectivity loss of LCOS SLM. (b) Wavefront compensated but non-steered laser beam with strehl ratio=0.82 using (a) as a reference. (c) Wavefront compensated and maximum steered beam with strehl ratio=0.846 using (b) as a reference.
A comparison of the DE value obtained from the simple model, the FDTD simulation, and the experimental results is carried out before in Chapter 2. The beam steering efficiency as function of the steering angle can be seen from Fig. 7. The experimental data shows excellent agreement with the FDTD simulation and the simple model. The diffraction efficiency of the LC OPA drops as deflection angle becomes larger. There is a maximum steering angle that if the LC OPA is programmed to steer to angle larger than the maximum steering angle, then the diffraction efficiency drops very quickly. Such maximum steering angle is defined to be the angle corresponding to having eight pixels within one reset. For the test device, the maximum steering angle is $\pm 4.07$ mrad.

The above discussion shows how well a LCOS SLM can be used for high resolution wavefront control. The performance of the device in terms of steering laser beam has been fully characterized and is close to the best expected performance. The next step in our work is to study using the LCOS SLM to correct for aberration in large aperture telescope.
4.3 Advanced wavefront control in large aperture deployable telescope

4.3.1 Type of aberration that can be corrected with LCOS SLM

In a long distance laser communication system as shown in Fig. 50, as Gruinisen pointed out, the dynamic range of wavefront correction needed to overcome thermal expansion, vibration etc is very large. Beyond this, high numerical aperture mirror is often used in such a system to reduce the size and weight. The severely aberrated wavefront will cause substantial aberration to the ray, which makes the design, analyze and performance evaluation of such system extremely difficult. In this section, type of aberration that can be corrected by a LC SLM is discussed.

The first question regarding high resolution wavefront control in large optics is what type and amplitude of aberration can be corrected with a LCOS SLM. For primary mirror made of manbrane type of material, if the surface of the primary mirror is a scattering surface, the loss induced by the surface roughness of the primary mirror could not be corrected by the LCOS SLM. Even if the surface is well polished surface, the spatial frequency of the local aberration on the primary optics can be very large for a membrane mirror. Assuming the pixel pitch of the LCOS is $\chi$, and the total magnification ratio of the telescope is $\beta=66.7$, then the highest spatial frequency of surface deformation of the primary mirror can be corrected by LC SLM is $1/(8\chi\beta)$ assuming at least eight sampling point to sample one wave of aberration. This is similar to the previous discussion of eight steps blazed grating in previously chapters.
Fig. 50: Free space laser communication transmitter with LCOS SLM as wavefront corrector and beam steerer.
Fig. 51: Illustration of effect of local surface deformation on the wavefront correction.
The maximum local slope of wavefront is another important factor to consider. Again, the number of pixels required to generate one wave of tilt is at least \( m = 8 \) according to previous report, otherwise, strong diffraction loss will occur\(^8\). This requirement limits the maximum tilt that can be produced on our current LCOS to be

\[ \gamma = \sin^{-1}\left( \frac{\lambda}{m \chi} \right) = 4.07 \text{ mrad}. \]

The corresponding maximum local slope of wavefront aberration on the primary mirror is \( \kappa = \gamma / \beta = 61.0 \mu\text{rad} \).

If the local wavefront slope of the aberration is large, it may cause substantial ray aberration that reduces the efficiency of the correction. For example, the ray missing the correction aperture or two separated ray may go to the same active element on the correction device, as shown in Fig. 51. For a better understanding, we can trace an uniformly spaced ray boundle with 50×50 rays across the clear aperture is traced throught all surfaces in the system. The position of each ray intercept the LC SLM correction plane is ploted in Fig. 52. For low order Zernike mode, even if larger magnitude of aberration is present in the system, for example in Fig. 52 (a), 60 waves rms of primary coma is introduced to the primary mirror of the transmitter and the ray intersection plot is shown, no serious ray crossing problem is observed. However, ray crossing problem is observed in higher order Zernike modes at much smaller magnitude. For the standard Zernike term \( Z_{33} \), about 20 waves rms of wavefront aberration will induce serious ray crossing problem.
Fig. 52: Ray Intersection plot on LCOS device plane. (a) With 60 waves rms of primary coma $Z_8$ on primary mirror, no serious ray cross problem is observed. (b) With 60 waves rms of high order coma $Z_{33}$ on primary mirror, serious ray crossing problem is observed.
4.3.2 Optical throughput of the system

A comprehensive method is required to evaluate how well a wavefront correction system works in terms of restoring the wavefront to diffraction limited. Since the strehl ratio of the system after wavefront correction is a core performance metric, we can use a model to describe the Strehl Ratio of the system considering four major factors as shown in Equ. 4.5. These influence factors are based on very different physical phenomenon, and we treat them as independent factors in this article.

\[ \eta_{\text{total}} = \eta_s \eta_{\text{ray}} \eta_{\text{aber}} \eta_{\text{SLM}} \]  \hspace{1cm} (4.5)

As an introduction to these factors: The first factor, \( \eta_s \), describes the losses from scattering and absorption of any optical surfaces. The second factor, \( \eta_{\text{ray}} \), describes how well the optical system can map an area on the distorted optical element to a corresponding unique area on the wavefront corrector. Its value would be one if the aberration producing surface is in an optically conjugate position to the corrector. The third factor, \( \eta_{\text{aber}} \), describes how well an ideal phase plate, with the resolution of the wavefront corrector, can correct an aberrated wavefront passing through it. Its value would be one if the corrector had infinite resolution and phase control. The last factor, \( \eta_{\text{SLM}} \), is related to how much the phase profile of the electrically controllable liquid crystal device deviates from the desired phase plate. In the next several paragraphs, we will describe the definition and effect of these terms in more detail.
The first factor, $\eta_1$, is the loss associated with the passive loss in the system such as the imperfection in the mirror surface, scattering, absorption and front surface reflection loss etc. This factor mainly depends on the material and process that is used to make the optical elements.

The second efficiency factor, $\eta_{\text{ray}}$, is related to the non-conjugate position of the element being corrected and the corrector. As a simple example, shown in Fig. 51, if there is a substantial aberration in the primary mirror, a ray A can miss the clear aperture of the correction device. In another case, two rays, ray B and C could cross each other and hit the same pixel on the correction device. When such things happen, the correction device would not be able to correct perfectly for the wavefront aberration, even if an infinitely high-resolution correction device is used.

First of all, $\eta_{\text{ray}}$ depends on the optical system design. In an ideal perfect conjugate system, where the correction device is placed at the conjugate position of the primary optical element, the position of any ray that hits a particular point on the primary mirror will hit a corresponding point on the LC-SLM. There is a one to one relationship of the ray interception position on the primary mirror and the correction device, and it doesn’t matter what is the magnitude or order of the aberration on the primary mirror. In this case, $\eta_{\text{ray}} = 1$ always holds true. However, this ideal conjugate relationship may not always hold true for a high numerical aperture telescope with large magnification. The conjugate
image of the primary mirror is not a flat surface, but a spherical surface instead. It is not possible for a LC-SLM with flat surface to satisfy the conjugate relationship for the entire aperture on the device. In this case, the wavefront aberration could cause substantial shift of the ray interception position on the correction device for different aberration, and the efficiency $\eta_{\text{ray}}$ will be low.

Second, $\eta_{\text{ray}}$ depends strongly on the magnitude and order of the wavefront aberration. For example, CODE V optical design software is used to trace a uniformly spaced ray bundle through a particular optical system as shown in Table 13. The position of each ray intercepting the LC-SLM correction plane is plotted in Fig. 52. In case A, a low order Zernike mode with 60 waves rms of primary coma on the primary mirror of the transmitter is shown. In case B, a high order Zernike term, the standard Zernike term $Z_{33}$ with 20 waves rms of wavefront aberration is shown. It is clear that the second case has a much stronger ray aberration than the first case, and $\eta_{\text{ray}}$ will be much smaller for the second case.

Third, $\eta_{\text{ray}}$ also depends on the resolution of the correction device. While other terms that govern the overall efficiency increase as the resolution of the correction device increases, this term drops because the significance of the non-conjugate nature of the system is greater if the considered resolution is higher. It can be seen that a ray will be more likely to shift to a wrong pixel on the correction device, if the pixel size of the
correction device is small; which means, this efficiency term drops as the resolution of the correction device increases.

It is extremely hard to quantify the efficiency term $\eta_{\text{ray}}$ with an accurate analytical method. But we can use a simple model to describe this term in a physically meaningful way. Consider a certain aberration in a certain optical system, where we can trace a $m \times m$ bundle of rays through it. The correction device in the system has $m \times m$ pixels across the clear aperture. For each pixel on the correction device, we can count how many rays intercept the correction device on that pixel. When there is no aberration present in the system, the number of rays intercepting a pixel on the correction device should be one. However, when aberration is present in the system, the number of rays intercepting a certain pixel is no longer one. We define $n_0$ to be the number of pixels on the correction device that have no ray intercepting that pixel; $n_1$ to be the number of pixels on the correction device that have one ray intercepting that pixel; $n_2$ to be the number of pixels on the correction device that have two rays intercepting that pixel; and $n_k$ to be the number of pixels that have $k$ rays intercepting that pixel.
Fig. 53: The efficiency of correction for ray aberration as function of the resolution of the correction device.
However, we may want to trace more than one ray through a certain pixel to be accurate. In this case, we may have \( j \times j \) rays in the bundle, and \( m \times m \) pixels on the correction device \((j > m)\). There should be \( j^2/m^2 \) rays intercepting one pixel on the correction device, when there is no aberration in the system. We can normalize the number of rays intercepting one pixel on the correction device by the factor of \( j^2/m^2 \) in later calculation. If there is an aberration in the system, we can still define \( n_0 \) to be the number of pixels that has no ray intercepting the pixel, but \( n_1 \) will the number of pixel that has a number of normalized rays intercepting the pixel in the range of \((0 \ 1]\). The same way, \( n_k \) is the number of pixels that have a normalized number of rays in the range of \((n_{k-1} \ n_k]\). Then the percentage of pixels that have a normalized \( k \) rays intercepting the pixel is \( \mu_k = n_k / m^2 \). For a telescope system shown in Table 13, if the aberration on the primary optics is a primary spherical aberration \( Z_{13} \), and the correction device is a 50×50 resolution device. \( \mu_0 = 12.2\% \), \( \mu_1 = 73.8\% \), \( \mu_2 = 13.9\% \), \( \mu_3 = 0.3\% \), \( \mu_4 = 0.0\% \) can be obtained by tracing 500×500 rays through the system. Since the efficiency of the system will be a direct function of how many rays will miss the desired pixel, which is simply by \( \mu_0 \), it can be expressed in Equ. 4.6.

\[
\eta_{ray} = 1 - \mu_0
\]  

(4.6)

In this case, we can obtain \( \eta_{ray} = 88\% \) for a 50×50 correction device. On the other hand, if the correction device is 500×500 resolution, the \( \mu_0 = 25.3\% \), \( \mu_1 = 51.6\% \), \( \mu_2 = 22.3\% \), \( \mu_3 = 0.3\% \), \( \mu_4 = 0.0\% \), can be obtained similarly. In this case, the \( \eta_{ray} = 74.7\% \).

We can also vary the resolution of the correction device and the aberration on the primary
telescope to perform the same calculation. The relationship between the $\eta_{ray}$ and the resolution of the correcting device obtained is shown in . We can see a clear trend showing the efficiency drops as the resolution of the correction device increases, and the trend tend to saturate as the resolution of the correction device becomes very high.

The third efficiency factor $\eta_{aber}$ is related to the resolution of the corrector. This term becomes larger as the resolution of the device becomes higher. If we assume an ideal piston-phase-plate correction device with finite resolution, the correction efficiency for random high order aberration is not 100%. Consider the simplest case of correcting a simple tilt, and assume $q$ is the number of steps for every wave of tilt, the efficiency factor $\eta_{aber}$ is the same as the diffraction efficiency for a stair-like blazed grating as in Equ. 4.7.

$$\eta_{aber} = \left(\frac{\sin(\pi / q)}{\pi / q}\right)^2$$ (4.7)

We would like to estimate the efficiency factor that is related to the resolution of the correction device, but is applicable to the more general case of an arbitrary aberration. To implement this concept of Equ. 4.7 for a 2-D aberration, consider again the telescope system shown in Table 13. Any aberration on the primary mirror will induce a corresponding but different aberration on the correction device. The aberration profile on the correcting device can be obtained by diffractive beam propagation of a Guassian beam from the primary optics to the correction device. (More details about the CODE V diffractive beam propagation calculation will be shown in later section). The whole
aperture is divided into \( l \times l \) small regions. Within region \( \Omega \), if the region is very small, the aberration \( P(x, y)_{x, y \in \Omega} \) can be approximated by a simple tilt, where the maximum difference in the phase across the region is:

\[
\Delta_{\Omega} = \max(P(x, y)_{x, y \in \Omega}) - \min(P(x, y)_{x, y \in \Omega})
\]  

(4.8)

The number of steps along either horizontal or vertical step is \( S = m/l \). Then the number of steps for one wave of tilt \( q \) in region \( \Omega \) is approximately

\[
q_{\Omega} = S / \Delta_{\Omega} = \frac{m}{l \Delta_{\Omega}}.
\]  

(4.9)

With such approximation, the efficiency term \( \eta_{\text{aberr}, \Omega} \) within region \( \Omega \) can be estimated for a 2-D aberration.

\[
\eta_{\text{aberr}, \Omega} = \left( \frac{\sin(\pi / q_{\Omega})}{\pi / q_{\Omega}} \right)^{2} = \left( \frac{\sin(\pi l \Delta_{\Omega} / m)}{\pi l \Delta_{\Omega} / m} \right)^{2}
\]  

(4.10)

If we assume the fractional intensity of the beam on region \( \Omega \) is \( W_{\Omega} \), then the total efficiency across the whole aperture is the weighted average of \( \eta_{\text{aberr}, \Omega} \) across the whole aperture as in Equ. 4.11.

\[
\eta_{\text{aberr}} = \sum_{\Omega} W_{\Omega} \eta_{\text{aberr}, \Omega} = \sum_{\Omega} W_{\Omega} \left( \frac{\sin(\pi / q_{\Omega})}{\pi / q_{\Omega}} \right)^{2} = \sum_{\Omega} W_{\Omega} \left( \frac{\sin(\pi l \Delta_{\Omega} / m)}{\pi l \Delta_{\Omega} / m} \right)^{2}
\]  

(4.11)

Following this approach, we can calculate the efficiency term \( \eta_{\text{aberr}} \) in a 2-D case. In Fig. 54, the calculated efficiency for different aberration is shown as a function of the resolution of the correction device. For a particular resolution of device, the correction
efficiency is different for different aberration. Generally speaking, the larger than magnitude of the aberration, the higher order the aberration, the lower the efficiency. However, it is also clear that if the resolution of the correction device is high enough, this efficiency $\eta_{aberr}$ can be very high.

The fourth factor $\eta_{SLM}$ is the efficiency associated with the LC SLM. This factor has been extensively discussed in Chapter 3, and there is not need to repeat here any more.
Fig. 54: The efficiency of correction for wavefront aberration as function of the resolution of the correction device.
Fig. 55: Optical layout of one meter diameter telescope used in the simulation.
4.3.3 Modeling of the correction of the global aberration

The correction of the global aberration is the most important issue we focused on. A modeling to study the correction of global aberration is carried out with CODE V software. The layout of the lasercom transmitter is shown in Fig. 55 and Table 13. A compact design of Ritchey-Chretien telescope with a parabolic primary and secondary mirror is considered, with a LCOS wavefront corrector positioned at the conjugate plane of the primary mirror. The clear aperture of the primary mirror is 1 m with a focal length f=300 mm. The secondary mirror has a clear aperture of 20 mm with f=4.5 mm. The LCOS device has a clear aperture of 15 mm. The total magnification of the telescope is 66.7x. The initial system is aberration free. An ideal lens module is introduced behind the LCOS SLM to help analyzing the afocal system. The point spread function at the focus of the ideal lens module is evaluated to obtain the Strehl ratio of the telescope system.

Table 13: Free space laser communication transmitter telescope design.

<table>
<thead>
<tr>
<th>Surface No.</th>
<th>Surface Name</th>
<th>Surface Type</th>
<th>Y Radius</th>
<th>Thickness</th>
<th>Glass Refract Mode</th>
<th>Y Semi Aperture</th>
</tr>
</thead>
<tbody>
<tr>
<td>Object</td>
<td></td>
<td>Sphere</td>
<td>Infinity</td>
<td>Infinity</td>
<td>Refract</td>
<td>500.00</td>
</tr>
<tr>
<td>1</td>
<td></td>
<td>Sphere</td>
<td>Infinity</td>
<td>400.00</td>
<td>Refract</td>
<td>500.00</td>
</tr>
<tr>
<td>Stop</td>
<td>Primary Mirror</td>
<td>Conic</td>
<td>-600.00</td>
<td>-250.00</td>
<td>Reflect</td>
<td>500.00</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>Sphere</td>
<td>Infinity</td>
<td>-45.500</td>
<td>Refract</td>
<td>10.00</td>
</tr>
<tr>
<td>4</td>
<td>Secondary Mirror</td>
<td>Conic</td>
<td>-9.0000</td>
<td>2.00</td>
<td>Reflect</td>
<td>7.500</td>
</tr>
<tr>
<td>5</td>
<td></td>
<td>Sphere</td>
<td>Infinity</td>
<td>2.56</td>
<td>Refract</td>
<td>7.500</td>
</tr>
<tr>
<td>6</td>
<td>Correction phase plane</td>
<td>Sphere</td>
<td>Infinity</td>
<td>0.01</td>
<td>BK7</td>
<td>7.500</td>
</tr>
<tr>
<td>7</td>
<td></td>
<td>Sphere</td>
<td>Infinity</td>
<td>20.00</td>
<td>Refract</td>
<td>7.500</td>
</tr>
<tr>
<td>8</td>
<td>Ideal Lens Modular</td>
<td>Sphere</td>
<td>Infinity</td>
<td>50.00</td>
<td>Refract</td>
<td>7.500</td>
</tr>
<tr>
<td>Image</td>
<td></td>
<td>Sphere</td>
<td>Infinity</td>
<td>0.00</td>
<td>Refract</td>
<td>0.200</td>
</tr>
</tbody>
</table>


First of all, a surface deformation (10 waves rms, or 16 waves P-V of primary defocus) is introduced to the primary mirror, which will introduce a wavefront aberration of 20 waves rms, or 32 waves P-V of primary defocus to the optical system. With such large aberration applied to the primary mirror, sequential ray tracing is not accurate enough to determine the wavefront aberration in the LCOS plane. Instead, the Diffractive Beam Propagation (BPR function) in CODE V is used to obtain the phase and intensity of light at any given position in the system. The Diffractive Beam Propagation function in CODE V is a combined method of ray tracing and beam propagation algorithm, with geometrical ray tracing algorithm for the rays passing through any non-air surface; and near/far field beam propagation algorithm for all air paths. To our knowledge, this method is the best optical simulation available that can deal with both diffractive optical element and large aperture lens system. In Fig. 56, the wavefront aberration at the LCOS plane obtained using Diffractive Beam Propagation is shown. Since every optical element and input beam is rotationally symmetric, the wavefront aberration should be rotationally symmetrical as well. However, some non-rotationally symmetrical pattern is observed in the wavefront map. The reason for this is the input 1/e^2 Guassian beam diameter is half the clear aperture of the primary optical element. The intensity of the beam at the edge of the clear aperture is close to zero. This leads to computational errors in calculating the phase of light, and such error is negligible for our purpose because the intensity of light is very small at the edge of the clear aperture. The intensity profile at the LCOS plane is illustrated in the upper figure of Fig. 56. After the introduction of the aberration on the primary mirror, the strehl ratio of the whole system decreases from 1.0 to 0.0000005.
Fig. 56: Wavefront aberration at LCOS SLM plane obtained by diffractive beam propagation. Upper graph is the intensity distribution of light at LCOS SLM.
Fig. 57: Simulated phase of beam after wavefront correction.
Fig. 58: Point Spread Function at the focus of the idea lens modular. (a) Before wavefront compensation (b) After wavefront compensation.
A conjugate phase plate with 500 x 500 active elements over the 15 mm x 15 mm clear aperture is generated by changing the sign of the aberration on the LC SLM plane and take the modulo of $2\pi$. Such modulo $2\pi$ version of the conjugate phase plate is introduced to the LC SLM plane as the correction phase plate. Diffractive beam propagation is performed after introducing the correction phase plate. As shown in Fig. 57, the residual wavefront error after correction is zero within the beam waist, except for some very high spatial frequency noise at the wavefront resets. The point spread function before and after the wavefront compensation is shown in Fig. 58. After wavefront correction, the strehl ratio of the system improved from 0.0000005 to 0.63. A strehl ratio improvement factor of $\gamma = 0.63/0.0000005 = 1.26 \times 10^6$ is obtained.

With this technique, correction of different Zernike modes of different magnitude is studied. First, the magnitude of the aberration is fixed to be 10 waves rms while different Zernike mode of aberration is introduced to the primary mirror. As shown in Fig. 59, strehl ratio after correction is very different. The coma and the spherical aberration can decrease the system strehl ratio much faster than other terms. Even with a resolution of 500 x 500, the strehl ratio after correction can sometimes be as low as 0.2 (for the 25th standard Zernike term $Z_{25}$). For a particular Zernike mode, the strehl ratio after correction for different magnitude is shown in Fig. 60. For up to 25 waves rms of low order astigmatism $Z_4$ and $Z_6$, strehl ratio after correction can be higher than 0.65. On the other hand, the strehl ratio after correction for primary spherical aberration $Z_{13}$ drops very fast as the magnitude of aberration gets larger and larger.
Fig. 59: Strehl ratio after correction for different Zernike terms. Assuming all wavefront aberration is 10 waves rms.
Fig. 60: Strehl Ratio after wavefront correction for different magnitude of primary Astigmatism, Defocus, Coma and Spherical aberration. Here the Zernike coefficient of 1 wave rms is the surface deformation in primary optical element, it is equivalent to 2 waves of wavefront aberration.
Fig. 61: Strehl ratio after correction of different magnitude of primary defocus and spherical aberration versus resolution of the LCOS device.
Fig. 62: Comparison of CODE V ray tracing results with system analyze results using Equ. 4.6 and Equ. 4.11.
The resolution of the LC SLM also places a limitation on the maximum amount of aberration that can be corrected. In Fig. 61, the correction of primary defocus and spherical aberration with different resolution is shown. The strehl ratio after correction is not a linear function of the resolution of the LC SLM device, but has a critical value. If the resolution of the LC SLM is smaller than this value, the strehl ratio decreases very fast as the resolution of the correction phase plates becomes smaller. On the other hand, if the resolution of the LC SLM is smaller than this value, the improvement of the strehl ratio is small. Such critical resolution is related to the type of aberration and the magnitude of the aberration. Generally speaking, the larger the magnitude of the aberration, the larger the critical resolution would be. For example, to correct for 10 waves rms of primary spherical aberration $Z_{13}$, such critical resolution is about $150 \times 150$. However, for 15 waves of primary spherical aberration, such critical resolution is about $300 \times 300$. The type of aberration also plays an important role. For example, the primary defocus is much easier to correct as compared with spherical aberration. The critical resolution is lower for the primary defocus. In any case, high resolution correction device has higher correction efficiency and larger dynamic range of correction. If we plot $\eta_{ray} \eta_{aber}$ obtained earlier by Equ. 4.6 and 4.11, as well as the strehl ratio after correction obtained by CODE V simulation The comparison is shown in Fig. 62, both data agrees very well. The result implies that it is always possible to obtain larger correction efficiency of $\eta_{aber}$ by increasing the resolution of the LCOS SLM. Especially if the system is designed to be a conjugate system where $\eta_{ray} = 1$. 

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Another important factor that could influence the correction efficiency is the pupil apodization (the intensity distribution of beam at the input aperture) at the primary optical element. In the system discussed above, the \(1/e^2\) beam diameter of beam on the LCOS plane is 7.5 mm, which is only half the size of the clear aperture of the LCOS SLM. The active elements outside of the \(1/e^2\) beam diameter contribute little to wavefront compensation because the light intensity is very low. More than half of the resolution of the LCOS device is not used efficiently. One can imaging there is a trade off between the filling factor of the beam on LCOS plane versus the truncation loss of Guassian beam. We will not discuss this in full detail because it strongly depends on the system design.

4.3.5 Comparison of the numerical modeling results with the simple model

\[
\eta_{\text{total}} = \eta_s \eta_{\text{ray}} \eta_{\text{ave}} \eta_{\text{SLM}}
\]

\[
= \eta_s (1-u_0) \left[ \sum_{\Omega} W_{\Omega} \left( \frac{\sin(\pi l \Delta_{\Omega} / m)}{\pi l \Delta_{\Omega} / m} \right)^2 \right] \left( 1 - \frac{a (d / PS)^\beta}{N} \right)^2
\]  

(4.12)

If we summarize the discussion in Chapter 3 and Chapter 4 regarding the diffraction efficiency expression for different term, it is possible to relate the total optical throughput of the system to many design parameters as in Equ. 4.12. For example, the total optical throughput is a function of the scattering and reflection loss in the system \(\eta_s\), the extent of ray missing corresponding pixel \(u_0\), the resolution of the correction device \(m\), the complexity of the wavefront \(\Delta_{\Omega}\), the pixel spacing of the correction device \(PS\) and
cell thickness of the device (d), etc. It is possible to estimate the efficiency by using the empirical model described in Equ. 4.12, or by numerical calculation of the four efficiency terms.

Let us compare the two methods considering a system has no passive loss; and 32 waves P-V (16.6 waves rms) of primary defocus is corrected by a 500×500 resolution correction device with 9.7×9.7 mm aperture. The pixel spacing of the 2-D LC-SLM is 19.4 µm, and the LC cell thickness is d=6.0 µm. (The LC-SLM used in the experimental section has a pixel spacing is 19.4 µm, and a cell thickness of d=6.0 µm. The resolution is 1024×768, and the aperture is 20×15 mm. However, only part of the aperture is used, which is 9.7×9.7 mm with 500×500 resolution.). The LC material used has Δn=0.20. The average wavefront slope of the aberration is about 0.004 rad for 32 waves P-V of primary defocus. If we use Equ. 4.12 to calculate the total optical throughput, the first factor η_s = 1.0. The second factor η_ray = 82% as previously considered in Fig. 53 and the third factor is η_ray = 70%, as previously considered in Fig. 54. The fourth factor here

$$\eta_{SLM} = \left(1 - \frac{a(d/PS)}{N}\right)^2 = (1-1.4*(6.0/19.4)^{0.7}/(500/(2*32)))^2 = 0.84.$$  

So the total optical throughput of the system calculated by the analytical method is

$$\eta_{total} = \eta_s \eta_{ray} \eta_{aberr} \eta_{SLM} = 1.0 \times 0.82 \times 0.70 \times 0.84 = 0.48.$$ 

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If we use the CODE V numerical modeling method, the Strehl Ratio after correcting the 32 waves of aberration is 0.63. This is equivalent to the product of the second and third efficiency factor in 4.12. So \( \eta_{\text{ray}} \eta_{\text{aberr}} = 0.63 \). The first factor is still \( \eta_s = 1.0 \) for a system with no passive loss. To obtain the fourth efficiency term, consider the case, where the pixel spacing is 19.4 \( \mu \text{m} \), and there are eight pixels per blaze, the wavefront slope produced by the LC-SLM is also about 0.004 rad. The diffraction efficiency low bound value (Corresponds to a surface alignment parallel to the electrode case) is \( \Gamma_{\text{min}} = 81.5\% \), and the diffraction efficiency high bound value (Corresponds to a surface alignment perpendicular to the electrode case) is \( \Gamma_{\text{max}} = 85.8\% \). An average of diffraction efficiency for the 2-D LC-SLM is \( \eta_{\text{SLM}} = 83.7\% \) in this case, which is very close to the estimation with Equ. 4.12 in the last paragraph. The total optical throughput as calculated by numerical modeling for the considered system is then \( \eta_{\text{total}} = \eta_s \eta_{\text{ray}} \eta_{\text{aberr}} \eta_{\text{SLM}} = 1.0 \times 0.63 \times 0.837 \times 0.52 \). This demonstrates that the concepts of the simple model are consistent with a more detailed numerical calculation.

4.3.6 Correction of aberration in 8 inch mirror

Experimental study is carried out to verify the results of the above mentioned modelling. The specification of the LCOS wavefront corrector used in the experiment is listed in Table 1. It consists of thin layers of liquid crystal material sanwiched between top glass and silicon backplane. Both the top and the bottom substrate are coated with polyimide alignment layer with parallel rubbing. On the silicon backplane, CMOS gate
on each pixel is hidden behind the segmented aluminum mirror. The size of each mirror is 19 µm square with 0.4 µm gap between mirrors. The filling factor of the mirror is as high as 96% and the diffraction loss from the discontinuity of the mirror is small due to the small gap between mirrors. Measured reflectivity is 80% since the aluminum mirror is not coated with dielectric enhancement layer. The reflectivity can be improved if dielectric enhancement layer is added to the aluminum mirror. The non-uniformity of the liquid crystal layer is less than 1/10 λ at 632.8 nm\textsuperscript{48}. 
Fig. 63: Measure and correcting of aberration in 8 inch mirror.
A wavefront measurement and correction system is shown in Fig. 63. The system consists of three parts, an 8 inch telescope, a phase shifting Mach-Zehnder interferometer to measure the wavefront aberration, and a LCOS correction device. For the telescope, since the mirror is a diffraction limited mirror with transmitted wavefront aberration less than $1/20 \lambda$ rms, a window glass is introduced in front of the mirror to simulate severally aberrated primary optical element. Several aberration sources are present in the optical system, for example, the aberration introduce by the silicon backplane of the LCOS device, misalignment of the optics and the aberration introduced by the window glass. The surface shape of the silicon backplane is not an optical flat, but will introduce a wavefront aberration of 18.7 waves P-V. The aberration at the exit pupil is measured by interfering a reference beam with the aberrated beam. The standard phase shifting algorithm is used to extract the phase information of the aberrated beam. The phase profile is subsequently unwrapped and filtered with noise removal filter as shown in Fig. 64. The measured aberration is decomposed to Zernike component as listed in Table 14. (Here instead of stander Zernike polynomial, Fringe Zernike polynomial developed by University of Arizona is used.) The most significant Zernike mode is 7.75 waves rms of primary defocus and 2.1 waves rms of astigmatism. The magnitude of the aberration is 34 waves P-V.
Table 14: Zernike mode of the transmitted wavefront aberration on LCOS clear aperture introduced by the large aperture telescope. Here we use Fringe Zernike polynomials developed by University of Arizona, which is a subset of standard Zernike polynomial with the terms of the Zernike mode arranged in a different order.

<table>
<thead>
<tr>
<th>Zernike term</th>
<th>Order</th>
<th>Zernike Coefficient (waves at 632.8 nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Piston</td>
<td>0</td>
<td>7.781</td>
</tr>
<tr>
<td>2 Tilt</td>
<td>1</td>
<td>1.603</td>
</tr>
<tr>
<td>3 Tilt</td>
<td>1</td>
<td>-0.583</td>
</tr>
<tr>
<td>4 Focus</td>
<td>1</td>
<td>7.751</td>
</tr>
<tr>
<td>5 Astig.</td>
<td>2</td>
<td>2.097</td>
</tr>
<tr>
<td>6 Astig.</td>
<td>2</td>
<td>0.776</td>
</tr>
<tr>
<td>7 Coma</td>
<td>2</td>
<td>0.640</td>
</tr>
<tr>
<td>8 Coma</td>
<td>2</td>
<td>-0.130</td>
</tr>
<tr>
<td>9 Spherical</td>
<td>2</td>
<td>0.0783</td>
</tr>
<tr>
<td>10 Astig.</td>
<td>3</td>
<td>0.195</td>
</tr>
<tr>
<td>11 Astig.</td>
<td>3</td>
<td>-0.052</td>
</tr>
<tr>
<td>12</td>
<td>3</td>
<td>0.295</td>
</tr>
<tr>
<td>13</td>
<td>3</td>
<td>-0.031</td>
</tr>
<tr>
<td>14 Coma</td>
<td>3</td>
<td>0.056</td>
</tr>
<tr>
<td>15 Coma</td>
<td>3</td>
<td>-0.045</td>
</tr>
<tr>
<td>16 Astig.</td>
<td>3</td>
<td>-0.060</td>
</tr>
</tbody>
</table>
Fig. 64: Measured aberration at exit aperture of the telescope system before wavefront correction.
The conjugate phase profile is introduced to the LCOS device to correct for the aberration. However, this direct conjugate phase plate fails to correct for the aberration to diffraction limited because of the complexity of the system. Instead, a multi-step optimization approach is taken to obtain the best correction phase plate. The optimization process consists of several steps as following. First, the wavefront aberration is measured and a conjugate correction phase to put on the LCOS SLM. Second, the residual wavefront error is measured and added to the correction phase of the previous step. Then, the residual aberration is measured again and this procedure is repeated until the residual aberration at the exit pupil at the interferometer is minimum. Most times, within several of such steps, the residual aberration is minimum. In Fig. 65, the phase map introduced to LCOS device at the final iteration is shown.

The residual wavefront map after three loops of the above mentioned iteration is shown in Fig. 66. The wavefront at the exit pupil of the telescope is well corrected as the magnitude of the residual wavefront error is less than $1/10 \lambda$ P-V or $1/30\lambda$ rms. Diffraction limited performance is reached after the correction. It is also noticeable that the residuals wavefront map has very similar ring like pattern to the reset pattern on correction phase plate. The wavefront of the front surface reflection is aberrated and could not be corrected because this portion of light does not go through the liquid crystal layer. Thus, in the captured interferogram, such front surface reflection will show up as the above mentioned ring like patterns.
Fig. 65: Correction phase ramp introduced on LCOS SLM.
Fig. 66: Residual wavefront aberration after correction at the exit aperture.
If we focus the laser beam to a CCD camera, the far field beam diameter of the compensated beam can be obtained to be 136.4 µm, or 1.31x diffraction limited beam waist. In Fig. 67, the point spread function captured by the CCD camera is shown before wavefront compensation and after wavefront compensation. However, it is hard to determine the Strehl Ratio of the system due to the difficulty in measuring the peak intensity of the aberration free system, because several aberration sources present and there are front surface losses from many optical components. We can only measure the peak intensity of the compensated beam, which is 339 times higher than the non-compensated beam.

If we try to approximate the Strehl Ratio of the system by the encircled energy of the far field beam. The amount of energy passing through a 120 µm pinhole is 51% that of the total laser energy at far field (The detector collects all light at the focus of the lens at 1170 mm. The size of the detector is 5×5 mm. The intensity of the beam with or without the pinhole is measured. When the pinhole is in the optical path, it is directly mounted on the detector to reduce loss. The reason we choose a 120 µm pinhole is that the diffraction limited spot size of the beam is $\frac{4 \lambda f}{\pi D}$=4*0.6328*1170/8.5/3.1415=98.7 µm. For our system, there is no truncation to the Guassian Beam, the point spread function is a Guassian profile instead of Airy disc. In ideal situation where there is no aberration in the system, all light should go into the pinhole, and the amount of energy collected by the detector should be 100% of the total laser energy.)
Then the experimentally measured Strehl Ratio of the system is $\eta_{\text{total}} = 51\%$. This measured total optical throughput is in line with our analytical estimation results of $\eta_{\text{total}} = 48\%$ and the numerical estimation results of $\eta_{\text{total}} = 52\%$ in section 4.3.5.
Fig. 67: Compensated beam (left) and non-compensated beam (right) at far field.
4.4 Conclusion

The performance limits of diffractive wavefront compensation of the free space laser communication transmitter with severely aberrated meter class primary mirror are studied by modeling the wavefront compensation in the system level and the device level. The aberration correction efficiency for different magnitude and type of aberration is discussed, as well as the influence of the resolution of LCOS on the correction efficiency. The viability of a large aperture deployable telescope is greatly improved by utilizing the correction power of the LCOS SLM to greatly lower the tolerance placed on primary mirror of a lasercom system. Up to several tens of waves of aberration can be corrected efficiently with current LCOS device. Experimentally, the correction of severally aberrated large optics to diffraction limited is demonstrated.
Chapter 5

Liquid Crystal Binary Gratings in Digital Holography

5.1 Introduction to 3-D displays based on digital holography

There are several approaches to achieve 3D visualization effects: stereoscopic display\(^6^2\), volumetric system\(^6^3\), integral photography (integral imaging)\(^6^4\) and holography\(^6^5\). Each of these technologies has advantages and disadvantages. Holography is particularly attractive because a single hologram is capable of creating authentic illusion of volumetric objects by naked eye\(^6^6\). While conventional holography technique has demonstrated the most realistic 3D visualization effect by direct recording the scene on a holographic film, to replace the holographic film with a digital holographic media is still a very challenging task. The recent advances in CCD camera, high efficiency liquid crystal on silicon spatial light modulators have provided a new tool to realize real time 3D display based on digitally recorded hologram and opto-electronic reconstruction. Such a 3D display system is illustrated in the Fig. 68.

The key factor to the success of such a system is the quality of the opto-electronic reconstruction. Several important factors, such as the field of view of reconstruction, image multiplication at reconstruction plane, diffraction efficiency, contrast, spatial resolution of image, speckle from coherent illumination, fidelity of phase object etc, have to be considered in order to get satisfactory reconstruction. In this chapter, we will try to address the first three, which are related to the spatial resolution of the spatial light modulator used for opto-electronic reconstruction.
Fig. 68: Holographic recording of 3D object and opto-electronic reconstruction system.
As shown in Fig. 68, if we define the angle $\alpha$ to be the maximum angle between the object ray and the reference ray, $\alpha$ needs to be large in order to record big objects. If we consider the minimum requirement for the sampling of digitally recorded hologram to be two sampling points per wave of phase modulation (Nyquist criterion). It means the field angle $\alpha$ has to satisfy:

$$\alpha \leq \frac{\lambda}{2\Delta}$$

(5.1)

Where $\Delta$ is the pixel spacing on spatial light modulator and $\lambda$ is the wavelength. This means for a CCD camera with pixel spacing of 5 µm, only 3.62° field of view can be recorded for 632.8 nm wavelength. For recording larger field of view scenes, smaller pixel spacing is required for the CCD used to record the hologram.

On the opto-electronic reconstruction side, we define the maximum angle between reconstruction beam and the 1st order diffraction peak to be $\beta$. Similar requirement is posed on the SLM for reconstruction of large field of view scene. In this case, things are more complicated because as the pixel spacing becomes smaller and smaller, the inter-pixel coupling between neighboring pixel becomes stronger and stronger due to the fringing electric field. This results in reduced phase modulation depth and higher diffraction loss to unwanted diffraction orders. A limitation of spatial resolution of liquid crystal SLM can be expected. How to alleviate such effect as well as understanding the spatial resolution limits of LCoS SLM becomes very important for opto-electronic reconstruction.
5.2 Spatial resolution limitation of LC binary gratings

If we consider a simple case of two beam interfere in space, the phase difference between dark and bright fringe is $\pi$, suppose the two interfering beam have same intensity. In an imaging hologram, the light intensity on the recorded hologram represents a summation of contribution of point sources on the object and the reference beam. The hologram is recorded directly by taking a snap shot of the intensity distribution with a holographic film or CCD camera, and then transferred to the LCoS SLM directly. In this case, it is very hard to understand the physics of this process without simplified consideration.

Let us start with considering a simple liquid crystal diffractive grating, where by control the graylevel of each pixel on the SLM, different gratings are formed which diffract light to different diffraction orders. The diffraction angle for a LC grating is corresponding to the field of view of opto-electronic reconstruction. 2D liquid crystal director simulation and 2D Finite Difference Time Domain simulation is carried out to simulate the phase profile of LCoS SLM and light propagation in LCoS SLM with previously developed software. Liquid crystal binary grating is simulated with alternating high/low voltage applied to array of pixels. As a starting point, the simulation parameter of liquid crystal (LC) is chosen to reflect the property of the LC material used in the current LCoS SLM. Later on, an improved design of LC cell is shown to optimize field of view of LCoS SLM. Liquid crystal parameter used in the first series of simulation is: elastic constant $K_{11} = 14.1 \times 10^{-12}$ N, $K_{22} = 7.1 \times 10^{-12}$ N, $K_{33} = 19.1 \times 10^{-12}$ N, dielectric constant $\varepsilon_// = 12.1 \varepsilon_o$, $\varepsilon_\perp = 4.1 \varepsilon_o$, refractive index $n_o = 1.5035$, $n_e = 1.6742$. A reflective device
with cell thickness $d=4 \ \mu m$ is used in the simulation. Liquid crystal material used in the optimized LC design is BL015 with elastic constant $K_{11}= 14.1 \times 10^{-12} \text{N}$, $K_{22}= 7.1 \times 10^{-12} \text{N}$, $K_{33}= 19.1 \times 10^{-12} \text{N}$, dielectric constant $\varepsilon_{//}=25.3 \ \varepsilon_o$, $\varepsilon_{\perp}=6.9 \ \varepsilon_o$, refractive index $n_o=1.533$, $n_e=1.814$. Cell thickness $d=0.8 \ \mu m$. Different spatial resolution of SLM is simulated with pixel spacing of $19.4 \ \mu m$, $10.5 \ \mu m$, $7.5 \ \mu m$, $4.5 \ \mu m$, $2.5 \ \mu m$ and $1.5 \ \mu m$ with inter-pixel gap between electrodes $0.4 \ \mu m$ for the $19.4 \ \mu m$ pixel spacing and $0.5 \ \mu m$ for all other pixel spacing.

In this case, a binary phase grating with maximum phase difference of $\pi$ is simulated. The single pass phase profile of such a binary grating is shown in Fig. 69 for different spatial resolution LCoS with different pixel spacing. As the pixel spacing becomes smaller and smaller, the modulation depth becomes smaller and smaller. When the pixel spacing is less than $4.5 \ \mu m$, the modulation depth is less than half required value. This result suggests that for small pixel spacing scheme, the dominant factor of the modulation depth is the fringe field, as apposed to normal scheme where pixel spacing is big and the dominant factor is cell thickness and applied voltage.
Table 15: Simulated diffraction efficiency of LC binary grating with different pixel size

<table>
<thead>
<tr>
<th>Diffraction angle $\beta_{\lambda=632.8 \text{ nm}}$</th>
<th>0.94°</th>
<th>1.73°</th>
<th>2.42°</th>
<th>4.02°</th>
<th>7.21°</th>
<th>11.91°</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pixel Spacing (µm)</td>
<td>19.4</td>
<td>10.5</td>
<td>7.5</td>
<td>4.5</td>
<td>2.5</td>
<td>1.5</td>
</tr>
<tr>
<td>$\Delta n=0.1707$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$d=4 \mu m$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-1 order</td>
<td>35.1%</td>
<td>31.7%</td>
<td>27.7%</td>
<td>14.5%</td>
<td>2.1%</td>
<td>0.1%</td>
</tr>
<tr>
<td>0 order</td>
<td>4.3%</td>
<td>16.3%</td>
<td>31.9%</td>
<td>68.4%</td>
<td>95.5%</td>
<td>99.6%</td>
</tr>
<tr>
<td>+1 order</td>
<td>42.7%</td>
<td>38.8%</td>
<td>32.2%</td>
<td>15.5%</td>
<td>2.2%</td>
<td>0.1%</td>
</tr>
</tbody>
</table>
Fig. 69: Single pass phase profile of binary liquid crystal grating. \( \pi \) Phase difference between neighboring electrodes. \( \Delta n=0.1707 \), cell thickness \( d=4 \, \mu m \), for wavelength=632.8 nm. (a) 7.5 \( \mu m \) pixel spacing. (b) 4.5 \( \mu m \) pixel spacing. (c) 1.5 \( \mu m \) pixel spacing. Far field diffraction efficiency of LC binary grating, \( \lambda=632.8 \, \text{nm} \). (d) 7.5 \( \mu m \) pixel spacing. (e) 4.5 \( \mu m \) pixel spacing. (f) 1.5 \( \mu m \) pixel spacing.
The simulated director configuration is fed into FDTD software for near field propagation of a coherent beam. Far field diffraction pattern is obtained by Fresnel diffraction using complex field obtained from FDTD. The main interest is in the percentage of energy goes into \(-1\) or \(+1\) diffraction peak, since that’s the desirable diffraction peak for a holographic reconstruction. In the following discussion, the diffraction efficiency \(DE\) is chosen as the percentage of energy goes into \(+1\) diffraction order, because the percentage of energy goes into \(+1\) order is higher than \(-1\) order. As shown in Table 15, for pixel spacing greater or equal to 7.5 µm, the simulated phase profile shows good phase modulation with \(DE\) of 32.2%. For pixels size smaller than 4.5 µm, phase modulation depth is seriously reduced that the \(DE\) is only 15.5%.

In Table 15, the energy goes into \(-1\), 0, \(+1\) diffraction order is listed. The corresponding diffraction angle is in agreement with what calculated by Equ. 5.1. For 632.8 nm wavelength, if diffraction efficiency \(DE=30\%\) is required for opto-electronic reconstruction, the maximum angular field of view can be obtained is 2.42°. In this case, 3 strong peaks and several weaker peaks will be observed at the far field, which corresponds to the image multiplication at far field. The reason for low \(DE\) with very small pixel spacing is that the dominant factor in this case is the fringe field effect, which strongly reduces the phase modulation depth.

A trade off between the maximum field of view and diffraction efficiency has to be made. As the pixel spacing becomes smaller and smaller, the separation between multiple images become wider, but the unwanted images from high order diffraction peaks become brighter. Another interesting behavior observed is the highly non-
symmetrical diffraction to +1 and –1 diffraction order. The source of this non-symmetric is the pretilt of liquid crystal at top and bottom alignment layer. In some cases, we noted that the difference of energy between –1 and +1 order is over 17% in Table 16.

5.3 Opto-electronic reconstruction of digitally recorded hologram.

To understand how the limitation of the diffraction efficiency and diffraction angle of the current available LC SLM influence the Opto-electronic reconstruction of 3-D image, experiments have been carried out to study the quality of the reconstruction. In Fig. 70 (a), the recorded hologram of the toy bear is shown. In Fig. 70 (b), the computer simulated reconstruction of such electronic hologram is shown. Although the reconstructed image clearly represents the toy bear, the quality of the reconstruction is not perfect. First of all, in the reconstruction algorithm, the zero order diffraction peak is artificially removed due to the algorithm being used. Secondly, the recorded hologram is a Fourier hologram that has the same image in -1 diffraction order.

In Fig. 71, the reconstructed image using LCOS device is shown. The image is reconstructed at different field of view. When the toy bear is reconstructed at an angle of 0.35°, the quality of the reconstruction is very good. Speckles are presented and the zero order diffraction peak is very strong. As the image is reconstructed at larger and larger angle, the image becomes dimmer and dimmer. The quality of the image decreases dramatically. Clearly, a wide angle spatial light modulator is required in order to achieve better performance.
Fig. 70: (a) A digitally recorded hologram of a toy bear. (b) Computer simulated reconstructed image from the digitally recorded hologram.
Fig. 71: Electro-Opto reconstruction of a digitally recorded hologram at different field of view. (a) 0.35° (b) 0.44° (c) 0.60°
Given the current generation of the LC SLM has small diffraction angle and the zero order diffraction peak is very strong. One possibility to improve the image quality is to suppress one of the 1st order diffraction peak in non-imaging holography is to use multilevel phase steps instead of simple binary grating and choose the maximum phase difference to be $2\pi$ instead of $\pi$, as shown in Fig. 72. The advantage is the other 1st order diffraction peak will be much higher. However, this also poses some burden by requiring more pixels for the same wavefront information and wavefront reconstruction. Kinoform, a computer generated phase plate to maximized certain intensity distribution at Fourier plane is generated to demonstrate this idea. In some sense, kinoform is very similar to the blazed grating since both have multilevel grayscale blazed profile as shown in Fig. 73. The reconstructed image is shown in Fig. 74. The amplitude object of letter “KINOFORM” is reconstructed with high brightness. Also some image multiplication can also be observed with more than one image of the text observed in the reconstruction.
Fig. 72: Phase profile of a 4, 8 step LC grating with $2\pi$ phase difference. (a) 4.5 µm pixel spacing. (b) 1.5 pixel spacing. Far field of a 4, 8 step LC grating with $2\pi$ phase difference. (c) 4.5 µm pixel spacing. (d) 1.5 pixel spacing.
Fig. 73: Kinoform used to perform opto-electronic reconstruction (left) and magnified view of kinoform (right)
Fig. 74: Reconstructed amplitude object with computer generated kinoform.
Fig. 75: Single pass phase profile of binary liquid crystal grating. $\pi$ Phase difference between neighboring electrodes. $\Delta n=0.281$, cell thickness $d=0.8 \, \mu m$, for wavelength=632.8nm. (a) 7.5 $\mu$m pixel spacing. (b) 4.5 $\mu$m pixel spacing. (c) 1.5 $\mu$m pixel spacing. Far field diffraction efficiency of LC binary grating, $\Delta n=0.281$, cell thickness $d=0.8 \, \mu m$, $\lambda=632.8 \, nm$. (a) 7.5 $\mu$m pixel spacing. (b) 4.5 $\mu$m pixel spacing. (c) 1.5 $\mu$m pixel spacing.
5.3 Wide field of view LCoS SLM for Digital Holography

Another possibility to improve the diffraction efficiency at large diffraction angle is by reducing the cell thickness to alleviate the fringing field effect. In Chapter 3, we already discussed this issue for a LC OPA. In our case, LC binary grating needs to be considered for the LCoS SLM with LC material BL015 from Merck. Simulation is carried out for different LC materials. A high $\Delta n=0.281$ material is considered to reduce the cell thickness to $d=0.8 \mu m$. The retardation of the LC cell is enough to produce half wave phase modulation for 632.8 nm wavelength. Pixel spacing of 1.5, 2.5, 4.5 and 7.5 $\mu m$ is simulated like before. Even though the $\Delta n*d/\lambda$ decreased significantly, the phase modulation depth increased as compared with LC cell with $d=4 \mu m$. Even for a 1.5 $\mu m$ pixel spacing LC grating, the DE is 39.5% as shown in Fig. 75. The corresponding field of view for opto-electronic reconstruction is 11.91°. The diffraction efficiency for a LC binary grating with different pixel size is shown in Table 16.

Here we see substantial improvement of DE as we use higher $\Delta n$ liquid crystal material while reducing the cell thickness. But the question is, what is the limit and how far can we push in this direction? S.T. Wu et al\textsuperscript{68} reported, a LC mixture with $\Delta n=0.45$. To produce half wave of phase modulation, the cell thickness of the device needs to be only $d=0.352 \mu m$. With $\Delta n=0.45$ LC material, the viscosity is high and the stability of the material haven’t been confirmed. In our case, we choose a $\Delta n=0.35$, $d=0.6 \mu m$ as a very representative liquid crystal device design. The diffraction efficiency for a LC binary grating with $\Delta n=0.35$, $d=0.6 \mu m$ LC cell design is shown in Table 16. DE=44.4% is
observed in the simulation for a 1.5 µm pixel spacing LCoS SLM with a field view of 11.91°.

Table 16: Simulated diffraction efficiency of LC binary grating with different pixel size

| Diffraction angle β _λ=632.8 nm_ | 2.42° | 4.02° | 7.21° | 11.91° |
| Pixel Spacing (µm) | 7.5 | 4.5 | 2.5 | 1.5 |

| Δn=0.281 d=0.8 µm | -1 order | 35.6% | 33.7% | 30.5% | 26.9% |
| 0 order | 1.7% | 3.5% | 12.2% | 26.6% |
| +1 order | 46.5% | 44.9% | 42.7% | 39.5% |

| Δn=0.35 d=0.6 µm | -1 order | 35.6% | 33.7% | 30.9% | 27.1% |
| 0 order | 1.7% | 3.5% | 8.3% | 23.2% |
| +1 order | 50.8% | 48.2% | 46.2% | 44.4% |

For real digitally recorded hologram, whether the diffraction efficiency will be as high as simulation results still need confirmation from experimental results. However, the general physics tells a story that with the use of high Δn material to reduce fringing field is a very promising approach. LCoS device with 1-D line shape electrodes has been developed by Boulder Nonlinear System with pixel spacing as small as 1.6 µm. This suggests LCoS SLM with half angular field of view in the order of low ten degrees with high DE may be available in the foreseeable future.
5.4 Non-symmetrical LC binary gratings

An electronic switchable grating can find applications in many areas such as: laser beam steering, electronic holography, optical communication, active interferometer, hyper-spectral imaging, etc. Although there are many ways to achieve electronic switchability of a diffractive grating, for example binary gratings and Bragg reflectors based on Holographic Polymer Dispersed Liquid Crystal (HPDLC), Photo-elastic gratings, Photo-refractive gratings, acoustic optics, cholesteric liquid crystals etc., it is still very challenging to make a binary grating of high diffraction efficiency at large diffraction angle and still preserve the possibility of varying the periodicity of the grating. This is particularly true when the periodicity of the grating is very close to the wavelength of light. In this section, we describe a variable period liquid crystal binary grating that has highly non-symmetrical -1 and +1 diffraction order for diffraction angle ranging from about 5° ~ 32°. This LC binary grating allows high diffraction efficiency for +1 diffraction order for wide range of achievable diffraction angle.

The LC binary grating consists of two glass substrates with transparent line shape electrodes along X axis on one substrate and common electrode on the other substrate, as shown in Fig. 76 (a). Polyimide alignment layer or other organic or inorganic alignment layer is coated on top of the transparent electrodes, to induce homogenous, or homeotropic alignment of LC director in XZ plane. Glass fibers or spheres with constant diameter are sprayed or printed between the top and bottom glass substrate to create a chamber of constant thickness for filling in LC material. Because of the 1-D line shape electrodes on one of the substrate, the fringing fields between electrodes are in the same
plane of the LC director (the XZ plane). When positive dielectric LC material is used to fill in the gap between the top substrate and bottom substrate, the LC director will align along the electric field, thus remains in XZ plane. This configuration is important because it prevents the LC director to rotate out of XZ plane to form twist structure. Moreover, the LC director at the alignment layer surface has a small angle with respect to the cell surface, which is called the pretilt angle. The pretilt angle is desirable to be 3°~5° for our application. The reason for having non-zero pretilt angle is that it gives LC director a preferred rotation direction upon applying electric field. If the pretilt angle is zero, the LC director on the left and right side of an electrode can rotate in different direction, either clockwise or counter-clockwise, thus form a trapped tilt wall. In a low spatial resolution LC device where the electrode size is larger than 10 µm, such trapped tilt wall is stable. However, for our application where less than 1 µm electrode is used, such trapped tilt wall becomes meta-stable and will rotate out of XZ plane to form a twist structure. Such twist structure will introduce polarization to the grating, thus should be avoided in order to achieve high diffraction efficiency.

An alternating high and low voltage is applied to the electrodes, thus producing the director configuration as shown in Fig. 76 (b). If an incident light is polarized along X direction, the optical path difference (OPD) of the light is a binary phase profile as shown in Fig. 77. The LC binary grating has a highly non-symmetrical -1 and +1 diffraction order according to Finite Difference Time Domain (FDTD) simulation. As shown in this example, the +1 order diffraction peak can be about twice as high as the -1 peak. The
The diffraction efficiency to the +1 diffraction order is 58.0%. The origin of this highly non-symmetrical behavior of the LC binary grating is the most interesting thing to understand.

First of all, the fringing electric field plays a very important role in a high resolution LC device. Generally, the fringing electric field would reduce the phase modulation depth of LC device which lowers the diffraction efficiency of the device. The fringing field effect strongly depends on the cell thickness of the LC device. If the LC device with pixel spacing of the LC binary grating much smaller than the cell thickness of the LC cell, the fringing electric field effect is very strong. The resulting diffraction efficiency for a binary grating that can deflect light to larger than 5° is close to zero, as shown in Table 15. This limitation severely limits the application potential of a LC binary grating.
Fig. 76: Symmetry broken by fringing electric field and tilting angle in a reflective LC binary grating. Here the cell thickness $d=0.4 \ \mu\text{m}$, electrode size $w_e=0.4 \ \mu\text{m}$, gap between electrode $w_g=0.4 \ \mu\text{m}$. LC material used is a high birefringence LC material with $\Delta n=0.50$.

(a) Electrode configuration and rubbing direction of the LC binary grating. (b) Liquid crystal director configuration in X-Z plane. (c) Iso-potential line in the LC binary grating.
In our case, the fringing field is utilized in a beneficial way. If we consider a reflective LC binary grating for He-Ne wavelength, and the double pass phase modulation depth $\frac{2\Delta n d}{\lambda}$ needs to be slightly larger than $1/2$ to maximize the diffraction efficiency. The director configuration in region A and B in Fig. 76 (b) is not a mirror image of each other as the tilting of the LC director is both positive. Because the presence of fringing electric field, the field direction in region A and B is pointing to left-up and right-up direction instead of perpendicular to the cell surface. The angle between the electric field and the director is not identical in region A and B. In region A, such angle is much larger than in region B. Thus, the electric torque applied to the LC director in these two regions is not the same. The resulting phase profile of the grating as showing in Fig. 77 (a) is non-symmetrical. However, this non-symmetrical phase profile leads to only small difference between the +1 and -1 diffraction peak if the pixel spacing of the binary grating is not optimized. Only when the periodicity of the phase profile is compatible with wavelength of light, should a strong non-symmetrical +1 and -1 diffraction peak become obvious. This can be illustrated in, where different pixel spacing of binary grating is simulated. The diffraction efficiency Fig. 78 is plotted in Fig. 78 (a) as function of the corresponding steering angle of the grating. The peak intensity ratio of the +1 and -1 diffraction order is plotted the same fashion in Fig. 78 (b). For pixel size smaller than 4.5 µm, the steering angle of the binary grating is larger than 4°, and the peak intensity ratio of the +1 and -1 diffraction order can be very large.
Fig. 77: Non-symmetrical phase profile and far field diffraction pattern of LC binary grating. ($\lambda=632.8$ nm) (a) Phase profile of a binary grating with cell thickness $d=0.4$ µm, electrode size $w_e=0.4$ µm, gap between electrode $w_g=0.4$ µm, LC material $\Delta n=0.50$. (b) Simulated far field diffraction pattern of the binary grating.
Fig. 78: Diffraction efficiency and non-symmetrical behavior as function of diffraction angle and electrode size. ($\lambda=632.8$ nm) (a) Diffraction efficiency and angle for different pixel spacing and cell thickness. Here the electrode size $w_e=6, 4, 2, 1, 0.5, 0.4, 0.3$ µm, gap between electrode $w_g=0.5, 0.5, 0.5, 0.5, 0.5, 0.4, 0.3$ µm respectively. (b) The peak intensity ratio between $+1$ diffraction order and $-1$ diffraction order for the corresponding cell parameter.
The peak intensity ratio also strongly depends on the cell thickness of the LC cell. For cell thickness larger than 0.5 \( \mu \text{m} \), such non-symmetrical behavior is not apparent. Only when the cell thickness of the device is less than 0.5 \( \mu \text{m} \), the peak intensity ratio is very large. Because of the highly non-symmetrical peak intensity, the diffraction efficiency for the +1 diffraction order can be higher than 50\%. There is an optimum pixel spacing that gives the highest peak intensity ratio. Such optimum pixel spacing is a function of the cell thickness. The smaller the cell thickness, the smaller the optimum pixel spacing and the wider the pixel spacing range that can produce the non-symmetrical behavior. In order for a thin LC device to have \( \frac{2\Delta n d}{\lambda} \) value larger than 1/4, a high birefringence LC material is critical.

At the mean time, this liquid crystal binary grating can be a variable period grating if each of the electrode is independently addressable. However, to make a relative large clear aperture, the total number of electrodes for the grating is very large. A more efficient way to achieve variable period grating can be bridged every 2N electrode of the LC binary grating together, similarly to Ref.\(^7\). The whole clear aperture is divided to sub-apertures with each sub-aperture has 2N electrodes. Every 2N electrodes are electrically connected together. If the pixel size of the grating is \( W_e \) and the gap between the electrode is \( W_g \). With current photolithograph technology, the pixel spacing of the grating \( W_e + W_g \) can be smaller than wavelength of light. In this case, depends on the driving voltage applied to the 2N electrode, a binary grating with grating period ranging from \( 2*( W_e + W_g) \) to \( 2N*( W_e + W_g) \) is achievable. Such a variable period grating with
high diffraction efficiency can be very attractive for many applications. Especially for wide angle beam steering for NIR wavelength, a reflective binary gratings requires only 1/4 wave of total phase modulation depth, as compared with 1/2 wave of a reflective blazed grating. The reduction in the cell thickness greatly alleviates the fringing field problem, thus can achieve higher diffraction efficiency as compared with a blazed grating that steers to the same angle. The speed of the device can also be much higher than the blazed grating because of the reduction in cell thickness.

5.5 Conclusion

Using LC SLM to realized electronic hologram faces challenges in the limitation of diffraction efficiency and diffraction angle of the liquid crystal diffractive optical element. Methods to improve the diffraction efficiency and angle are proposed. Simulations show it is possible to achieve over 30° of diffraction angle with efficiency higher than 50%, by utilizing the strong non-symmetrical behavior of the LC binary grating. The physics behind such non-symmetrical behavior is studied.
Chapter 6

Conclusions and Suggestions for Future Works

6.1 Summaries

This dissertation is related to the fundamental physics of liquid crystal (LC) diffractive optical element (DOE) and its application in beam steering, wavefront control in large optics, electronic holography etc.

Extensive computer modeling is performed to study the fundamental physics of LC DOE, in terms of its physical property, that involves advanced simulation method such as: Finite Difference Time Domain (FDTD) simulation, CODE V ray tracing and diffractive beam propagation, 2-D and 3-D liquid crystal director simulation etc. As a result, fringing electric field effect, defect formation, diffraction efficiency, polarization effect in a high resolution OPA is quantitatively studied. Many new device structure and concepts that can substantially improve the efficiency and diffraction angle of a LC DOE is proposed, for example, an optimized OPA, a pinned electrode OPA, a non-symmetrical variable period binary grating etc. FDTD simulation with both TE and TM mode is carried out, light propagation in LC DOE with complicated 3-D director distribution is studied.

Experimental study is carried out to verify the modeling results. 2-D birefringence measurement, Electro-Optical response of the device, as well as the diffraction efficiency, near field phase distribution, wavefront quality, far field beam profile is carried out to
study the optical performance of the LC DOE. High resolution wavefront control system for large aperture telescope based on a LC DOE is demonstrated. Active laser beam control for multiple target tracking and acquisition is performed. Opto-electronic reconstruction of a digitally recorded hologram is also demonstrated with the best quality so far observed in this field.
References


San Jose, Calif., 489, (1999).


Appendix A: Detailed implementation of 3D director modeling

This is the "Feni.msw" Maple worksheet that derives the functional derivatives of the electric free energy with respect to \( n_x \), \( n_y \), and \( n_z \).

This part of LCSD © 2000 Kent State University
Jim Anderson 1/21/99

Some info on notation: \( \tilde{n}(x,y,z) \) is the \( 3 \times 3 \) component of the q tensor, \( e \) is the q tensor, \( F_e \) is the electric free energy, \( V_a \) is the derivative of the voltage with respect to a.

This resets everything.

> restart;
This brings in some linear algebra subroutines such as dsvr and dotprod.

> with(linalg):
Warning, new definition for norm
Warning, new definition for trace

Define each of the components of the dielectric tensor.

> e11(x,y,z) := e0* (epsilon + Dielectric(x,y,z) * n(x,y,z));
> e12(x,y,z) := e0* (epsilon + Dielectric(x,y,z) * n(y,x,z));
> e13(x,y,z) := e0* (epsilon + Dielectric(x,y,z) * n(z,x,y));
> e21(x,y,z) := e0* (epsilon + Dielectric(x,y,z) * n(x,y,z));
> e22(x,y,z) := e0* (epsilon + Dielectric(x,y,z) * n(y,x,z));
> e23(x,y,z) := e0* (epsilon + Dielectric(x,y,z) * n(z,x,y));
> e31(x,y,z) := e0* (epsilon + Dielectric(x,y,z) * n(x,y,z));
> e32(x,y,z) := e0* (epsilon + Dielectric(x,y,z) * n(y,x,z));
> e33(x,y,z) := e0* (epsilon + Dielectric(x,y,z) * n(z,x,y));

Make the dielectric tensor.

> m := linalg(matrix)(3,3, [e11(x,y,z), e12(x,y,z), e13(x,y,z), e21(x,y,z), e22(x,y,z), e23(x,y,z), e31(x,y,z), e32(x,y,z), e33(x,y,z)));

Form the gradient of \( V_a \), which is the negative of the electric field.

> gradV := grad(V_a(x,y,z), [x,y,z]);

Form the electric displacement (negative of \( \mathbf{E} \)).

> e := (epsilon + Dielectric(x,y,z) * n(x,y,z));

Helmholtz free energy is 1/2 (E dot D).

> gradVgradD := dotprod(gradient(gradV, x), e * gradient(D, x));

Form the electric displacement.

> gradVgradD := dotprod(D, gradV);

Helmholtz free energy is 1/2 (E dot D).

> gradVgradD := dotprod(gradient(gradV, x), e * gradient(D, x));

Form the electric displacement.

> Fe := 1/2 * gradVgradD;

Helmholtz free energy is 1/2 (E dot D).

> gradVgradD := dotprod(gradient(gradV, x), e * gradient(D, x));
\[
\left( \frac{\partial}{\partial y} V(x,y,z) \right) \left( \epsilon_0 \frac{\partial}{\partial x} w(x,y,z) \eta(x,y,z) \right) + \epsilon_0 \left( \frac{\partial}{\partial z} V(x,y,z) \right) \frac{\partial}{\partial y} V(x,y,z) \right)
\]

\[
+ \epsilon_0 \left( \frac{\partial}{\partial y} V(x,y,z) \right) \left( \epsilon_0 \frac{\partial}{\partial x} w(x,y,z) \eta(x,y,z) \right) + \epsilon_0 \frac{\partial}{\partial z} V(x,y,z) \left( \frac{\partial}{\partial y} V(x,y,z) \right)
\]

\[
+ \epsilon_0 \left( \frac{\partial}{\partial y} V(x,y,z) \right) \left( \epsilon_0 \frac{\partial}{\partial x} w(x,y,z) \eta(x,y,z) \right) + \epsilon_0 \frac{\partial}{\partial z} V(x,y,z) \left( \frac{\partial}{\partial y} V(x,y,z) \right)
\]

\[
+ \epsilon_0 \left( \frac{\partial}{\partial y} V(x,y,z) \right) \left( \epsilon_0 \frac{\partial}{\partial x} w(x,y,z) \eta(x,y,z) \right) + \epsilon_0 \frac{\partial}{\partial z} V(x,y,z) \left( \frac{\partial}{\partial y} V(x,y,z) \right)
\]

\]
\[
\frac{1}{2} \left( (Y_0 - V_{100}) \frac{\partial m(x,y,z)}{\partial x} (V_{100} - V_0 - 1) \right) + \frac{1}{2} \left( (Y_0 - V_{100}) \frac{\partial m(x,y,z)}{\partial y} (V_{100} - V_0 - 1) \right) + \frac{1}{2} \left( n \frac{\partial m(x,y,z)}{\partial z} (V_{100} - V_0 - 1) \right)
\]

Output the Fortran code for the update formula for \(m\):

```fortran
fortran (m = dFm, optimised, precision = double);
```

1. Take the derivative of \(F\) with respect to \(n\).

```fortran
dFncey := \frac{1}{2} \left( (Y_0 - V_{100}) \frac{\partial n(x,y,z)}{\partial x} (V_{100} - V_0 - 1) \right) + \frac{1}{2} \left( (Y_0 - V_{100}) \frac{\partial n(x,y,z)}{\partial y} (V_{100} - V_0 - 1) \right) + \frac{1}{2} \left( n \frac{\partial n(x,y,z)}{\partial z} (V_{100} - V_0 - 1) \right)
```

Rearrange this so as to be able to take derivatives with respect to \(n\):

```fortran
dFncey := \frac{1}{2} \left( (Y_0 - V_{100}) \frac{\partial n(x,y,z)}{\partial x} (V_{100} - V_0 - 1) \right) + \frac{1}{2} \left( (Y_0 - V_{100}) \frac{\partial n(x,y,z)}{\partial y} (V_{100} - V_0 - 1) \right) + \frac{1}{2} \left( n \frac{\partial n(x,y,z)}{\partial z} (V_{100} - V_0 - 1) \right)
```

Output the Fortran code for the update formula for \(n\):

```fortran
fortran (n = dFm, optimised, precision = double);
```

1. Take the derivative of \(F\) with respect to \(y\).

```fortran
dFncy := \frac{1}{2} \left( (Y_0 - V_{100}) \frac{\partial n(x,y,z)}{\partial x} (V_{100} - V_0 - 1) \right) + \frac{1}{2} \left( (Y_0 - V_{100}) \frac{\partial n(x,y,z)}{\partial y} (V_{100} - V_0 - 1) \right) + \frac{1}{2} \left( n \frac{\partial n(x,y,z)}{\partial z} (V_{100} - V_0 - 1) \right)
```

Rearrange this so as to be able to take derivatives with respect to \(y\):

```fortran
dFncy := \frac{1}{2} \left( (Y_0 - V_{100}) \frac{\partial n(x,y,z)}{\partial x} (V_{100} - V_0 - 1) \right) + \frac{1}{2} \left( (Y_0 - V_{100}) \frac{\partial n(x,y,z)}{\partial y} (V_{100} - V_0 - 1) \right) + \frac{1}{2} \left( n \frac{\partial n(x,y,z)}{\partial z} (V_{100} - V_0 - 1) \right)
```

Output the Fortran code for the update formula for \(y\):

```fortran
fortran (y = dFm, optimised, precision = double);
```

1. Take the derivative of \(F\) with respect to \(z\).

```fortran
dFcz := \frac{1}{2} \left( (Y_0 - V_{100}) \frac{\partial n(x,y,z)}{\partial x} (V_{100} - V_0 - 1) \right) + \frac{1}{2} \left( (Y_0 - V_{100}) \frac{\partial n(x,y,z)}{\partial y} (V_{100} - V_0 - 1) \right) + \frac{1}{2} \left( n \frac{\partial n(x,y,z)}{\partial z} (V_{100} - V_0 - 1) \right)
```

Rearrange this so as to be able to take derivatives with respect to \(z\):

```fortran
dFcz := \frac{1}{2} \left( (Y_0 - V_{100}) \frac{\partial n(x,y,z)}{\partial x} (V_{100} - V_0 - 1) \right) + \frac{1}{2} \left( (Y_0 - V_{100}) \frac{\partial n(x,y,z)}{\partial y} (V_{100} - V_0 - 1) \right) + \frac{1}{2} \left( n \frac{\partial n(x,y,z)}{\partial z} (V_{100} - V_0 - 1) \right)
```
This is the "Voltage.mws" Maple worksheet that derives the formula for the new value of the potential at the current grid point, based on the potentials at the surrounding grid points.

Some info on notation:
- \( \epsilon \) = the epsilon tensor
- \( \mathbf{a} \) = the electric displacement, \( \mathbf{V} = \frac{\partial \mathbf{V}}{\partial y} \) at \( y \), and \( \mathbf{V}_0 = \frac{\partial \mathbf{V}}{\partial x} \) at \( x \)

This needs everything:

> restart;

This brings in some linear algebra subroutines such as diverge and dotprod.

> with(LinearAlgebra):

Working, new definition for \( \nabla \mathbf{V} \):

> Define the gradient of the voltage:

\[
\mathbf{grad} \mathbf{V} := \left( \frac{\partial}{\partial x} \mathbf{V}(x, y, z), \frac{\partial}{\partial y} \mathbf{V}(x, y, z), \frac{\partial}{\partial z} \mathbf{V}(x, y, z) \right)
\]

> Define the dielectric tensor:

\[
\epsilon := \begin{bmatrix}
\epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\
\epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\
\epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz}
\end{bmatrix}
\]

> Define the electric displacement:

\[
\mathbf{E} := \mathbf{grad} \mathbf{V} \cdot \epsilon
\]

Define the divergence of \( \mathbf{D} \) equal to 0 (Maxwell's equations):

\[

\mathbf{div} \mathbf{D} := \frac{\partial}{\partial x} (\epsilon_{xx} \mathbf{E}_x + \epsilon_{xy} \mathbf{E}_y + \epsilon_{xz} \mathbf{E}_z) + \frac{\partial}{\partial y} (\epsilon_{yx} \mathbf{E}_x + \epsilon_{yy} \mathbf{E}_y + \epsilon_{yz} \mathbf{E}_z) + \frac{\partial}{\partial z} (\epsilon_{zx} \mathbf{E}_x + \epsilon_{zy} \mathbf{E}_y + \epsilon_{zz} \mathbf{E}_z) = 0
\]
\[ V_x = -\frac{\partial}{\partial x} (v_0 + v_0) - 2v_0 \delta y \]

Define the second derivative of the voltage with respect to \( z \), with respect to \( y \), \( \frac{d^2 V}{dy^2} \): 
\[ \frac{d^2 V}{dy^2} = \frac{v_0 + v_0 - v_0 - v_0}{4} \]

Define the second derivative of the voltage with respect to \( z \), \( \frac{d^2 V}{dz^2} \): 
\[ V_{zz} = \frac{v_0 + v_0 - v_0 - v_0}{2} \]

Define the Euler-Lagrange equation (grad \( D \)).
\[ E \cdot N = \nabla \cdot (v_0 + v_0) - \frac{1}{2} \int \left( \frac{1}{2} c_1 (v_0 + v_0) - c_1 (v_0 + v_0) \right) \frac{d^2}{dy^2} V \]

\[ E \cdot V = \frac{1}{2} c_2 (v_0 + v_0) - c_2 (v_0 + v_0) \]

\[ \frac{d}{dy} \frac{\partial}{\partial y} (v_0 + v_0) + \frac{\partial}{\partial y} \frac{\partial}{\partial y} (v_0 + v_0) \]

\[ \frac{d^2}{dy^2} (v_0 + v_0) - \frac{1}{2} \int \left( \frac{1}{2} c_1 (v_0 + v_0) - c_1 (v_0 + v_0) \right) \frac{d^2}{dy^2} V \]

\[ \frac{d}{dy} \frac{\partial}{\partial y} (v_0 + v_0) + \frac{\partial}{\partial y} \frac{\partial}{\partial y} (v_0 + v_0) \]

\[ \frac{d^2}{dy^2} (v_0 + v_0) - \frac{1}{2} \int \left( \frac{1}{2} c_1 (v_0 + v_0) - c_1 (v_0 + v_0) \right) \frac{d^2}{dy^2} V \]

\[ \frac{d^2}{dy^2} (v_0 + v_0) - \frac{1}{2} \int \left( \frac{1}{2} c_1 (v_0 + v_0) - c_1 (v_0 + v_0) \right) \frac{d^2}{dy^2} V \]

Output this in Fortran. This is what would be used if one would want to relax on voltage.

\[ \text{fortran (ELECTROFLUIDS), precision=double):} \]
1. \( v_0 = 0.0 \)\( \times 100 \)
2. \( v_0 = 0.0 \)\( \times 100 \)
3. \( v_0 = 0.0 \)\( \times 100 \)

\[ \text{Solve this equation for the voltage at the current point.} \]
1. \( \text{solve}(v_0, 0.000); \]
2. \( \text{beta} = 1.0 \times 100 \)
3. \( \text{beta} = 1.0 \times 100 \)
4. \( \text{beta} = 1.0 \times 100 \)
5. \( \text{beta} = 1.0 \times 100 \)
This is the "vectorenergy mws" Maple worksheet that derives and outputs Fortran code for splay, twist, bend and strain free energies as well as the functional derivatives of Fs with respect to nx, ny and nz, the three components of the liquid crystal director.

This is part of LCD © 2000 Kent State University

Jim Anderson 9/2/99

Some info on notation: \( v \) is the \((x,y,z)\) volume element, \( n \) is the liquid crystal director (consisting of \( nx, ny \) and \( nz \)); \( K11, K22, K33 \) are the splay, twist and bend elastic constants respectively; \( Fs \) is the strain free energy and derivatives are written directly (which means the derivative of \( Fs \) with respect to \( n \)).

This resets everything.

> restart;

This brings in some linear algebra subroutines such as diverge and dotprod.

> with(linalg);

Warning, new definition for norm
Warning, new definition for trace

Define the volume element.

> \( v := \{x, y, z\} \);

Define the liquid crystal director.

> \( n := \) vector([[nx(x,y,z), ny(x,y,z), nz(x,y,z)]]);

Define the Splay free energy.

> splay := \( (1/2)*K11*(\text{div}(n, v))^2 \);

\[
\text{div}(n, v) = \frac{1}{2} K11 \left( \frac{\partial nx(x,y,z)}{\partial x} + \frac{\partial ny(x,y,z)}{\partial y} + \frac{\partial nz(x,y,z)}{\partial z} \right)
\]

Expand this out to see all terms.

> splay := \( \text{expand('splay')} \);

\[
\text{exp}(n, v) = \frac{1}{2} K11 \left( \frac{\partial nx(x,y,z)}{\partial x} + \frac{\partial ny(x,y,z)}{\partial y} + \frac{\partial nz(x,y,z)}{\partial z} \right)
\]

Define the twist free energy.

> twist := \( (1/2)*K22*(\text{curl}(n, v))^2 \);

\[
\text{curl}(n, v) = \frac{1}{2} K22 \left( \frac{\partial nz(x,y,z)}{\partial y} - \frac{\partial ny(x,y,z)}{\partial z} \right)
\]

Expand this out to see all terms.

> twist := \( \text{expand('twist')} \);

\[
\text{exp}(n, v) = \frac{1}{2} K22 \left( \frac{\partial nz(x,y,z)}{\partial y} - \frac{\partial ny(x,y,z)}{\partial z} \right)
\]
\[ - \frac{1}{2} k_{22} \frac{\partial^2 n(x, y, z)}{\partial x^2} + \frac{1}{2} k_{22} \frac{\partial^2 n(x, y, z)}{\partial y^2} + \frac{1}{2} k_{22} \frac{\partial^2 n(x, y, z)}{\partial z^2} \]

\[ - \frac{1}{2} k_{22} \frac{\partial^2 n(x, y, z)}{\partial x^2} + \frac{1}{2} k_{22} \frac{\partial^2 n(x, y, z)}{\partial y^2} + \frac{1}{2} k_{22} \frac{\partial^2 n(x, y, z)}{\partial z^2} \]

\[ - k_{22} n(x, y, z) \frac{\partial^2 n(x, y, z)}{\partial x^2} + k_{22} n(x, y, z) \frac{\partial^2 n(x, y, z)}{\partial y^2} - k_{22} n(x, y, z) \frac{\partial^2 n(x, y, z)}{\partial z^2} \]

\[ - k_{22} n(x, y, z) \frac{\partial^2 n(x, y, z)}{\partial x^2} + k_{22} n(x, y, z) \frac{\partial^2 n(x, y, z)}{\partial y^2} - k_{22} n(x, y, z) \frac{\partial^2 n(x, y, z)}{\partial z^2} \]
\[-K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial x} n_i(x, y, z) \right) - \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial y} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right)\]

\[+ \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial y} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right)\]

\[+ \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial x} n_i(x, y, z) \right)\]

\[= K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial x} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial y} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right)\]

\[+ \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial y} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right)\]

\[+ \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial x} n_i(x, y, z) \right)\]

\[= K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial x} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial y} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right)\]

\[+ \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial y} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right)\]

\[+ \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial x} n_i(x, y, z) \right)\]

\[= K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial x} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial y} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right)\]

\[+ \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial y} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right)\]

\[+ \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial x} n_i(x, y, z) \right)\]

\[= K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial x} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial y} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right)\]

\[+ \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial y} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right)\]

\[+ \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial x} n_i(x, y, z) \right)\]

\[= K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial x} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial y} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right)\]

\[+ \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial y} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right)\]

\[+ \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial x} n_i(x, y, z) \right)\]

\[= K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial x} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial y} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right)\]

\[+ \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial y} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right)\]

\[+ \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial z} n_i(x, y, z) \right) + \frac{1}{2} K_{IJ} n_i(x, y, z) \left( \frac{\partial}{\partial x} n_i(x, y, z) \right)\]
Now we have all three elastic free energies defined, let's output them separately.

Output the twist free energy in Fortran code. Note: After this is copied and pasted into the Fortran program, the user will have to define some variables. \( \text{Diff}(A,B) \) is the derivative of \( A \) with respect to \( B \), and \( K_{ij} \) are the elastic constants.

```fortran
> fortran ([(answer=row), optimized, precision=double]);
```

Output the bend free energy in Fortran code. Again, some variables have to be defined.

```fortran
> fortran ([(answer=twist), optimized, precision=double]);
```

We have computed the elastic constants that appear in the energy definitions. The constants are:

- \( K_{11} = \frac{3E'}{3(1-\nu)} \)
- \( K_{12} = \frac{E'}{3(1-\nu)} \)
- \( K_{22} = \frac{E'}{3(1-\nu)} \)
- \( K_{13} = \frac{E'}{3(1-\nu)} \)
- \( K_{23} = \frac{E'}{3(1-\nu)} \)
- \( K_{33} = \frac{E'}{3(1-\nu)} \)
- \( K_{14} = \frac{E'}{3(1-\nu)} \)
- \( K_{24} = \frac{E'}{3(1-\nu)} \)
- \( K_{34} = \frac{E'}{3(1-\nu)} \)
- \( K_{44} = \frac{E'}{3(1-\nu)} \)
- \( K_{15} = \frac{E'}{3(1-\nu)} \)
- \( K_{25} = \frac{E'}{3(1-\nu)} \)
- \( K_{35} = \frac{E'}{3(1-\nu)} \)
- \( K_{45} = \frac{E'}{3(1-\nu)} \)
- \( K_{55} = \frac{E'}{3(1-\nu)} \)
- \( K_{16} = \frac{E'}{3(1-\nu)} \)
- \( K_{26} = \frac{E'}{3(1-\nu)} \)
- \( K_{36} = \frac{E'}{3(1-\nu)} \)
- \( K_{46} = \frac{E'}{3(1-\nu)} \)
- \( K_{56} = \frac{E'}{3(1-\nu)} \)

We have also computed the elastic constants that appear in the energy definitions. The constants are:

- \( K_{11} = \frac{3E'}{3(1-\nu)} \)
- \( K_{12} = \frac{E'}{3(1-\nu)} \)
- \( K_{22} = \frac{E'}{3(1-\nu)} \)
- \( K_{13} = \frac{E'}{3(1-\nu)} \)
- \( K_{23} = \frac{E'}{3(1-\nu)} \)
- \( K_{33} = \frac{E'}{3(1-\nu)} \)
- \( K_{14} = \frac{E'}{3(1-\nu)} \)
- \( K_{24} = \frac{E'}{3(1-\nu)} \)
- \( K_{34} = \frac{E'}{3(1-\nu)} \)
- \( K_{44} = \frac{E'}{3(1-\nu)} \)
- \( K_{15} = \frac{E'}{3(1-\nu)} \)
- \( K_{25} = \frac{E'}{3(1-\nu)} \)
- \( K_{35} = \frac{E'}{3(1-\nu)} \)
- \( K_{45} = \frac{E'}{3(1-\nu)} \)
- \( K_{55} = \frac{E'}{3(1-\nu)} \)
- \( K_{16} = \frac{E'}{3(1-\nu)} \)
- \( K_{26} = \frac{E'}{3(1-\nu)} \)
- \( K_{36} = \frac{E'}{3(1-\nu)} \)
- \( K_{46} = \frac{E'}{3(1-\nu)} \)
- \( K_{56} = \frac{E'}{3(1-\nu)} \)

We have also computed the elastic constants that appear in the energy definitions. The constants are:

- \( K_{11} = \frac{3E'}{3(1-\nu)} \)
- \( K_{12} = \frac{E'}{3(1-\nu)} \)
- \( K_{22} = \frac{E'}{3(1-\nu)} \)
- \( K_{13} = \frac{E'}{3(1-\nu)} \)
- \( K_{23} = \frac{E'}{3(1-\nu)} \)
- \( K_{33} = \frac{E'}{3(1-\nu)} \)
- \( K_{14} = \frac{E'}{3(1-\nu)} \)
- \( K_{24} = \frac{E'}{3(1-\nu)} \)
- \( K_{34} = \frac{E'}{3(1-\nu)} \)
- \( K_{44} = \frac{E'}{3(1-\nu)} \)
- \( K_{15} = \frac{E'}{3(1-\nu)} \)
- \( K_{25} = \frac{E'}{3(1-\nu)} \)
- \( K_{35} = \frac{E'}{3(1-\nu)} \)
- \( K_{45} = \frac{E'}{3(1-\nu)} \)
- \( K_{55} = \frac{E'}{3(1-\nu)} \)
- \( K_{16} = \frac{E'}{3(1-\nu)} \)
- \( K_{26} = \frac{E'}{3(1-\nu)} \)
- \( K_{36} = \frac{E'}{3(1-\nu)} \)
- \( K_{46} = \frac{E'}{3(1-\nu)} \)
- \( K_{56} = \frac{E'}{3(1-\nu)} \)
Define the total "strain" free energy, which is the sum of the splay, twist and bend free energies.

\[ F_s = \frac{1}{2} K_{1s} \left( \frac{\partial^2}{\partial x^2} \psi(x, y, z) + \frac{\partial^2}{\partial y^2} \psi(x, y, z) \right) + K_{1t} \left( \frac{\partial^2}{\partial x \partial y} \psi(x, y, z) \right)^2 + K_{1b} \left( \frac{\partial^2}{\partial x \partial z} \psi(x, y, z) \right)^2 + \frac{1}{2} K_{2s} \frac{\partial^2}{\partial y \partial z} \psi(x, y, z) \]

\[ + \frac{1}{2} K_{2t} \frac{\partial^2}{\partial x \partial y} \psi(x, y, z) \]

\[ + \frac{1}{2} K_{2b} \frac{\partial^2}{\partial x \partial z} \psi(x, y, z) \]

\[ - K_{22} \frac{\partial^2}{\partial x \partial y} \psi(x, y, z) \]

\[ - K_{22} \frac{\partial^2}{\partial x \partial z} \psi(x, y, z) \]

\[ - K_{22} \frac{\partial^2}{\partial y \partial z} \psi(x, y, z) \]

\[ + K_{22} \frac{\partial^2}{\partial x \partial y} \psi(x, y, z) \]

\[ + K_{22} \frac{\partial^2}{\partial x \partial z} \psi(x, y, z) \]

\[ + K_{22} \frac{\partial^2}{\partial y \partial z} \psi(x, y, z) \]
\[ F_s = -{1 \over 2} K_1 \nu \frac{\partial \phi}{\partial t} - {K_2 q}^2 \]

We need to rewrite this so as to be able to take derivatives with respect to derivatives.

\[ F_s = -{1 \over 2} K_1 \nu \frac{\partial \phi}{\partial t} - {K_2 q}^2 \]

This is the derivative of \( F_s \) with respect to \( (\nu, t) \) derivative.

\[ \text{diff} = \text{diff}(F_s, \nu, t) \]

\[ \text{diff} = K_1 \nu \cdot K_1 \nu = K_1^2 \nu^2 \]

Rewrite this in terms of \( x, y \), and \( z \) and put the derivatives back in.

\[ \text{diff} = - \]
This is the derivative with respect to \( x \):

\[
dP_{\text{dF}x} = K_{1} \left( \frac{\partial}{\partial x} n(x, y, z) \right) + K_{1} \left( \frac{\partial}{\partial y} n(x, y, z) \right) + K_{1} \left( \frac{\partial}{\partial z} n(x, y, z) \right)
\]

\[
dP_{\text{dF}y} = K_{2} \left( \frac{\partial}{\partial x} n(x, y, z) \right) + K_{2} \left( \frac{\partial}{\partial y} n(x, y, z) \right) + K_{2} \left( \frac{\partial}{\partial z} n(x, y, z) \right)
\]

\[
dP_{\text{dF}z} = K_{3} \left( \frac{\partial}{\partial x} n(x, y, z) \right) + K_{3} \left( \frac{\partial}{\partial y} n(x, y, z) \right) + K_{3} \left( \frac{\partial}{\partial z} n(x, y, z) \right)
\]

This is the derivative of \( P \) with respect to \( x \):

\[
dP_{\text{dF}x} = K_{1} \left( \frac{\partial}{\partial x} n(x, y, z) \right)
\]

\[
dP_{\text{dF}x} = K_{2} \left( \frac{\partial}{\partial x} n(x, y, z) \right)
\]

\[
dP_{\text{dF}x} = K_{3} \left( \frac{\partial}{\partial x} n(x, y, z) \right)
\]

\[
dP_{\text{dF}x} = K_{1} \left( \frac{\partial}{\partial x} n(x, y, z) \right) + K_{1} \left( \frac{\partial}{\partial y} n(x, y, z) \right) + K_{1} \left( \frac{\partial}{\partial z} n(x, y, z) \right)
\]

\[
dP_{\text{dF}x} = K_{2} \left( \frac{\partial}{\partial x} n(x, y, z) \right) + K_{2} \left( \frac{\partial}{\partial y} n(x, y, z) \right) + K_{2} \left( \frac{\partial}{\partial z} n(x, y, z) \right)
\]

\[
dP_{\text{dF}x} = K_{3} \left( \frac{\partial}{\partial x} n(x, y, z) \right) + K_{3} \left( \frac{\partial}{\partial y} n(x, y, z) \right) + K_{3} \left( \frac{\partial}{\partial z} n(x, y, z) \right)
\]

\[
dP_{\text{dF}x} = K_{1} \left( \frac{\partial}{\partial x} n(x, y, z) \right) + K_{1} \left( \frac{\partial}{\partial y} n(x, y, z) \right) + K_{1} \left( \frac{\partial}{\partial z} n(x, y, z) \right)
\]

\[
dP_{\text{dF}x} = K_{2} \left( \frac{\partial}{\partial x} n(x, y, z) \right) + K_{2} \left( \frac{\partial}{\partial y} n(x, y, z) \right) + K_{2} \left( \frac{\partial}{\partial z} n(x, y, z) \right)
\]

\[
dP_{\text{dF}x} = K_{3} \left( \frac{\partial}{\partial x} n(x, y, z) \right) + K_{3} \left( \frac{\partial}{\partial y} n(x, y, z) \right) + K_{3} \left( \frac{\partial}{\partial z} n(x, y, z) \right)
\]

\[
dP_{\text{dF}x} = K_{1} \left( \frac{\partial}{\partial x} n(x, y, z) \right) + K_{1} \left( \frac{\partial}{\partial y} n(x, y, z) \right) + K_{1} \left( \frac{\partial}{\partial z} n(x, y, z) \right)
\]

\[
dP_{\text{dF}x} = K_{2} \left( \frac{\partial}{\partial x} n(x, y, z) \right) + K_{2} \left( \frac{\partial}{\partial y} n(x, y, z) \right) + K_{2} \left( \frac{\partial}{\partial z} n(x, y, z) \right)
\]

\[
dP_{\text{dF}x} = K_{3} \left( \frac{\partial}{\partial x} n(x, y, z) \right) + K_{3} \left( \frac{\partial}{\partial y} n(x, y, z) \right) + K_{3} \left( \frac{\partial}{\partial z} n(x, y, z) \right)
\]

\[
dP_{\text{dF}x} = K_{1} \left( \frac{\partial}{\partial x} n(x, y, z) \right) + K_{1} \left( \frac{\partial}{\partial y} n(x, y, z) \right) + K_{1} \left( \frac{\partial}{\partial z} n(x, y, z) \right)
\]
\[ \begin{align*}
&+ K_{13} \left( \frac{\partial}{\partial x} n_{13}(x, y, z) \right) \left( \frac{\partial}{\partial y} n_{13}(x, y, z) \right) + K_{13} \left( \frac{\partial}{\partial z} n_{13}(x, y, z) \right) + K_{13} \left( \frac{\partial}{\partial x} n_{13}(x, y, z) \right) + K_{13} \left( \frac{\partial}{\partial y} n_{13}(x, y, z) \right) + K_{13} \left( \frac{\partial}{\partial z} n_{13}(x, y, z) \right) \\
&+ K_{13} \left( \frac{\partial}{\partial x} n_{13}(x, y, z) \right) + K_{13} \left( \frac{\partial}{\partial y} n_{13}(x, y, z) \right) + K_{13} \left( \frac{\partial}{\partial z} n_{13}(x, y, z) \right) \\
&+ K_{13} \left( \frac{\partial}{\partial x} n_{13}(x, y, z) \right) + K_{13} \left( \frac{\partial}{\partial y} n_{13}(x, y, z) \right) + K_{13} \left( \frac{\partial}{\partial z} n_{13}(x, y, z) \right) \\
&+ K_{13} \left( \frac{\partial}{\partial x} n_{13}(x, y, z) \right) + K_{13} \left( \frac{\partial}{\partial y} n_{13}(x, y, z) \right) + K_{13} \left( \frac{\partial}{\partial z} n_{13}(x, y, z) \right) \\
&+ K_{13} \left( \frac{\partial}{\partial x} n_{13}(x, y, z) \right) + K_{13} \left( \frac{\partial}{\partial y} n_{13}(x, y, z) \right) + K_{13} \left( \frac{\partial}{\partial z} n_{13}(x, y, z) \right) \\
&+ K_{13} \left( \frac{\partial}{\partial x} n_{13}(x, y, z) \right) + K_{13} \left( \frac{\partial}{\partial y} n_{13}(x, y, z) \right) + K_{13} \left( \frac{\partial}{\partial z} n_{13}(x, y, z) \right)
\end{align*} \]

Take the derivative of \( F \) with respect to each variable.

\[ \text{\textbf{Problem:}} \]

\[ \text{\textbf{Equation:}} \]

\[ \text{\textbf{Solution:}} \]

\[ \text{\textbf{Conclusion:}} \]

\[ \text{\textbf{Discussion:}} \]
Now we have all the terms for the Euler-Lagrange equation. Here we define \( F \) as the functional derivative of \( P \) with respect to \( \phi \).

\[ F = \frac{\partial P}{\partial \phi} + \frac{\partial E}{\partial \phi} \]

Euler-Lagrange equation:

\[ \frac{\partial}{\partial y} \frac{\partial F}{\partial \phi_y} - \frac{\partial}{\partial x} \frac{\partial F}{\partial \phi_x} = 0 \]
- \( \frac{\partial}{\partial t} \psi(x, y, z) + \frac{\partial}{\partial x} \nabla_x \cdot \mathbf{u}(x, y, z) + \frac{\partial}{\partial y} \nabla_y \cdot \mathbf{u}(x, y, z) + \frac{\partial}{\partial z} \nabla_z \cdot \mathbf{u}(x, y, z) = 0 \)

+ \( \mathbf{u}(x, y, z) \cdot \nabla \psi(x, y, z) = 0 \)

- \( \mathbf{u}(x, y, z) \cdot \nabla \cdot \mathbf{u}(x, y, z) = 0 \)

- \( \frac{\partial}{\partial t} \psi(x, y, z) + \frac{\partial}{\partial x} \nabla_x \cdot \mathbf{u}(x, y, z) + \frac{\partial}{\partial y} \nabla_y \cdot \mathbf{u}(x, y, z) + \frac{\partial}{\partial z} \nabla_z \cdot \mathbf{u}(x, y, z) = 0 \)

+ \( \mathbf{u}(x, y, z) \cdot \nabla \psi(x, y, z) = 0 \)

- \( \mathbf{u}(x, y, z) \cdot \nabla \cdot \mathbf{u}(x, y, z) = 0 \)

- \( \frac{\partial}{\partial t} \psi(x, y, z) + \frac{\partial}{\partial x} \nabla_x \cdot \mathbf{u}(x, y, z) + \frac{\partial}{\partial y} \nabla_y \cdot \mathbf{u}(x, y, z) + \frac{\partial}{\partial z} \nabla_z \cdot \mathbf{u}(x, y, z) = 0 \)

+ \( \mathbf{u}(x, y, z) \cdot \nabla \psi(x, y, z) = 0 \)

- \( \mathbf{u}(x, y, z) \cdot \nabla \cdot \mathbf{u}(x, y, z) = 0 \)

- \( \frac{\partial}{\partial t} \psi(x, y, z) + \frac{\partial}{\partial x} \nabla_x \cdot \mathbf{u}(x, y, z) + \frac{\partial}{\partial y} \nabla_y \cdot \mathbf{u}(x, y, z) + \frac{\partial}{\partial z} \nabla_z \cdot \mathbf{u}(x, y, z) = 0 \)

+ \( \mathbf{u}(x, y, z) \cdot \nabla \psi(x, y, z) = 0 \)

- \( \mathbf{u}(x, y, z) \cdot \nabla \cdot \mathbf{u}(x, y, z) = 0 \)
\[ f(x, y) = g(x) \cdot h(y) \]

where \( g(x) \) and \( h(y) \) are functions of \( x \) and \( y \) respectively. The derivative of \( f(x, y) \) with respect to \( x \) is:

\[ \frac{\partial f}{\partial x} = g(x) \cdot \frac{\partial h}{\partial y} \]

And the derivative with respect to \( y \) is:

\[ \frac{\partial f}{\partial y} = h(y) \cdot \frac{\partial g}{\partial x} \]

For a more complex function, we can use the chain rule:

\[ \frac{\partial f}{\partial x} = \frac{\partial f}{\partial u} \cdot \frac{\partial u}{\partial x} \]

where \( u = g(x) \cdot h(y) \).

This is the derivative of \( f(x, y) \) with respect to \( x \):

\[ \frac{\partial f}{\partial x} = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial x} + \frac{\partial f}{\partial h} \cdot \frac{\partial h}{\partial x} \]

Rewrite this in terms of \( x, y, z, u \) and put the derivatives back in:

\[ \frac{\partial f}{\partial x} = \frac{\partial f}{\partial u} \cdot \frac{\partial u}{\partial x} + \frac{\partial f}{\partial u} \cdot \frac{\partial u}{\partial y} \cdot \frac{\partial y}{\partial x} \]

This is the derivative of \( f(x, y) \) with respect to \( y \):

\[ \frac{\partial f}{\partial y} = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial y} + \frac{\partial f}{\partial h} \cdot \frac{\partial h}{\partial y} \]

Rewrite this in terms of \( x, y, z, u \) and put the derivatives back in:

\[ \frac{\partial f}{\partial y} = \frac{\partial f}{\partial u} \cdot \frac{\partial u}{\partial y} + \frac{\partial f}{\partial u} \cdot \frac{\partial u}{\partial x} \cdot \frac{\partial x}{\partial y} \]
\[ dF/dn = K31 m(x, y, z) n(x, y, z) \]
\[ - K31 m(x, y, z) n(x, y, z) \frac{\partial m(x, y, z)}{\partial x} - K31 m(x, y, z) n(x, y, z) \frac{\partial m(x, y, z)}{\partial y} - K31 m(x, y, z) n(x, y, z) \frac{\partial m(x, y, z)}{\partial z} \]
\[ + K31 m(x, y, z) n(x, y, z) \frac{\partial n(x, y, z)}{\partial x} + K31 m(x, y, z) n(x, y, z) \frac{\partial n(x, y, z)}{\partial y} + K31 m(x, y, z) n(x, y, z) \frac{\partial n(x, y, z)}{\partial z} \]
\[ - K33 m(x, y, z) n(x, y, z) \frac{\partial m(x, y, z)}{\partial x} - K33 m(x, y, z) n(x, y, z) \frac{\partial m(x, y, z)}{\partial y} - K33 m(x, y, z) n(x, y, z) \frac{\partial m(x, y, z)}{\partial z} \]
\[ + K33 m(x, y, z) n(x, y, z) \frac{\partial n(x, y, z)}{\partial x} + K33 m(x, y, z) n(x, y, z) \frac{\partial n(x, y, z)}{\partial y} + K33 m(x, y, z) n(x, y, z) \frac{\partial n(x, y, z)}{\partial z} \]
\[ - K22 m(x, y, z) n(x, y, z) \frac{\partial m(x, y, z)}{\partial x} - K22 m(x, y, z) n(x, y, z) \frac{\partial m(x, y, z)}{\partial y} - K22 m(x, y, z) n(x, y, z) \frac{\partial m(x, y, z)}{\partial z} \]
\[ + K22 m(x, y, z) n(x, y, z) \frac{\partial n(x, y, z)}{\partial x} + K22 m(x, y, z) n(x, y, z) \frac{\partial n(x, y, z)}{\partial y} + K22 m(x, y, z) n(x, y, z) \frac{\partial n(x, y, z)}{\partial z} \]
\[ - K33 m(x, y, z) n(x, y, z) \frac{\partial m(x, y, z)}{\partial x} - K33 m(x, y, z) n(x, y, z) \frac{\partial m(x, y, z)}{\partial y} - K33 m(x, y, z) n(x, y, z) \frac{\partial m(x, y, z)}{\partial z} \]
\[ + K33 m(x, y, z) n(x, y, z) \frac{\partial n(x, y, z)}{\partial x} + K33 m(x, y, z) n(x, y, z) \frac{\partial n(x, y, z)}{\partial y} + K33 m(x, y, z) n(x, y, z) \frac{\partial n(x, y, z)}{\partial z} \]

This is the derivative of the function \( F(x, y, z) \).
Rewrite this in terms of x, y and z and put the derivatives back in.

\[
\begin{align*}
\frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} \right) &= K22 \mu(x,y,z) \frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} \right) + K23 \mu(x,y,z) \\
\frac{\partial}{\partial y} \left( \frac{\partial}{\partial y} \right) &= K22 \mu(x,y,z) \frac{\partial}{\partial y} \left( \frac{\partial}{\partial y} \right) + K23 \mu(x,y,z) \\
\frac{\partial}{\partial z} \left( \frac{\partial}{\partial z} \right) &= K22 \mu(x,y,z) \frac{\partial}{\partial z} \left( \frac{\partial}{\partial z} \right) + K23 \mu(x,y,z)
\end{align*}
\]

Now we have all the terms for the Euler-Lagrange equation. Here we define \( F \) as the functional derivative of \( F \) with \( \mu \).

\[
\frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} \right) = K22 \mu(x,y,z) \frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} \right) + K23 \mu(x,y,z)
\]

\[
\frac{\partial}{\partial y} \left( \frac{\partial}{\partial y} \right) = K22 \mu(x,y,z) \frac{\partial}{\partial y} \left( \frac{\partial}{\partial y} \right) + K23 \mu(x,y,z)
\]

\[
\frac{\partial}{\partial z} \left( \frac{\partial}{\partial z} \right) = K22 \mu(x,y,z) \frac{\partial}{\partial z} \left( \frac{\partial}{\partial z} \right) + K23 \mu(x,y,z)
\]
Compute the functional derivatives in Fermion. This will be used for the update for ny.

> Fermion (\texttt{Feny2} = \texttt{Feml}), optimized, precision=double):

\[
\frac{\partial}{\partial y} \mathcal{N}(x, y, z) \quad \frac{\partial}{\partial z} \mathcal{N}(x, y, z) - \mathcal{N}(x, y, z) \quad \frac{\partial}{\partial y} \mathcal{N}(x, y, z) \quad \frac{\partial}{\partial z} \mathcal{N}(x, y, z) - \mathcal{N}(x, y, z)
\]

\[
3 \mathcal{K}_2 \mathfrak{w}(x, y, z) \quad \frac{\partial}{\partial y} \mathcal{N}(x, y, z) \quad \frac{\partial}{\partial y} \mathcal{N}(x, y, z) - \mathcal{K}_3 \mathfrak{w}(x, y, z) \quad \frac{\partial}{\partial y} \mathcal{N}(x, y, z) \quad \frac{\partial}{\partial y} \mathcal{N}(x, y, z)
\]

\[
\mathfrak{g}_1 = \frac{\partial}{\partial y} \mathcal{N}(x, y, z)
\]

\[
\mathfrak{g}_2 = \frac{\partial}{\partial y} \mathcal{N}(x, y, z)
\]

This is the derivative of \texttt{Feml} w.r.t. \texttt{ny}.

> \texttt{diffeml} = \texttt{diffeml} (max):

\[
\texttt{diffeml} := \mathcal{K}_2 \mathfrak{w}(x, y, z) + \mathcal{K}_2 \mathfrak{w}(x, y, z) - \mathcal{K}_3 \mathfrak{w}(x, y, z) + \mathcal{K}_3 \mathfrak{w}(x, y, z) + \mathcal{K}_2 \mathfrak{w}(x, y, z) + \mathcal{K}_3 \mathfrak{w}(x, y, z)
\]

Rewrite this in terms of x, y and z and put the derivatives back in.

> \texttt{diffeml} = \texttt{diffeml} (max):

\[
- \mathcal{K}_2 \mathfrak{w}(x, y, z) + \mathcal{K}_3 \mathfrak{w}(x, y, z) + \mathcal{K}_2 \mathfrak{w}(x, y, z) + \mathcal{K}_3 \mathfrak{w}(x, y, z) + \mathcal{K}_2 \mathfrak{w}(x, y, z) + \mathcal{K}_3 \mathfrak{w}(x, y, z)
\]

\[
- \mathcal{K}_2 \mathfrak{w}(x, y, z) + \mathcal{K}_3 \mathfrak{w}(x, y, z) + \mathcal{K}_2 \mathfrak{w}(x, y, z) + \mathcal{K}_3 \mathfrak{w}(x, y, z) + \mathcal{K}_2 \mathfrak{w}(x, y, z) + \mathcal{K}_3 \mathfrak{w}(x, y, z)
\]
\[
\begin{align*}
  y_{,y} &= \delta(x,y,z) X_{,x}(x,y,z) + X_{,y}(x,y,z) Y - X_{,x}(x,y,z) Y_{,y} + X_{,y}(x,y,z) Y_{,y} \\
  y_{,z} &= \delta(x,y,z) X_{,z}(x,y,z) + X_{,y}(x,y,z) Y_{,z} - X_{,x}(x,y,z) Y_{,z} + X_{,y}(x,y,z) Y_{,z} \\
  dF/dx &= -K_2 y(x,y,z) + K_2 y(x,y,z) \\
  &= -K_2 y(x,y,z) \\
  &= -K_2 y(x,y,z)
\end{align*}
\]
\[ \text{d}
abla V \left( x, y, z \right) = \frac{\partial}{\partial x} \nabla V \left( x, y, z \right) + \frac{\partial}{\partial y} \nabla V \left( x, y, z \right) + \frac{\partial}{\partial z} \nabla V \left( x, y, z \right) \]

This is the derivative w.r.t. of the derivative of \( F \). Let's simplify it. Let: \( d \text{diff}(\nabla V) \). Then:

\[ \text{diff}(\nabla V) = \text{diff}(\nabla V) \]

This is the derivative of \( F \) w.r.t. \( x \).

\[ d \text{diff}(\nabla V) = \text{diff}(\nabla V) \]

This is the derivative of \( F \) w.r.t. \( x \).

\[ d \text{diff}(\nabla V) = \text{diff}(\nabla V) \]

This is the derivative of \( F \) w.r.t. \( x \).
Now we are done, the functional derivatives can be copied and pasted into Fortran code, the variables defined, a user interface made, and director configurations calculated.

Appendix B : The Finite Difference Time Domain simulation algorithm

B.1 Discretizing the Maxwell’s equations and the Yee’s FDTD algorithm

To solve the Maxwell’s equations for a linear, isotropic, non-dispersive and lossy media, the Maxwell curl equation is given by:

\[
\frac{\partial \vec{H}}{\partial t} = -\frac{1}{\mu} \nabla \times \vec{E} - \frac{1}{\mu} (\vec{M}_{\text{source}} + \sigma^* \vec{H}) \tag{B.1a}
\]

\[
\frac{\partial \vec{E}}{\partial t} = \frac{1}{\varepsilon} \nabla \times \vec{H} - \frac{1}{\varepsilon} (\vec{J}_{\text{source}} + \sigma \vec{E}) \tag{B.1b}
\]

Where \(\varepsilon\) is the dielectric constant, \(\mu\) is the magnetic permeability, \(\sigma\) is the electric conductivity, \(\sigma^*\) is the equivalent magnetic loss. The scalar representation of Equ. B.1a and Equ. B.1b is:

\[
\frac{\partial H_x}{\partial t} = \frac{1}{\mu} \left[ \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} - (M_{\text{source}_x} + \sigma^* H_x) \right] \tag{B.2a}
\]

\[
\frac{\partial H_y}{\partial t} = \frac{1}{\mu} \left[ \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} - (M_{\text{source}_y} + \sigma^* H_y) \right] \tag{B.2b}
\]

\[
\frac{\partial H_z}{\partial t} = \frac{1}{\mu} \left[ \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - (M_{\text{source}_z} + \sigma^* H_z) \right] \tag{B.2c}
\]

\[
\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon} \left[ \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - (J_{\text{source}_x} + \sigma E_x) \right] \tag{B.3a}
\]

\[
\frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon} \left[ \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} - (J_{\text{source}_y} + \sigma E_y) \right] \tag{B.3b}
\]

\[
\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon} \left[ \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - (J_{\text{source}_z} + \sigma E_z) \right] \tag{B.3c}
\]
Fig. B.1: Yee space lattice in 3-D space and the arrangements of the electric and magnetic field vector components.
For a 2D medium invariant in the z direction, all partial derivatives with respect to z is zero. There are two possible propagating modes. This first one is the transverse-magnetic mode, TM$_z$ mode. It involves $H_x$, $H_y$, and $E_z$ fields as in Equ. B.2a, Equ. B.2b and Equ. B.2c. The other one is the transverse-electric mode, TE$_z$ mode, which the equations only involve $E_x$, $E_y$, and $H_z$, as in Equ. B.3a, Equ. B.3b and Equ. B.3c.

In order to obtain the solution of the Maxwell’s equations numerically, the computational grid has to be defined properly. Yee provided a unit cubic lattice where the electric and magnetic field vector components are interleaved with each other as shown in Fig. A.1. to satisfy the Faraday’s Law and Ampere’s Law. This grid structure can also be reduced to 2-D and 1-D cases when system possesses z-direction invariant property.

For 1-D case, Equ. B.2a-B.2c can be simplified to be:

$$\frac{\partial E_z}{\partial t} = \frac{1}{\mu} \left[ \frac{\partial E_z}{\partial x} - (M_{source, z} + \sigma H_y) \right] \quad (B.4a)$$

$$\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon} \left[ \frac{\partial H_y}{\partial x} - (J_{source, z} + \sigma E_z) \right] \quad (B.4b)$$

Discretization of the Equ. B.4b can be discretized by following steps:

$$\frac{E_{z, i}^{n+\frac12} - E_{z, i}^{n-\frac12}}{\Delta t} = \frac{1}{\varepsilon} \left( \frac{H_y_{i+\frac12}^{n} - H_y_{i-\frac12}^{n}}{\Delta x} - (J_{source, z}^{n} + \sigma E_z^{n}) \right) \quad (B.5)$$

The numerical implementation of such discretization follows a leapfrog scheme as shown in Fig. B.2, the space-time chart of the Yee algorithm for a 1D wave propagation.
Fig. B.2: Space-time chart of the Yee’s algorithm for 1D wave propagation, showing the use of central differences for the space derivatives and leapfrog for the time derivatives.

\[ \vec{E} = E_z \hat{k}, \quad \vec{H} = H_y \hat{j} \]
At the left hand side of Equ. B.5, the time derivative of $E_z$ at time-step $n$ is evaluated by the central difference scheme that uses $E_z$ at time-step $n+1/2$ and $n-1/2$. The quantities in right hand side of Equ. B.5 are evaluated at time-step $n$, including the electric field $E_z$ due to the non-zero material conductivity $\sigma$. Since $E_z$ values at time-step $n$ are not assumed to be stored in the computer’s memory (only the previous values of $E_z$ at time-step $n-1/2$ are assumed to be in memory), so this term needs to be estimated. A very good way is as follow, using what we call a semi-implicit approximation:

$$E_z |_{i}^{n} = \frac{E_z |_{i}^{n+1/2} + E_z |_{i}^{n-1/2}}{2} \quad (B.6)$$

Here $E_z$ values at time–step $n$ are assumed to be simply the arithmetic average of the stored values of $E_z$ at time-step $n-1/2$ and the yet-to-be computed new values of $E_z$ at time-step $n+1/2$. Substituting Equ. B.6 into Equ. B.5 after multiplying both sides by $\Delta t$, we obtain

$$E_z |_{i}^{n+1/2} - E_z |_{i}^{n-1/2} = \frac{\Delta t}{\varepsilon_l} \left( \frac{H_y |_{i+1/2}^{n} - H_y |_{i-1/2}^{n}}{\Delta x} - (J_{source_x} + \sigma |_{i}^{n+1/2} + E_z |_{i}^{n+1/2}) \right) \quad (B.7)$$

Solving term $E_z |_{i}^{n+1/2}$ from Equ. A.7, we obtain

$$E_z |_{i}^{n+1/2} = \left( 1 - \frac{\sigma |_{i}^{n} \Delta t}{2 \varepsilon_l} \right) E_z |_{i}^{n-1/2} + \left( \frac{\Delta t}{\varepsilon_l} + \frac{\sigma |_{i}^{n} \Delta t}{2 \varepsilon_l} \right) \left( \frac{H_y |_{i+1/2}^{n} - H_y |_{i-1/2}^{n}}{\Delta x} - J_{source_x} |_{i}^{n} \right) \quad (B.8)$$

By following the same procedure to the Equ. B.4a, $H_y |_{i-1/2}^{n+1}$ can be obtained
\[ H_{y, l, \frac{\nu + 1}{2}} = \left( 1 - \frac{\sigma_{1} \Delta t}{2 \mu_{l, \frac{\nu + 1}{2}}} \right) H_{y, l, \frac{\nu}{2}} + \left( \frac{\Delta t}{1 + \frac{\sigma_{1} \Delta t}{2 \mu_{l, \frac{\nu + 1}{2}}} \mu_{l, \frac{\nu}{2}}} \right) \left( \frac{E_{z, l, \frac{\nu + 1}{2}} - E_{z, l, \frac{\nu + 1}{2}}}{\Delta x} - M_{\text{source}, l, \frac{\nu + 1}{2}} \right) \quad (B.9) \]

With the systems of finite-difference expressions of Equ. B.8 and Equ. B.9, the new value of an electromagnetic field vector component at any grid point depends only on its previous value, the previous values of the components of the other field vector at adjacent points, and the known electric and magnetic current sources. Therefore, at any given time-step, the computation of all field components can be proceeded.

B.2 The Maxwell’s equations in an inhomogeneous, anisotropic, sourceless media

The Maxwell’s equations in an inhomogeneous, anisotropic, sourceless media is showed in Equ. B.10 and Equ. B.11:

\[ \frac{\partial \vec{D}}{\partial t} = \nabla \times \vec{H}(r) \quad \rightarrow \quad \frac{\partial \vec{E}}{\partial t} = \varepsilon^{-1}(r) \cdot [\nabla \times \vec{H}(r)] \quad (B.10) \]

\[ -\mu \frac{\partial \vec{H}}{\partial t} = \nabla \times \vec{E}(r) \quad \rightarrow \quad -\frac{\partial \vec{E}}{\partial t} = \mu^{-1} \cdot [\nabla \times \vec{E}(r)] \quad (B.11) \]

\[ \varepsilon(r) \vec{E} = \vec{D} \quad \rightarrow \quad \vec{E} = \varepsilon^{-1}(r) \vec{D} \quad (B.12) \]

\( \vec{D} \) is the electric displacement and \( \varepsilon^{-1} \) is the inverse of the spatially varying dielectric tensor. If we define the spatially varying dielectric tensor to be:

\[ \varepsilon(r) = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{bmatrix} \quad (B.12) \]

Then the inverse of the dielectric tensor is:
\[
E^{-1}(r) = \begin{bmatrix}
\varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\
\varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\
\varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz}
\end{bmatrix}^{-1} = \begin{bmatrix}
\varepsilon_{xx}^{-1} & \varepsilon_{xy}^{-1} & \varepsilon_{xz}^{-1} \\
\varepsilon_{yx}^{-1} & \varepsilon_{yy}^{-1} & \varepsilon_{yz}^{-1} \\
\varepsilon_{zx}^{-1} & \varepsilon_{zy}^{-1} & \varepsilon_{zz}^{-1}
\end{bmatrix}
\] (B.13)

Note here \( \varepsilon_{ij}^{-1} \) means elements of inversion matrix of \( \varepsilon(r) \), doesn’t mean \( \varepsilon_{ij}^{-1} = \frac{1}{\varepsilon_{ij}} \), \( i,j=x, y, z \).

Combine Equ. B.10, Equ. B.11, Equ. B.12, all the electric and magnetic component and its time-step update formulas in 3D can be derived as Equ. B.14 and Equ. B.15.

\[
E^{n+1}_x = E^n_x + \Delta t[\varepsilon_{xx}^{-1}\left(\frac{\partial H_z^{n+\frac{1}{2}}}{\partial y} - \frac{\partial H_y^{n+\frac{1}{2}}}{\partial z}\right) + \varepsilon_{xy}^{-1}\left(\frac{\partial H_z^{n+\frac{1}{2}}}{\partial x} - \frac{\partial H_x^{n+\frac{1}{2}}}{\partial z}\right) + \varepsilon_{xz}^{-1}\left(\frac{\partial H_y^{n+\frac{1}{2}}}{\partial x} - \frac{\partial H_x^{n+\frac{1}{2}}}{\partial y}\right)]
\] (B.14a)

\[
E^{n+1}_y = E^n_y + \Delta t[\varepsilon_{yx}^{-1}\left(\frac{\partial H_z^{n+\frac{1}{2}}}{\partial z} - \frac{\partial H_z^{n+\frac{1}{2}}}{\partial x}\right) + \varepsilon_{yy}^{-1}\left(\frac{\partial H_z^{n+\frac{1}{2}}}{\partial y} - \frac{\partial H_x^{n+\frac{1}{2}}}{\partial x}\right) + \varepsilon_{yz}^{-1}\left(\frac{\partial H_z^{n+\frac{1}{2}}}{\partial y} - \frac{\partial H_x^{n+\frac{1}{2}}}{\partial z}\right)]
\] (B.14b)

\[
E^{n+1}_z = E^n_z + \Delta t[\varepsilon_{zx}^{-1}\left(\frac{\partial H_z^{n+\frac{1}{2}}}{\partial x} - \frac{\partial H_z^{n+\frac{1}{2}}}{\partial y}\right) + \varepsilon_{zy}^{-1}\left(\frac{\partial H_z^{n+\frac{1}{2}}}{\partial z} - \frac{\partial H_x^{n+\frac{1}{2}}}{\partial y}\right) + \varepsilon_{zz}^{-1}\left(\frac{\partial H_z^{n+\frac{1}{2}}}{\partial z} - \frac{\partial H_x^{n+\frac{1}{2}}}{\partial z}\right)]
\] (B.14c)

\[
H^{n+\frac{1}{2}}_x = H^{n-\frac{1}{2}}_x + \frac{\Delta t}{\mu}\left(\frac{\partial E^n_y}{\partial z} - \frac{\partial E^n_z}{\partial y}\right)
\] (B.15a)

\[
H^{n+\frac{1}{2}}_y = H^{n-\frac{1}{2}}_y + \frac{\Delta t}{\mu}\left(\frac{\partial E^n_z}{\partial x} - \frac{\partial E^n_x}{\partial z}\right)
\] (B.15b)

\[
H^{n+\frac{1}{2}}_z = H^{n-\frac{1}{2}}_z + \frac{\Delta t}{\mu}\left(\frac{\partial E^n_x}{\partial y} - \frac{\partial E^n_y}{\partial x}\right)
\] (B.15c)
B.3 The Perfectly Matched Layer absorption boundary condition

To solve the differential equation, one still needs to consider the boundary condition at edge of the computation grid. If a FDTD program directly uses the above mentioned updating rules to simulate the light propagation in free space without any treatment at the boundary layer, one may find that when the optical wave meets the computational grid, the energy of light will be strongly reflected from the boundary. This creates non physical observations as normally the electromagnetic wave propagation in opened or unbounded space is desired. To efficiently use the computer memory and save computation time, a desired approach is to include the structures we are interested in the main computation grid and a suitable boundary condition on the outer perimeter of the domain that simulates an extension to infinity.

Many grid termination techniques have been proposed to achieve this purpose, the most accurate and effective method is the Perfectly Matched Layer (PML) proposed by Jean-Pierre Berenger. This technique uses a special designed fictitious lossy media to absorb electromagnetic waves. A thin layer of this kind of medium surrounding the computational domain can theoretically absorb any kind of wave traveling towards boundaries without reflection, so it can be regarded as a perfectly matched layer, like shown in Fig. B.3. We will save the lengthy derivations for this technique and please see Ref for more details.
Fig. B.3: Perfectly Matched Layer (PML) surrounding the main calculation domain, the wave traveled in all different directions in the main calculation domain will be absorbed by the PML without reflections.
B.4 Numerical dispersion, stability and order of accuracy

The FDTD algorithm for Maxwell’s curl equations discussed previously may cause nonphysical dispersion of the simulated waves in a free-space computational grid. That is, the phase velocity of numerical wave modes can differ from light speed $c$ by an amount varying with the wavelength, direction of propagation in the grid and grid discretization.

Studies have shown that the numerical dispersion may come from approximation of the equation derivatives. The amount of error caused by a numerical approximation of a spatial derivative will depend on grid size, an approximation of time derivative will depend on the size of the time step. The amount of error also depends on the different forms (forward, backward, central, etc.) of numerical approximation to a first derivative and the accuracy (second order and fourth order). Equ. B.16 is the general numerical dispersion relation of the Yee algorithm for the TM$_z$ mode $^{39}$.

\[ \left[ \frac{1}{vt} \sin \left( \frac{\omega \Delta t}{2} \right) \right]^2 = \left[ \frac{1}{\Delta x} \sin \left( \frac{\tilde{k}_x \Delta x}{2} \right) \right]^2 + \left[ \frac{1}{\Delta y} \sin \left( \frac{\tilde{k}_y \Delta y}{2} \right) \right]^2 \]  

(B.16)

where $v = 1/\sqrt{\mu \varepsilon}$ is the speed of light in the material being modeled, $\tilde{k}_x$ and $\tilde{k}_y$ are the x-and y-components of the numerical wave vector and $\omega$ is the wave angular frequency, $x$ and $y$ are grid spacing, $t$ is size of time step. You can see from Equ. B.16 that the numerical dispersion not only depends on grid size and time step size, but also depends on material properties and the frequency of the propagating wave. Among those factors, the grid size and time step size need to be determined. It has been confirmed that reducing grid size can reduce the calculation error, but
reducing time step, to which is smaller than its maximum stable value, will increase the error. This may be due to the fact that as time step decrease, more time steps are needed to reach steady state and increase the impact of round off error.

We have known that the choice of grid size and time step size will affect the propagation characteristic of numerical waves in the Yee space lattice. Studies have also shown that the limited time step is necessary to prevent numerical instability.

The limit for 3D cubic-cell space lattice with $\Delta x=\Delta y=\Delta z=\Delta$ is

$$\Delta t \leq \frac{1}{v \sqrt{ \frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2} }} = \frac{\Delta}{v \sqrt{3}}$$

(B.17)

For 2D case with $\Delta x=\Delta y=\Delta$

$$\Delta t \leq \frac{1}{v \sqrt{ \frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} }} = \frac{\Delta}{v \sqrt{2}}$$

(B.18)

where $\Delta t$ is the size of time step, $v = 1/\sqrt{\mu \varepsilon}$ is the phase velocity of light in the material being modeled. The spatial step $\Delta$ is the size of the standard Yee grid, normally defined as $\lambda/N$, $N$ is an integer. When $N$ increasing, the computational accuracy will increase. $N$ is usually larger than 10.

In order to get accurate solution of Maxwell’s equation by FDTD method, the better scheme of approximation of the first order derivatives for Maxwell’s curl equations needs to be applied. The forward and backward difference formulas to approximate a derivative are of only first order of accuracy $O(\Delta x)$. Central finite difference formula to approximate the first derivative has second order accuracy $O(\Delta x^2)$ iii. So far in this chapter the FDTD
calculation discussed has second order accuracy. One of them used in our simulation program is called staggered fourth-order $O(\Delta x^4)$ accuracy explicit finite difference scheme \textsuperscript{iv}.

A study \textsuperscript{34} has shown for a cholestiric liquid crystal device, the spatial variation of the dielectric constant is very fast. In this case, for second order scheme to get accurate result, the grid size needs to be $\lambda/60$, but to achieve same calculation accuracy by fourth order scheme, the grid space can be $\lambda/20$.

![Fig. B.4: Geometry of 2D diffraction problem. The diffracting object lies in the $y' = 0$ plane between $x' = -d$ and $x' = d$. Diffracted light is observed at $(x, y, z)$.](image-url)
B.5 Near Field to Far Field Transformation

For LC DOE, to obtain the diffraction pattern and efficiency is of the most important goal. The FDTD simulation is a near field simulation program and is not efficient for calculating the diffraction pattern at far field. Calculating the diffraction pattern of the DOE is achieved by calculating the diffraction integrals from Helmholtz and Kirchhoff diffraction theory.

\[
\Psi^{\text{far}}(r) = \frac{1}{4\pi} \iint_{S'} \mathbf{n} \left[ \Psi^{\text{near}}(r') \mathbf{\nabla}' \mathbf{G} - \mathbf{G}' \mathbf{\nabla} \Psi^{\text{near}}(r') \right] ds' \tag{B.19}
\]

According to Charles M. Titus’s Ph. D dissertation, the 2D scaler form of the Helmholtz Kirchhoff surface integral is given by:

\[
\Psi(x, y) = \frac{e^{-ikx}}{\sqrt{8\pi k}} \int_{-d}^{d} \frac{e^{ikR_{||}}}{\sqrt{R_{||}}} \left\{ \frac{\partial \Psi(x')}{\partial y} + \frac{iky}{R_{||}} \Psi(x') \right\} \cdot dx' \tag{B.20}
\]

where \(\Psi(x, y)\) is electric or magnetic component at far field, \(k\) is wave vector. Other parameters are showed in Fig. B.4. The light intensity for far field diffraction pattern can be calculated as: for TM_{z} wave far field intensity \(I \propto E_{z}^{2}\), for TE_{z} wave far field intensity \(I \propto Z_{0}^{2} H_{z}^{2}\), where \(Z_{0}\) is the impedance of free space.
Appendix C: Demonstration system for advanced wavefront control and beam steering

An 2-D LC SLM can be used in many places such as a non-mechanical beam steering, adaptive and active optics, electronic hologram for free space laser communication, laser beam steering/shaping, IR missile countermeasure, advanced wavefront control, 3-D holographic display system etc.

In this document, a XVGA resolution Liquid Crystal On Silicon (LCOS) Spatial Light Modulator (SLM) manufactured by Hana MicroDisplay Inc. is described. The device specification, calibration procedure, optical setup for system demonstration as well as device calibration and programming is described.

<table>
<thead>
<tr>
<th>Cell Type</th>
<th>Electric controlled birefringence (ECB) liquid crystal on Silicon LCOS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Active Area</td>
<td>20mm*15mm</td>
</tr>
<tr>
<td>Resolution</td>
<td>1024*768</td>
</tr>
<tr>
<td>Pixel Size</td>
<td>19.0×19.0µm</td>
</tr>
<tr>
<td>Electrode Gap</td>
<td>0.4µm</td>
</tr>
<tr>
<td>Pixel spacing</td>
<td>19.4µm</td>
</tr>
<tr>
<td>Filling factor</td>
<td>96.0%</td>
</tr>
<tr>
<td>Input signal bit depth</td>
<td>8 bit 256 grayscale</td>
</tr>
<tr>
<td>Frame rate</td>
<td>60Hz</td>
</tr>
</tbody>
</table>

Table C.1: LCOS Device specification
The 2-D LCOS SLM system consists of the LCOS device (Fig. C.1) and its driver (Fig. C.2). The specification of the LCOS device is listed in Table C.1. Depending on the LC material and the cell thickness used for the LCOS device, there are several different types of device for visible or NIR application. Performance of different types of LCOS device is listed in Table C.2.
Table C.2: Performance summary of different type of LCOS device

<table>
<thead>
<tr>
<th>Device Type</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>LC material</td>
<td>Hana Fluid</td>
<td>MLC 6080</td>
<td>E44</td>
</tr>
<tr>
<td>Cell Thickness</td>
<td>4.0 µm</td>
<td>4.0 µm</td>
<td>6.0 µm</td>
</tr>
<tr>
<td>Operation wavelength range</td>
<td>Visible</td>
<td>Visible/NIR</td>
<td>Visible/NIR</td>
</tr>
<tr>
<td>Effective stroke length</td>
<td>650 nm</td>
<td>1000 nm</td>
<td>2000 nm</td>
</tr>
<tr>
<td>Liquid crystal layer uniformity</td>
<td>1/10λ Peak-Valley at 632.8nm</td>
<td>1/5λ Peak-Valley at 632.8nm</td>
<td>1/5λ Peak-Valley at 632.8nm</td>
</tr>
<tr>
<td>Transmitted Wavefront Aberration before self correction¹</td>
<td>Depends on device: Typical value 20 µm</td>
<td>Depends on device: Typical value 3 µm</td>
<td>Depends on device: Typical value 20 µm</td>
</tr>
<tr>
<td>Transmitted Wavefront Aberration after self correction¹</td>
<td>1/10λ Peak-Valley at 632.8nm</td>
<td>1/10λ Peak-Valley at 632.8nm</td>
<td>1/10λ Peak-Valley at 632.8nm</td>
</tr>
<tr>
<td>AR coating</td>
<td>Visible broadband</td>
<td>Visible broadband</td>
<td>Visible broadband</td>
</tr>
<tr>
<td>Mirror material</td>
<td>Aluminum</td>
<td>Aluminum</td>
<td>Aluminum</td>
</tr>
<tr>
<td>Beam steering range</td>
<td>±4 mrad on both X and Y axis for 632.8nm</td>
<td>±4 mrad on both X and Y axis for 632.8nm</td>
<td>±10 mrad on both X and Y axis for 1550 nm</td>
</tr>
<tr>
<td>Response Speed</td>
<td>0.02 ms</td>
<td>0.05 ms</td>
<td>0.2 ms</td>
</tr>
<tr>
<td>Steering efficiency² (At maximum steering angle)</td>
<td>77.2%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Steering Accuracy (Open Loop)</td>
<td>Better than 10 µrad</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Notes:
1. The transmitted aberration is introduced by the shape of the silicon backplane of the LCOS device. Such aberration can be compensated by introducing a correction phase profile to the device. After self-correction, diffraction limited performance can be reached.
2. The steering efficiency is defined as the strehl ratio of the far field beam bounced on the LCOS device after steering versus before steering.
C.3 Typical optical system for demonstration

A complete demonstration of using LCOS as a wavefront corrector and beam steerer can be carried out by setting up the system in the following way. First set up the optical system as shown in Fig. C.3. First, a He-Ne laser is beam expanded to provide a high quality 10 mm diameter beam. Two polarizer, P1 and P2 is placed in the optical path so the intensity of the beam can be easily adjusted by rotation P1. The orientation of P2 needs to be along the rubbing direction of the LCOS panel. The expanded beam is bounced by the LCOS device, and then a far field lens L3 is placed in the system to focus the beam. Sometimes, another polarizer P3 is also placed in the optical path to block unwanted polarization of light. A screen is placed at the focus of the far field lens L3 for observation purpose.

<table>
<thead>
<tr>
<th>Component</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>He-Ne Laser</td>
<td>1/e^2 beam diameter=1.0 mm, power 1mw, beam divergence&lt;1mrad, wavelength 632.8nm at vacuum</td>
</tr>
<tr>
<td>P1</td>
<td>Polarizer 1, used for beam intensity adjustment, transmitted wavefront aberration&lt;1/20λ rms</td>
</tr>
<tr>
<td>P2</td>
<td>Polarizer 2, used for polarization control, optical axis aligned along rubbing direction of LCOS panel</td>
</tr>
<tr>
<td>P3</td>
<td>Polarizer 3, optical axis aligned along rubbing direction of LCOS panel, used to block unwanted polarization after the LCOS device. (There may be small mount of depolarized light coming out of LCOS device)</td>
</tr>
<tr>
<td>10X beam expander</td>
<td>To provide 10mm 1/e^2 beam diameter laser beam with pure TEM00 mode. L1: Low aberration precision objective, infinity corrected, EFL=16.5mm, NA=0.20 H1: 30 μm precision pinhole L2: Precision double let lens, EFL=150mm, Dia=50.8 mm, transmitted wavefront aberration&lt; 1/20λ rms</td>
</tr>
<tr>
<td>L3</td>
<td>Precision double let lens, EFL=1170mm, Dia=76.2 mm, transmitted wavefront aberration&lt; 1/20λ rms</td>
</tr>
</tbody>
</table>

Table C.3: Optical components in the demonstration system
C.4. Operation of the system and demonstration sequence

After the optical system is set up, a demonstration can be shown by carrying out the following procedure.

Operation of the system:

1. Setup optical system like shown in the system illustration.
2. Connect video output from computer to “Video In” port on the demo unit.
3. Connect “Video Out” port to computer driver.
4. Connect input power.
5. Wait for the Panel Power green LED indicator to start blinking and push the yellow Panel Power button. If the green LED stay on, then the panel is successfully powered up.

6. Wait for the demo unit for at least 20 mins before doing any measurement for the device to stabilize.

7. Check the alignment again to make sure each component is correctly aligned. Make sure the polarization direction is along the rubbing direction of LCOS panel.

8. Put a compensation image (compensator.bmp file in the demonstration disk) on the screen in full screen mode, and then put a screen at the focus of the laser beam at around 1170mm away from Lens 3.

9. Play demonstration video LCOSsteer.avi or put steering image on the screen and make sure the computer is display in full screen mode that no windows frame should be seen.

Note: The LCOS panel is using the green channel of the computer, the gamma curve should be set to default value. Changing the gamma curve of computer setting could also change the E-O curve.

C.5. Demonstration

The demonstration of the wavefront correction system consists of five major parts.

a. Wavefront compensation demonstration

The first demonstration is the wavefront compensation demonstration. The image sent to LCOS device is a uniform gray scale image (no compensation case) followed by an image with ring like structure (compensation case). This process will repeat 3 times for a comparison of compensated far field and non-compensated far field. At the far field, when the compensation image is on, the far field pattern is a sharp spot represents a focused laser beam when the optical system is correctly aligned. When the no
compensation image is on, the far field pattern is a big spot with low intensity. In this case, the aberration introduced by the silicon backplane of the LCOS severely aberrated the beam.

b. 2-D beam steering demonstration

The second demonstration is for 2-D target tracking. The focused beam is steered to horizontal and vertical direction so that the far field spot would travel along the spiral trajectory as showing in the Fig. B.4. In this case, the phase profile introduced to the LCOS device is the wavefront compensation image superimposed with a steering image. Thus the wavefront compensation and the beam steering is achieved at the same time. Unwanted higher order diffraction peak may be observed during the demonstration. If the alignment of the optical system is accurate, the total energy in these peaks are small. Since the beam steering angle is very small, the beam steering is carried out at very close to maximum steering angle where the diffraction efficient is at it’s worse point. For details regarding the steering efficiency please see later sections.
Fig. C.4: 2-D 1 beam target tracking along a spiral trajectory
c. Focusing and de-focusing

The third demonstration is the focusing and defocusing of the beam. This is achieved by superimposing the wavefront correction image with certain focusing and defocusing image to the image send to the LCOS device. When the beam is defocused, the spot on the far field screen becomes larger and larger. When the beam is focusing, the spot on the far field screen becomes smaller and smaller. It is possible to move the screen to the correct focus during the focusing and defocusing, however, this is hard to do because of the dynamic change of the focus.

d. Two beam steering

The fourth demonstration is to show in a multiple communication channel system, two independently controlled beam is steered to different angle. This is achieved by equally split the compensation image into two region, each half has a independent steering direction. At the far field, you will see the beam is split into two spot and each has an independent movement following the trajectory as shown in Fig. B.5. Since the illumination on both half may not be exactly the same, the intensity of the two beam may not be the same. Side-lopes are larger in this case because of the diffraction from the two beams.
Fig. C.5: 2-D 2 beam target tracking along a spiral trajectory
e. Four beam steering

The fifth is to show controlling of four independent beams. Similar to the two beam control case, the compensation image is equally split into four regions, each region has a independent steering direction. At the far field, you will see the beam is split into four beams and each has an independent movement following trajectory as shown in Fig. B.6.

![Fig. C.6: 2-D 4 beam target tracking along a spiral trajectory](image)

Fig. C.6: 2-D 4 beam target tracking along a spiral trajectory
Appendix D: Detailed software codes and hardware used in the above calibration procedure

D.1 2-D Birefringence and Electro-Optical curve measurement

Hardware:
   a. PULNIX 1320-15CL digital camera with NI image grabbing card
   b. NI-DAQ SCB-100 digital/Analog input output card

This software:
   a. The automation and data collection software written in LabWindows CVI 5.0
      which includes files:

```
  2DBirefMap.c
  2DBirefMap.h
  2DBirefMap.uir
  ansi_c.h
  dataacq.h
  niimaq.h
  nitypes.h
```

Since these header files can be easily found on National Instrument support disk, they are not listed in this document.
Fig. D.1. User interface of the Phase Shifting Polarimeter data collection software

The source code of the data collection software is:
/* Phase shifting polarimeter: 2-D birefringence and E-O response measurement software */
/* Copyright (c) BOSLab Creation. All Rights Reserved. */

#include "2DBirefMap.h"
#include <ansi_c.h>
#include <formatio.h>
#include <cvirte.h> /* Needed if linking in external compiler; harmless otherwise */
#include <userint.h>
#include "2DBirefMap.h"
#include "niimaq.h"
#include "nitypes.h"
#include "ansi_c.h"
#include <utility.h>
#include <dataacq.h>
#include <formatio.h>
#include <string.h>

#define MIN_DELTA_V 0.0048828125 // 10.0/2048

// global data type
typedef struct
{
    int compstep;
    int compcurrstep;
    int grayinc;
    double startv;
    double endv;
    double Vapp[1000];
    int rampsteps;
    int grayorvolts;
    char filename[100];
    int devicenumber;
    short devicenumbercode;
    short chanvect[2];
    int NIDAQboardstatus;
    double frequency;
    double samplingfrequency;
    short *waveformbuffer;
    short timebase;
    int amplifiersgain;
    int bufferlength;
    unsigned long int interval;
}
BIREFDATA;
BIREFDATA birefdata;

// function
void loaddatafrompanel (int panel);
static int birefmain;
void SnapAndSave (int i, int j);
double RoundVoltage(double v);
int ShutDownDAQ(void);
int InitializeDAQ(void);
int OutPutSquareWaveForm(double v);
int IniOutPutSquareWaveForm(double v);
int SaveLog(void);

int main (int argc, char *argv[])
{
    if (InitCVIRTE (0, argv, 0) == 0) /* Needed if linking in external compiler; harmless otherwise */
        return -1; /* out of memory */
    if ((birefmain = LoadPanel (0, "2DBirefMap.uir", BirefMain)) < 0)
        return -1;
    DisplayPanel (birefmain);
    RunUserInterface ();
    return 0;
}

int CVICALLBACK CompCurrSteps (int panel, int control, int event,
    void *callbackData, int eventData1, int eventData2)
{
    switch (event)
    {
    case EVENT_COMMIT:
        GetCtrlVal(panel, BirefMain_CompCurrSteps, &birefdata.compcurrstep);
        break;
    }
    return 0;
}

int CVICALLBACK Frequency (int panel, int control, int event,
    void *callbackData, int eventData1, int eventData2)
{
    switch (event)
    {
    case EVENT_COMMIT:
        GetCtrlVal(panel, BirefMain_Frequency, &birefdata.frequency);
        break;
    }
    return 0;
}
int CVICALLBACK SamplingFrequency (int panel, int control, int event, void *callbackData, int eventData1, int eventData2)
{
    switch (event)
    {
    case EVENT_COMMIT:
        GetCtrlVal(panel, BirefMain_SamplingFrequency, &birefdata.samplingfrequency);
        break;
    }
    return 0;
}

int CVICALLBACK GrayInc (int panel, int control, int event, void *callbackData, int eventData1, int eventData2)
{
    switch (event)
    {
    case EVENT_COMMIT:
        GetCtrlVal(panel, BirefMain_GrayInc, &birefdata.grayinc);
        break;
    }
    return 0;
}

int CVICALLBACK AmplifierGain (int panel, int control, int event, void *callbackData, int eventData1, int eventData2)
{
    switch (event)
    {
    case EVENT_COMMIT:
        GetCtrlVal(panel, BirefMain_AmplifierGain, &birefdata.amplifiergain);
        break;
    }
    return 0;
}

int CVICALLBACK StartVoltage (int panel, int control, int event, void *callbackData, int eventData1, int eventData2)
{
    switch (event)
    {
    case EVENT_COMMIT:
        GetCtrlVal(panel, BirefMain_StartVNUMERIC, &birefdata.startv);
        break;
    }
    return 0;
}

int CVICALLBACK EndVoltage (int panel, int control, int event, void *callbackData, int eventData1, int eventData2)
switch (event)
{
    case EVENT_COMMIT:
        GetCtrlVal(panel, BirefMain_EndVNUMERIC, &birefdata.endv);
        break;
}
return 0;
}

int CVICALLBACK RampSteps (int panel, int control, int event, void *callbackData, int eventData1, int eventData2)
{
    switch (event)
    {
        case EVENT_COMMIT:
            GetCtrlVal(panel, BirefMain_VstepsNUMERIC, &birefdata.rampsteps);
            break;
    }
    return 0;
}

int CVICALLBACK FileName (int panel, int control, int event, void *callbackData, int eventData1, int eventData2)
{
    switch (event)
    {
        case EVENT_COMMIT:
            GetCtrlVal(panel, BirefMain_FileName, &birefdata.filename);
            break;
    }
    return 0;
}

int CVICALLBACK Quit (int panel, int control, int event, void *callbackData, int eventData1, int eventData2)
{
    switch (event)
    {
        case EVENT_COMMIT:
            DiscardPanel (panel);
            QuitUserInterface (0);
            break;
    }
    return 0;
}

int CVICALLBACK StartGrayscaleRamp (int panel, int control, int event, void *callbackData, int eventData1, int eventData2)
{
    int bufSize,j,count;

switch (event)
{
    case EVENT_COMMIT:
        loaddatafrompanel(panel);
        GetPanelAttribute (panel, BirefMain_CANVAS, &CVIWndHndl);
        DispBuffer = malloc (1024*768);
        Delay(5);

        for (j=0;j<256;j=j+birefdata.grayinc)
        {
            DispBuffer[count]=j;
            for (count=0;count<1024*768;count++)
                DispBuffer[count]=j;
        }

        imgPlot (CVIWndHndl, DispBuffer, 0, 0, 1024,
                768, 0, 0, IMG_PLOT_MONO_8);
        Delay(0.5);
        SnapAndSave(birefdata.compcurrstep,j);

        //free(DispBuffer);
        //DisplayPanel (panel);
        ProcessSystemEvents();
        MinimizeAllWindows ();
        break;
}

return 0;

int CVICALLBACK StartVoltageRamp (int panel, int control, int event,
                                 void *callbackData, int eventData1, int eventData2)
{
    int bufSize,i,j,count,status;
    double dv,v,currentv;

    switch (event)
    {
        case EVENT_COMMIT:
            loaddatafrompanel(panel);
            if (InitializeDAQ())
                return 1;
            else
            {
                dv=(birefdata.endv-birefdata.startv)/(birefdata.rampsteps-1);
                j=1;
                IniOutPutSquareWaveForm(0.0);

                for (v=birefdata.startv;v<=birefdata.endv;v=v+dv)
                {
                    currentv=RoundVoltage(v);
                    birefdata.Vapp[j]=currentv;
                    if (OutPutSquareWaveForm(birefdata.Vapp[j]))
                    {
                        MessagePopup("Voltage OutPut Error",
                                     "Analog output failed!");
                        return 1;
                    }
                }

            }
    }

    return 0;
}
else
{
    SetCtrlVal(panel, BirefMain_VoltageDisp, currentv);
    SnapAndSave(birefdata.compcurrstep, j);
    j = j + 1;
}
ShutDownDAQ();
SaveLog();
DisplayPanel(panel);
ProcessSystemEvents();
break;
}
return 0;

void loaddatafrompanel (int panel)
{
    GetCtrlVal(panel, BirefMain_CompCurrSteps, &birefdata.compcurrstep);
    GetCtrlVal(panel, BirefMain_FileName, birefdata.filename);
    GetCtrlVal(panel, BirefMain_GrayInc, &birefdata.grayinc);
    GetCtrlVal(panel, BirefMain_EndVNUMERIC, &birefdata.endv);
    GetCtrlVal(panel, BirefMain_AmplifierGain, &birefdata.amplifiergain);
    GetCtrlVal(panel, BirefMain_EndVNUMERIC, &birefdata.endv);
    GetCtrlVal(panel, BirefMain_StartVNUMERIC, &birefdata.startv);
    GetCtrlVal(panel, BirefMain_VstepsNUMERIC, &birefdata.rampsteps);
    GetCtrlVal(panel, BirefMain_Frequency, &birefdata.frequency);
    GetCtrlVal(panel, BirefMain_SamplingFrequency, &birefdata.samplingfrequency);
}
void SnapAndSave (int i, int j)
{
int    acqWinWidth, acqWinHeight;
unsigned int bufSize, bytesPerPixel, plotFlag, bitDepth;
char    intfName[10], filename[50];
char    SaveName[100];
acqWinWidth = 320;
acqWinHeight = 240;
bytesPerPixel = 1;
Fmt(intfName, "%s<%s","img1");
// Open an interface and a session
imgInterfaceOpen (intfName, &Iid);
imgSessionOpen (Iid, &Sid);

// Let's check that the Acquisition window is not smaller than the Canvas
imgGetAttribute (Sid, IMG_ATTR_ROI_WIDTH, &acqWinWidth);
imgGetAttribute (Sid, IMG_ATTR_ROI_HEIGHT, &acqWinHeight);
imgGetAttribute (Sid, IMG_ATTR_BYTESPERPIXEL, &bytesPerPixel);
imgGetAttribute (Sid, IMG_ATTR_BITSPERPIXEL, &bitDepth);
// if(CanvasWidth < acqWinWidth)
//    acqWinWidth = CanvasWidth;
// if(CanvasHeight < acqWinHeight)
//    acqWinHeight = CanvasHeight;

    // Set the ROI to the size of the Canvas so that it will fit nicely
    imgSetAttribute(Sid, IMG_ATTR_ROI_WIDTH, acqWinWidth);
    imgSetAttribute(Sid, IMG_ATTR_ROI_HEIGHT, acqWinHeight);
    imgSetAttribute(Sid, IMG_ATTR_ROWPIXELS, acqWinWidth);

    // create a buffer list with one element
    imgCreateBufList(1, &Bid);

    // compute the size of the required buffer
    bufSize = acqWinWidth * acqWinHeight * bytesPerPixel;

    // create a buffer and configure the buffer list
    imgCreateBuffer(Sid, FALSE, bufSize, &ImaqBuffer);

    /* the following configuration assigns the following to buffer list
    element 0:
       1) buffer pointer that will contain the image
       2) size of the buffer for buffer element 0
       3) command to stop acquisition when this element is reached
    */
    imgSetBufferElement(Bid, 0, IMG_BUFF_ADDRESS, (uInt32)ImaqBuffer);
    imgSetBufferElement(Bid, 0, IMG_BUFF_SIZE, bufSize);
    imgSetBufferElement(Bid, 0, IMG_BUFF_COMMAND, IMG_CMD_STOP);

    // lock down the buffers contained in the buffer list
    imgMemLock(Bid);

    // configure the session to use this buffer list
    imgSessionConfigure(Sid, Bid);

    // start the acquisition (synchronous function)
    imgSessionAcquire(Sid, FALSE, NULL);

    // Fetch image name and save image
    Fmt(SaveImageName, "%s<%s%d%s%d%s", birefdata.filename, i, "_", j, ".bmp");
    imgSessionSaveBuffer(Sid, 0, SaveImageName);

    // unlock the buffers in the buffer list
    if (Bid != 0)
        imgMemUnlock(Bid);

    // dispose the buffer
    if (ImaqBuffer != NULL)
        imgDisposeBuffer(ImaqBuffer);

    // close this buffer list
    if (Bid != 0)
        imgDisposeBufList(Bid, FALSE);
// Close the interface and the session
    imgClose (Sid, TRUE);
    imgClose (Iid, TRUE);
}

int IniOutPutSquareWaveForm(double v)
{
    int err,i,tempv;
    short wfmStopped;
    unsigned long int iterDone,pointsDone;
    short half_ready;

    tempv=v/MIN_DELTA_V;
    if ((tempv>2047) | (tempv<-2048))
    {
        MessagePopup("Voltage Out of Range", "Check you voltage to be within 10v*External Amplifier Gain!");
        return 1;
    }

    birefdata.waveformbuffer[0]=tempv;
    birefdata.waveformbuffer[1]=-1*tempv;

    err=WFM_Group_Setup(birefdata.devicenumber, 2, birefdata.chanvect, 1);
    err=WFM_DB_Config(birefdata.devicenumber, 2, birefdata.chanvect, 1, 0, 0);
    err = WFM_Load(birefdata.devicenumber, 1, birefdata.chanvect, birefdata.waveformbuffer, 
                    birefdata.bufferlength, 0, 0);
    err = WFM_Rate(2*birefdata.frequency, 0, &birefdata.timebase, &birefdata.interval);
    err = WFM_ClockRate(birefdata.devicenumber, 1, 0, birefdata.timebase, birefdata.interval, 0);
    err = WFM_Group_Control(birefdata.devicenumber, 1, 1);
    err = WFM_Check(birefdata.devicenumber, 0, &wfmStopped, &iterDone, &pointsDone);

    if (err)
    {
        MessagePopup("Waveform Generator Error!", "Check validity of your input data!");
        WFM_Group_Control(birefdata.devicenumber, 1, 0);
        return 1;
    }

    half_ready = 0;
    while (half_ready == 0)
    {
        err = WFM_DB_HalfReady (birefdata.devicenumber, 1, birefdata.chanvect, 
                                &half_ready);
        if (half_ready == 1){
            err = WFM_DB_Transfer(birefdata.devicenumber,1,birefdata.chanvect, 
                                  birefdata.waveformbuffer, 
                                  birefdata.bufferlength/2);
        }
    }
    half_ready = 0;
    while (half_ready == 0)
{ 
    err = WFM_DB_HalfReady (birefdata.devicenumber, 1, birefdata.chanvect, 
    &half_ready);
     
    if (half_ready == 1) {
        err = WFM_DB_Transfer(birefdata.devicenumber, 1, birefdata.chanvect, 
                              birefdata.waveformbuffer, 
                              birefdata.bufferlength/2);
    }
}

Delay(birefdata.samplingfrequency);
// err = WFM_Group_Control(birefdata.devicenumber, 1, 0);

return 0;
}

int OutPutSquareWaveForm(double v) 
{
    int err, i, tempv;
    short wfmStopped;
    unsigned long int iterDone, pointsDone;
    short half_ready;

    tempv = v/MIN_DELTA_V;
    if ((tempv>2047) | (tempv<2048))
    {MessagePopup("Voltage Out of Range", "Check you voltage to be within 5v*External Amplifier
    Gain!");
        return 1;
    }

    birefdata.waveformbuffer[0]=tempv;
    birefdata.waveformbuffer[1]=-1*tempv;

    // err = WFM_Rate(birefdata.frequency, 0, &birefdata.timebase, &birefdata.interval);
    // err = WFM_ClockRate(birefdata.devicenumber, 1, 0, birefdata.timebase, birefdata.interval, 0);
    err = WFM_Group_Control(birefdata.devicenumber, 1, 1);
    err = WFM_Clock(birefdata.devicenumber, 0, &wfmStopped, &iterDone, &pointsDone);

    half_ready = 0;
    while (half_ready == 0)
    {
        err = WFM_DB_HalfReady (birefdata.devicenumber, 1, birefdata.chanvect, 
                        &half_ready);
        if (half_ready == 1) {
            err = WFM_DB_Transfer(birefdata.devicenumber, 1, birefdata.chanvect, 
                                  birefdata.waveformbuffer, 
                                  birefdata.bufferlength/2);
        }
    }
    half_ready = 0;
    while (half_ready == 0)
    {

err = WFM_DB_HalfReady (birefdata.devicenumber, 1, birefdata.chanvect, &half_ready);
if (half_ready == 1){
    err = WFM_DB_Transfer(birefdata.devicenumber, 1, birefdata.chanvect, birefdata.waveformbuffer, birefdata.bufferlength/2);
}
}
Delay(birefdata.samplingfrequency);
return 0;

int InitializeDAQ(void)
{
    int i, temp;
    int devicenumber;
    short devicenumbercode;
    birefdata.bufferlength=2;
    birefdata.waveformbuffer=calloc(birefdata.bufferlength,sizeof(short));

    devicenumber = 0;
    devicenumbercode = -1;
    while((devicenumber < 16) && (devicenumbercode < 0)){
        devicenumber++;
        Init_DA_Brds(devicenumber, &devicenumbercode);
    }
    if((devicenumber == 16) && (devicenumbercode < 0))
        {MessagePopup ("Initialized DAQ error", "Can not initialize DAQ board!");
            return 1;
        }
    else
        { birefdata.NIDAQboardstatus = TRUE;

            birefdata.devicenumber = devicenumber;
            birefdata.devicenumbercode = devicenumbercode;
            birefdata.chanvect[0]=0;
            birefdata.chanvect[1]=1;
        }

    return 0;
}

double RoundVoltage(double v)
{
    double intv;
    double outv;

    intv=RoundRealToNearestInteger (v/MIN_DELTA_V);
outv = intv * MIN_DELTA_V;
return outv;
}

int ShutDownDAQ(void)
{
    short half_ready;
    int err;
    half_ready = 0;
    while (half_ready == 0)
    {
        err = WFM_DB_HalfReady (birefdata.devicenumber, 1, birefdata.chanvect, &half_ready);
        if (half_ready == 1){
            err = WFM_DB_Transfer(birefdata.devicenumber, 1, birefdata.chanvect,
                                   birefdata.waveformbuffer,
                                   birefdata.bufferlength/2);
        }
    }
    half_ready = 0;
    while (half_ready == 0)
    {
        err = WFM_DB_HalfReady (birefdata.devicenumber, 1, birefdata.chanvect, &half_ready);
        if (half_ready == 1){
            err = WFM_DB_Transfer(birefdata.devicenumber, 1, birefdata.chanvect,
                                   birefdata.waveformbuffer,
                                   birefdata.bufferlength/2);
        }
    }
    Delay(birefdata.samplingfrequency);
    err = WFM_Group_Control(birefdata.devicenumber, 1, 0);
    AO_VWrite(birefdata.devicenumber, 0, 0);
    free(birefdata.waveformbuffer);
    return 0;
}

int SaveLog (void)
{
    int i;
    char SaveFileName[100];

    Fmt(SaveFileName,"%s<%s%ss", birefdata.filename, ",.DAT");
    fid = fopen(SaveFileName, "w+");
    fprintf(fid,"%s %n","Phase Shift Polarimeter Log File: ");

    fprintf(fid,"%s %n", TimeStr());
    fprintf(fid,"%s %n", DateStr());
    fprintf(fid,"%s %s %n","Voltage Ramp No., " Voltage Applied (V) ");
for (i=1;i<=birefdata.rampsteps;i++)
fprintf(fid,"     %i                   %f
",i,birefdata.Vapp[i]);
fclose(fid);

return 0;
}

---2DbirefMap.h---
/***************************************************************************/
/* Phase shifting polarimeter: User Interface header file */
/* Copyright (c) BOSLab Creation. All Rights Reserved. */
/***************************************************************************/
#include <userint.h>
#ifdef __cplusplus
extern "C" {
#endif
/* Panels and Controls: */
#define  BirefMain                          1 /* callback function: */
#define  BirefMain_GrayInc                  2 /* callback function: GrayInc */
#define  BirefMain_CompCurrSteps            3 /* callback function: CompCurrSteps */
#define  BirefMain_FileName                 4 /* callback function: FileName */
#define  BirefMain_Qui                       5 /* callback function: Quit */
#define  BirefMain_StartVoltageRamp         6 /* callback function: StartVoltageRamp */
#define  BirefMain_StartGrayscaleRamp       7 /* callback function: StartGrayscaleRamp */
#define  BirefMain_CANVAS                    8
#define  BirefMain_EndVNUMERIC              9 /* callback function: EndVoltage */
#define  BirefMain_StartVNUMERIC            10 /* callback function: StartVoltage */
#define  BirefMain_VstepsNUMERIC            11 /* callback function: RampSteps */
#define  BirefMain_SamplingFrequency        12 /* callback function: SamplingFrequency */
#define  BirefMain_Frequency                13 /* callback function: Frequency */
#define  BirefMain_AmplifierGain            14 /* callback function: AmplifierGain */
#define  BirefMain_text                     15
#define  BirefMain_DECORATION               16
#define  BirefMain_TEXTMSG                  17
#define  BirefMain_TEXTMSG_2                18
#define  BirefMain_TEXTMSG_3                19
#define  BirefMain_TEXTMSG_4                20
#define  BirefMain_DECORATION_3             21
#define  BirefMain_DECORATION_2             22
#define  BirefMain_TEXTMSG_5                23
#define  BirefMain_TEXTMSG_6                24
#define  BirefMain_TEXTMSG_7                25
#define  BirefMain_TEXTMSG_8                26
#define  BirefMain_TEXTMSG_9                27
/* Menu Bars, Menus, and Menu Items: */
/* (no menu bars in the resource file) */
/* Callback Prototypes: */

int CVICALLBACK AmplifierGain(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK CompCurrSteps(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK EndVoltage(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK FileNm(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK FileName(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK Frequency(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK GrayInc(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK Quit(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK RampSteps(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK SamplingFrequency(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK StartGrayscaleRamp(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK StartVoltage(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK StartVoltageRamp(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);

#ifdef __cplusplus
}
#endif

b. The data analyze software that reads the image collected by 2DBirefMap.exe and plot the 2-D birefringence map and E-O response curves.

function Biref2Danaylze

%2-D Birefringence of LCOS device analyze program

%---------------------------------------------- Parameters -----------------------------
dir='C:\2DBiref\data\';
filename='Img';
SmoothenOriginal=1; % whether to smooth the original image file or not
SmoothenFinal=1; % whether to smooth the final image file or not
DefMask=0; % whether to define the mask or not
resizeon=1; % whether to resize the image to smaller image
finalimagesize=100; % resolution of the final grid size
TotalPhaseSteps=2; % phase shifting steps

%---------------------------------------------- Define Mask Region-----------------------
graphread=imread('C:\2DBiref\data\Img0_1.bmp','bmp');
if (DefMask==1)
    n=figure;
    imshow(graphread);
[ Y X]=ginput(2);
else
    break
end

282
Y=[352.7071 791.4835];
X=[478.2247 656.1071];
end

Mnew=graphread(ceil(X(1)):ceil(X(2)),ceil(Y(1)):ceil(Y(2)));
%Mimshow(Mnew);
disp('Input Image Size=');
[SizeX SizeY]=size(Mnew)
tic
%------------------------ Read image ------------------------
for compstep=1:totalcompstep
count=1;
for grayscale=1:6

readfilename=['dir filename num2str(compstep-1) '_num2str(grayscale) '.bmp'];
graph=imread(readfilename,'bmp');
graphread=graph(ceil(X(1)):ceil(X(2)),ceil(Y(1)):ceil(Y(2)));

%------------------------ Phase Map smoothing----------------
if (SmoothOnOriginal==1)
%graphread=wiener2(graphread,[5 5]);
graphread=wiener2(graphread,[10 10]);
graphread=wiener2(graphread,[20 20]);
end

%----------------------------------
if (resizeornot==1)
rsgraph=imresize(graphread,[finalimagesize finalimagesize],'bicubic',5);
SizeX=finalimagesize;SizeY=finalimagesize;
else
rsgraph=graphread;
end
%------------------------ Phase Map smoothing----------------
if (SmoothOnFinal==1)
rsgraph=wiener2(rsgraph,[2 2]);
rsg=wiener2(rsgraph,[2 2]);
rsg=wiener2(rsgraph,[3 3]);
rsg=wiener2(rsgraph,[4 4]);
rsg=wiener2(rsgraph,[5 5]);
end

M(:,:,compstep,count)=rsgraph;
count=count+1;
%Mimshow(rsgraph);
end
end

%-------------------------------Plot figure-----------------------------
%for steps=1:7
% s=M(:,:,steps,1);
% figure
% imshow(s)
M=double(M); imshow(rsgraph);

%---------------------------- Plot intensity change on sample pixel----
drawsample=1;
if (drawsample==1)
    SampleX=40;
    SampleY=50;
    intensi(1:totalcompstep)=M(SampleX,SampleY,1:totalcompstep,1);
    n=figure;
    plot(1:totalcompstep,intensi(1:totalcompstep));
end

%----------------------------phase analyze using 7 step algorithm------
usemethod1=1;
if (usemethod1==1)

    for countx=1:SizeX %SizeX
        for county=1:SizeY %SizeY
            for grayscale=1:6
                I(1:totalcompstep)=M(countx,county,:,grayscale);
                theta=sqrt(3)/3*(-1*I(1)+3*I(2)+3*I(3)-3*I(5)-3*I(6)+I(7))/(-1*I(1)-I(2)+I(3)+2*I(4)+I(5)-I(6)-I(7)+1e-32);    %5 step algorithm
                surf(countx,county,grayscale)=atan(theta)/pi;
            end
        end
    end

save 2Dbirefcurve.mat surf

start=1;                          % Starting grayscale or voltage
endd=256;        % Endding grayscale or voltage
Vapp=[1:256;0:1:255]';            % Vapp is voltage copied from the log file
V=Vapp(:,2);

if (1==1)
    figure
    count=0;
    S_ave=0;                      % Averged E-O response curve for certain pixel
    for i=20:2:80
        for j=20:2:80
            s(1:endd-start+1)=surf(i,j,start:endd);    % E-O response curve for certain pixel
            if (s(1)<-0.2)
                s(1)=s(1)-1;
            end
        end
    end

end
s=-1*s*2*pi;
s=unwrap(s,pi/4);
s=s/2/pi/2;
%surf(i,j,1:52)=s;

s(33:256)=s(33:256)-0.5;
s(37:256)=s(37:256)-0.5;
s(41:256)=s(41:256)-0.5;

%A=polyfit(0:2:255,s,6);
%sfit=polyval(A,10:2:255);
%plot(s(1:length(s)),0:5:255,'r');hold on;
plot(V,s,'r');hold on;

count=count+1;
S_ave=(S_ave+s);
end
end
S_ave=S_ave/count;
nS_ave=S_ave(1:endd-start+1)

%nS_ave=nS_ave+[0 0 0 0 0 -0.5 -0.5 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1]

plot(V,nS_ave,'b.');hold on;
title('100*100 E-O response curve across aperture');
xtitle('Applied Voltage (v)');
ytitle('Absolute retardation (wave at 632.8nm)');
plot(S_ave(11:length(s)-3),50:5:240,'b');hold on;
plot(nS_ave,19:2:215,'b');hold on;
end
figure
%----------------------Plotting and results reporting------------------
if (1==1)
x=0;

count=1;
figure;

for i=start:endd
x(1:81,1:81)=surf(10:90,10:90,i);
x=x*2*pi;
x=unwrap(x,[],1);
x=unwrap(x,[],2);
x=x/2/pi/2;
peak2valley(count)=max(max(x))-min(min(x));
surfunwrap(1:81,1:81,i)=x;
surf(1:81,1:81,i)=surf(10:90,10:90,i);
rms(count)=std2(x);

%figure;
%surf(x);
%mesh(x);%Hold on
if (i==1) figure; end;

    count=count+1;
    drawnow;
end
end

figure
plot(V,peak2valley)
title('Maximum peak-valley non-uniformity vs. voltage')
figure
plot(V,rms)
title('Maximum rms non-uniformity vs. voltage')

disp('Maximum peak-valley non-uniformity');
max(peak2valley)
disp('Maximum R.M.S. non-uniformity');
max(rms)

save 2Dbirefmap.mat surf surfunwrap
b. Interferometer control/data analyze and wavefront compensation measurement

Hardware:
   c. PULNIX 1320-15CL digital camera with NI image grabbing card
   d. PI-750.CP Nano-positioning stage

Software contains two main parts:
   a) The automation and data collection software written in LabWindows CVI 5.0 which includes files:

      Interf.c
      Interf.h
      Interf.uir
      as well as some header files from LabWindows or NI-IMAQ 3.0

      dataacq.h
      niimaq.h
      nitypes.h

      and static linked librarie and header files for the camera and the Peizo stage

      alphacs.h
      alphacs.lib
      alphadll.c
      alphadll.lib
      niimaq.lib

      Since these header files and support files can be easily found on National Instrument support disk, they are not listed in this documents.
Fig. C.2: Main user interface for interferometer data collection software

---Interf.c---
/**********************************************
/* Interferometer controller: Main source code */
/*                                        */
/* Copyright (c) BOSLab Creation. All Rights Reserved. */
/***********************************************/

#include <ansi_c.h>
#include <cviyte.h>  /* Needed if linking in external compiler; harmless otherwise */
#include <userint.h>
#include <formatio.h>
#include <string.h>
#include <niimaq.h>
#include <nitypes.h>
#include <Interf.h>
#include <alphacs.h>

#define ENABLE 0
#define DISABLE 1
#define FALSE 0
# define TRUE 1

FILE *fid;

static BUFLIST_ID Bid;
static SESSION_ID Sid;
static INTERFACE_ID lid;
static Int8* ImaqBuffer=NULL;
static double* ImaqAveBuffer=NULL;
static Int8* ImaqDispBuffer=NULL;
static unsigned int CanvasWidth, CanvasHeight, CanvasTop, CanvasLeft;
static int CVIWndHndl;

typedef struct
{
    int   delay;
    int    portno;
    int    baudrate;
    float currentposition;
    float PZTposition[200];
    float startposition;
    float endposition;
    float targetposition;
    int    steps;
    int    aveframe;
    char   workingdir[50];
    char   filename[50];
    char   error[50];
}InterfDataType;

InterfDataType interfdata;

static int panelHandle, pnlSconf;

 /*-------------------------------------------------------------------------*/
/* Internal function prototypes                                          */
 /*-------------------------------------------------------------------------*/
void CheckStatus (void);
void EnablePanelControls (void);
void SnapAndSave (int);
void Snap (int);
void ParameterInput(void);

 /*-------------------------------------------------------------------------*/
/* Updat parameters.                                    */
 /*-------------------------------------------------------------------------*/
void ParameterInput (void) {
    char cDispPosition[50];
    GetCtrlVal (panelHandle, PANEL_NUMERIC_Port, &interfdata.portno);
    GetCtrlVal (panelHandle, PANEL_NUMERIC_BaudRate, &interfdata.baudrate);
    GetCtrlVal (panelHandle, PANEL_NUMERIC_StartPosition, &interfdata.startposition);
    GetCtrlVal (panelHandle, PANEL_NUMERIC_EndPosition, &interfdata.endposition);
}
GetCtrlVal (panelHandle, PANEL_NUMERIC_ToPosition, &interfdata.targetposition);
GetCtrlVal (panelHandle, PANEL_NUMERIC_TotalSteps, &interfdata.steps);
GetCtrlVal (panelHandle, PANEL_NUMERIC_AveFrame, &interfdata.aveframe);
GetCtrlVal (panelHandle, PANEL_TextBox_WorkingDir, interfdata.workingdir);
GetCtrlVal (panelHandle, PANEL_TextBox_FileName, interfdata.filename);
GetCtrlVal (panelHandle, PANEL_NUMERIC_DelayTime, &interfdata.delay);

void EnablePanelControls (void)
{
    SetCtrlAttribute (panelHandle, PANEL_COM_BUT_Initialize, ATTR_DIMMED, DISABLE);
    SetCtrlAttribute (panelHandle, PANEL_COM_BUT_Move2position, ATTR_DIMMED, ENABLE);
    SetCtrlAttribute (panelHandle, PANEL_COM_BUT_Grab1Frame, ATTR_DIMMED, ENABLE);
    SetCtrlAttribute (panelHandle, PANEL_COM_BUT_StartInterf, ATTR_DIMMED, ENABLE);
    SetCtrlAttribute (panelHandle, PANEL_COM_BUT_PrintPNL, ATTR_DIMMED, ENABLE);
}

/*--------------------------------------------------------------------------------*/
/* Display error information to the user.                                      */
/*--------------------------------------------------------------------------------*/

void CheckStatus (void)
{
    long sByte;
    int dllerror;
    Dll_ErrStatus(&dllerror);
    if(StatusByte(&sByte))
    {
        if (sByte&0x08)
        {
            switch (dllerror)
            {
            case 0:
                MessagePopup ("Error Message", "DLL interface function was called although there is no connection!");
                break;
            case -1:
                MessagePopup ("Error Message", "DLL interface function was called although there is no connection!");
                break;
            case -2:
                MessagePopup ("Error Message", "The connection of the DLL to the E-750.CP system can not be established");
                break;
            case -3:
                MessagePopup ("Error Message", "DLL can not create required internal object, memory problems");
                break;
            case -4:
                MessagePopup ("Error Message", "parameter of DLL interface function is out of range");
                break;
            case -5:
                MessagePopup ("Error Message", "an internal object cannot be deleted");
                break;
            default:
                MessagePopup ("Error Message", "unknown error");
                break;
            }
        }
    }
}
MessagePopup ("Error Message", "Interface ID is not known");
    break;
case -6:
    MessagePopup ("Error Message", "Implementation DLL can not be linked");
    break;
case -7:
    MessagePopup ("Error Message", "COM-port can not be accessed by DLL");
    break;
case -8:
    MessagePopup ("Error Message", "During sending or receiving a communication error occurred");
    break;
case -9:
    MessagePopup ("Error Message", "An E-750.CP controller could not be identified as connected device");
    break;
case -10:
    MessagePopup ("Error Message", "General parser error");
    break;
case -19:
    MessagePopup ("Error Message", "the DLL is in a non expected state");
    break;
case -20:
    MessagePopup ("Error Message", "the DLL execution failed but no error can be detected");
    break;
}
}

int main (int argc, char *argv[])
{
    if (InitCVIRTE (0, argv, 0) == 0) /* Needed if linking in external compiler; harmless otherwise */
        return -1; /* out of memory */
    if ((panelHandle = LoadPanel (0, "Interf.uir", PANEL)) < 0)
        return -1;
    DisplayPanel (panelHandle);
    RunUserInterface ();
    return 0;
}

int CVICALLBACK Initialize (int panel, int control, int event,
    void *callbackData, int eventData1, int eventData2)
{
    int err;
    char position[50];
    switch (event)
    {
    case EVENT_COMMIT:
        ParameterInput();
    }
err = rs232_connect(interfdata.portno, interfdata.baudrate);

    if (err==FALSE)
    {
        MessagePopup ("Error Message", "RS232 communication connection error!");
        CheckStatus ();
        MessagePopup ("PZT Controller Message", "Status Checked!");
    }
    else
    {
        err = SetServo(TRUE);
        if (err==FALSE)
        {
            MessagePopup ("Error Message", "Set Servo Error on E-750 controller!");
        }

        err = TellPosition(&interfdata.currentposition);
        if (err==FALSE)
        {
            MessagePopup ("Error Message", "TellPosition() Error on E-750 controller!");
            Fmt(position, "%s<%f", interfdata.currentposition);
            ResetTextBox (panelHandle,PANEL_TEXTBOX_DispPosition , position);
        }

        SetCtrlVal (panelHandle, PANEL_LED_Communication,TRUE);
        ResetTextBox (panelHandle,PANEL_TEXTBOX_Info , "Piezo Stage in Remote control State!");
        EnablePanelControls();
        break;
    }

return 0;

int CVICALLBACK Move2position (int panel, int control, int event,
    void *callbackData, int eventData1, int eventData2)
{
    int err;
    char position[50];

    switch (event)
    {
    case EVENT_COMMIT:

        CheckStatus();
        err = SetPosition(interfdata.targetposition);
        Delay(0.01);
        if (err==FALSE)
        {
            MessagePopup ("Error Message", "Cannot go to position!");
            SetCtrlAttribute (panelHandle, PANEL_TEXTBOX_DispPosition, ATTR_DIMMED, DISABLE);
        }
        else
        {
            TellPosition(&interfdata.currentposition);
            SetCtrlAttribute (panelHandle, PANEL_TEXTBOX_DispPosition, ATTR_DIMMED, ENABLE);
            Fmt(position, "%s<%f", interfdata.currentposition);
        }

        break;
    }
ResetTextBox (panelHandle,PANEL_TEXTBOX_DispPosition , position);

if (fabs(interfdata.targetposition-interfdata.currentposition)<0.005)
  ResetTextBox (panelHandle,PANEL_TEXTBOX_Info , "Piezo Electric Stage in Position!");
else
  ResetTextBox (panelHandle,PANEL_TEXTBOX_Info , "Warning:Piezo Electric Stage Position Error >0.005 micron !");
}
break;
return 0;
}

void SnapAndSave (int img_count)
{
  int    acqWinWidth, acqWinHeight,i,j,count,err;
  unsigned int bufSize, bytesPerPixel, plotFlag, bitDepth;
  char    intfName[10],filename[50];
  char    SaveImageName[100];
  acqWinWidth=1000;
  acqWinHeight=1000;
  Fmt(intfName, "%s<%s","img0");

  // Open an interface and a session
  imgInterfaceOpen (intfName, &Iid);
  imgSessionOpen (Iid, &Sid);
  // Get the Acquisition window and plot window On Canvas
  GetCtrlAttribute (panelHandle, PANEL_CANVAS, ATTR_TOP, &CanvasTop);
  GetCtrlAttribute (panelHandle, PANEL_CANVAS, ATTR_LEFT, &CanvasLeft);
  imgGetAttribute (Sid, IMG_ATTR_BYTESPERPIXEL, &bytesPerPixel);
  imgGetAttribute (Sid, IMG_ATTR_BITSPERPIXEL, &bitDepth);
  // Set the ROI to the size of the Canvas so that it will fit nicely
  imgSetAttribute (Sid, IMG_ATTR_ROI_WIDTH, acqWinWidth);
  imgSetAttribute (Sid, IMG_ATTR_ROI_HEIGHT, acqWinHeight);
  imgSetAttribute (Sid, IMG_ATTR_ROWPIXELS, acqWinWidth);
  // create a buffer list with one element
  imgCreateBufList(1, &BId);
  // compute the size of the required buffer
  bufSize = acqWinWidth * acqWinHeight * bytesPerPixel;
  // create a buffer and configure the buffer list
  imgCreateBuffer(Sid, FALSE, bufSize, &ImaqBuffer);
  ImaqAveBuffer=calloc(acqWinWidth * acqWinHeight,sizeof(double));
  ImaqDispBuffer=calloc(acqWinWidth * acqWinHeight/4,sizeof(Int8));
}

/* the following configuration assigns the following to buffer list
element 0:
1) buffer pointer that will contain the image
2) size of the buffer for buffer element 0
3) command to stop acquisition when this element is reached

```c
imgSetBufferElement(Bid, 0, IMG_BUFF_ADDRESS, (uInt32)ImaqBuffer);
imgSetBufferElement(Bid, 0, IMG_BUFF_SIZE, bufSize);
imgSetBufferElement(Bid, 0, IMG_BUFF_COMMAND, IMG_CMD_STOP);
```

// lock down the buffers contained in the buffer list
imgMemLock(Bid);

// configure the session to use this buffer list
imgSessionConfigure(Sid, Bid);

// start the acquisition and averaging several frames and reduce the size of image
// by half for display purpose

```c
imgSessionAcquire(Sid, FALSE, NULL);
for (j=0;j<500;j++)
{
    for (i=0;i<500;i++)
    {
    }
}
```

// Display using NI-IMAQ
// set the plot Flag depending on the bitDepth
switch(bitDepth)
{
    case 10:
        plotFlag = IMGPLOT_MONO_10;
        break;
    case 12:
        plotFlag = IMGPLOT_MONO_12;
        break;
    case 14:
        plotFlag = IMGPLOT_MONO_14;
        break;
    case 16:
        plotFlag = IMGPLOT_MONO_16;
        break;
    case 24:
    case 32:
        plotFlag = IMGPLOT_COLOR_RGB32;
    }
break;
    default:
        plotFlag = IMGPLOT_MONO_8;
        break;
    }
}

imgPlot(CVIWndHndl, ImaqDispBuffer, 0, 0, acqWinWidth/2, acqWinHeight/2, CanvasLeft, CanvasTop, plotFlag);

Fmt(SaveImageName,"%s<%s%s%d%s",interfdata.workingdir,interfdata.filename,img_count,".bmp");

imgSessionSaveBufferEx(Sid, ImaqBuffer, SaveImageName);

    // unlock the buffers in the buffer list
    if (Bid != 0)
        imgMemUnlock(Bid);
    
    // dispose the buffer
    if (ImaqBuffer != NULL)
        imgDisposeBuffer(ImaqBuffer);
    
    // close this buffer list
    if (Bid != 0)
        imgDisposeBufList(Bid, FALSE);
    
    // Close the interface and the session
    imgClose (Sid, TRUE);
    imgClose (Iid, TRUE);
    free(ImaqAveBuffer);
    free(ImaqDispBuffer);
}

void Snap (int img_count)
{
    int acqWinWidth, acqWinHeight,i,j,count,err;
    unsigned int bufSize, bytesPerPixel, plotFlag, bitDepth;
    char intfName[10],filename[50];
    char SaveImageName[100];
    acqWinWidth=1000;
    acqWinHeight=1000;
    Fmt(intfName, "%s<%s","img0");
    // Open an interface and a session
    ImaqAveBuffer=malloc(acqWinWidth * acqWinHeight,sizeof(double));
    ImaqDispBuffer=malloc(acqWinWidth * acqWinHeight/4,sizeof(Int8));
    
    for (count=0;count<1000000;count++)
        ImaqAveBuffer[count]=0;

    for (i=0;i<acqWinHeight;i++)
        for (j=0;j<acqWinWidth;j++)
            ImaqAveBuffer[i*acqWinWidth+j]=0;

    for (i=0;i<acqWinHeight;i++)
        for (j=0;j<acqWinWidth;j++)
            ImaqDispBuffer[i*acqWinWidth/4+j]=0;

    for (count=0;count<1000000;count++)
        ImaqAveBuffer[count]=0;

    for (i=0;i<acqWinHeight;i++)
        for (j=0;j<acqWinWidth;j++)
            ImaqDispBuffer[i*acqWinWidth/4+j]=0;

    for (count=0;count<1000000;count++)
        ImaqAveBuffer[count]=0;

    for (i=0;i<acqWinHeight;i++)
        for (j=0;j<acqWinWidth;j++)
            ImaqdispBuffer[i*acqWinWidth/4+j]=0;

    for (count=0;count<1000000;count++)
        ImaqAveBuffer[count]=0;

    for (i=0;i<acqWinHeight;i++)
        for (j=0;j<acqWinWidth;j++)
            ImaqDispBuffer[i*acqWinWidth/4+j]=0;

    for (count=0;count<1000000;count++)
        ImaqAveBuffer[count]=0;
for (j=1;j<=interfdata.aveframe;j++)
{
    imgInterfaceOpen (intfName, &Iid);
    imgSessionOpen (Iid, &Sid);
    // Get the Acquisition window and plot window On Canvas
    GetCtrlAttribute (panelHandle, PANEL_CANVAS,
    ATTR_TOP, &CanvasTop);
    GetCtrlAttribute (panelHandle, PANEL_CANVAS,
    ATTR_LEFT, &CanvasLeft);
    imgGetAttribute (Sid, IMG_ATTR_BYTESPERPIXEL,
    &bytesPerPixel);
    imgGetAttribute (Sid, IMG_ATTR_BITSPERPIXEL,
    &bitDepth);
    // Set the ROI to the size of the Canvas so that it will fit nicely
    imgSetAttribute (Sid, IMG_ATTR_ROI_WIDTH,
    acqWinWidth);
    imgSetAttribute (Sid, IMG_ATTR_ROI_HEIGHT,
    acqWinHeight);
    imgSetAttribute (Sid, IMG_ATTR_ROWPIXELS,
    acqWinWidth);
    // create a buffer list with one element
    imgCreateBufList(1, &Bid);
    // compute the size of the required buffer
    bufSize = acqWinWidth * acqWinHeight * bytesPerPixel;
    // create a buffer and configure the buffer list
    imgCreateBuffer(Sid, FALSE, bufSize, &ImaqBuffer);
    /* the following configuration assigns the following to buffer list
    element 0:
    1) buffer pointer that will contain the image
    2) size of the buffer for buffer element 0
    3) command to stop acquisition when this element is reached
    */
    imgSetBufferElement(Bid, 0, IMG_BUFF_ADDRESS,
    (uInt32)ImaqBuffer);
    imgSetBufferElement(Bid, 0, IMG_BUFF_SIZE, bufSize);
    imgSetBufferElement(Bid, 0, IMG_BUFF_COMMAND,
    IMG_CMD_STOP);
    // lock down the buffers contained in the buffer list
    imgMemLock(Bid);
    // configure the session to use this buffer list
    imgSessionConfigure(Sid, Bid);
    // start the acquisition and averaging several frames and reduce the
    size of image
    // by half for display purpose
imgSessionAcquire(Sid, FALSE, NULL);

for (count=0; count<1000000; count++)

ImaqAveBuffer[count] = ImaqAveBuffer[count] + ImaqBuffer[count];

// Display using NI-IMAQ
// set the plot Flag depending on the bitDepth
switch(bitDepth)
{
    case 10:
        plotFlag = IMGPLOT_MONO_10;
        break;
    case 12:
        plotFlag = IMGPLOT_MONO_12;
        break;
    case 14:
        plotFlag = IMGPLOT_MONO_14;
        break;
    case 16:
        plotFlag = IMGPLOT_MONO_16;
        break;
    case 24:
    case 32:
        plotFlag = IMGPLOT_COLOR_RGB32;
        break;
    default:
        plotFlag = IMGPLOT_MONO_8;
        break;
}

Fmt(SaveImageName, "%s<%s%dd%s", interfdata.workingdir, interfdata.filename, img_count, ".bmp");

err = imgSessionSaveBufferEx(Sid, ImaqBuffer, SaveImageName);

if (err)
    MessagePopup ("Error Message", "Image Saving Error!");

// unlock the buffers in the buffer list
if (Bid != 0)
    imgMemUnlock(Bid);

// dispose the buffer
if (ImaqBuffer != NULL)
    imgDisposeBuffer(ImaqBuffer);
// close this buffer list
if (Bid != 0)
    imgDisposeBufList(Bid, FALSE);
// Close the interface and the session
imgClose (Sid, TRUE);
imgClose (Iid, TRUE);
}

imgInterfaceOpen (intfName, &Iid);

imgSessionOpen (Iid, &Sid);
imgCreateBufList(1, &Bid);
// Get the Acquisition window and plot window On Canvas
GetCtrlAttribute (panelHandle, PANEL_CANVAS,
ATTR_TOP, &CanvasTop);
GetCtrlAttribute (panelHandle, PANEL_CANVAS,
ATTR_LEFT, &CanvasLeft);
imgGetAttribute (Sid, IMG_ATTR_BYTESPERPIXEL,
&bytesPerPixel);
imgGetAttribute (Sid, IMG_ATTR_BITSPERPIXEL,
&bitDepth);

// Set the ROI to the size of the Canvas so that it will fit nicely
imgSetAttribute (Sid, IMG_ATTR_ROI_WIDTH,
acqWinWidth);
imgSetAttribute (Sid, IMG_ATTR_ROI_HEIGHT,
acqWinHeight);
imgSetAttribute (Sid, IMG_ATTR_ROWPIXELS,
acqWinWidth);

// create a buffer list with one element

// compute the size of the required buffer
bufSize = acqWinWidth * acqWinHeight * bytesPerPixel;

// create a buffer and configure the buffer list
imaqCreateBuffer(Sid, FALSE, 1000000, &ImaqBuffer);

// configure the session to use this buffer list
imgSessionConfigure(Sid, Bid);

for (count=0; count<1000000; count++)
ImaqBuffer[count]=(Int8)(ImaqAveBuffer[count]/interfdata.aveframe);

for (j=0; j<500; j++)
{
    for (i=0; i<500; i++)
    {
+ImaqBuffer[2000*i+2*j+1]+ImaqBuffer[2000*i+2*j+1001])/4.0000);
    }
}
imgPlot (CVIWindowHndl, ImaqDispBuffer, 0, 0, acqWinWidth/2, acqWinHeight/2, CanvasLeft, CanvasTop, plotFlag);

   imgSessionSaveBufferEx(Sid, ImaqBuffer, SaveImageName);

   // dispose the buffer
   if (ImaqBuffer != NULL)
      imgDisposeBuffer(ImaqBuffer);
   // close this buffer list
   if (Bid != 0)
      imgDisposeBufList(Bid, FALSE);
   // Close the interface and the session
   imgClose (Sid, TRUE);
   imgClose (Iid, TRUE);

   free(ImaqAveBuffer);
   free(ImaqDispBuffer);

}

int CVICALLBACK Grab1Frame (int panel, int control, int event,
void *callbackData, int eventData1, int eventData2)
{
   switch (event)
   {
   case EVENT_COMMIT:
      
      ResetTextBox (panelHandle,PANEL_TEXTBOX_Info, "Grabbing frame!");
      SnapAndSave(0);
      ResetTextBox (panelHandle,PANEL_TEXTBOX_Info, "Image grabbed and
saved as serial No 0!");
      break;
   }
   return 0;
}

int CVICALLBACK StartInterf (int panel, int control, int event,
void *callbackData, int eventData1, int eventData2)
{
   int i,j,count;
   float tempPosition;
   char SavelImageName[100],infostring[100],positionchar[100];

   switch (event)
   {
   case EVENT_COMMIT:
      
      ParameterInput();
      CheckStatus();
      SetCtrlAttribute (panelHandle, PANEL_TEXTBOX_DispPosition,
   ATTR_DIMMED, ENABLE);
ResetTextBox (panelHandle,PANEL_TEXTBOX_Info , "Start Taking Phase Shift Interferogram!");
Delay(interfdata.delay);
for (i=1;i<=interfdata.steps;i++)
{
    temptposition=interfdata.startposition+(interfdata.endposition-
            interfdata.startposition)*(i-1)/(interfdata.steps-1);
    SetPosition(temptposition);
    Delay(0.01);
    TellPosition(&interfdata.PZTposition[i]);
    if (abs(interfdata.PZTposition[i]-temptposition)>0.005)
        MessagePopup ("Warning Message", "Actual position differ from
target position by larger than 0.005 micron!");
    Fmt(positionchar, "%s<%f",interfdata.PZTposition[i]);
    ResetTextBox (panelHandle,PANEL_TEXTBOX_DispPosition ,
            positionchar);
    Fmt(infostring,"%s%s%i%s%i","Steps No ",i," Of total
            ",interfdata.steps);
    ResetTextBox (panelHandle,PANEL_TEXTBOX_Info , infostring);
    if (interfdata.aveframe>1)
        Snap(i);
    else
        SnapAndSave(i);
    ProcessSystemEvents();
}
ResetTextBox (panelHandle,PANEL_TEXTBOX_Info , "Finished Taking Phase Shift Interferogram!");
break;
return 0;

int CVICALLBACK PrintPNL (int panel, int control, int event, 
    void *callbackData, int eventData1, int eventData2)
{
    switch (event)
    {
    case EVENT_COMMIT:
        PrintPanel (panelHandle,"", 1, VAL_FULL_PANEL, 1);
        break;
    }
    return 0;
}
int CVICALLBACK Port (int panel, int control, int event, void *callbackData, int eventData1, int eventData2)
{
    char cTPosition[50];
    switch (event)
    {
    case EVENT_COMMIT:
        GetCtrlVal (panelHandle, PANEL_NUMERIC_Port, &interfdata.portno);
        ResetTextBox (panelHandle, PANEL_TEXTBOX_Info, "New Port No!");
        break;
    }
    return 0;
}

int CVICALLBACK BaudRate (int panel, int control, int event, void *callbackData, int eventData1, int eventData2)
{
    char cTVoltage[50];
    switch (event)
    {
    case EVENT_COMMIT:
        GetCtrlVal (panelHandle, PANEL_NUMERIC_BaudRate, &interfdata.baudrate);
        ResetTextBox (panelHandle, PANEL_TEXTBOX_Info, "New Baud Rate!");
        break;
    }
    return 0;
}

int CVICALLBACK StartPosition (int panel, int control, int event, void *callbackData, int eventData1, int eventData2)
{
    char cStartPosition[50];
    switch (event)
    {
    case EVENT_COMMIT:
        GetCtrlVal (panelHandle, PANEL_NUMERIC_StartPosition, &interfdata.startposition);
        ResetTextBox (panelHandle, PANEL_TEXTBOX_Info, "New Start Position!");
        break;
    }
    return 0;
}

int CVICALLBACK EndPosition (int panel, int control, int event, void *callbackData, int eventData1, int eventData2)
{
    char cEndPosition[50];
    switch (event)
    {
    case EVENT_COMMIT:
        GetCtrlVal (panelHandle, PANEL_NUMERIC_EndPosition, &interfdata.endposition);
        ResetTextBox (panelHandle, PANEL_TEXTBOX_Info, "New End Position!");
        break;
    }
int CVICALLBACK ToPosition (int panel, int control, int event, 
    void *callbackData, int eventData1, int eventData2)
} char cEndPosition[50];
    switch (event)
    {
        case EVENT_COMMIT:
            GetCtrlVal (panelHandle, PANEL_NUMERIC_ToPosition, 
            &interfdata.targetposition);
            ResetTextBox (panelHandle,PANEL_TEXTBOX_Info , "New target Position!");
            break;
    }
    return 0;
}

int CVICALLBACK TotalSteps (int panel, int control, int event, 
    void *callbackData, int eventData1, int eventData2)
} char cSteps[50];
    switch (event)
    {
        case EVENT_COMMIT:
            GetCtrlVal (panelHandle, PANEL_NUMERIC_TotalSteps, &interfdata.steps);
            ResetTextBox (panelHandle,PANEL_TEXTBOX_Info , "New phase shifting 
            steps!");
            break;
    }
    return 0;
}

int CVICALLBACK AveFrame (int panel, int control, int event, 
    void *callbackData, int eventData1, int eventData2)
} char cSteps[50];
    switch (event)
    {
        case EVENT_COMMIT:
            GetCtrlVal (panelHandle, PANEL_NUMERIC_AveFrame,
            &interfdata.aveframe);
            ResetTextBox (panelHandle,PANEL_TEXTBOX_Info , "New averaging 
            frames!");
            break;
    }
    return 0;
}

int CVICALLBACK WorkingDir (int panel, int control, int event, 
    void *callbackData, int eventData1, int eventData2)
} int err;
    switch (event)
    {
        case EVENT_COMMIT:
            GetCtrlVal (panelHandle, PANEL_TextBox_WorkingDir, 
            &interfdata.workingdir);
break;
    
return 0;
}

int CVICALLBACK DelayTime (int panel, int control, int event,
    void *callbackData, int eventData1, int eventData2)
{
    switch (event)
    {
    case EVENT_COMMIT:
        GetCtrlVal (panelHandle, PANEL_NUMERIC_DelayTime, &interfdata.delay);
        break;
    }
    return 0;
}

int CVICALLBACK FileName (int panel, int control, int event,
    void *callbackData, int eventData1, int eventData2)
{
    switch (event)
    {
    case EVENT_COMMIT:
        GetCtrlVal (panelHandle, PANEL_TextBox_FileName, &interfdata.filename);
        ResetTextBox (panelHandle,PANEL_TEXTBOX_Info , "New File Name!");
        break;
    }
    return 0;
}

int CVICALLBACK SaveData (int panel, int control, int event,
    void *callbackData, int eventData1, int eventData2)
{
    int i;
    char SaveFileName[100];

    switch (event)
    {
    case EVENT_COMMIT:
        ParameterInput();
        Fmt(SaveFileName,"%s<%s%<%s",interfdata.workingdir,interfdata.filename," DAT");
        fid=fopen(SaveFileName, "w+");
        fprintf(fid,"%s \n","Phase Shifting Interferogram Data.");

        fprintf(fid," %s \n","TimeStr());
        fprintf(fid," %s \n","DateStr()");
        fprintf(fid," %s %s ","Step No."," Piezo Stage Position (micron )");

        for (i=1;i<=interfdata.steps;i++)
        {
        
        }
    
    return 0;
    
    }
fprintf(fid," %i %f\n",i,interfdata.PZTposition[i]);
fclose(fid);

ResetTextBox (panelHandle,PANEL_TEXTBOX_Info , "Data File Saved!");
break;
}
return 0;
}

//------------------------Input parameter from Panel------------------------
int CVICALLBACK QUIT (int panel, int control, int event,
void *callbackData, int eventData1, int eventData2)
{
switch (event)
{
case EVENT_COMMIT:
    DII_FreeInterface();
    QuitUserInterface (0);
    break;
}
return 0;
}

**************************************************************************
/* Interferometer controller: User Interface header file                  */
/* Copyright (c) BOSLab Creation. All Rights Reserved.                    */
**************************************************************************
#include <userint.h>
#endif __cplusplus

#define  PANEL                           1
#define  PANEL_CANVAS                    2
#define  PANEL_COM_BUT_StartInterf       3       /* callback function: StartInterf */
#define  PANEL_TextBox_FileName          4       /* callback function: FileName */
#define  PANEL_TextBox_WorkingDir        5       /* callback function: WorkingDir */
#define  PANEL_TEXTBOX_DispPosition      6
#define  PANEL_COM_BUT_Grab1Frame        7       /* callback function: Grab1Frame */
#define  PANEL_COM_BUT_Move2position     8       /* callback function: Move2position */
#define  PANEL_COM_BUT_PrintPNL          9       /* callback function: PrintPNL */
#define  PANEL_COM_BUT_SaveData          10      /* callback function: SaveData */
#define  PANEL_COM_BUT_QUIT              11      /* callback function: QUIT */
#define  PANEL_TEXTBOX_Info              12
#define  PANEL_NUMERIC_Port              13      /* callback function: Port */
#define PANEL_NUMERIC_EndPosition       14      /* callback function: EndPosition */
#define PANEL_NUMERIC_StartPosition     15      /* callback function: StartPosition */
#define PANEL_NUMERIC_ToPosition        16      /* callback function: ToPosition */
#define PANEL_NUMERIC_BaudRate          17      /* callback function: BaudRate */
#define PANEL_COM_BUT_Initialize        18      /* callback function: Initialize */
#define PANEL_NUMERIC_TotalSteps        19      /* callback function: TotalSteps */
#define PANEL_NUMERIC_DelayTime         20      /* callback function: DelayTime */
#define PANEL_NUMERIC_AveFrame          21      /* callback function: AveFrame */
#define PANEL_LITERAL                    22
#define PANEL_LED_Communication         23
#define PANEL_TEXTMSG_2                 24
#define PANEL_DECORATION                25
#define PANEL_DECORATION_3              26
#define PANEL_TEXTMSG_7                 27
#define PANEL_TEXTMSG_6                 28
#define PANEL_TEXTMSG_10                29
#define PANEL_TEXTMSG_13                30
#define PANEL_TEXTMSG_14                31
#define PANEL_TEXTMSG_15                32
#define PANEL_DECORATION_5              33
#define PANEL_TEXTMSG_8                 34
#define PANEL_TEXTMSG_16                35
#define PANEL_TEXTMSG_11                36
#define PANEL_TEXTMSG_12                37
#define PANEL_TEXTMSG_17                38

/* Menu Bars, Menus, and Menu Items: */

/* (no menu bars in the resource file) */

/* Callback Prototypes: */

int CVICALLBACK AveFrame(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK BaudRate(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK DelayTime(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK EndPosition(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK FileName(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK Grab1Frame(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK Initialize(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK Move2position(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK Port(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK PrintPNL(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK SaveData(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK StartInterf(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK StartPosition(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK ToPosition(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK TotalSteps(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);
int CVICALLBACK WorkingDir(int panel, int control, int event, void *callbackData, int eventData1, int eventData2);

#endif
b. The data analyze software reads the image collected by Interf.exe and generates the compensation image for wavefront compensation.

function Interferometer

% Function to extract wavefront map from image collected by interf.exe
% Xinghua (Mark) Wang Version 2.0 Oct. 2004
% Copyright (c) BOSLab Creation. All Rights Reserved.

dir=['C:\Xinghua\LCOS_wavefront\NInterferometer\fringeAnaylze\'; % Directory of the stored image
filename='Interferograph'; % File names of the collected image
NoOfSteps=7; % Number of phase shifting stages
SizeX=1010; % Image resolution of camera
SizeY=1008; % Image resolution of camera
SizeZ=3; % True Color image as in .bmp file format
wavelength=0.6328; % Wavelength of the laser used

%----------------------------- Read Image File-----------------------------
a=imread('C:\Xinghua\LCOS_wavefront\NInterferometer\fringeAnaylze\Interferograph1.bmp','bmp');

for count=1:NoOfSteps
    graphread=imread([dir filename num2str(count)],'bmp');
    M(:,:,count)=graphread(:,:);
end
%---------------------------- Select Mask Region-----------------------
UseMask=1;
if (UseMask==1)
    defMask=0;
    if (defMask==1)
        n=figure;
        imshow(a);
        [Y X]=ginput(2)
        break
    end
    Y=[143.8649 887.9408];
    X=[219.6943 790.7844];
    Mnew=double(M(ceil(X(1)):ceil(X(2)),ceil(Y(1)):ceil(Y(2)),:));
end

[SizeX SizeY SizeZ]=size(Mnew)
clear M;

smoothornot=1;
if (smoothornot==1)
    for count=1:NoOfSteps
        M(:,:,count)=Mnew(:,:,count);
    end
end
M = wiener2(M,[2 2]);
M = wiener2(M,[5 5]);
M = wiener2(M,[7 7]);
M = wiener2(M,[9 9]);
Mnew(:,:,count) = M(:,:);
end
end

%---------------------------- Plot intensity change on sample pixel----
drawsample = 0;
if (drawsample == 1)
SampleX = 300;
SampleY = 300;
intensi(1:NoOfSteps) = Mnew(SampleX,SampleY,1:NoOfSteps);
n = figure;
plot(1:NoOfSteps,intensi(1:NoOfSteps));
end

%---------------------------- Fringe analyze with different algorithms--
algorithm = 7
for countx = 1:SizeX
  for county = 1:SizeY
    I(1:NoOfSteps) = Mnew(countx,county,1:NoOfSteps);
    if (algorithm == 91)
      theta = -0.5*(I(1)-2*I(2)+4*I(4)+I(1)-18*I(6)+14*I(7)+2*I(8)-I(9))... /
        (I(1)+4*I(2)-4*I(3)+4*I(4)-4*I(5)-4*I(6)+4*I(7)+4*I(8)+I(9)+1e-20);
      %9 step 90 degree algorithm
    end
    if (algorithm == 92)
      theta = (-4*I(2)+12*I(4)-12*I(6)+4*I(8))/(-4*I(2)-16*I(3)+14*I(5)-8*I(7)+I(9)+1e-20);
      %9 step 90 degree algorithm
    end
    if (algorithm == 3)
      theta = (I(3)-I(2))/(I(1)+I(2)+1e-20);
      %9 step 90 degree algorithm
    end
    if (algorithm == 5)
      theta = 2*Mnew(countx,county,2)-Mnew(countx,county,4)+0.0000001;
      %5 step algorithm
    end
    if (algorithm == 7)
      I(1:NoOfSteps) = Mnew(countx,county,:);
      theta = sqrt(3)/3*(-1*I(1)+3*I(2)+3*I(3)-3*I(5)+3*I(6)+I(7))/(-1*I(1)-I(2)+I(3)+2*I(4)+I(5)-I(6)-I(7));
      %7 step 60 degree algorithm
    end
    surf0(countx,county) = atan(theta)/2/pi;
  end
end
figure;
mesh(surf0);
title('wavefront surface map');

%---------------------------- Phase Map unwrapping---------------------
unwrapornot = 1;
if (unwrapornot == 1)
tol=pi;
surf=surf0*4*pi;
[SizeX SizeY]=size(surf);

halfx=ceil(SizeX/2);
halfy=ceil(SizeY/2);

quasisurf1(1:halfx,1:halfy)=surf(halfx:-1:1,halfy:-1:1);
quasisurf2((halfx+1:SizeX)-halfx,1:halfy)=surf(halfx+1:SizeX,halfy:-1:1);
%quasisurf2((halfx+1:SizeX)-halfx,1:halfy)=surf(halfx+1:SizeX,halfy:-1:1);
quasisurf3(halfx+1:SizeX,halfy)=surf(halfx+1:SizeX,halfy:-1:1);
quasisurf4((halfx+1:SizeX)-halfx,(halfy+1:SizeY)-halfy)=surf(halfx+1:SizeX,halfy+1:SizeY);
quasisurf1=unwrap(quasisurf1,tol,1);
quasisurf1=unwrap(quasisurf1,tol,2);
quasisurf2=unwrap(quasisurf2,tol,1);
quasisurf2=unwrap(quasisurf2,tol,2);
quasisurf3=unwrap(quasisurf3,tol,1);
quasisurf3=unwrap(quasisurf3,tol,2);
quasisurf4=unwrap(quasisurf4,tol,1);
quasisurf4=unwrap(quasisurf4,tol,2);

surf(halfx:-1:1,halfy:-1:1)=quasisurf1(1:halfx,1:halfy);
%quasisurf2(halfx+1:SizeX,halfy)=surf(halfx+1:SizeX,halfy:-1:1);
%quasisurf2((halfx+1:SizeX)-halfx,1:halfy)=surf(halfx+1:SizeX,halfy:-1:1);
%quasisurf3((halfx+1:SizeY,1:halfy)=surf(halfx+1:SizeY,halfy:-1:1);
quasisurf4((halfx+1:SizeX)-halfx,(halfy+1:SizeY)-halfy)=surf(halfx+1:SizeX,halfy+1:SizeY);
surf1=surf/4/pi;

figure;
mesh(surf1);
title('wavefront surface after unwrapping');
end

figure
mesh(surf1)
clear surf0 Mnew;

save phasemap.mat surf1

%------------------------ Fit the surface for noise removal---------
[SizeX SizeY]=size(surf1);
x=linspace(0,15,SizeY);
y=linspace(0,20,SizeX);

%------------------------ Remove Border noisy data---------------------
removeborderornot=0;
if (removeborderornot==1)
    border=50;
surf1(1:border,:)=surf1(border+1,ceil(SizeY/2));
surf1(1:border,:)=surf1(border+1,ceil(SizeY/2));
surf1(:,1:border)=surf1(ceil(SizeX/2),border+1);
surf1(:,SizeY-border:SizeY)=surf1(ceil(SizeX/2),SizeY-border-1);
surf1(:,SizeY-border:SizeY)=surf1(ceil(SizeX/2),SizeY-border-1);
end

%----------------------------- fit with 36 order zernike polynomial-----
fitornot=0;
if (fitornot==1)
readtxtdata=0;
fitorder=36;

if (readtxtdata==1)
A = dlmread('zernikefitmatrix.dat','*');
save zernike491-754.mat A;             % Read Zernike data file
disp('okay');
break;
end

load zernike491-754.mat;
	surf1=surf1';
size(A)

lineold=surf1(300,1:424);
S0 = reshape(surf1,SizeX*SizeY,1);

pack;
zernike_coef=A\S0;
%zernike_coef=inv(A'*A)*A'*S0;
zernike_coef

surfnewarray=A*zernike_coef;
surfnew=reshape(surfnewarray,SizeY,SizeX);
surfnew=surfnew;

n=figure;
mesh(surfnew);
title('zernike fittion surface');

linenew=surfnew(300,1:424);
n=figure;
plot(1:424,lineold,'r',1:424,linenew)
figure;
mesh(y,x,wiener2((surf1-surfnew),[20 20]))
title('zernike fittion residual');
surf1=surfnew;
else
surf1=surf1;
end
surf0=surf1;

%----------------------------- Smooth profile-----------------------------
smoothornot=1;

if ( smoothornot==1)
surf1=wiener2(surf1,[2 2]);
surf1=wiener2(surf1,[3 3]);
surf1=wiener2(surf1,[4 4]);
surf1=wiener2(surf1,[5 5]);
surf1=wiener2(surf1,[6 6]);

mesh(surf1);
title('surface after smoothing');
figure;
mesh(x,y,(surf1-surf0));
title('residual after smoothing');

end

surffinal=(surf1-surf0)/2;
%---------------------------- generate compensator---------------------
SizeX=1024;         % required resolution of the output image for wavefront compensation
SizeY=768;
surf1=imresize(surf1',[SizeX SizeY],'bicubic');
save surfmapfit3.mat surf1

load surfmapfit1.mat surf1;
surf1=surf1;
%load surfmapfit2.mat surf1;
%surf1=surf1;
%load surfmapfit3.mat surf1;
%surf1=surf1;
%load surfmapfit4.mat surf1;
%surf1=surf1;
surf1=surf1; %+surf1;   % adding multipule compensation images
%---------------------------- generate compensator--------------------- [SizeX SizeY]=size(surf1);
surf=1-mod(surf1,1);

%------------------------ compensation curve obtained earlier----------
p1 = -37.902
p2 = 132.76
p3 = -80.601
p4 = -159.38
p5 = 192.63
p=[p1 p2 p3 p4 p5];

%------------------------ compensation curve-----------------------

x=-0.5:0.01:2;
y=polyval(p,x);
figure;
plot(y,x,'g');

for countx=1:SizeX  %SizeX
    for county=1:SizeY  %SizeY
comp(SizeY-county+1,countx)=polyval(p,(surf(countx,county)))/255;
    end
    end
end

figure

imwrite(comp,'comp.bmp','bmp')
imshow(comp')

%%---------------------------- results----------------------------
disp('End of calculation');
function EOcurvecalcu

% -----------------1-D simulation to find out E-O curve-------------------
Donewsimulation=0;
if (Donewsimulation==1)
d=2.3e-6;
LCmaterial=7;              % 1:MLC6080,       2:Hanafluid
tic
count=1;
for V=0:0.1:5
    V
    [phase,theta]=dir_conf(V,d,LCmaterial);
    %plot(theta*180/pi),hold on;
    retardation(count)=phase/1e-6;
    count=count+1;
end
toc
V1=0:0.1:5;
plot(V1,retardation)
V
break
end

% -----------------0-5v MLC6080 3degree pretilt-------------------
V=0:0.1:5;
retardationMLC6080_6um=[ 10.2560 10.2560 10.2559 10.2557 10.2555 10.2551 10.2546 10.2539...
10.2528 10.2512 10.2485 10.2439 10.2353 10.2184 10.1881 10.1439...
9.2631 9.2578 9.2528];
retardationMLC6080_ninetenth=[1.5384 1.5384 1.5384 1.5384 1.5383 1.5383 1.5382 1.5381...
1.5379 1.5377 1.5373 1.5366 1.5353 1.5328 1.5282 1.5216 1.5136...
1.5048 1.4959 1.4870 1.4785 1.4704 1.4627 1.4557 1.4491 1.4432...
1.4377 1.4328 1.4283 1.4242 1.4206 1.4173 1.4142 1.4115...
1.4090 1.4068 1.4047 1.4028 1.4011 1.3995 1.3981 1.3967 1.3954...
1.3943 1.3932 1.3922 1.3912 1.3903 1.3895 1.3887 1.3879];
12.6960 12.6599 12.6273 12.5978 12.5711 12.5468 12.5248...
12.5047 12.4864 12.4697 12.4543 12.4402 12.4272 12.4151...
12.4039 12.3935 12.3838 12.3748 12.3663 12.3583 12.3508...
12.3437 12.3370];

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4.1955 ...

3.8130 ...

3.6294 ...

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retardation_dn35_23_lowkbend=[    4.2520    4.2520    4.2519    4.2517    4.2512    4.2512 ...
4.2491  4.2474  4.2446  4.2391  4.2275  4.2100  4.1601  4.1039 ...
4.0420  3.9802  3.9226  3.8716  3.8279  3.7607  3.7353 ...
3.7140  3.6961  3.6807  3.6675  3.6563  3.6464  3.6375 ...
3.6214  3.6148  3.6087  3.5980  3.5887  3.5846 ...
3.5807  3.5771  3.5736  3.5673  3.5644  3.5617  3.5591 ...
3.5460  5.5460  5.5459  5.5457  5.5455  5.5451  5.5445 ...
5.5402 ...
5.5366  5.5299  5.5165  5.4908  5.4505  5.3998  5.3442 ...
5.1291  5.0830  5.0407  5.0023  4.9675  4.9361  4.8826 ...
4.8212  4.8048  4.7899  4.7765  4.7643  4.7532  4.7431 ...
4.7103  4.7037  4.6975  4.6863  4.6764  4.6672  4.6638 ...
4.2901 ...
4.7383  4.7254  4.7176 ...
4.7103  4.7037  4.6975  4.6863  4.6764  4.6672  4.6638 ...
4.6000];

retardation_dn35_4um=[7.3947  7.3947  7.3946  7.3943  7.3943  7.3943  7.3943 ...
7.3822  7.3732  7.3554  7.3211  7.2673  7.1997  7.1257 ...
6.8388  6.7774  6.7210  6.6697  6.6233  6.5815  6.5439 ...
6.2183  6.2133 ];

8.5486  8.4717  8.4012  8.3371  8.2791  8.2269  8.1799 ...
8.0354  8.0079  7.9832  7.9608  7.9405  7.9220  7.9052 ...
7.8506  7.8394  7.8291  7.8194  7.8104  7.8020  7.7941 ...
7.7666];

retardation_dn35_6um=[11.0921  11.0920  11.0920  11.0918  11.0918  11.0909  11.0901 ...
11.0890  11.0872  11.0846  11.0804 ...
11.0733  11.0599  11.0331  10.9817  10.9010  10.7996  10.6885 ...
9.3275  9.3200];
12.9598 12.8566 12.7372 12.7047 12.6752 12.6483 12.6236...
12.6010 12.5802 12.5609 12.5431 12.5265 12.5111 12.4967...
12.4832 12.4705 12.4473 12.4367 12.4266];

retardation_dn35_6_10thum=[1.1092 1.1092 1.1092 1.1091 1.1091 1.1090 1.1090...
1.1085 1.1080 1.1073 1.1060...
1.1033 1.0982 1.0901 1.0800 1.0688 1.0575 1.0464 1.0358 1.0258 1.0166 1.0081...
0.9935 0.9872 0.9816 0.9765 0.9720 0.9679 0.9642 0.9610 0.9580 0.9553 0.9529...
0.9506...
0.9486 0.9468 0.9451 0.9435 0.9421 0.9407 0.9395 0.9383 0.9373...
0.9362 0.9353 0.9344 0.9335 0.9328 0.9320];

retardation_dn35_8_10thum=[1.4789 1.4789 1.4789 1.4789 1.4788 1.4787 1.4785...
1.4779 1.4774 1.4764 1.4746...
1.4711 1.4642 1.4535 1.4399 1.4251 1.4100 1.3952 1.3811 1.3678 1.3555 1.3442...
1.3339...
1.3247 1.3163 1.3088 1.3020 1.2960 1.2905 1.2857 1.2813 1.2773 1.2737 1.2705...
1.2675...
1.2648 1.2624 1.2601 1.2580 1.2561 1.2543 1.2527 1.2511 1.2497 1.2483 1.2471...
1.2459...
1.2447 1.2437 1.2427];

retardation_dn35_7_10thum=[1.2941 1.2941 1.2940 1.2940 1.2939 1.2938 1.2937...
1.2932 1.2927 1.2919 1.2903...
1.2872 1.2812 1.2718 1.2599 1.2470 1.2338 1.2208 1.2084 1.1968 1.1860 1.1762...
1.1672...
1.1591 1.1518 1.1452 1.1393 1.1340 1.1292 1.1250 1.1211 1.1176 1.1145 1.1117...
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1.1067 1.1046 1.1026 1.1008 1.0991 1.0975 1.0961 1.0947 1.0935 1.0923 1.0912...
1.0901...
1.0891 1.0882 1.0873];

%-------------------0-5v dn=0.30 material d=2um 3 degree pretilt---------------------
retardation_dn30_3um=[5.3967 5.3967 5.3966 5.3965 5.3963 5.3959 5.3955 5.3948...
5.3937 5.3920 5.3890 5.3835 5.3725 5.3512 5.3178 5.2755...
5.2290 5.1813 5.1343 5.0891 5.0466 5.0070 4.9706 4.9374...
4.9074 4.8802 4.8557 4.8337 4.8139 4.7962 4.7802 4.7658...
4.7529 4.7411 4.7305 4.7208 4.7120 4.7039 4.6965 4.6897...
4.6834 4.6776 4.6721 4.6671 4.6624 4.6579 4.6538 4.6499...
4.6462 4.6427 4.6394];

7.1939 7.1930 7.1916 7.1893 7.1853 7.1780...
7.1633 7.1350 7.0904 7.0341 6.9720 6.9084...
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6.3736 6.3545 6.3372 6.3215 6.3073 6.2944...
6.2827 6.2719 6.2620 6.2529 6.2445 6.2367...
6.1949 6.1903 6.1859];

retardation_dn30_5um=[8.9946 8.9946 8.9944 8.9942 8.9938 8.9932 8.9924 8.9913...
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8.1789  8.1336  8.0928  8.0232  7.9936  7.9670  7.9431...  
7.9214  7.9019  7.8842  7.8680  7.8533  7.8399  7.8275  7.8162...  
7.8056  7.7959  7.7869  7.7785  7.7706  7.7632  7.7563  7.7498...  
7.7437  7.7378  7.7323];

3.8796  3.8781...  
3.4951  3.4616  3.4337  3.4105  3.3911  3.3747  3.3607  3.3486  3.3381  3.3288...  

if (1==1)
reflective=2;        % 1 is transmission  2 is reflective device
rampdirection=-1;    % -1 means steer to minus directin   1 means steer to plus direction
NoOfPixel=96;
wavelength=1.55;
pixelspacing=1.5;
steerangle_factor=0.6;
Maxsteeringangle=asin(wavelength/(8*pixelspacing));
steerangle=steerangle_factor*Maxsteeringangle;
disp([’steering angle=’num2str(steerangle*180/pi)  ’  degree’])
for count=1:NoOfPixel
ramp(count)=(count-1)*sin(steerangle)*pixelspacing/wavelength;
end
if (rampdirection==-1)
    Mod2piRamp=mod(ramp,1)/reflective;
else
    Mod2piRamp=(1-mod(ramp,1))/reflective;
end
startc=10;endc=51-startc;
x=retardationhana_4um;
x1=x(startc:endc);
y1=V(startc:endc);
phaseramp=x(5)-Mod2piRamp*wavelength
plot(phaseramp,'-o')
for count=1:NoOfPixel
    if (phaseramp(count)<x(51))
        phaseramp(count)=x(51);
    end
end
v_ini=interp1(x1,y1,phaseramp,'cubic')
figure
plot(v_ini,phaseramp,'ro',V,x,'r');
if (1==0)

startc=10; endc=51-startc;
x1=retardation_dn35_23um_p1(startc:endc);
x2=retardation_dn35_23um_p2(startc:endc);
x3=retardation_dn35_23um(startc:endc);
x4=retardation_dn35_23um_p5(startc:endc);
x5=retardation_dn35_23um_p10(startc:endc);
y=V(startc:endc);
%plo(V,retardationhana)

% -----------------retadation profile-------------------
elementNo=20;
%phaseramp=linspace(6.6,6.6-0.5/2,11)
%phaseramp=2.7-0.6328/2*(1+cos((2*pi*((1:elementNo)-1))/(elementNo-1))))/2
%max(phaseramp)-min(phaseramp)
%plot(phaseramp)
%figure
phaseramp=linspace(4.222,4.222-1.55/2,9)
phaseramp=phaseramp(1:8)

v_ini1=interp1(x1,y,phaseramp,'cubic')
v_ini2=interp1(x2,y,phaseramp,'cubic')
v_ini3=interp1(x3,y,phaseramp,'cubic')
v_ini4=interp1(x4,y,phaseramp,'cubic')
v_ini5=interp1(x5,y,phaseramp,'cubic')

plot(v_ini1,phaseramp,'ro',V,retardation_dn35_23um_p1,'r');hold on;
plot(v_ini2,phaseramp,'bo',V,retardation_dn35_23um_p2,'b');hold on;
plot(v_ini3,phaseramp,'go',V,retardation_dn35_23um_p5,'g');hold on;
plot(v_ini4,phaseramp,'yo',V,retardation_dn35_23um_p10,'y');hold on;
plot(v_ini5,phaseramp,'ko',V,retardation_dn35_23um_p10,'k');hold on;
break

v_ini1=interp1(x1,y,phaseramp,'cubic');
plo(v_ini1,phaseramp,'ro',V,retardation_dn35_23um_p10,'r');hold on;
end
Appendix E: Detailed software codes for Liquid Crystal diffractive optical element modeling

Manual for 2-D director simulation of Optical Phase Array (OPA) devices

Xinghua Wang, BosLab, Kent State University
version 2.0, June, 2004

1. System requirement and general setup:

Due to the fact that the calculation is very memory consuming, in order to run the current setup properly, an memory of at least 256M is required. Also to run the director configuration simulation, both Matlab 6.0 and Fortran 5.0 is required to be installed on the computer.

To setup the program, just copy the required program to a working directory where Matlab can find the path. Also if check to make sure Matlab compiler is properly setup. To setup Matlab compiler, type "mbuild -setup" under matlab command window. Then select the default compiler to Fortran 5.0 Compiler.

2. Calculation:

Before run the director configuration simulation, push the bottom "Edit Director Simulation Parameter" to input correct simulation parameter. Several things has to mentioned is that, make sure the parameter width_electrode/dx, width_gap/dx and totalwidthz/dz is integer, or error could occur.

Also the default size of matrix passed to Fortran calculation engine is sizex=2000, sizey=1, sizez=100. If Numx, Numy, Numz is larger than any of the corresponding value, error could also occur. To change the size of matrix passed to Fortran routine or simply to build new "DirEngine.dll" file. First make changes to the "DirEngine.for" program. Replace any line like:

parameter (sizex =2000, sizey = 1, sizez = 100)

to what ever you want. Second make changes to Dir_simu.m, of sizex, sizey, sizez. Then type command "mex DirEngine.for" in Matlab command window. The new "DirEngine.dll" will be generated automatically to the current matlab folder.

Parameter "idealphasex" is used for calibration use only, it doesn't influence the calculation at all, the purpose of it is only to make some mark on the phase profile. If you want to adjust the voltage on the electrode to provide a wanted phase on the electrode, you can mark the wanted phase profile on the figure for a comparision.

The "workspace1.mat" "workspace2.mat" "workspace3.mat" "workspace4.mat" are used to store the calculation results of each program, and provide the input data for the next calculation. Detail info please refer to the notes on the original code.

If you want to do a new simulation use last times results as a initial guess of director profile, change the name of "workspace2.mat" to "initialguess.mat" and also make "use_saved_initial_guess=1" (Dir_ini).

For any detailed information on the algorism on the "DirEngine.for" see chapter "Algorism".

When you initialized the simulation parameters, you can run the director configuration simulation. When the
simulation ended, the number of successful iteration and the error of the liquid crystal relaxation process is
display to Matlab command window. Figures show the director profile as well as the phase profile and
voltage profile of the final time step. Also the parameter "Xsample_rate" and "Zsample_rate" is used, so every
graph on at the final time step, the data in the whole matrix may not be shown, but only reduce to a fraction
by those 2 sample rate parameters.

When you are done with the director simulation program, you can go ahead with FDTD optical
simulation.

3. Algorism:

Then Fortran calculation routine is based on Jim Anderson's LC3D equilibrium.for program. But
several modification is made.

1. Add a voltage relaxation process before relax the director of liquid crystal in main grid. This
provide the safe guard when the initial guess of voltage profile is very bad and may cause the
relaxation process to go unstable.
2. Add a backward relaxation to voltage on glass.
3. Put the electrode on the second layer in glass next to liquid crystal layer. Which makes it more
close to the real situation of one layer of alignment layer lay on top of those electrode. Of course here
we assume the dielectric constant of alignment layer is very close to that of glass. Especially when the
grid resolution is choses to be very small and dz is close to 0.05 micron--"The thickness of alignment
layer and ito", the voltage profile close to the electrode should be close to a real situation.
4. change the dz in glass from 4*dz to dz, the same as in the liquid crystal grid, so a dz close to 0.05
micron could be achieved with 100 grid in z direction. And as long as a voltage boundary condition in
z direction "Vbc" is set to 1, it is more intutive to use the same grid size in glass and liquid crystal grid.
5. An Matlab MexFuncion is added to the fortran code to drive it in Matlab envirement, also some
variable type change is also performed to ensure the proper variable passing between two codes.

The main relaxation process is:
1. Relax the voltage on glass, interface and liquid crystal layer forward and backward until "maxViter"
is reached or "MaxVerr" is satisfied.
2. Relax voltage on bottom glass, bottom interface, liuqid crystal layer, top interface and then top
glass, then relax backward again to assume symmetry.
Manual for FDTD simulation of Optical Phase Array (OPA) devices

Xinghua Wang, BosLab, Kent State University
version 2.0, June, 2004

1. Memory requirement:

As FDTD simulation is extremely memory consuming, the device size we can simulate is limited mainly by the memory installed on the computer. As we measured, with current settings, a grid resolution=10 grid/wavelength, a cell of 10 micron, wavelength=630nm, every 100 micron meter of width of device will need a minimum of 100M memory and 200M of peak memory when the movie is on.
So to simulate a real size device generally need a huge memory installed on the computer.

2. Calculation:

Similar to the director configuration simulation, a input file is also written in M file and should be edit to input the right simulation parameter before run the FDTD simulation. In this simulation, only TM mode of the light is calculated. Which means the FDTD part of the simulation cannot simulate any liquid crystal cell will twist or any out of plane configuration. The program can simulate the situation when the polarization of light is in plane with the director of liquid crystal.

Also the FDTD simulation is based on 4th order finit-difference approximation. To avoid serious numerical dispersion, a grid resolution of 20 grid/wavelength is guaranteed to give highly accurate results. And we find as we currently setted, a grid resolution of 10 grid/wavelength produced almost exactly the same results as 20 grid/wavelength as we observed, but lower grid resolution than that is not guaranteed.

The program can simulate a transmissive device as well as a reflective one. In later case, a mental layer is added next to the liquid crystal cell, and we cut off the light source after half of the simulation time and cleaned the collecting region to get the reflected light. The simulation works well when off axis light source is used.

In both end of the grid on X direction, we didn't use a periodical boundary condition, we use a perfect matching layer to absorb any light going out of the boundary. A free boundary condition used to simulate a free space condition. Due to the fact, the light source is not a plane wave anymore (but rather a point source) on the two end point of the grid, some small distortion on the wavefront could be seen when we use a plane wave light source. In most cases, a gaussian beam with a beam waist less than 0.4 of the total width of OPA is used, and because in that case the intensity at the end point is small, it actually didn't influence the far field result at all.

A important point is that, the director simulation process generally simulate only 1 reset. But when doing FDTD simulation, we need to interpolate the director profile to the FDTD grid. A linear interpolation method is used. If the director profile resolution to too low on director simulation, the interpolation process could introduce error. And though the director simulation generally simulate only one reset, the FDTD program can put multiple resets on the grid see parameter "number_of_wedge".

Finally, when the FDTD simulation is done. You can also use the bottom "Calculate Peak Efficiency", to calculate the percent of energy on any selected region. Just click on mouse and select two point on the graph Matlab generated and the results will be showing the energy fraction of the region between the two points.
function varargout = OPASimu(varargin)
% OPASIMU Application M-file for OPASimu.fig
% FIG = OPASIMU launch OPASimu GUI.
% OPASIMU('callback_name', ...) invoke the named callback.

% Last Modified by GUIDE v2.0 21-Jun-2004 23:44:37

if nargin == 0  % LAUNCH GUI
    fig = openfig(mfilename,'reuse');
    set(fig,'HandleVisibility','On');
    set(fig,'Resize','Off');
    h1 = axes;
    image(imread('nasa.jpg'));
    set(h1,'position',[0.78 0.70 0.077 0.1]);
    axis off;
    h2 = axes;
    image(imread('FrontPage.jpg'));
    set(h2,'position',[0.08 0.1 0.5 0.6]);
    axis off;

    % Use system color scheme for figure:
    set(fig,'Color',get(0,'defaultUicontrolBackgroundColor'));

    % Generate a structure of handles to pass to callbacks, and store it.
    handles = guihandles(fig);
    guidata(fig, handles);

    if nargout > 0
        varargout{1} = fig;
    end
elseif ischar(varargin{1}) % INVOKE NAMED SUBFUNCTION OR CALLBACK
    try
        if (nargout)
            [varargout{1:nargout}] = feval(varargin{:}); % FEVAL switchyard
        else
            feval(varargin{:}); % FEVAL switchyard
        end
    catch
        disp(lasterr);
    end
end

% function varargout = pushbutton.Dir_ini_Callback(hObject, eventdata, handles, varargin)
% edit('Dir_ini.m');
%---------------------------------------------------------------
function varargout = pushbutton_FDTD_ini_Callback(hObject, eventdata, handles, varargin)
edit('FDTD_ini.m');

function varargout = pushbutton_Dir_Callback(hObject, eventdata, handles, varargin)
Dir_simu;

function varargout = pushbutton_FDTD_Callback(hObject, eventdata, handles, varargin)
FDTD;

function varargout = Status_Callback(hObject, eventdata, handles, varargin)

function varargout = Simu_menu_Callback(hObject, eventdata, handles, varargin)

function varargout = Dir_Callback(hObject, eventdata, handles, varargin)
Dir_simu;

function varargout = FDTD_Cancelback(hObject, eventdata, handles, varargin)
FDTD;

function varargout = Manual_menu_Callback(hObject, eventdata, handles, varargin)

function varargout = Dir_doc_Callback(hObject, eventdata, handles, varargin)
edit('Dir_doc.txt');

function varargout = FDTD_doc_Callback(hObject, eventdata, handles, varargin)
edit('FDTD_doc.txt');

function varargout = About_Callback(hObject, eventdata, handles, varargin)
h = helpdlg('Version 1.0, Author: Xinghua Wang BosLab,Liquid Crystal Institute','Info');

function Dir_ini

% 2-D director configuration simulation parameter input file for Director Simulation (Dir_Simu.m)
% Part of Optical Phase Array simulation (OPASimu.m)
% Xinghua Wang, BosLab,Kent State University
% version 2.0, April,2004

%-------------------Liquid Crysta parameters and-----------------------------------------------
LCmaterial=7; %"1" MLC6080 "2" Hanafluide "3" High birefringence LC

if (LCmaterial==1)
%Merck MLC-6080
K11=14.1e-12; %Splay elastic constant of liquid crystal material
K22=7.1e-12; %Twist elastic constant of liquid crystal material
K33=19.1e-12; %Bend elastic constant of liquid crystal material
ep=[11.1 3.9]; %dielectric constant of liquid crystal material
epglass=4.5; %dielectric constant of glass substrate
ne_LC=1.7100; %extraordinary refractive index of liquid crystal material
no_LC=1.5076; %ordinary refractive index of liquid crystal material
e0=8.85e-12; %permittivity constant
q0=-1/4*5e-6; %nematic twisting power of chiral dopant
q0=0;

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if (LCmaterial==2) %Hana fluid
K11=14.1e-12; %Splay elastic constant of liquid crystal material
K22=7.1e-12; %Twist elastic constant of liquid crystal material
K33=19.1e-12; %Bend elastic constant of liquid crystal material
ep=[12.1 4.1]; %dielectric constant of liquid crystal material
epglass=4.5; %dielectric constant of glass substrate
ne_LC=1.6742; %extraordinary refractive index of liquid crystal material
no_LC=1.5035; %ordinary refractive index of liquid crystal material
e0=8.85e-12; %permittivity constant
q0=0;
end

if (LCmaterial==3) %Hana fluid
K11=14.1e-12; %Splay elastic constant of liquid crystal material
K22=7.1e-12; %Twist elastic constant of liquid crystal material
K33=19.1e-12; %Bend elastic constant of liquid crystal material
ep=[12.1 4.1]; %dielectric constant of liquid crystal material
epglass=4.5; %dielectric constant of glass substrate
ne_LC=1.85; %extraordinary refractive index of liquid crystal material
no_LC=1.50; %ordinary refractive index of liquid crystal material
e0=8.85e-12; %permittivity constant
q0=0;
end

if (LCmaterial==7) % 3: High birefringence material BL015, dn=0.28, Tni=87c Vis=58
K11=14.1e-12;
K22=7.1e-12;
K33=19.1e-12;
ep=[12.1 4.1]; %dielectric constant of liquid crystal material
epglass=4.5; %dielectric constant of glass substrate
ne_LC=2.0; %extraordinary refractive index of liquid crystal material
no_LC=1.5; %ordinary refractive index of liquid crystal material
e0=8.85e-12; %permittivity constant
q0=0;
end

%-----------------------Cell parameters ------------------------------
width_electrode=0.5e-6; %width of each electrode
width_gap=0.5e-6; %width of gap between electrodes
number_electrode=2; %total number of electrodes

totalwidthx=(width_electrode+width_gap)*number_electrode; %total width of OPA device within one
reset
totalwidthy=1e-6; %Doesn't matter here for 2-D simulation
totalwidthz=0.4e-6; %Thickness of Liquid Crystal cell

%V_electrode=[ 0.7468  1.4624  1.6897  1.9233  2.2003  2.5767 3.2145 4.7830 ]; % 1th iteration
%-----------------------Calibration phase profile ------------------------

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V_electrode=[0.8855  3.8780];

%--------------------Calibration phase profile -----------------------------------------------
idealphasex=[0.7980   0.6398];

%--------------------simulation parameters  -----------------------------------------------
D=2;                                                 % Dimension of LC3D simulation (Don't Change)
dx=0.005e-6;                                           % Grid resolution in X direction  (Warning: Make sure
   width_electrode/dx width_gap/dx is integer)
dy=1e-6;                                           % Doesn't matter here for 2-D simulation
dz=0.005e-6;                                           % Grid resolution in Z direction  (Warning: Make sure
   totalwidthZ/dz is integer)
Numx=round(totalwidthx/dx)                           %Maximum value 3500
Numy=1;                                              % Doesn't matter here for 2-D simulation
Numz=round(totalwidthz/dz)                           %Maximum value 100
C=0.001;                                               %relaxation speed of liquid crystal director
w=0.7;                                                %relaxation speed of votage
tol=1e-4;                                             %maximum tolerance of err in director simulation
maxloops=1;                                          %maximum director simulation iteration allowed
maxViter=1500;                                           %maximum votage iteration loops allowed
maxVerr=1e-6;                                            %maximum err in voltage relaxation process allowed

xmir=0;                         %Boundary condition for x:         "0" Periodical Boundary Condition, "1" Mirror Image BC
ymir=0;                         %Boundary condition for y:         "0" Periodical Boundary Condition, "1" Mirror Image BC
Vbc=1;                          %Boundary condition for Voltage on z:   "0" V|BC=0,                        "1"
dV/dz|BC=0
rubbingparallel=0;                       % is rubbing direction parallel or perpendicular to electrodes "1" parallel
"0" perpendicular "2" other
pretilt_top=3*pi/180;                    %pretilt of top plate (top means index large, here top ito don't have any
pattern on)
azimuthal_top=0*pi/180;                    % rubbing direction in top plate.
pretilt_bot=3*pi/180;                    %pretilt of bottom plate (bottom means index small, here bot ito have
pattern on!)
azimuthal_bot=0*pi/180;                    %rubbing direction in bottom plate.
total_twist=0*pi/180;                    %total twist of liquid crystal
Initial_twist=0*pi/180;                   %twist in the bulk but the surface is kept parallal. To study the influence
of out of plane twist by scratch in alignment layer

%-----------------------------Use Polymerization to fix director at certain pixel or not -----------------------------

usepolymerstablization=0;       % Whether to use polymerization to fix director configuration on particular pixel

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fixwholepixel=0;
fixpixelnumber=2;

if (fixwholepixel==1)
    xfixmax=(width_electrode/2+width_gap+(fixpixelnumber-1)*width_electrode)/dx  % Ending pixel
    position of the polymerized region
    xfixmin=(width_electrode/2+width_gap+(fixpixelnumber-2)*width_electrode)/dx  % Starting position
    of the polymerized region  Do not put the lowest voltage pixel at first pixel.
else
    xfixmax=0;  % Ending pixel position of the polymerized region
    xfixmin=0;  % Starting position of the polymerized region  Do not
    put the lowest voltage pixel at first pixel.
end

%--------------------Control parameters---------------------------------
use_saved_initial_guess=1;  % use saved director file as initial guess
Openoldinifiles=1;  % To open old ini files where ny is not saved
show_before_calcu=0;  % show profile before calculation and break
Xsample_rate=5;  % display sampling rate in x direction
Zsample_rate=2;  % display sampling rate in z direction

%-----------------------graphic function-------------------------------
textX=10;  % text position
textY=2.4;
dv=0.1;  % dv for iso-potential line
Visocontour=[0:dv:5];  % iso potential lines
plotVLCisocurve=1;  % plot isopotential curve or not
plotdirconfigure=1;  % plot director configuration or not

plotelasticenergy=0;  % plot elastic energy distribution in computation grid or
not
plotsplay=0;  % plot splay elastic energy distribution in computation grid
plottwist=0;  % plot twist elastic energy distribution in computation grid
plotbend=0;  % plot bend elastic energy distribution in computation grid
plottotalelasticenergy=0;  % plot total elastic energy distribution in computation

%--------------------file parameters---------------------------------
textoutput_filename='Output8.dat';  % Output text file for LCDraw
saveoutput=0;  %
save workspace1.mat  % workspace1 saves initial parameter for director
simulation (Dir_simu.m)  % workspace1 saves initial parameter for director
% Liquid Crystal Configuration 3D simulation
% Originally written by J. E. Anderson and P. Watson, 1998 - 1999
% This subroutine is part of LC3D ?Kent State University 2000
%
% Changes in core routine:
% 1. Put ITO within glass to avoid problem on the interface
% 2. First relax voltage on glass to avoid bad initial guess to affect relaxation in LC
% 3. Add symmetric voltage relaxation process to glass
% 4. Add Matlab driver so it can be run at Matlab
% 5. Add option to fix director at particular position to simulate polymerization on certain pixel
%
% Matlab (API Interface) Gateway subroutine

subroutine mexFunction(nlhs, pllhs, nrhs, prhs)
C--------------------------------------------------------------
C     (pointer) Replace integer by integer*8 on the DEC Alpha
C     platform.
C
integer sizex,sizey,sizez,x,y
integer dims(0:2)
parameter (sizex =500,sizey = 1,sizez =100)
real*8 D         ! Number of dimensions:
real*8 xmir,ymir  ! B.C.s in x and y
real*8 numloops,maxloops,successIter,maxViter     ! Loops so far, max allowed
real*8 usepolymerstabilization,xfixmax,xfixmin
real*8 Numx,Numy,Numz     ! Lattice dimensions
real*8 V(0:sizex,0:sizey,0:3*sizez)  ! Voltage array
real*8 dx,dy,dz        ! Grid spacing
real*8 ep(2)       ! Epsilon par and perp
real*8 nx(0:sizex,0:sizey,0:sizez)  ! nx array (director)
real*8 ny(0:sizex,0:sizey,0:sizez)  ! ny array (director)
real*8 nz(0:sizex,0:sizey,0:sizez)  ! nz array (director)
real*8 K11,K22,K33  ! Elastic constants
real*8 e0        ! Perm. of free
real*8 q0        ! Chiral
wavevector (2 pi/P)
real*8 C
real*8 err,maxVerr  ! Maximum uncertainty
real*8 w
parameter
real*8 epglass
   !Dielectric constant of the glass
real*8 topito(0:sizex,0:sizey)
   !2D array (where ITO on top)
real*8 botito(0:sizex,0:sizey)
   !2D array (where ITO on bottom)
real*8 tol
   !Stopping tolerance
real*8 Vbc
   !Voltage

boundary condition:
   ! a 0

means V=0, a 1 means dV/dz=0

integer plhs(*), prhs(*)
integer mxCreateFull
integer nx_pr,ny_pr,nz_pr,V_pr,topito_pr,botito_pr,real_pr
integer nlhs, nrhs
integer m, n, size
integer mxGetM, mxGetN, mxIsNumeric

dims(0)=sizex+1
 dims(1)=sizey+1
 dims(2)=3*sizez+1

c Check for proper number of arguments.
if (nrhs .ne. 32) then
   call mexErrMsgTxt('Number of inputs incorrect.')
elseif (nlhs .ne. 9) then
   call mexErrMsgTxt('Number of outputs incorrect.')
endif

c feed input and output matrix V.
 size = mxGetNumberOfElements(prhs(1))
 plhs(1) = mxCreateNumericArray(3, dims, #mxGetClassID(prhs(1)), 0)
 V_pr = mxGetPr(prhs(1))
 call mxCopyPtrToReal8(V_pr, V, size)

C feed input and output matrix nx.
 dims(2)=sizez+1
 size = mxGetNumberOfElements(prhs(2))
 plhs(2) = mxCreateNumericArray(3, dims, #mxGetClassID(prhs(2)), 0)
 nx_pr = mxGetPr(prhs(2))
 call mxCopyPtrToReal8(nx_pr, nx, size)

C feed input and output matrix ny.
 size = mxGetNumberOfElements(prhs(3))
 plhs(3) = mxCreateNumericArray(3, dims, #mxGetClassID(prhs(3)), 0)
 ny_pr = mxGetPr(prhs(3))
 call mxCopyPtrToReal8(ny_pr, ny, size)

C feed input and output matrix nz.
 size = mxGetNumberOfElements(prhs(4))
plhs(4) = mxCreateNumericArray(3, dims, 
mxGetClassID(prhs(4)), 0)
nz_pr = mxGetPr(prhs(4))
call mxCopyPtrToReal8(nz_pr, nz, size)

 feed input and output matrix topito.
 size = mxGetNumberOfElements(prhs(5))
topito_pr = mxGetPr(prhs(5))
call mxCopyPtrToReal8(topito_pr, topito, size)

 feed input and output matrix botito.
 size = mxGetNumberOfElements(prhs(6))
botito_pr = mxGetPr(prhs(6))
call mxCopyPtrToReal8(botito_pr, botito, size)

 feed input argument.
 real_pr = mxGetPr(prhs(7))
call mxCopyPtrToReal8(real_pr, NumX, 1)
real_pr = mxGetPr(prhs(8))
call mxCopyPtrToReal8(real_pr, NumY, 1)
real_pr = mxGetPr(prhs(9))
call mxCopyPtrToReal8(real_pr, NumZ, 1)
real_pr = mxGetPr(prhs(10))
call mxCopyPtrToReal8(real_pr, dx, 1)
real_pr = mxGetPr(prhs(11))
call mxCopyPtrToReal8(real_pr, dy, 1)
real_pr = mxGetPr(prhs(12))
call mxCopyPtrToReal8(real_pr, dz, 1)
real_pr = mxGetPr(prhs(13))
call mxCopyPtrToReal8(real_pr, K11, 1)
real_pr = mxGetPr(prhs(14))
call mxCopyPtrToReal8(real_pr, K22, 1)
real_pr = mxGetPr(prhs(15))
call mxCopyPtrToReal8(real_pr, K33, 1)
real_pr = mxGetPr(prhs(16))
call mxCopyPtrToReal8(real_pr, e0, 1)
real_pr = mxGetPr(prhs(17))
call mxCopyPtrToReal8(real_pr, q0, 1)
real_pr = mxGetPr(prhs(18))
call mxCopyPtrToReal8(real_pr, C, 1)
real_pr = mxGetPr(prhs(19))
call mxCopyPtrToReal8(real_pr, w, 1)
real_pr = mxGetPr(prhs(20))
call mxCopyPtrToReal8(real_pr, ep, 2)
real_pr = mxGetPr(prhs(21))
call mxCopyPtrToReal8(real_pr, epglass, 1)
real_pr = mxGetPr(prhs(22))
call mxCopyPtrToReal8(real_pr, xmir, 1)
real_pr = mxGetPr(prhs(23))
call mxCopyPtrToReal8(real_pr, ymir, 1)
real_pr = mxGetPr(prhs(24))
call mxCopyPtrToReal8(real_pr, Vbc, 1)
real_pr = mxGetPr(prhs(25))
call mxCopyPtrToReal8(real_pr, D, 1)
real_pr = mxGetPr(prhs(26))
call mxCopyPtrToReal8(real_pr, tol, 1)
real_pr = mxGetPr(prhs(27))
call mxCopyPtrToReal8(real_pr, maxloops, 1)
real_pr = mxGetPr(prhs(28))
call mxCopyPtrToReal8(real_pr, maxViter, 1)
real_pr = mxGetPr(prhs(29))
call mxCopyPtrToReal8(real_pr, maxVerr, 1)
real_pr = mxGetPr(prhs(30))
call mxCopyPtrToReal8(real_pr, usepolymerstablization, 1)
real_pr = mxGetPr(prhs(31))
call mxCopyPtrToReal8(real_pr, xfixmax, 1)
real_pr = mxGetPr(prhs(32))
call mxCopyPtrToReal8(real_pr, xfixmin, 1)

C output argumant for successIter.
plhs(5) = mxCreateFull(1, 1, 0)
C output argumant for totalloops.
plhs(6) = mxCreateFull(1, 1, 0)
C output argumant for Viter.
plhs(7) = mxCreateFull(1, 1, 0)
C output argumant for err.
plhs(8) = mxCreateFull(1, 1, 0)
C output argumant for Verr.
plhs(9) = mxCreateFull(1, 1, 0)

numloops=0.d0
er=1.d0
successIter=0.d0
C Call the computational subroutine
    call LC2D(V,nx,ny,nz,topito,botito,Numx,Numy,Numz,dx,
#dy,dz,K11,K22,K33,e0,q0,C,w,ep,epglass,xmir,ymir,Vbc,D,numloops,
#tol,err,maxloops,successIter,maxViter,maxVerr,
#usepolymerstablization,xfixmax,xfixmin)
C
C Load the output into a MATLAB array.
size = mxGetNumberOfElements(plhs(1))
V_pr = mxGetPr(plhs(1))
call mxCopyReal8ToPtr(V, V_pr, size)

nx_pr = mxGetPr(plhs(2))
ny_pr = mxGetPr(plhs(3))
nz_pr = mxGetPr(plhs(4))

size = mxGetNumberOfElements(plhs(2))
call mxCopyReal8ToPtr(nx, nx_pr, size)
size = mxGetNumberOfElements(plhs(3))
call mxCopyReal8ToPtr(ny, ny_pr, size)

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size = mxGetNumberOfElements(plhs(4))
call mxCopyReal8ToPtr(nz, nz_pr, size)

real_pr = mxGetPr(plhs(5))
call mxCopyReal8ToPtr(successIter, real_pr, 1)
real_pr = mxGetPr(plhs(6))
call mxCopyReal8ToPtr(numloops, real_pr, 1)
real_pr = mxGetPr(plhs(7))
call mxCopyReal8ToPtr(maxViter, real_pr, 1)
real_pr = mxGetPr(plhs(8))
call mxCopyReal8ToPtr(err, real_pr, 1)
real_pr = mxGetPr(plhs(9))
call mxCopyReal8ToPtr(maxVerr, real_pr, 1)

return
end

Subroutine LC2D(V, nx, ny, nz, rtopito, rbotito, rNumx, rNumy, rNumz,
#dx, dy, dz, K11, K22, K33, e0, q0, C, w, ep, epglass, rxmir, rymir, rVbc, rD,
#rnumloops, tol, err, rmaxloops, rsuccessIter, rmaxViter, maxVerr,
#usepolymerstabilization, xfixmax, xfixmin)

c c This subroutine is the calculation engine for the equilibrium program
c c It takes a set of liquid crystal system parameters and calculation
parameters, and simulates the equilibrium state of a system based on Euler-Lagrange
equations. It is intended to be compiled into a DLL which may be called
c by a control program. For more information on the variables passed to
c and from this routine, see the documentation for LC3D.
c
Program Outline:
c --> Declare Variables
c --> Form initial dielectric tensor
c --> Set Voltage boundary conditions
c -->Loop until tolerance or max loops reached
    -->Store old director and dielectric tensor
    -->Reset damping variables
    -->Reset steady state variables
    -->Loop over all lattice points
        -->Calculate voltage for current lattice point
        -->Apply over-relaxation method for voltage
        -->Calculate Fgni's for current lattice point
        -->get new ni's for current lattice point
        -->Rescale director for unit length
        -->Calculate damping and stopping variables
        -->End Loop over all lattice points
        -->Check if unstable, if so damp and redo last iteration
        -->Update Time
    -->End Loop until tolerance or max loops is reached
    -->Exit subroutine

Included Subroutines:
    -->Voltage: Determines the voltage at a given gridpoint
               Uses code based on maple sheet Voltage.mws
    -->Calceps: Determines the epsilon tensor at a gridpoint
    -->Fgni: Determines the derivative of the Gibbs free
            energy with respect to a specified ni
            (that is, nx, ny, or nz).
            Uses code based on maple sheet VectorEnergy.mws

*** Set DLL Attributes ***

*** Declare Variables ***
implicit real*8 (r-w)
integer*4 sizex,sizey,sizez
parameter (sizex =500,sizey = 1,sizez =100)

c *** Variables passed from the control routine ***
integer*4 xmir,ymir                          !B.C.s in x and y
integer*4 D                                  !Number of dimensions
integer*4 numloops,maxloops,maxViter,successIter                     !Loops number,max successful loops,
real*8 usepolymerstabilization,xfixmax,xfixmin
integer*4 Numx,Numy,Numz                        !Lattice dimensions
real*8 V(0:sizex,0:sizey,0:3*sizez)               !Voltage array
real*8 dx,dy,dz                                   !Grid spacing
real*8 ep(2)                                      !epsilon par and perp
real*8 nx(0:sizex,0:sizey,0:sizez)                !nx array (director)
real*8 ny(0:sizex,0:sizey,0:sizez)                !ny array (director)
real*8 nz(0:sizex,0:sizey,0:sizez)                !nz array (director)
real*8 K11,K22,K33                               !Elastic constants
real*8 e0                                       !Perm. of free space (8.85E-12)

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real*8 q0        !Chiral
wavevector (2 π/P)
real*8 C        !Normalized time step
real*8 err,maxVerr,Verr      !total error in LC layer, and in
Voltage iterations
real*8 w        !Voltage over-relaxation
parameter
real*8 epglass     !Dielectric constant of the
glass
integer*4 topito(0:sizex,0:sizey)  !2D array (where ITO on top)
integer*4 botito(0:sizex,0:sizey)  !2D array (where ITO on bottom)
real*8 tol        !Stopping tolerance in LC layer and in Voltage iterations
integer*4 Vbc       !Voltage boundary condition:
real*8 rmaxViter,rsuccessIter
real*8 rxmir,rymir     !B.C.s in x and y
real*8 rnumloops,rmaxloops  !Loops so far, max allowed
real*8 rNumx,rNumy,rNumz    !Lattice dimensions
real*8 rtopito(0:sizex,0:sizey)  !2D array (where ITO on top)
real*8 rbotito(0:sizex,0:sizey)  !2D array (where ITO on bottom)
real*8 rVbc        !Voltage boundary condition:
real*8 rD        !Number of dimensions:
c
*** Other variables used in this subroutine ***
c
integer*4 x,y,z     !Spatial looping variables
integer*4 j        !Generic looping variable
variable
real*8 nxnew,nynew,nznew    !New director components
real*8 Vnew        !New voltage
real*8 epst(1:3,1:3,0:sizex,0:sizey,0:sizez)  !Epsilon tensor
real*8 length      !Length of director (for norm.)
real*8 Fgnx,Fgny,Fgnz     !Functional derivatives
real*8 De        !Delta Epsilon
real*8 errold,errnew    !Old and new uncertainty
real*8 checkx,checky,checkz  !Sum of changes in director
real*8 check(1:3,1:3,0:sizex,0:sizey,0:sizez)  !Changes in director
real*8 Vold(0:sizex,0:sizey,0:3*sizez)    !Voltage array
real*8 nxold(0:sizex,0:sizey,0:sizez)      !Old nx (used when damping)
real*8 nyold(0:sizex,0:sizey,0:sizez)      !Old ny (used when damping)
real*8 nzold(0:sizex,0:sizey,0:sizez)      !Old nz (used when damping)
real*8 epstold(1:3,1:3,0:sizex,0:sizey,0:sizez)  !Old dielectric tensor
real*8 maxC        !Maximum relaxation parameter
real*8 maxcheck,dVmax    !Max change in any dir. component
integer*4 num        !Number to avg (stopping cond.)
c
conver double type in Matlab to Int in Fortran
Numx=int(rNumx)
Numy=int(rNumy)
Numz=int(rNumz)
do x = 0,Numx
  do y = 0,Numy
    topito(x,y)=int(rtopito(x,y))
    botito(x,y)=int(rbotito(x,y))
  end do
end do

numloops=0
maxViter=int(rmaxViter)
successIter=0
maxloops=int(rmaxloops)
xmir=int(rxmir)
ymir=int(rymir)
Vbc=int(rVbc)
D=int(rD)

*** Form the initial dielectric tensor ***

De = ep(1)-ep(2) !Calculate Delta epsilon
do x = 0,Numx
do y = 0,Numy
do z= 0,Numz
call Calceps(epst,e0,ep,nx(x,y,z),ny(x,y,z),nz(x,y,z),x,y,z)
end do
end do

*** Set the boundary conditions at the computational boundary. ***

if (Vbc .eq. 0) then
  do x = 0,Numx
    do y = 0,Numy
      V(x,y,0) = 0.d0
      V(x,y,3*Numz) = 0.d0
    end do
  end do
end if

*** Set the number of loops to 0, this is used so the control routine ***
*** can have this subroutine return after a certain number of loops. ***

*** First relax the voltage ***

Verr=1000
do while ((Verr .LT. maxVerr .and. numloops .LT. maxViter)
  #.or. numloops .LT. maxViter/2)

dVmax=0.d0
do x = 0,Numx  !Loop over all x
do y = 0,Numy  !Loop over all y
if (numloops .EQ. 1) then
   do z=1,Numz-1
      Vold(x,y,z)=V(x,y,z)
   end do
   do z=2*Numz+1,3*Numz-1
      Vold(x,y,z)=V(x,y,z)
   end do
else
   do z=1,Numz-1
      dVmax=dVmax+dabs(Vold(x,y,z)-V(x,y,z));
      Vold(x,y,z)=V(x,y,z)
   end do
   do z=2*Numz+1,3*Numz-1
      dVmax=dVmax+dabs(Vold(x,y,z)-V(x,y,z));
      Vold(x,y,z)=V(x,y,z)
   end do
endif
end do
end do
Verr=dVmax/(sizex*sizey*sizez)
c *** relax bottom glass to find voltage profile ***
do x = 0,Numx
   do y = 0,Numy
      if (Vbc .eq. 1) then
         V(x,y,0) = V(x,y,2)
         V(x,y,1) = V(x,y,2)
      end if
      do z = 1,Numz-1
         if (z .EQ. Numz-2) then ! bottom ITO layer is placed here
            if (botito(x,y) .EQ. 0) then
               Call Voltageglass(V,dx,dy,dz,x,y,z,#Numx,Numy,Numz,Vnew,xmir,ymir,D)
               V(x,y,z) = V(x,y,z)+w*(Vnew-V(x,y,z))
            else
               Call Voltageglass(V,dx,dy,dz,x,y,z,#Numx,Numy,Numz,Vnew,xmir,ymir,D)
               V(x,y,z) = V(x,y,z)+w*(Vnew-V(x,y,z))
            end if
         else
            Call Voltageglass(V,dx,dy,dz,x,y,z,#Numx,Numy,Numz,Vnew,xmir,ymir,D)
            V(x,y,z) = V(x,y,z)+w*(Vnew-V(x,y,z))
         end if
      end do
   end do
end do
c *** relax top glass to find voltage profile ***
do x = 0,Numx
   do y = 0,Numy
      if (Vbc .eq. 1) then
         V(x,y,3*Numz) = V(x,y,3*Numz-2)
         V(x,y,3*Numz-1) = V(x,y,3*Numz-2)
      end if
do z = 2*Numz+1,3*Numz-1  
    if (z .EQ. 2*Numz+2) then             ! top ITO layer is place here  
      if (topito(x,y) .EQ. 0) then  
        Call Voltageglass(V,dx,dy,dz,x,y,z,  
        #Numx,Numy,Numz,Vnew,xmir,ymir,D)  
        V(x,y,z) = V(x,y,z)+w*(Vnew-V(x,y,z))  
        end if  
    else  
      Call Voltageglass(V,dx,dy,dz,x,y,z,  
        #Numx,Numy,Numz,Vnew,xmir,ymir,D)  
      V(x,y,z) = V(x,y,z)+w*(Vnew-V(x,y,z))  
      end if  
    end do  
  end do  
end do  

c *** relax interface and LC layer to find voltage profile ***  
do x = 0,Numx                     !Loop over all x  
do y = 0,Numy                     !Loop over all y  
call Voltageinterfbot(V,dx,dy,dz,x,y,0,  
#Vnew,epst,epglass,Numx,Numy,Numz,xmir,ymir,D)  
V(x,y,Numz) = V(x,y,Numz)+w*(Vnew-V(x,y,Numz))  

do z = 1,Numz-1  
call VoltageLC(V,dx,dy,dz,x,y,z,  
#Vnew,epst,Numx,Numy,Numz,xmir,ymir,D)  
V(x,y,z+Numz) = V(x,y,z+Numz) + w*(Vnew-V(x,y,z+Numz))  
end do  
call Voltageinterftop(V,dx,dy,dz,x,y,Numz,  
#Vnew,epst,Numx,Numy,Numz,xmir,ymir,D)  
V(x,y,2*Numz) = V(x,y,2*Numz)+w*(Vnew-V(x,y,2*Numz))  
end do  
c *** relax interface and LC layer backward to assume symmetry ***  
do x = Numx,0,-1              !Loop over all x  
do y = Numy,0,-1              !Loop over all y  
call Voltageinterftop(V,dx,dy,dz,x,y,Numz,  
#Vnew,epst,epglass,Numx,Numy,Numz,xmir,ymir,D)  
V(x,y,2*Numz) = V(x,y,2*Numz)+w*(Vnew-V(x,y,2*Numz))  

do z = Numz-1,1,-1  
call VoltageLC(V,dx,dy,dz,x,y,z,  
#Vnew,epst,Numx,Numy,Numz,xmir,ymir,D)  
V(x,y,z+Numz) = V(x,y,z+Numz) + w*(Vnew-V(x,y,z+Numz))  
end do  
call Voltageinterfbot(V,dx,dy,dz,x,y,0,  
#Vnew,epst,epglass,Numx,Numy,Numz,xmir,ymir,D)  
V(x,y,Numz) = V(x,y,Numz)+w*(Vnew-V(x,y,Numz))  
end do  
end do
c *** relax top glass to find voltage profile ***
do x = Numx,0,-1
  do y = Numy,0,-1
    if (Vbc eq 1) then
      V(x,y,3*Numz) = V(x,y,3*Numz-2)
      V(x,y,3*Numz-1) = V(x,y,3*Numz-2)
    end if
    do z = 3*Numz-1,2*Numz+1,-1
      if (z .EQ. 2*Numz+2) then            ! top ITO layer is place here
        if (topito(x,y) .EQ. 0) then
          Call Voltageglass(V,dx,dy,dz,x,y,z,
#Numx,Numy,Numz,Vnew,xmir,ymir,D)
          V(x,y,z) = V(x,y,z)+w*(Vnew-V(x,y,z))
        end if
      else
        Call Voltageglass(V,dx,dy,dz,x,y,z,
#Numx,Numy,Numz,Vnew,xmir,ymir,D)
        V(x,y,z) = V(x,y,z)+w*(Vnew-V(x,y,z))
      end if
    end do
  end do
end do

numloops=numloops+1
end do
maxVerr=Verr
rmaxViter=dfloat(numloops)

c open(101,FILE="E:\Matlab6\work\LCMod\Fortran_Log.txt")
c write (101,*) "ep(1)",ep(1)
c close(101)
numloops = 0

**** main loop starts here ****

do while (err .gt. tol .and. numloops .lt. maxloops) ! loops <= maxloops

*** relax bottom glass to find voltage profile ***

do x = 0,Numx
  do y = 0,Numy
    if (Vbc .eq. 1) then
      V(x,y,0) = V(x,y,2)
      V(x,y,1) = V(x,y,2)
    end if
    do z = 1,Numz-1
      if (z .EQ. Numz-2) then ! bottom ITO layer is place here
        if (botito(x,y) .EQ. 0) then
          Call Voltageglass(V,dx,dy,dz,x,y,z,
#Numx,Numy,Numz,Vnew,xmir,ymir,D)
          V(x,y,z) = V(x,y,z)+w*(Vnew-V(x,y,z))
        end if
        else
          Call Voltageglass(V,dx,dy,dz,x,y,z,
#Numx,Numy,Numz,Vnew,xmir,ymir,D)
          V(x,y,z) = V(x,y,z)+w*(Vnew-V(x,y,z))
      endif
    end do
  end do
end do

*** Loop over Liquid Crystal ***

*** Put values from previous time step into variables. ***

*** If the simulation goes unstable, we will need to ***

*** redo the last iteration with a smaller time step. ***

*** To do this, we need to know the previous state. ***

*** Therefore, we need to store the director and the ***

*** dielectric tensor. ***

call storeoldn(nx,ny,nz,nxold,nyold,nzold,Numx,Numy,Numz)
call storeolddens(epst,epstold,Numx,Numy,Numz)

100 check = 0.d0

*** Reinitialize variables which will be used to deter-

*** mine if damping is neccessary. ***

errold = errnew
  errnew = 0.d0
num = 0
do x = 0,Numx    !Loop over all x
doy = 0,Numy    !Loop over all y

c
c*** If there is no ITO on the bottom plate at this x, y location ***
c*** then we need to calculate the voltage at the interface. ***
c
call Voltageinterfbot(V,dx,dy,dz,x,y,0,#Vnew,epst,epglass,Numx,Numy,Numz,xmir,ymir,D)
V(x,y,Numz) = V(x,y,Numz)+w*(Vnew-V(x,y,Numz))
c
do z = 1,Numz-1  !Loop over just inside layers
Vnew = 0.d0   !reinitialize all temporary variables
nxnew = 0.d0
nynew = 0.d0
nznew = 0.d0
length = 0.d0
Fgnx = 0.d0
Fgny = 0.d0
Fgnz = 0.d0
c
c*** Find new value of voltage at current point ***
c
call VoltageLC(V,dx,dy,dz,x,y,z,#Vnew,epst,Numx,Numy,Numz,xmir,ymir,D)
c
c*** Apply the over-relaxation method ***
c
V(x,y,z+Numz) = V(x,y,z+Numz) + w*(Vnew-V(x,y,z+Numz))
c
c*** Get the [Fg]ni s (The functional der. of Fg w.r.t. ni) ***
c
c*** Get [Fg]nx at the current point. ***
call Fgni(K11,K22,K33,e0,De,dx,dy,dz,q0,V,x,y,z,#Fgnx,nx,ny,nz,1,Numx,Numy,Numz,xmir,ymir,D)
c
c*** Get [Fg]ny at the current point. ***
call Fgni(K11,K22,K33,e0,De,dx,dy,dz,q0,V,x,y,z,#Fgny,nx,ny,nz,2,Numx,Numy,Numz,xmir,ymir,D)
c
c*** Get [Fg]nz at the current point. ***
call Fgni(K11,K22,K33,e0,De,dx,dy,dz,q0,V,x,y,z,#Fgnz,nx,ny,nz,3,Numx,Numy,Numz,xmir,ymir,D)
c
c*** Update stopping condition variables ***
c
errnew = errnew+dabs(Fgnx)+dabs(Fgny) 
#+dabs(Fgnz)
num = num+1
c
c*** Update the director. Have to rescale length. ***
c-------------------------  !modified to fix director at particular position ------------
c-------as if the director in the particular pixel is fixed by polymer stablization--------------
if (usepolymerstablization  .eq. 1) then
if (x .lt. xfixmax) then
  if (x .gt. xfixmin) then
    nxnew = nx(x,y,z)
    nynew = ny(x,y,z)
    nznew = nz(x,y,z)
  else
    nxnew = nx(x,y,z)-C*Fgnx
    nynew = ny(x,y,z)-C*Fgny
    nznew = nz(x,y,z)-C*Fgnz
  end if
else
  nxnew = nx(x,y,z)-C*Fgnx
  nynew = ny(x,y,z)-C*Fgny
  nznew = nz(x,y,z)-C*Fgnz
endif

else
  nxnew = nx(x,y,z)-C*Fgnx
  nynew = ny(x,y,z)-C*Fgny
  nznew = nz(x,y,z)-C*Fgnz
endif

c-------------------------  !modified to fix director at particular position ------------
c-------as if the director in the particular pixel is fixed by polymer stablization--------------

c    *** Rescale new n to be a unit vector ***

c length = dsqrt((nxnew**2.d0)+(nynew**2.d0)+(nznew**2.d0))
nxnew = nxnew/length
nynew = nynew/length
nznew = nznew/length

c    *** Calculate changes to be used for damping and stopping ***

c check(1,x,y,z) = dabs(nxnew-nx(x,y,z)) !1 means nx
check(2,x,y,z) = dabs(nynew-ny(x,y,z)) !2 means ny
check(3,x,y,z) = dabs(nznew-nz(x,y,z)) !3 means nz

c    *** Use the successive Displacement method ***

c nx(x,y,z) = nxnew
ny(x,y,z) = nynew
nz(x,y,z) = nznew

c    *** Form the new dielectric tensor at this point (Succ. Disp.) ***
call Calceps(epst,e0,ep,nx(x,y,z),ny(x,y,z),
nz(x,y,z),x,y,z)

end do !End z loop

c    *** If there is no ITO on the top plate at this x, y location ***
c    *** then we need to calculate the voltage at the interface. ***
call Voltageinterftop(V,dx,dy,dz,x,y,Numz,
#Vnew, epst, epglass, Numx, Numy, Numz, xmir, ymir, D)
V(x,y,2*Numz) = V(x,y,2*Numz) + w*(Vnew-V(x,y,2*Numz))
end do  !End y loop
end do  !End x loop
c
*** In this next section of code, we determine if the system ***
*** to be damped. If it does, we go back a time step and ***
*** reduce C by 1.5. It if does not, we finish calculating ***
*** the stopping variable, and proceed to the next iteration. ***
checkx = 0.d0
checky = 0.d0
checkz = 0.d0
maxcheck = 0.d0
do x = 0, Numx
do y = 0, Numy
do z = 1, Numz-1
  if (check(1,x,y,z) .gt. checkx) then
    checkx = check(1,x,y,z)
  end if
  if (check(2,x,y,z) .gt. checky) then
    checky = check(2,x,y,z)
  end if
  if (check(3,x,y,z) .gt. checkz) then
    checkz = check(3,x,y,z)
  end if
  if (checkx .gt. maxcheck) then
    maxcheck = checkx
  end if
  if (checky .gt. maxcheck) then
    maxcheck = checky
  end if
  if (checkz .gt. maxcheck) then
    maxcheck = checkz
  end if
end do
end do
end do
c
*** To damp, check to see if the max of the changes of ***
*** any one component is bigger than .004. ***
if (maxcheck .GT. .004d0) then
  C = C/1.5d0  !If have to damp, go back to previous time step
  call storeoldn(nxold, nyold, nzold, nx, ny, nz, Numx, Numy, Numz)
call storeoldtens(epstold, epst, Numx, Numy, Numz)
err = 10000
errnew = errold
numloops = numloops+1  !Increment loop counter
if (numloops .LT. maxloops) then
goto 100
end if
else

c
else
**maxC** is derived using the heat equation. It is only meant as a safeguard against the simulation going unstable. If the simulation goes unstable, the director dynamics no longer follow physical laws, and this can introduce errors that lead to non-physical results.

\[ \text{maxC} = \frac{dz*dz}{2*K33} \]

If \( C < \text{maxC} \)
\[
C = C*1.005d0
\]

\[ \text{err} = 0.d0 \]
\[ \text{errnew} = \frac{\text{errnew}}{\text{num}} \]
\[ \text{err} = \frac{\text{dabs} (\text{errnew}-\text{errold})}{C} \]

\[ \text{successIter} = \text{successIter} + 1 \]
\[ \text{numloops} = \text{numloops} + 1 \]

*** relax top glass to find voltage profile ***

\[ \text{do } x = 0, \text{Numx} \]
\[ \text{do } y = 0, \text{Numy} \]
\[ \text{if (Vbc eq. 1) then} \]
\[ V(x,y,3*\text{Numz}) = V(x,y,3*\text{Numz}-2) \]
\[ V(x,y,3*\text{Numz}-1) = V(x,y,3*\text{Numz}-2) \]
\[ \text{end if} \]
\[ \text{do } z = 2*\text{Numz}+1, 3*\text{Numz}-1 \]
\[ \text{if (z .EQ. 2*\text{Numz}+2) then} \]
\[ \text{if (topito(x,y) .EQ. 0) then} \]
\[ \text{Call Voltageglass}(V,dx,dy,dz,x,y,z, \#\text{Numx,Numy,Numz,Vnew,xmir,ymir,D}) \]
\[ V(x,y,z) = V(x,y,z)+w*(Vnew-V(x,y,z)) \]
\[ \text{end if} \]
\[ \text{else} \]
\[ \text{Call Voltageglass}(V,dx,dy,dz,x,y,z, \#\text{Numx,Numy,Numz,Vnew,xmir,ymir,D}) \]
\[ V(x,y,z) = V(x,y,z)+w*(Vnew-V(x,y,z)) \]
\[ \text{end if} \]
\[ \text{end do} \]
\[ \text{end do} \]
\[ \text{end do} \]

*** The successive displacement method speeds up the calculation, but does introduce some asymmetry.***

*** We will now loop over Liquid Crystal Backwards to try to keep the simulation as symmetric as possible.***

*** Put values from previous time step into variables.***

*** If the simulation goes unstable, we will need to redo the last iteration with a smaller time step.***

*** To do this, we need to know the previous state.***

*** Therefore, we need to store the director and the dielectric tensor.***

200 call storeoldn(nx,ny,nz,nxold,nyold,nzold,Numx,Numy,Numz)
call storeoldtens(epst,epstold,Numx,Numy,Numz)

*** Reinitialize variables which will be used to deter-
*** mine if damping is neccessary.

check = 0.d0

*** Reinitialize variables which will be used to deter-
*** mine if simulation has reached steady state.

errold = errnew
ernew = 0.d0
num = 0

*** relax top glass to find voltage profile ***
do x = Numx,0,-1
  do y = Numy,0,-1
    if(Vbc .eq. 1) then
      V(x,y,3*Numz) = V(x,y,3*Numz-2)
      V(x,y,3*Numz-1) = V(x,y,3*Numz-2)
    end if
    do z = 3*Numz-1,2*Numz+1,-1
      if(z .EQ. 2*Numz+2) then ! top ITO layer is place here
        if (topito(x,y) .EQ. 0) then
          call Voltageglass(V,dx,dy,dz,x,y,z,#
          Numx,Numy,Numz,Vnew,xmir,ymir,D)
          V(x,y,z) = V(x,y,z)+w*(Vnew-V(x,y,z))
        end if
        else
          call Voltageglass(V,dx,dy,dz,x,y,z,#
          Numx,Numy,Numz,Vnew,xmir,ymir,D)
          V(x,y,z) = V(x,y,z)+w*(Vnew-V(x,y,z))
        end if
      end do
    end do
  end do
end do

*** If there is no ITO on the top plate at this x, y location ***
*** then we need to calculate the voltage at the interface. ***
do x = 0,Numx !Loop over all x
do y = 0,Numy !Loop over all y

call Voltageinterftop(V,dx,dy,dz,x,y,Numz,
#Vnew,epst,epglass,Numx,Numy,Numz,xmir,ymir,D)
V(x,y,2*Numz) = V(x,y,2*Numz)+w*(Vnew-V(x,y,2*Numz))

do z = Numz-1,1,-1 !Loop over just inside layers
Vnew = 0.d0
nxnew = 0.d0
nynew = 0.d0
nznew = 0.d0
length = 0.d0
Fgnx = 0.d0
Fgny = 0.d0
Fgnz = 0.d0

c
*** Find new value of voltage at current point ***

call VoltageLC(V,dx,dy,dz,x,y,z,
    #Vnew,epst,Numx,Numy,Numz,xmir,ymir,D)

c
*** Apply the over-relaxation method ***

V(x,y,z+Numz) = V(x,y,z+Numz) + w*(Vnew-V(x,y,z+Numz))

c
*** Get the [Fg]ni s (The functional der. of Fg w.r.t. ni) ***

c
*** Get [Fg]nx at the current point. ***
call Fgni(K11,K22,K33,e0,De,dx,dy,dz,q0,V,x,y,z,
    #Fgnx,nx,ny,nz,1,Numx,Numy,Numz,xmir,ymir,D)

c
*** Get [Fg]ny at the current point. ***
call Fgni(K11,K22,K33,e0,De,dx,dy,dz,q0,V,x,y,z,
    #Fgny,nx,ny,nz,2,Numx,Numy,Numz,xmir,ymir,D)

c
*** Get [Fg]nz at the current point. ***
call Fgni(K11,K22,K33,e0,De,dx,dy,dz,q0,V,x,y,z,
    #Fgznz,nx,ny,nz,3,Numx,Numy,Numz,xmir,ymir,D)

c
*** Update stopping condition variables ***

ernew = errnew+dabs(Fgnx)+dabs(Fgny)
    #+#dabs(Fgznz)
    num = num+1

c
*** Update the director. Have to rescale length. ***

c------------------------- !modified to fix director at particular position ------------

---as if the director in the particular pixel is fixed by polymer stablization----------

if (usepolymerstablization .eq. 1) then
    if (x .lt. xfixmax) then
        if (x .gt. xfixmin) then
            nxnew = nx(x,y,z)
            nynew = ny(x,y,z)
            nznew = nz(x,y,z)
        else
            nxnew = nx(x,y,z)-C*Fgnx
            nynew = ny(x,y,z)-C*Fgny
            nznew = nz(x,y,z)-C*Fgznz
        endif
    else
        nxnew = nx(x,y,z)-C*Fgnx
        nynew = ny(x,y,z)-C*Fgny
        nznew = nz(x,y,z)-C*Fgznz
    endif
else
    nxnew = nx(x,y,z)-C*Fgnx
    nynew = ny(x,y,z)-C*Fgny
    nznew = nz(x,y,z)-C*Fgznz
endif

c
else
    nxnew = nx(x,y,z)-C*Fgnx

344
nynew = ny(x,y,z)-C*Fgny  
nznew = nz(x,y,z)-C*Fg nz  
endif  

*e n d i f*  

!modified to fix director at particular position ------------
---as if the director in the particular pixel is fixed by polymer stablization---------

*** Rescale new n to be a unit vector ***

length = dsqrt(nxnew**2.0d0)+(nynew**2.0d0)+(nznew**2.0d0)  
nxnew = nxnew/length  
nynew = nynew/length  
nznew = nznew/length

*** Calculate changes to be used for damping and stopping ***

check(1,x,y,z) = dabs(nxnew-nx(x,y,z))  
check(2,x,y,z) = dabs(nynew-ny(x,y,z))  
check(3,x,y,z) = dabs(nznew-nz(x,y,z))

*** Use the successive Displacement method ***

nx(x,y,z) = nxnew  
ny(x,y,z) = nynew  
nz(x,y,z) = nznew

*** Form the new dielectric tensor at this point (Succ. Disp.) ***

call Calceps(epst,e0,ep,nx(x,y,z),ny(x,y,z),  
nz(x,y,z),x,y,z)

V(x,y,0) = V(x,y,2)  
V(x,y,1) = V(x,y,2)
end if

if (z .EQ. Numz-2) then           ! bottom ITO layer is place here
if (botito(x,y) .EQ. 0) then  
Call Voltageglass(V,dx,dy,dz,x,y,z,  
Numx,Numy,Numz,Vnew,xmir,ymir,D)  
V(x,y,z) = V(x,y,z)+w*(Vnew-V(x,y,z))
endif
else

*** relax bottom glass to find voltage profile ***

do x = Numx,0,-1  
do y = Numy,0,-1  
   if (Vbc .eq. 1) then  
      V(x,y,0) = V(x,y,2)  
      V(x,y,1) = V(x,y,2)
   end if
   do z = Numz-1,1,-1  
   if (z .EQ. Numz-2) then ! bottom ITO layer is place here
      if (botito(x,y) .EQ. 0) then  
       Call Voltageglass(V,dx,dy,dz,x,y,z,  
        Numx,Numy,Numz,Vnew,xmir,ymir,D)  
       V(x,y,z) = V(x,y,z)+w*(Vnew-V(x,y,z))
      end if
      else
Call Volfageglass(V,dx,dy,dz,x,y,z,
#Numx,Numy,Numz,Vnew,xmir,ymir,D)
V(x,y,z) = V(x,y,z)+w*(Vnew-V(x,y,z))
end if

end do
end do
end do

c
*** In this next section of code, we determine if the system ***
*** to be damped. If it does, we go back a time step and ***
*** reduce C by 1.5. If it does not, we finish calculating ***
*** the stopping variable, and proceed to the next iteration. ***
c
checkx = 0.d0
checky = 0.d0
checkz = 0.d0
maxcheck = 0.d0
do x = 0,Numx
do y = 0,Numy
do z = 1,Numz-1
  if (check(1,x,y,z) .gt. checkx) then
    checkx = check(1,x,y,z)
  end if
  if (check(2,x,y,z) .gt. checky) then
    checky = check(2,x,y,z)
  end if
  if (check(3,x,y,z) .gt. checkz) then
    checkz = check(3,x,y,z)
  end if
end do
end do
end do

c
*** To damp, check to see if the max of the changes of ***
*** any one component is bigger than .004. ***
c
if (maxcheck .GT. .004d0) then
  C = C/1.5d0   !If have to damp, go back to previous time step
  call storeoldn(nxold,nyold,nzold,nx,ny,nz,Numx,Numy,Numz)
call storeoldtens(epstold,epst,Numx,Numy,Numz)
err = 10000
errnew = errold
numloops = numloops+1
!Increment loop counter
if (numloops .lt. maxloops) then
goto 200
end if
else

  *** maxC is derived using the heat equation. It is only meant ***
  *** as a safeguard against the simulation going unstable. If ***
  *** the simulation goes unstable, the director dynamics no ***
  *** longer follow physical laws, and this can introduce errors***
  *** that lead to non-physical results.             ***

  maxC = dz*dz/(2*K33)
  if (C .lt. maxC) then
      C = C*1.005d0
  end if

  err = 0.d0
  errnew = ernew/num
  err = dabs(errnew-errold)/C !New stopping metric
  successIter=successIter+1 !successful steps
  numloops = numloops+1 !total Steps
end if

Now, we are done with this run. Return to VB.
end do
rsuccessIter=dfloat(successIter)
rnumloops=dfloat(numloops)
return
contains
! *** Subroutines used in main program ***
!
! *** Subroutine for calculating new Voltage ***
Subroutine VoltageLC(V,dx,dy,dz,x,y,z,Vnew,epst,#Numx,Numy,Numz,xmir,ymir,D)
!
! *******************************************
! ***  This subroutine calculates the new ***
! *** value of the potential at the point ***
! *** x,y,z (integers between 0 and Numx, ***
! *** Numy,Numz). The equation used is:  ***
! *** 0 = -[Fg] = div(e *e*gradV)     ***
! ***      V     0                     ***
! *** This equation can be directly       ***
! *** solved for V at the current point. ***
! *** (See Maple sheet "Voltage.mws")    ***
! *** Jim Anderson, Feb/1/98             ***
! *******************************************
!
! Declare Variables ***
implicit real*8 (r-w)
integer x,y,z,TV !lattice point, z
!
for V
integer Numx, Numy, Numz ! lattice dimensions
integer D
! # of spatial dimensions
integer sizex, sizey, sizez ! size of arrays
integer xmir, ymir
! boundary conditions
parameter (sizex = 500, sizey = 1, sizez = 100) ! set array size
real*8 V(0:sizex, 0:sizey, 0:(3*sizez)) ! Voltage array
real*8 dx, dy, dz ! grid spacing
real*8 epst(1:3, 1:3, 0:sizex, 0:sizey, 0:sizez) ! dielectric tensor array
real*8 mirrepst(1:3, 1:3, 0:sizex, 0:sizey, 0:sizez) ! holds mirror dielectric tensor
real*8 v001, v010, v011, v100, v101, v110, v111, v000 ! voltage at different grid points
real*8 v01_1, v0_10, v1_10, v_10_1, v_1_10, v0_1_1, v_10_1, v_1_10 ! hold dielectric derivatives
real*8 e11x, e12x, e13x, e21y, e22y, e23y, e31z, e32z, e33z ! rename dielectric tensor
c
zV = z + Numz ! voltage array starts at Numz in the LC layer
c
*** Voltages at neighboring gridpoints (needed for derivatives of V) ***
c
*** the voltage at a point is given the name "vijk" here, if i,j or k is 1, we are referring to a point with a lattice index 1
***
c
*** greater than the current gridpoint. If i,j or k is 0, that means we are referring to a point in the same plane as the gridpoint,
***
c
*** and if i,j, or k is -1 (_1), we are referring to a point with a lattice index 1 less than the current point.
***
c
*** Thus, if we are at gridpoint (x,y,z) = (137, 44, 34) then v_1_10 is the voltage at (138,43,35) and
***
c
*** v_10_1 is the voltage at (136,44,33).
***
c
*** This parts gets complicated with all the different possibilities that have to calculate the derivative different if at a boundary,
***
c
*** then have to determine which kind of boundary condition is used. Finally, if 2-D only need derivatives in x and z dimensions.
***
c
if (x .EQ. 0 .or. x .EQ. Numx) then ! is x at a boundary?
    if (xmir .EQ. 1) then ! is the x B.C. mirror?
        if (x .EQ. 0) then ! is x at 0?
            v_10_1 = V(1, y, zV)
            v_101 = V(1, y, (zV + 1)) ! define x and z
e1
            v10_1 = V(1, y, (zV - 1)) ! derivatives.
            v100 = V(1, y, zV)
            v101 = V(1, y, (zV + 1))
        else ! or is it at Numx?
            v_10_1 = V((Numx - 1), y, (zV - 1))
            v_100 = V((Numx - 1), y, zV)
            v_101 = V((Numx - 1), y, (zV + 1))
        endif!
    endif!
endif!
v10_1 = V((Numx-1),y,(zV-1)) !derivatives.
v100 = V((Numx-1),y,zV)
v101 = V((Numx-1),y,(zV+1))
end if

else  !or is the B.C.

v_10_1 = V((Numx-1),y,(zV-1))
v_100 = V((Numx-1),y,zV)
v_101 = V((Numx-1),y,(zV+1)) !define x and z
ev10_1 = V(1,y,(zV-1)) !derivatives.
v100 = V(1,y,zV)
v101 = V(1,y,(zV+1))
end if

if (y .EQ. 0 .or. y .eq. Numy) then  !is y at a boundary?
  if (ymir .EQ. 1) then      !is the y B.C. mirror?
    if (y .EQ. 0) then       !is y at 0?
      if (xmir .EQ. 1) then       !is the x B.C. mirror?
        if (x .EQ. 0) then        !is x at 0?
          if (D. eq. 3) then         !3-D?
            v_1_1_1 = V(1,1,(zV-1))
v_1_10 = V(1,1,zV)
v_1_11 = V(1,1,(zV+1))        !define derivatives
            v_11_1 = V(1,1,(zV-1))
v_110 = V(1,1,zV)
v_111 = V(1,1,(zV+1))
v1_1_1 = V(1,1,(zV-1))
v1_10 = V(1,1,zV)
v1_11 = V(1,1,(zV+1))
v11_1 = V(1,1,(zV-1))
v110 = V(1,1,zV)
v111 = V(1,1,(zV+1))
v0_1_1 = V(x,1,(zV-1))
v0_10 = V(x,1,zV)
v0_11 = V(x,1,(zV+1))
v01_1 = V(x,1,(zV-1))
v010 = V(x,1,zV)
v011 = V(x,1,(zV+1))
else            !or 2-D?
            v_1_1_1 = V(1,y,(zV-1))
v_1_10 = V(1,y,zV)
v_1_11 = V(1,y,(zV+1))
v_11_1 = V(1,y,(zV-1)) !define derivatives
            v_110 = V(1,y,zV)
v_111 = V(1,y,(zV+1))
v1_1_1 = V(1,y,(zV-1))
v1_10 = V(1,y,zV)
v1_11 = V(1,y,(zV+1))
v11_1 = V(1,y,(zV-1))
v110 = V(1,y,zV)
v111 = V(1,y,(zV+1))
v0_1_1 = V(x,y,(zV-1))
v0_10 = V(x,y,zV)
v0_11 = V(x,y,(zV+1))
v01_1 = V(x,y,(zV-1))
v010 = V(x,y,zV)
v011 = V(x,y,(zV+1))
else if (D .eq. 3) then !3-D?
  v_1_1_1 = V((Numx-1),1,(zV-1))
  v_1_10 = V((Numx-1),1,zV)
  v_1_11 = V((Numx-1),1,(zV+1))
  v_11_1 = V((Numx-1),1,(zV-1))
  v_110 = V((Numx-1),1,zV)
  v_111 = V((Numx-1),1,(zV+1))
  v1_1_1 = V((Numx-1),1,(zV-1))
  v1_10 = V((Numx-1),1,zV)
  v1_11 = V((Numx-1),1,(zV+1))
  v11_1 = V((Numx-1),1,(zV-1))
  v110 = V((Numx-1),1,zV)
  v111 = V((Numx-1),1,(zV+1))
end if
else
  !or is x at Numx?
  if (D .eq. 3) then !3-D?
    v_1_1_1 = V((Numx-1),y,(zV-1))
    v_1_10 = V((Numx-1),y,zV)
    v_1_11 = V((Numx-1),y,(zV+1))
    v_11_1 = V((Numx-1),y,(zV-1))
    v_110 = V((Numx-1),y,zV)
    v_111 = V((Numx-1),y,(zV+1))
    v1_1_1 = V(1,y,(zV-1))
    v1_10 = V(1,y,zV)
    v1_11 = V(1,y,(zV+1))
    v11_1 = V(1,y,(zV-1))
    v110 = V(1,y,zV)
    v111 = V(1,y,(zV+1))
  else !or 2-D?
    v_1_1_1 = V((Numx-1),y,(zV-1))
    v_1_10 = V((Numx-1),y,zV)
    v_1_11 = V((Numx-1),y,(zV+1))
    v_11_1 = V((Numx-1),y,(zV-1))
    v_110 = V((Numx-1),y,zV)
    v_111 = V((Numx-1),y,(zV+1))
    v0_1_1 = V(x,y,(zV-1))
    v0_10 = V(x,y,zV)
    v0_11 = V(x,y,(zV+1))
    v01_1 = V(x,y,(zV-1))
    v010 = V(x,y,zV)
    v011 = V(x,y,(zV+1))
  end if
else
  !or the x B.C. periodic?
  if (D .eq. 3) then !3-D?
    v_1_1_1 = V((Numx-1),1,(zV-1))
    v_1_10 = V((Numx-1),1,zV)
    v_1_11 = V((Numx-1),1,(zV+1))
    v_11_1 = V((Numx-1),1,(zV-1))
    v_110 = V((Numx-1),1,zV)
    v_111 = V((Numx-1),1,(zV+1))
    v1_1_1 = V(1,1,(zV-1))
    v1_10 = V(1,1,zV)
    v1_11 = V(1,1,(zV+1))
    v11_1 = V(1,1,(zV-1))
    v110 = V(1,1,zV)
    v111 = V(1,1,(zV+1))
  else
v0_1_1 = V(x,1,(zV-1))
v0_10 = V(x,1,zV)
v0_11 = V(x,1,(zV+1))
v01_1 = V(x,1,(zV-1))
v010 = V(x,1,zV)
v011 = V(x,1,(zV+1))

else

v1_1_1 = V((Numx-1),y,(zV-1))
v1_10 = V((Numx-1),y,zV)
v1_11 = V((Numx-1),y,(zV+1))
v1_11 = V((Numx-1),y,(zV-1))
!define derivatives
v1_10 = V((Numx-1),y,zV)
v1_11 = V((Numx-1),y,(zV+1))
v1_11 = V((Numx-1),y,(zV-1))

end if

else

if (xmir.EQ.1) then
  !is the x B.C. mirror?
  if (x .EQ. 0) then
    !is x at 0?
      if (D.eq.3) then
        !3-D?
          v1_1_1 = V(1,(Numy-1),(zV-1))
v1_10 = V(1,(Numy-1),zV)
v1_11 = V(1,(Numy-1),(zV+1))
v_11_1 = V(1,(Numy-1),(zV-1))
!define derivatives
v1_10 = V(1,(Numy-1),zV)
v1_11 = V(1,(Numy-1),(zV+1))
v1_11 = V(1,(Numy-1),(zV-1))
v1_10 = V(1,(Numy-1),zV)
v1_11 = V(1,(Numy-1),(zV+1))
v1_11 = V(1,(Numy-1),(zV-1))
v10 = V(1,(Numy-1),zV)
v11 = V(1,(Numy-1),(zV+1))
v0_1_1 = V(x,(Numy-1),(zV-1))
v0_10 = V(x,(Numy-1),zV)
v0_11 = V(x,(Numy-1),(zV+1))
v01_1 = V(x,(Numy-1),(zV-1))
v010 = V(x,(Numy-1),zV)
v011 = V(x,(Numy-1),(zV+1))
else
  !or 2-D?
    v1_1_1 = V(1,y,(zV-1))
v1_10 = V(1,y,zV)
v1_11 = V(1,y,(zV+1))
v1_11 = V(1,y,(zV-1))
!define derivatives
v1_10 = V(1,y,zV)
v1_11 = V(1,y,(zV+1))

else

end if

else

! or is y at Numy?

if (xmir.EQ.1) then
  !is the x B.C. mirror?
  if (x .EQ. 0) then
    !is x at 0?
      if (D.eq.3) then
        !3-D?
          v1_1_1 = V(1,(Numy-1),(zV-1))
v1_10 = V(1,(Numy-1),zV)
v1_11 = V(1,(Numy-1),(zV+1))
v_11_1 = V(1,(Numy-1),(zV-1))
!define derivatives
v1_10 = V(1,(Numy-1),zV)
v1_11 = V(1,(Numy-1),(zV+1))
v1_11 = V(1,(Numy-1),(zV-1))
v1_10 = V(1,(Numy-1),zV)
v1_11 = V(1,(Numy-1),(zV+1))
v1_11 = V(1,(Numy-1),(zV-1))
v10 = V(1,(Numy-1),zV)
v11 = V(1,(Numy-1),(zV+1))
v0_1_1 = V(x,(Numy-1),(zV-1))
v0_10 = V(x,(Numy-1),zV)
v0_11 = V(x,(Numy-1),(zV+1))
v01_1 = V(x,(Numy-1),(zV-1))
v010 = V(x,(Numy-1),zV)
v011 = V(x,(Numy-1),(zV+1))
else
  !or 2-D?
    v1_1_1 = V(1,y,(zV-1))
v1_10 = V(1,y,zV)
v1_11 = V(1,y,(zV+1))
v1_11 = V(1,y,(zV-1))
!define derivatives
v1_10 = V(1,y,zV)
v1_11 = V(1,y,(zV+1))
v1_1_1 = V(1,y,(zV-1))
v1_10 = V(1,y,zV)
v1_11 = V(1,y,(zV+1))
v11_1 = V(1,y,(zV-1))
v110 = V(1,y,zV)
v111 = V(1,y,(zV+1))
v0_1_1 = V(x,y,(zV-1))
v0_10 = V(x,y,zV)
v0_11 = V(x,y,(zV-1))
v01_1 = V(x,y,(zV-1))
v010 = V(x,y,zV)
v011 = V(x,y,(zV+1))
end if
else            !or is x at Numx?
else                  !or is the x B.C. periodic?
if (D .eq. 3) then         !3-D?
else            !or is x at Numx?
if (D .eq. 3) then         !3-D?
v_1_1_1 = V((Numx-1),(Numy-1),(zV-1))
v_1_10 = V((Numx-1),(Numy-1),zV)  
v_1_11 = V((Numx-1),(Numy-1),(zV+1))

v_11_1 = V((Numx-1),(Numy-1),(zV-1))
v_110 = V((Numx-1),(Numy-1),zV)  
v_111 = V((Numx-1),(Numy-1),(zV+1))
v_11_1 = V(1,(Numy-1),(zV-1))
  v1_10 = V(1,(Numy-1),zV)  
v_111 = V(1,(Numy-1),(zV+1))
v0_1_1 = V(x,(Numy-1),(zV-1))
v0_10 = V(x,(Numy-1),zV)  
v0_11 = V(x,(Numy-1),(zV+1))
v01_1 = V(x,(Numy-1),(zV-1))
v010 = V(x,(Numy-1),zV)  
v011 = V(x,(Numy-1),(zV+1))

v_11_1 = V((Numx-1),y,(zV-1))
v_110 = V((Numx-1),y,zV)  
v_111 = V((Numx-1),y,(zV+1))

v_11_1 = V((Numx-1),y,(zV-1))
v_110 = V((Numx-1),y,zV)  
v_111 = V((Numx-1),y,(zV+1))
v1_1_1 = V(1,y,(zV-1))
  v1_10 = V(1,y,zV)  
v11_1 = V(1,y,(zV+1))
v110 = V(1,y,zV)  
v111 = V(1,y,(zV+1))
v0_1_1 = V(x,y,(zV-1))
v0_10 = V(x,y,zV)  
v0_11 = V(x,y,(zV+1))
v01_1 = V(x,y,(zV-1))
v010 = V(x,y,zV)  
v011 = V(x,y,(zV+1))

end if
end if
else
  !or 2-D?

v_1_1_1 = V((Numx-1),y,(zV-1))
v_1_10 = V((Numx-1),y,zV)  
v_11_1 = V((Numx-1),y,(zV+1))
v_110 = V((Numx-1),y,zV)  
v_111 = V((Numx-1),y,(zV+1))
v1_1_1 = V(1,y,(zV-1))
  v1_10 = V(1,y,zV)  
v11_1 = V(1,y,(zV+1))
v110 = V(1,y,zV)  
v111 = V(1,y,(zV+1))
v0_1_1 = V(x,y,(zV-1))
v0_10 = V(x,y,zV)  
v0_11 = V(x,y,(zV+1))
v01_1 = V(x,y,(zV-1))
v010 = V(x,y,zV)  
v011 = V(x,y,(zV+1))

end if
end if
else
  !or is the y B.C. periodic?
  if (xmir .EQ. 1) then
    !is the x B.C. mirror?
      if (x .EQ. 0) then
        !is x at 0?
          if (D .eq. 3) then
            !3-D?

v_1_1_1 = V(1,(Numy-1),(zV-1))
v_1_10 = V(1,(Numy-1),zV)  
v_1_11 = V(1,(Numy-1),(zV+1))

v_11_1 = V(1,1,(zV-1))
v_110 = V(1,1,zV)  
v_111 = V(1,1,(zV+1))
v1_1_1 = V(1,1,(zV-1))
  v1_10 = V(1,1,zV)  
v11_1 = V(1,1,(zV+1))
v110 = V(1,1,zV)  
v111 = V(1,1,(zV+1))
v0_1_1 = V(x,(Numy-1),(zV-1))
v0_10 = V(x,(Numy-1),zV)
v0_11 = V(x,(Numy-1),(zV+1))
v01_1 = V(x,1,(zV-1))
v010 = V(x,1,zV)
v011 = V(x,1,(zV+1))

else
  v_1_1_1 = V(1,y,(zV-1))
v_1_10 = V(1,y,zV)
v_1_11 = V(1,y,(zV+1))
  v_11_1 = V(1,y,(zV-1))
  v_110 = V(1,y,zV)
  v_111 = V(1,y,(zV+1))
  v1_1_1 = V(1,y,(zV-1))
  v1_10 = V(1,y,zV)
  v1_11 = V(1,y,(zV+1))
  v0_1_1 = V(x,y,(zV-1))
  v0_10 = V(x,y,zV)
  v0_11 = V(x,y,(zV+1))
end if

else
  if (D .eq. 3) then
    !3-D?
    v_1_1_1 = V((Numx-1),(Numy-1),(zV-1))
    v_1_10 = V((Numx-1),(Numy-1),zV)
    v_1_11 = V((Numx-1),(Numy-1),(zV+1))
    v_11_1 = V((Numx-1),1,(zV-1))
    v_110 = V((Numx-1),1,zV)
    v_111 = V((Numx-1),1,(zV+1))
    v1_1_1 = V((Numx-1),y,(zV-1))
    v1_10 = V((Numx-1),y,zV)
    v1_11 = V((Numx-1),y,(zV+1))
  else
    !or is x at Numx?
    v_1_1_1 = V((Numx-1),(Numy-1),(zV-1))
    v_1_10 = V((Numx-1),(Numy-1),zV)
    v_1_11 = V((Numx-1),(Numy-1),(zV+1))
    v_11_1 = V((Numx-1),1,(zV-1))
    v_110 = V((Numx-1),1,zV)
    v_111 = V((Numx-1),1,(zV+1))
    v1_1_1 = V((Numx-1),y,(zV-1))
    v1_10 = V((Numx-1),y,zV)
    v1_11 = V((Numx-1),y,(zV+1))
  end if

else
  !or 2-D?
  v_1_1_1 = V((Numx-1),y,(zV-1))
  v_1_10 = V((Numx-1),y,zV)
  v_1_11 = V((Numx-1),y,(zV+1))
  v_11_1 = V((Numx-1),y,(zV-1))
  v_110 = V((Numx-1),y,zV)
  v_111 = V((Numx-1),y,(zV+1))
  v1_1_1 = V((Numx-1),y,(zV-1))
  v1_10 = V((Numx-1),y,zV)
  v1_11 = V((Numx-1),y,(zV+1))
v11_1 = V((Numx-1),y,(zV-1))
v110 = V((Numx-1),y,zV)
v111 = V((Numx-1),y,(zV+1))
v0_1_1 = V(x,y,(zV-1))
v0_10 = V(x,y,zV)
v0_11 = V(x,y,(zV+1))
end if
end if
else
    !or is the x B.C. periodic?
    if (D.eq.3) then
        !3-D?
        v_1_1_1 = V((Numx-1),(Numy-1),(zV-1))
v_1_10 = V((Numx-1),(Numy-1),zV)
v_1_11 = V((Numx-1),(Numy-1),(zV+1)) !define derivatives
        v_11_1 = V((Numx-1),1,(zV-1))
v_110 = V((Numx-1),1,zV)
v_111 = V((Numx-1),1,(zV+1))
v1_1_1 = V(1,(Numy-1),(zV-1))
v1_10 = V(1,(Numy-1),zV)
v1_11 = V(1,(Numy-1),(zV+1))
v11_1 = V(1,1,(zV-1))
v110 = V(1,1,zV)
v111 = V(1,1,(zV+1))
v0_1_1 = V(x,(Numy-1),(zV-1))
v0_10 = V(x,(Numy-1),zV)
v0_11 = V(x,(Numy-1),(zV+1))
v01_1 = V(x,1,(zV-1))
v010 = V(x,1,zV)
v011 = V(x,1,(zV+1))
    else
        !or 2-D?
        v_1_1_1 = V((Numx-1),y,(zV-1))
v_1_10 = V((Numx-1),y,zV)
v_1_11 = V((Numx-1),y,(zV+1))
v_11_1 = V((Numx-1),y,(zV-1)) !define derivatives
        v_110 = V((Numx-1),y,zV)
v_111 = V((Numx-1),y,(zV+1))
v1_1_1 = V(1,y,(zV-1))
v1_10 = V(1,y,zV)
v1_11 = V(1,y,(zV+1))
v11_1 = V(1,y,(zV-1))
v110 = V(1,y,zV)
v111 = V(1,y,(zV+1))
v0_1_1 = V(x,y,(zV-1))
v0_10 = V(x,y,zV)
v0_11 = V(x,y,(zV+1))
v01_1 = V(x,y,(zV-1))
v010 = V(x,y,zV)
v011 = V(x,y,(zV+1))
end if
end if
else
    !or is y not at a boundary?
    if (D.eq.3) then
        !3-D?
        v_1_1_1 = V((Numx-1),(y-1),(zV-1))
    end if
v_1_10 = V((Numx-1),(y-1),zV)
v_1_11 = V((Numx-1),(y-1),(zV+1))
!define derivatives
v_11_1 = V((Numx-1),(y+1),(zV-1))
v_110 = V((Numx-1),(y+1),zV)
v_111 = V((Numx-1),(y+1),(zV+1))

else
    !or 2-D?
    v_1_1_1 = V((Numx-1),y,(zV-1))
v_1_1_0 = V((Numx-1),y,zV)
v_1_1_1 = V((Numx-1),y,(zV+1))
    !define derivatives
    v_1_0_1 = V((x-1),y,(zV-1))
v_1_0_0 = V((x-1),y,zV)
v_1_0_1 = V((x-1),y,(zV+1))
v_1_1_1 = V((x-1),y,(zV-1))
v_1_1_0 = V((x-1),y,zV)
v_1_1_1 = V((x-1),y,(zV+1))

end if
v011 = V(x,1,(zV+1))
v1_1_1 = V((x+1),1,(zV-1))
v1_1_0 = V((x+1),1,zV)
v1_1_1 = V((x+1),1,(zV+1))
v10_1 = V((x+1),y,(zV-1))
v100 = V((x+1),y,zV)
v101 = V((x+1),y,(zV+1))
v11_1 = V((x+1),1,(zV-1))
v110 = V((x+1),1,zV)
v111 = V((x+1),1,(zV+1))
else

v_1_1_1 = V((x-1),y,(zV-1))
v_1_1_0 = V((x-1),y,zV)
v_1_1_1 = V((x-1),y,(zV+1))
v_10_1 = V((x-1),y,(zV-1))
v_100 = V((x-1),y,zV)
v_101 = V((x-1),y,(zV+1))
v_11_1 = V((x-1),y,(zV-1))
v_110 = V((x-1),y,zV)
v_111 = V((x-1),y,(zV+1))
end if

else

! or 2-D?

v_1_1_1 = V((x-1),y,(zV-1))
v_1_1_0 = V((x-1),y,zV)
v_1_1_1 = V((x-1),y,(zV+1))
v_10_1 = V((x-1),y,(zV-1))
v_100 = V((x-1),y,zV)
v_101 = V((x-1),y,(zV+1))
v_11_1 = V((x-1),y,(zV-1))
v_110 = V((x-1),y,zV)
v_111 = V((x-1),y,(zV+1))

else

! or is y at Numy?

v_1_1_1 = V((x-1),(Numy-1),(zV-1))
v_1_1_0 = V((x-1),(Numy-1),zV)
v_1_1_1 = V((x-1),(Numy-1),(zV+1))
v_10_1 = V((x-1),(Numy-1),(zV-1))
v_100 = V((x-1),(Numy-1),zV)
v_101 = V((x-1),(Numy-1),(zV+1))
v_11_1 = V((x-1),(Numy-1),(zV-1))
v_110 = V((x-1),(Numy-1),zV)
v_111 = V((x-1),(Numy-1),(zV+1))
end if

else

! 3-D?

v_1_1_1 = V((x),(Numy-1),(zV-1))
v_1_1_0 = V((x),(Numy-1),zV)
v_1_1_1 = V((x),(Numy-1),(zV+1))
v_10_1 = V((x),(Numy-1),(zV-1))
v_100 = V((x),(Numy-1),zV)
v_101 = V((x),(Numy-1),(zV+1))
v_11_1 = V((x),(Numy-1),(zV-1))
v_110 = V((x),(Numy-1),zV)
v_111 = V((x),(Numy-1),(zV+1))

end if

else
v_{10,1} = V((x+1),y,(zV-1))
v_{100} = V(x+1,y,zV)
v_{101} = V((x+1),y,(zV+1))
v_{11,1} = V((x+1),(Numy-1),(zV-1))
v_{110} = V(x+1,(Numy-1),zV)
v_{111} = V((x+1),(Numy-1),(zV+1))

\text{else} \quad \text{!or 2-D?}
\begin{align*}
v_{1,1,1} &= V((x-1),y,(zV-1)) \\
v_{1,10} &= V((x-1),y,zV) \\
v_{1,11} &= V((x-1),y,(zV+1)) \\
v_{1,0,1} &= V((x-1),y,(zV-1)) \\
v_{1,00} &= V((x-1),y,zV) \\
v_{1,01} &= V((x-1),y,(zV+1)) \\
v_{1,1,1} &= V((x-1),1,(zV-1)) \\
v_{1,10} &= V((x-1),1,zV) \\
v_{1,11} &= V((x-1),1,(zV+1)) \\
v_{0,1,1} &= V(x,(Numy-1),(zV-1)) \\
v_{0,10} &= V(x,(Numy-1),zV) \\
v_{0,11} &= V(x,(Numy-1),(zV+1)) \\
v_{0,0,1} &= V(x,1,(zV-1)) \\
v_{0,00} &= V(x,1,zV) \\
v_{0,01} &= V(x,1,(zV+1)) \\
v_{1,1,1} &= V((x+1),(Numy-1),(zV-1)) \\
v_{1,10} &= V((x+1),(Numy-1),zV) \\
v_{1,11} &= V((x+1),(Numy-1),(zV+1)) \\
v_{1,0,1} &= V((x+1),y,(zV-1)) \\
v_{1,00} &= V((x+1),y,zV)
\end{align*}

\text{end if} \quad \text{!or is the}
\begin{align*}
\text{y B.C. periodic?} \\
\text{if (D. eq. 3) then} \quad \text{!3-D?}
\begin{align*}
v_{1,1,1} &= V((x-1),(Numy-1),(zV-1)) \\
v_{1,10} &= V((x-1),(Numy-1),zV) \\
v_{1,11} &= V((x-1),(Numy-1),(zV+1)) \\
v_{1,0,1} &= V((x-1),1,(zV-1)) \\
v_{1,00} &= V((x-1),1,zV) \\
v_{1,01} &= V((x-1),1,(zV+1)) \\
v_{0,1,1} &= V(x,(Numy-1),(zV-1)) \\
v_{0,10} &= V(x,(Numy-1),zV) \\
v_{0,11} &= V(x,(Numy-1),(zV+1)) \\
v_{0,0,1} &= V(x,1,(zV-1)) \\
v_{0,00} &= V(x,1,zV) \\
v_{0,01} &= V(x,1,(zV+1)) \\
v_{1,1,1} &= V((x+1),(Numy-1),(zV-1)) \\
v_{1,10} &= V((x+1),(Numy-1),zV) \\
v_{1,11} &= V((x+1),(Numy-1),(zV+1)) \\
v_{1,0,1} &= V((x+1),y,(zV-1)) \\
v_{1,00} &= V((x+1),y,zV)
\end{align*}
\text{end if}

end if
\[ v_{101} = V((x+1),y,(zV+1)) \]
\[ v_{11_1} = V((x+1),1,(zV-1)) \]
\[ v_{110} = V((x+1),1,zV) \]
\[ v_{111} = V((x+1),1,(zV+1)) \]
else
\[ v_{1_1_1} = V((x-1),y,(zV-1)) \]
\[ v_{1_10} = V((x-1),y,zV) \]
\[ v_{1_11} = V((x-1),y,(zV+1)) \]
\[ v_{10_1} = V((x-1),y,(zV-1)) \]
\[ v_{100} = V((x-1),y,zV) \]
\[ v_{101} = V((x-1),y,(zV+1)) \]
\[ v_{11_1} = V((x-1),y,(zV-1)) \]
\[ v_{110} = V((x-1),y,zV) \]
\[ v_{111} = V((x-1),y,(zV+1)) \]
\[ v_{0_1_1} = V(x,y,(zV-1)) \]
\[ v_{0_10} = V(x,y,zV) \]
\[ v_{0_11} = V(x,y,(zV+1)) \]
\[ v_{01_1} = V(x,y,(zV-1)) \]
\[ v_{010} = V(x,y,zV) \]
else
\[ v_{1_1_1} = V((x-1),y,(zV-1)) \]
\[ v_{1_10} = V((x-1),y,zV) \]
\[ v_{1_11} = V((x-1),y,(zV+1)) \]
\[ v_{10_1} = V((x-1),y,(zV-1)) \]
\[ v_{100} = V((x-1),y,zV) \]
\[ v_{101} = V((x-1),y,(zV+1)) \]
\[ v_{11_1} = V((x-1),y,(zV-1)) \]
\[ v_{110} = V((x-1),y,zV) \]
\[ v_{111} = V((x-1),y,(zV+1)) \]
\[ v_{0_1_1} = V(x,y,(zV-1)) \]
\[ v_{0_10} = V(x,y,zV) \]
\[ v_{0_11} = V(x,y,(zV+1)) \]
\[ v_{01_1} = V(x,y,(zV-1)) \]
\[ v_{010} = V(x,y,zV) \]
\[ v_{011} = V(x,y,(zV+1)) \]
\[ v_{1_1_1} = V((x+1),y,(zV-1)) \]
\[ v_{1_10} = V((x+1),y,zV) \]
\[ v_{1_11} = V((x+1),y,(zV+1)) \]
\[ v_{10_1} = V((x+1),y,(zV-1)) \]
\[ v_{100} = V((x+1),y,zV) \]
\[ v_{101} = V((x+1),y,(zV+1)) \]
\[ v_{11_1} = V((x+1),y,(zV-1)) \]
\[ v_{110} = V((x+1),y,zV) \]
\[ v_{111} = V((x+1),y,(zV+1)) \]
\[ v_{0_1_1} = V(x,y,(zV-1)) \]
\[ v_{0_10} = V(x,y,zV) \]
\[ v_{0_11} = V(x,y,(zV+1)) \]
\[ v_{01_1} = V(x,y,(zV-1)) \]
\[ v_{010} = V(x,y,zV) \]
\[ v_{011} = V(x,y,(zV+1)) \]
\[ v_{1_1_1} = V((x+1),y,(zV-1)) \]
\[ v_{1_10} = V((x+1),y,zV) \]
\[ v_{1_11} = V((x+1),y,(zV+1)) \]
\[ v_{10_1} = V((x+1),y,(zV-1)) \]
\[ v_{100} = V((x+1),y,zV) \]
\[ v_{101} = V((x+1),y,(zV+1)) \]
\[ v_{11_1} = V((x+1),y,(zV-1)) \]
\[ v_{110} = V((x+1),y,zV) \]
\[ v_{111} = V((x+1),y,(zV+1)) \]
end if
end if
else
\[ v_{1_1_1} = V((x-1),y,(zV-1)) \]
\[ v_{1_10} = V((x-1),y,zV) \]
\[ v_{1_11} = V((x-1),y,(zV+1)) \]
\[ v_{10_1} = V((x-1),y,(zV-1)) \]
\[ v_{100} = V((x-1),y,zV) \]
\[ v_{101} = V((x-1),y,(zV+1)) \]
\[ v_{11_1} = V((x-1),y,(zV-1)) \]
\[ v_{110} = V((x-1),y,zV) \]
\[ v_{111} = V((x-1),y,(zV+1)) \]
end if
else
\[ v_{1_1_1} = V((x-1),y,(zV-1)) \]
\[ v_{1_10} = V((x-1),y,zV) \]
\[ v_{1_11} = V((x-1),y,(zV+1)) \]
\[ v_{10_1} = V((x-1),y,(zV-1)) \]
\[ v_{100} = V((x-1),y,zV) \]
\[ v_{101} = V((x-1),y,(zV+1)) \]
\[ v_{11_1} = V((x-1),y,(zV-1)) \]
\[ v_{110} = V((x-1),y,zV) \]
\[ v_{111} = V((x-1),y,(zV+1)) \]
else
\[ v_{1_1_1} = V((x-1),y,(zV-1)) \]
\[ v_{1_10} = V((x-1),y,zV) \]
\[ v_{1_11} = V((x-1),y,(zV+1)) \]
\[ v_{10_1} = V((x-1),y,(zV-1)) \]
\[ v_{100} = V((x-1),y,zV) \]
\[ v_{101} = V((x-1),y,(zV+1)) \]
\[ v_{11_1} = V((x-1),y,(zV-1)) \]
\[ v_{110} = V((x-1),y,zV) \]
\[ v_{111} = V((x-1),y,(zV+1)) \]
end if
v110 = V((x+1),(y+1),zV)
v111 = V((x+1),(y+1),(zV+1))
else
    v_1_1_1 = V((x-1),y,(zV-1))
v_1_10 = V((x-1),y,zV)
v_1_11 = V((x-1),y,(zV+1))
v_10_1 = V((x-1),y,(zV-1))
v_100 = V((x-1),y,zV)
v_101 = V((x-1),y,(zV+1))
v_11_1 = V((x-1),y,(zV-1))
v_110 = V((x-1),y,zV)
v_111 = V((x-1),y,(zV+1))
end if
end if
v001 = V(x,y,(zV+1))
v00_1 = V(x,y,(zV-1))
v000 = V(x,y,zV)
c
*** form the dielectric tensor ***
c
if (xmir .eq. 1) then
    if ((x .eq. 0) .or. (x .eq. Numx)) then
        call calceps(mirrepst,e0,ep,-nx(x,y,z),ny(x,y,z),
        nz(x,y,z),x,y,z)
    end if
end if
if (ymir .eq. 1) then
    if ((y .eq. 0) .or. (y .eq. Numx)) then
        call calceps(mirrepst,e0,em,-nx(x,y,z),-ny(x,y,z),
        nz(x,y,z),x,y,z)
    end if
end if

*** define dielectric derivatives ***
c
if ((x .eq. 0) .or. (x .eq. Numx)) then
    if (xmir .EQ. 1) then
        e11x = (eps((1,1),(x,y,z))-mirrepst((1,1),(x,y,z)))/'(dx)
        e12x = (eps((1,2),(x,y,z))-mirrepst((1,2),(x,y,z)))/'(dx)
        e13x = (eps((1,3),(x,y,z))-mirrepst((1,3),(x,y,z)))/'(dx)
    end if
end if
else !or is x at Numx?
e11x = (mirrepst(1,1,x,y,z)-epst(1,1,x,y,z))/(dx)
e12x = (mirrepst(1,2,x,y,z)-epst(1,2,x,y,z))/(dx)
e13x = (mirrepst(1,3,x,y,z)-epst(1,3,x,y,z))/(dx)
end if
else !or is the x B.C. periodic?
e11x = (epst(1,1,1,y,z)-epst(1,1,(Numx-1),y,z))/(2.d0*dx)
e12x = (epst(1,2,1,y,z)-epst(1,2,(Numx-1),y,z))/(2.d0*dx)
e13x = (epst(1,3,1,y,z)-epst(1,3,(Numx-1),y,z))/(2.d0*dx)
end if
else !x is not at a boundary
else !x is not at a boundary

e11x = (epst(1,1,(x+1),y,z)-epst(1,1,(x-1),y,z))/(2.d0*dx)
e12x = (epst(1,2,(x+1),y,z)-epst(1,2,(x-1),y,z))/(2.d0*dx)
e13x = (epst(1,3,(x+1),y,z)-epst(1,3,(x-1),y,z))/(2.d0*dx)
end if
if (D. eq. 2) then !2-D?
e21y = 0.d0
else !or 3-D?
e21y = (epst(2,1,x,y,z)-mirrepst(2,1,x,y,z))/(dy)
e22y = (epst(2,2,x,y,z)-mirrepst(2,2,x,y,z))/(dy) !form deriv's
else !or is the y B.C. mirror?
e21y = (epst(2,1,x,y,z)-mirrepst(2,1,x,y,z))/(dy)
e22y = (epst(2,2,x,y,z)-mirrepst(2,2,x,y,z))/(dy) !form deriv's
else !or is the y B.C. periodic
if ((y .eq. 0) .or. (y .eq. Numy)) then !is y at a boundary?
e21y = (epst(2,1,x,1,z)-epst(2,1,x,(Numy-1),z))/(2.d0*dy)
e22y = (epst(2,2,x,1,z)-epst(2,2,x,(Numy-1),z))/(2.d0*dy) !form deriv's
else !or is y at Numy?
e21y = (mirrepst(2,1,x,y,z)-epst(2,1,x,y,z))/(dy)
e22y = (mirrepst(2,2,x,y,z)-epst(2,2,x,y,z))/(dy) !form deriv's
end if
else !y is not at a boundary
else !y is not at a boundary

e21y = (epst(2,1,x,y,z)-mirrepst(2,1,x,y,z))/(dy)
e22y = (epst(2,2,x,y,z)-mirrepst(2,2,x,y,z))/(dy) !form deriv's
else !y is not at a boundary

e31z = (epst(3,1,x,y,(z+1))-epst(3,1,x,y,(z-1)))/(2.d0*dz)
e32z = (epst(3,2,x,y,(z+1))-epst(3,2,x,y,(z-1)))/(2.d0*dz) !form z deriv's
else !y is not at a boundary

e31z = (mirrepst(3,1,x,y,z)-epst(3,1,x,y,z))/(dz)
e32z = (mirrepst(3,2,x,y,z)-epst(3,2,x,y,z))/(dz) !form z deriv's
end if
end if

*** dielectric tensor renamed in terms for Maple ***
e11 = epst(1,1,x,y,z)
e12 = epst(1,2,x,y,z)
e13 = epst(1,3,x,y,z)
$e_{21} = \text{epst}(2,1,x,y,z)$

$e_{22} = \text{epst}(2,2,x,y,z)$

$e_{23} = \text{epst}(2,3,x,y,z)$

$e_{31} = \text{epst}(3,1,x,y,z)$

$e_{32} = \text{epst}(3,2,x,y,z)$

$e_{33} = \text{epst}(3,3,x,y,z)$

c

*** code output by Maple V5 R5 ***

*** (See Maple sheet "Voltage.mws") ***

c

$tt_1 = dx**2$

$tt_2 = c32z*tt_1$

$tt_3 = dz**2$

$tt_4 = tr3z*dy$

$tt_5 = tr4z*v0_10$

$tt_7 = c32z*tt_1$

$tt_8 = dz*dy$

$tt_9 = tr8z*vo11$

$tt_{11} = tr8z*v0_1_1$

$tt_{13} = e13z*tt_1$

$tt_{14} = dy**2$

$tt_{15} = dz*tt_{14}$

$tt_{16} = tr15z*v001$

$tt_{18} = tr15z*v00_1$

$tt_{20} = e13z*dx$

$tt_{21} = tr15z*v101$

$tt_{23} = tr15z*v_{10_1}$

$tt_{25} = e31z*dx$

$tt_{26} = tr3z*tt_{14}$

$tt_{27} = tr26z*v_{100}$

$tt_{29} = e23z*tt_1$

$tt_{30} = tr8z*v01_1$

$tt_{32} = tr26z*v100$

$tt_{35} = e23y*tt_1$

$tt_{37} = -2.D0*tt2*tt5+tt7*tt9+tt7*tt11+2.D0*tt13*tt16-2.D0*tt13$

$tt_{39} = e33z*tt_1$

$tt_{42} = e22z*tt_1$

$tt_{47} = e22y*tt_1$

$tt_{49} = e33z*tt_1$

$tt_{52} = tr8z*v0_1_1$

$tt_{55} = e31z*dx$

$tt_{56} = tr15z*v_{101}$

$tt_{58} = tr15z*v_{10_1}$

$tt_{60} = e11z*tt_3$

$tt_{63} = tt29z*tt9+4.D0*tt39*tt14*v00_1+4.D0*tt42z*tt3*v0_10+4.D0*$

$tt_{69} = e11x*dx$

$tt_{71} = e21z*dx$

$tt_{72} = tr4z*v_{110}$

$tt_{74} = tr4z*v_{10_1}$

$tt_{77} = tr4z*v_{110}$

$tt_{79} = tr4z*v_{1_1}$

$tt_{82} = tr4z*v010$
tt85 = tt55*t21+tt55*t23+4.0D0*tt60*tt14*v100-2.0D0*tt69*tt27-
#tt71*tt72-tt74+2.0D0*tt69*cos(ttt71*tt79+tt71*tt79-tt20)*tt54+
#2.0D0*tt47*tt82+2.0D0*tt2*tt82

\[ tt86 = e12^*dx \]
\[ tt89 = e12^*x*tt1 \]
\[ tt98 = e21^*y*tt3 \]

Vnew = (tt37+tt63+tt85+tt102)/(tt42*tt3+tt60*tt14+tt39*tt14)/8.0D0

end Subroutine VoltageLC

Subroutine Voltageglass(V,dx,dy,dz,x,y,z, Numx,Numy,Numz,Vnew,xmir,ymir,D)

*** Declare Variables ***
implicit real*8 (r-w)
integer x,y,z,Numx,Numy,Numz,xmir,ymir
integer sizex,sizey,sizez,D
parameter (sizex =500,sizey = 1,sizez =100)
real*8 V(0:sizex,0:sizey,0:(3*sizez)),dx,dy,dz
real*8 v001,v010,v100,Vnew
real*8 v00_1,v0_10,v_100

*** This subroutine is very similar to VoltageLC, but it is in the glass, which makes the problem easier. ***

*** Voltages at neighboring gridpoints (needed for derivatives of V) ***
the voltage at a point is given the name "vijk" here, if i,j or k is 1, we are referring to a point with a lattice index 1 greater than the current gridpoint. If i,j or k is 0, that means we are referring to a point in the same plane as the gridpoint, and if i,j, or k is -1 (_1), we are referring to a point with a lattice index 1 less than the current point.

*** Thus, if we are at gridpoint (x,y,z) = (137,44,34) then v_11 is the voltage at (138,43,35) and v_10_1 is the voltage at (136,44,33).

*** This parts gets complicated with all the different possibilities have to calculate the derivative differently if at a boundary, then have to determine which kind of boundary condition is used. Finally, if 2-D only need derivatives in x and z dimensions. ***

if (x.EQ.0 .or. x .EQ. Numx) then
  if (xmir.EQ.1) then
    v_100 = V(1,y,z)
    v100 = V(1,y,z)
    else
      v_100 = V((Numx-1),y,z)
v100 = V((Numx-1),y,z)
end if

else
v_100 = V((Numx-1),y,z)
v100 = V(1,y,z)
end if

if (D .eq. 3) then
if (y .EQ. 0 .or. y .eq. Numy) then
if (ymir .EQ. 1) then
if (y .EQ. 0) then
v0_10 = V(x,1,z)
v010 = V(x,1,z)
else
v0_10 = V(x,(Numy-1),z)
v010 = V(x,(Numy-1),z)
end if
else
v0_10 = V(x,(Numy-1),z)
v010 = V(x,1,z)
end if
else
v0_10 = V(x,y,z)
v010 = V(x,y,z)
end if
else if (y .EQ. 0 .or. y .eq. Numy) then
if (D .eq. 3) then
if (ymir .EQ. 1) then
if (y .EQ. 0) then
v_100 = V((x-1),y,z)
v0_10 = V(x,1,z)
v010 = V(x,1,z)
v100 = V((x+1),y,z)
else
v_100 = V((x-1),y,z)
v0_10 = V(x,(Numy-1),z)
v010 = V(x,(Numy-1),z)
v100 = V((x+1),y,z)
end if
else
v_100 = V((x-1),y,z)
v0_10 = V(x,(Numy-1),z)
v010 = V(x,(Numy-1),z)
v100 = V((x+1),y,z)
end if
else
v_100 = V((x-1),y,z)
v0_10 = V(x,y,z)
v010 = V(x,y,z)
v100 = V((x+1),y,z)
end if
else
if (D .eq. 3) then
v_100 = V((x-1),y,z)
v0_10 = V(x,(y-1),z)
v010 = V(x,(y+1),z)
v100 = V((x+1),y,z)
else
  v_100 = V((x-1),y,z)
v0_10 = V(x,y,z)
v010 = V(x,y,z)
v100 = V((x+1),y,z)
end if
end if
v001 = V(x,y,(z+1))
v00_1 = V(x,y,(z-1))

*** code output by Maple V5 R5 ***
*** (See Maple sheet "Vglass.mws") ***
t1 = dy**2
t2 = dz**2
t3 = t1*t2
t6 = dx**2
t7 = t6*t2
t10 = t6*t1
Vnew = (t3*v100+t3*v_100+t7*v010+t7*v0_10+t10*v001+t10*v00_1)/
  #(t3+t7+t10)/2.D0

return
end Subroutine Voltageglass

Subroutine Voltageinterftop(V,dx,dy,dz,x,y,z,Vnew,epst,#epglass,Numx,Numy,Numz,xmir,ymir,D)

*** Declare Variables ***
implicit real*8 (r-w)
integer x,y,z,Numx,Numy,Numz,zV,xmir,ymir
integer sizex,sizey,sizez,D
parameter (sizex =500,sizey =1,sizez =100)
real*8 V(0:sizex,0:sizey,0:(3*sizez)),dx,dy,dz
real*8 epst(1:3,1:3,0:sizex,0:sizey,0:sizez)
real*8 v001,v010,v100,Vnew
real*8 e31,e32,e33,epglass

zV = z+Numz

*** This subroutine is similar to VoltageLC, except that now the
*** boundary condition (the normal component of the electric displace-
*** ment is continuous) means that there are different grid spacings.
***
*** The grid spacing in the L.C. layer is dz, the spacing in the glass
*** is 4*dz.
***
*** Voltages at neighboring gridpoints (needed for derivatives of V)
***
*** the voltage at a point is given the name "vijk" here, if i,j or
*** k is 1, we are referring to a point with a lattice index 1
***
*** greater than the current gridpoint. If i,j or k is 0, that means
***
*** we are referring to a point in the same plane as the gridpoint,
***
*** and if i,j, or k is -1 (_1), we are referring to a point with a
***
*** This subroutine is similar to VoltageLC, except that now the
*** boundary condition (the normal component of the electric displace-
*** ment is continuous) means that there are different grid spacings.
***
*** The grid spacing in the L.C. layer is dz, the spacing in the glass
 *** is 4*dz.
 ***
 *** Voltages at neighboring gridpoints (needed for derivatives of V)
 ***
 *** the voltage at a point is given the name "vijk" here, if i,j or
 *** k is 1, we are referring to a point with a lattice index 1
 ***
 *** greater than the current gridpoint. If i,j or k is 0, that means
 ***
 *** we are referring to a point in the same plane as the gridpoint,
 ***
 *** and if i,j, or k is -1 (_1), we are referring to a point with a
 ***
c *** lattice index 1 less than the current point.
***

c *** Thus, if we are at gridpoint (x,y,z) = (137, 44, 34) then
*** v1_11 is the voltage at (138,43,35) and
***
*** v_10_1 is the voltage at (136,44,33).
***

c *** This parts gets complicated with all the different possibilities
***
*** have to calculate the dereivative differently if at a boundary,
***
*** then have to determine which kind of boundary condition is used.
***
*** Finally, if 2-D only need derivatives in x and z dimensions.
***

c if (x .EQ. 0 .or. x .eq. Numx) then
  if (xmir .EQ. 1) then
    if (x .EQ. 0) then
      v_100 = V(1,y,zV)
      v100 = V(1,y,zV)
    else
      v_100 = V((Numx-1),y,zV)
      v100 = V((Numx-1),y,zV)
    end if
  else
    v_100 = V((Numx-1),y,zV)
    v100 = V(1,y,zV)
  end if
if (y .EQ. 0 .or. y .eq. Numy) then
  if (ymir .EQ. 1) then
    if (y .EQ. 0) then
      v0_10 = V(x,1,zV)
      v010 = V(x,1,zV)
    else
      v0_10 = V(x,(Numy-1),zV)
      v010 = V(x,(Numy-1),zV)
    end if
  else
    v0_10 = V(x,(y-1),zV)
    v010 = V(x,(y+1),zV)
  end if
else
  v0_10 = V(x,(y-1),zV)
  v010 = V(x,(y+1),zV)
end if
else if (y .EQ. 0 .or. y .eq. Numy) then
  if (D .eq. 3) then
    if (ymir .EQ. 1) then
      if (y .EQ. 0) then
        v_100 = V((x-1),y,zV)
      end if
    else
      v_100 = V((x,(Numy-1),zV)
    end if
  else
    v_100 = V(x,(y-1),zV)
    v0_10 = V(x,1,zV)
  end if
else
  v_100 = V((x-1),y,zV)
  v0_10 = V(x,1,zV)
end if
v100 = V((x+1),y,zV)
else
v_100 = V((x-1),y,zV)
v0_10 = V(x,(Numy-1),zV)
v010 = V(x,(Numy-1),zV)
v100 = V((x+1),y,zV)
end if
else
v_100 = V((x-1),y,zV)
v0_10 = V(x,(Numy-1),zV)
v010 = V(x,(Numy-1),zV)
v100 = V((x+1),y,zV)
end if
else
if (D. eq. 3) then
v_100 = V((x-1),y,zV)
v0_10 = V(x,(y-1),zV)
v010 = V(x,(y+1),zV)
v100 = V((x+1),y,zV)
else
v_100 = V((x-1),y,zV)
v0_10 = V(x,y,zV)
v010 = V(x,y,zV)
v100 = V((x+1),y,zV)
end if
end if
v001 = V(x,y,(zV+1))
v00_1 = V(x,y,(zV-1))
c  *** dielectric tensor renamed in terms for Maple ***
e31 = epst(3,1,x,y,z)
e32 = epst(3,2,x,y,z)
e33 = epst(3,3,x,y,z)
c  *** code output by Maple ***
c  *** (See Maple sheet "Vinterflop.mws") ***  t1 = e31*dy
t2 = dz*(4*dz)
t7 = e32*dx
t13 = dx*dy
Vnew = (-t1*t2*v100+t1*t2*v_100+t7*t2*v010+t7*t2*v0_10+ #2.D0*e33*v00_1*t13*(4*dz)+2.D0*epglass*v001*t13*dz)/2.D0/##dx/dy/(e33*(4*dz)+epglass*dz)/2.D0

return
end Subroutine Voltageinterflop
c Subroutine Voltageinterfbot(V,dx,dy,dz,x,y,z,Vnew,epst, #epglass,Numx,Numy,Numz,xmir,ymir,D)
c  *** Declare Variables ***
implicit real*8 (r-w)
integer x,y,z,Numx,Numy,Numz,zV,xmir,ymir
integer sizex,sizey,sizez,D
parameter (sizex =500,sizey = 1,sizez =100)
real*8 V(0:sizex,0:sizey,0:(3*sizez)),dx,dy,dz
real*8 epst(1:3,1:3,0:sizex,0:sizey,0:sizez)
real*8 v001,v010,v100,Vnew
real*8 v00_1,v0_10,v_100
real*8 e31,e32,e33,epglass

c
zV = z+Numz

c
*** This subroutine is similar to VoltageLC, except that now the  ***
c
*** boundary condition (the normal component of the electric displace-***
c
*** ment is continuous) means that there are different grid spacings.***
c
*** The grid spacing in the L.C. layer is dz, the spacing in the glass***
c
*** is 4*dz.  ***
***
c
*** Voltages at neighboring gridpoints (needed for derivatives of V) ***
c
*** the voltage at a point is given the name "vijk" here, if i,j or ***
c
*** k is 1, we are referring to a point with a lattice index 1 ***
c
*** greater than the current gridpoint. If i,j or k is 0, that means***
c
*** we are referring to a point in the same plane as the gridpoint, ***
c
*** and if i,j, or k is -1 (_1), we are referring to a point with a ***
c
*** lattice index 1 less than the current point. ***
***
c
*** Thus, if we are at gridpoint (x,y,z) = (137, 44, 34) then ***
c
*** v1_11 is the voltage at (138,43,35) and ***
c
*** v_10_1 is the voltage at (136,44,33). ***
***
c
*** This parts gets complicated with all the different possiblities ***
c
*** have to calculate the derervative differently if at a boundary, ***
c
*** then have to determine which kind of boundary condition is used. ***
c
*** Finally, if 2-D only need derivatives in x and z dimensions. ***

if (x.EQ. 0 .or. x .eq. Numx) then
  if (xmir .EQ. 1) then
    v_100 = V(1,y,zV)
  else
    v_100 = V((Numx-1),y,zV)
  end if
else
  v_100 = V((Numx-1),y,zV)
end if

if (y .EQ. 0 .or. y .eq. Numy) then
  if (ymir .EQ. 1) then
    v_100 = V(1,y,zV)
  else
    v_100 = V((Numy-1),y,zV)
  end if
else
  v_100 = V((Numy-1),y,zV)
end if

if (D. eq. 3) then
  if (y .EQ. 0 .or. y .eq. Numy) then
    if (ymir .EQ. 1) then
      v_100 = V(1,y,zV)
    else
      v_100 = V((Numy-1),y,zV)
    end if
  else
    if (y .EQ. 0 .or. y .eq. Numy) then
      if (ymir .EQ. 1) then
        v_100 = V(1,y,zV)
      else
        v_100 = V((Numy-1),y,zV)
      end if
    else
      v_100 = V((Numy-1),y,zV)
```plaintext
v0_10 = V(x,1,zV)
v010 = V(x,1,zV)
else
v0_10 = V(x,(Numy-1),zV)
v010 = V(x,(Numy-1),zV)
end if
else
v0_10 = V(x,(Numy-1),zV)
v010 = V(x,1,zV)
end if
else
v0_10 = V(x,(y-1),zV)
v010 = V(x,(y+1),zV)
end if
else
v0_10 = V(x,(y-1),zV)
v010 = V(x,(y+1),zV)
else if (y .EQ. 0 .or. y .eq. Numy) then
if (D .eq. 3) then
if (ymir .EQ. 1) then
if (y .EQ. 0) then
v_100 = V((x-1),y,zV)
v0_10 = V(x,1,zV)
v010 = V(x,1,zV)
v100 = V((x+1),y,zV)
else
v_100 = V((x-1),y,zV)
v0_10 = V(x,(Numy-1),zV)
v010 = V(x,(Numy-1),zV)
v100 = V((x+1),y,zV)
end if
else
v_100 = V((x-1),y,zV)
v0_10 = V(x,(y-1),zV)
v010 = V(x,(y+1),zV)
v100 = V((x+1),y,zV)
else
v_100 = V((x-1),y,zV)
v0_10 = V(x,y,zV)
v010 = V(x,y,zV)
v100 = V((x+1),y,zV)
end if
else
v_100 = V((x-1),y,zV)
v0_10 = V(x,(y-1),zV)
v010 = V(x,(y+1),zV)
v100 = V((x+1),y,zV)
else if (D .eq. 3) then
v_100 = V((x-1),y,zV)
v0_10 = V(x,(y-1),zV)
v010 = V(x,(y+1),zV)
v100 = V((x+1),y,zV)
else
v_100 = V((x-1),y,zV)
v0_10 = V(x,y,zV)
v010 = V(x,y,zV)
v100 = V((x+1),y,zV)
end if
```
end if
v001 = V(x,y,(zV+1))
v00._1 = V(x,y,(zV-1))

*** dielectric tensor renamed in terms for Maple ***
e31 = epst(3,1,x,y,z)
e32 = epst(3,2,x,y,z)
e33 = epst(3,3,x,y,z)

*** code output by Maple ***
(See Maple sheet "Vinterfbot")

t1 = e31*dy
t2 = dz*(4*dz)
t7 = e32*dx
t13 = dx*dy
Vnew = (t1*t2*v100-t1*t2*v_100+t7*t2*v010-t7*t2*v0_10+2.D0*e33
#*v001*t13*(4*dz)+2.D0*epglass*v00_1*t13*dz)/dx/dy/(e33*(4*dz)+
 #epglass*dz)/2.D0

return
dontroutine Voltageinterfbot

Subroutine Calceps(epst,e0,epx,epy,epz,i,j,k)

*****************************************
***  This subroutine calculates the ***
*** dielectric tensor at the current ***
*** point.       ***
James Anderson  Feb/7/98   ***
*****************************************

*** Declare Variables ***
integer i,j,k
integer sizex,sizey,sizez
parameter (sizex = 500,sizey = 1,sizez = 100)
real*8 e0,ep(2),epst(1:3,1:3,0:sizex,0:sizey,0:sizez)
real*8 newx,ney,newz,De

*** form the dielectric tensor ***
epst(1:3,i,j,k) = e0*(ep(0)+epx*epy)
epst(2:3,i,j,k) = e0*(epx*epy)
epst(1:2,i,j,k) = e0*(epx*epy)
epst(1,3,i,j,k) = e0*(epx*epy)
epst(2,3,i,j,k) = e0*(epx*epy)
epst(1,3,i,j,k) = e0*(epx*epy)
epst(2,3,i,j,k) = e0*(epx*epy)
epst(3,1,i,j,k) = e0*(epx*epy)
epst(3,2,i,j,k) = e0*(epx*epy)
epst(3,3,i,j,k) = e0*(epx*epy)

return
end subroutine Calceps

*** Subroutine for calculating the functional derivative of ***
Subroutine Fgni(K11,K22,K33,e0,De,dx,dy,dz,q0,V,x,y,z,#FinAns,nx,ny,nz,m,Numx,Numy,Numz,xmir,ymir,D)

*** Declare Variables ***
implicit real*8 (p-w)
integer m,x,y,z,xmir,ymir
integer sizex,sizey,sizez,D
parameter (sizex =500,sizey =1,sizez =100)
real*8 K11,K22,K33,e0,De,dx,dy,dz,q0
integer Numx,Numy,Numz
real*8 nx(0:sizex,0:sizey,0:sizez)
real*8 ny(0:sizex,0:sizey,0:sizez)
real*8 nz(0:sizex,0:sizey,0:sizez)
real*8 V(0:sizex,0:sizey,0:3*sizez)
real*8 FinAns,Fenx,Feny,Fenz,Fsnx,Fsny,Fsnz
real*8 diff1(1:3,1:3),diff2(1:3,1:3,1:3)
real*8 V100,V_100,V010,V0_10,V001,V00_1

zV = z+Numz

*** Now we will form all of our spatial derivatives ***

*** First derivatives ***

***note that diff1(A,B) means 1st derivative of nA with respect to B.***
***the indices are set so that 1=x, 2=y, 3=z, so that ***
***diff1(3,2) means ***

dnz / dy

if ((x .eq. Numx) .or. (x .eq. 0)) then
if (xmir .eq. 1) then
if (x .eq. 0) then
diff1(1,1) = (nx(x,y,z)+nx(x,y,z))/(dx)
diff1(2,1) = (ny(x,y,z)-ny(x,y,z))/(dx)
diff1(3,1) = (nz(x,y,z)-nz(x,y,z))/(dx)
else
diff1(1,1) = (-nx(x,y,z)-nx(x,y,z))/(dx)
diff1(2,1) = (ny(x,y,z)-ny(x,y,z))/(dx)
diff1(3,1) = (nz(x,y,z)-nz(x,y,z))/(dx)
end if
if (x .eq. 0) then
V100 = V(1,y,zV)
V_100 = V(1,y,zV)
else
V100 = V(Numx-1,y,zV)
V_100 = V(Numx-1,y,zV)
end if
else
diff1(1,1) = (nx(1,y,z)-nx(Numx-1,y,z))/(2.D0*dx)
diff1(2,1) = (ny(1,y,z)-ny(Numx-1,y,z))/(2.D0*dx)
diff1(3,1) = (nz(1,y,z)-nz(Numx-1,y,z))/(2.D0*dx)
V100 = V(1,y,zV)
V_100 = V(Numx-1,y,zV)
end if
else
diff1(1,1) = (nx(x+1,y,z)-nx(x-1,y,z))/(2.D0*dx)
diff1(2,1) = (ny(x+1,y,z)-ny(x-1,y,z))/(2.D0*dx)
diff1(3,1) = (nz(x+1,y,z)-nz(x-1,y,z))/(2.D0*dx)
V100 = V(x+1,y,zV)
V_.100 = V(x-1,y,zV)
end if
if (D .eq. 3) then
if ((y .eq. Numy) .or. (y .eq. 0)) then
if (ymir .eq. 1) then
if (x .eq. 0) then
diff1(1,2) = (nx(x,y,z)-nx(x,y,z))/(dy)
diff1(2,2) = (ny(x,y,z)+ny(x,y,z))/(dy)
diff1(3,2) = (nz(x,y,z)-nz(x,y,z))/(dy)
else
diff1(1,2) = (nx(x,y,z)-nx(x,y,z))/(dy)
diff1(2,2) = (-ny(x,y,z)-ny(x,y,z))/(dy)
diff1(3,2) = (nz(x,y,z)-nz(x,y,z))/(dy)
end if
if (y .eq. 0) then
V010 = V(x,1,zV)
V0_10 = V(x,1,zV)
else
V010 = V(x,Numy-1,zV)
V0_10 = V(x,Numy-1,zV)
end if
else
diff1(1,2) = (nx(x,1,z)-nx(x,Numy-1,z))/(2.D0*dy)
diff1(2,2) = (ny(x,1,z)-ny(x,Numy-1,z))/(2.D0*dy)
diff1(3,2) = (nz(x,1,z)-nz(x,Numy-1,z))/(2.D0*dy)
V010 = V(x,1,zV)
V0_10 = V(x,Numy-1,zV)
end if
else
diff1(1,2) = (nx(x,y+1,z)-nx(x,y-1,z))/(2.D0*dy)
diff1(2,2) = (ny(x,y+1,z)-ny(x,y-1,z))/(2.D0*dy)
diff1(3,2) = (nz(x,y+1,z)-nz(x,y-1,z))/(2.D0*dy)
V010 = V(x,y+1,zV)
V0_10 = V(x,y-1,zV)
end if
else
diff1(1,2) = 0.d0
diff1(2,2) = 0.d0
diff1(3,2) = 0.d0
V010 = V(x,y,zV)
V0_10 = V(x,y,zV)
end if
diff1(1,3) = (nx(x,y,z+1)-nx(x,y,z-1))/(2.D0*dz)
diff1(2,3) = (ny(x,y,z+1)-ny(x,y,z-1))/(2.D0*dz)
diff1(3,3) = (nz(x,y,z+1)-nz(x,y,z-1))/(2.D0*dz)
V001 = V(x,y,zV+1)
V00_1 = V(x,y,zV-1)
c
 *** Second Derivatives ***
c
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***note that diff2(A,B,C) means 1st derivative of nA with respect to B and C.***

***the indices are set so that 1=x, 2=y, 3=z, so that***

***diff2(2,3,1) means***

\[
\begin{align*}
\text{diff2}(1,1,1) &= \frac{nx(x+1,y,z)-2.0*nx(x,y,z)+nx(x-1,y,z)}{(dx*dx)} \\
\text{diff2}(2,1,1) &= \frac{ny(x+1,y,z)-2.0*ny(x,y,z)+ny(x-1,y,z)}{(dx*dx)} \\
\text{diff2}(3,1,1) &= \frac{nz(x+1,y,z)-2.0*nz(x,y,z)+nz(x-1,y,z)}{(dx*dx)} \\
\end{align*}
\]

\[
\begin{align*}
\text{diff2}(1,1,3) &= \frac{nx(x+1,y,z+1)+nx(x-1,y,z-1)-nx(x-1,y,z+1)-nx(x+1,y,z-1)}{4.0*(dx*dz)} \\
\text{diff2}(1,3,1) &= \text{diff2}(1,1,3) \\
\text{diff2}(2,1,3) &= \frac{ny(x+1,y,z+1)+ny(x-1,y,z-1)-ny(x-1,y,z+1)-ny(x+1,y,z-1)}{4.0*(dx*dz)} \\
\text{diff2}(2,3,1) &= \text{diff2}(2,1,3) \\
\text{diff2}(3,1,3) &= \frac{nz(x+1,y,z+1)+nz(x-1,y,z-1)-nz(x-1,y,z+1)-nz(x+1,y,z-1)}{4.0*(dx*dz)} \\
\text{diff2}(3,3,1) &= \text{diff2}(3,1,3) \\
\end{align*}
\]

\[
\begin{align*}
\text{diff2}(1,1,2) &= \frac{nx(x+1,1,z)+nx(x-1,1,z)-nx(x-1,1,z)-nx(x+1,1,z)}{4.0*(dx*dy)} \\
\text{diff2}(1,2,1) &= \text{diff2}(1,1,2) \\
\text{diff2}(2,1,2) &= \frac{ny(x+1,1,z)+ny(x-1,1,z)-ny(x-1,1,z)-ny(x+1,1,z)}{4.0*(dx*dy)} \\
\text{diff2}(2,2,1) &= \text{diff2}(2,1,2) \\
\text{diff2}(3,1,2) &= \frac{nz(x+1,1,z)+nz(x-1,1,z)-nz(x-1,1,z)-nz(x+1,1,z)}{4.0*(dx*dy)} \\
\text{diff2}(3,2,1) &= \text{diff2}(3,1,2) \\
\end{align*}
\]

end if

else

\[
\begin{align*}
\text{diff2}(1,1,2) &= \frac{(nx(x+1,y,z)+nx(x,y,z)+nx(x-1,y,z))}{(dx*dx)} \\
\text{diff2}(2,1,2) &= \frac{(ny(x+1,y,z)+ny(x,y,z)+ny(x-1,y,z))}{(dx*dx)} \\
\text{diff2}(3,1,2) &= \frac{(nz(x+1,y,z)+nz(x,y,z)+nz(x-1,y,z))}{(dx*dx)} \\
\text{diff2}(1,1,3) &= \frac{(nx(x+1,y,z)+nx(x,y,z)+nx(x-1,y,z))}{(dx*dx)} \\
\text{diff2}(2,1,3) &= \frac{(ny(x+1,y,z)+ny(x,y,z)+ny(x-1,y,z))}{(dx*dx)} \\
\text{diff2}(3,1,3) &= \frac{(nz(x+1,y,z)+nz(x,y,z)+nz(x-1,y,z))}{(dx*dx)} \\
\end{align*}
\]
\texttt{#nx(x+1,y,z-1))/(4.d0*dx*dz) diff2(1,3,1) = diff2(1,1,3) diff2(2,1,3) = (ny(x+1,y,z+1)+ny(x-1,y,z-1)-ny(x-1,y,z+1)-\texttt{#ny(x+1,y,z-1))/(4.d0*dx*dz) diff2(2,3,1) = diff2(2,1,3) diff2(3,1,3) = (nz(x+1,y,z+1)+nz(x-1,y,z-1)-nz(x-1,y,z+1)-\texttt{#nz(x+1,y,z-1))/(4.d0*dx*dz) diff2(3,3,1) = diff2(3,1,3) if (D. eq. 3) then if (y .eq. Numy) .or. (y .eq. 0) then diff2(1,1,2) = (nx(x+1,1,z)+nx(x-1,Numy-1,z)-nx(x-1,1,z)-\texttt{#nx(x+1,Numy-1,z))/(4.d0*dx*dy) diff2(1,2,1) = diff2(1,1,2) diff2(2,1,2) = (ny(x+1,1,z)+ny(x-1,Numy-1,z)-ny(x-1,1,z)-\texttt{#ny(x+1,Numy-1,z))/(4.d0*dx*dy) diff2(2,2,1) = diff2(2,1,2) diff2(3,1,2) = (nz(x+1,1,z)+nz(x-1,Numy-1,z)-nz(x-1,1,z)-\texttt{#nz(x+1,Numy-1,z))/(4.d0*dx*dy) diff2(3,2,1) = diff2(3,1,2) else diff2(1,1,2) = (nx(x+1,y+1,z)+nx(x-1,y-1,z)-nx(x-1,y+1,z)-\texttt{#nx(x+1,y-1,z))/(4.d0*dx*dy) diff2(1,2,1) = diff2(1,1,2) diff2(2,1,2) = (ny(x+1,y+1,z)+ny(x-1,y-1,z)-ny(x-1,y+1,z)-\texttt{#ny(x+1,y-1,z))/(4.d0*dx*dy) diff2(2,2,1) = diff2(2,1,2) diff2(3,1,2) = (nz(x+1,y+1,z)+nz(x-1,y-1,z)-nz(x-1,y+1,z)-\texttt{#nz(x+1,y-1,z))/(4.d0*dx*dy) diff2(3,2,1) = diff2(3,1,2) end if else diff2(1,1,2) = 0.d0 diff2(1,2,1) = 0.d0 diff2(2,1,2) = 0.d0 diff2(2,2,1) = 0.d0 diff2(3,1,2) = 0.d0 diff2(3,2,1) = 0.d0 end if end if if (D. eq. 3) then if (y .eq. Numy) .or. (y .eq. 0) then diff2(1,2,2) = (nx(x,1,z)-2.d0*nx(x,y,z)+nx(x,Numy-1,z))/\texttt{(dy*dy)} diff2(2,2,2) = (ny(x,1,z)-2.d0*ny(x,y,z)+ny(x,Numy-1,z))/\texttt{(dy*dy)} diff2(3,2,2) = (nz(x,1,z)-2.d0*nz(x,y,z)+nz(x,Numy-1,z))/\texttt{(dy*dy)} diff2(1,2,3) = (nx(x,1,z+1)+nx(x,Numy-1,z-1)-nx(x,1,z-1)-\texttt{#nx(x,Numy-1,z+1))/(4.d0*dy*dz) diff2(2,2,3) = (ny(x,1,z+1)+ny(x,Numy-1,z-1)-ny(x,1,z-1)-\texttt{#ny(x,Numy-1,z+1))/(4.d0*dy*dz) diff2(3,2,3) = (nz(x,1,z+1)+nz(x,Numy-1,z-1)-nz(x,1,z-1)-\texttt{#nz(x,Numy-1,z+1))/(4.d0*dy*dz) diff2(1,3,2) = diff2(1,2,3) diff2(2,3,2) = diff2(2,2,3) diff2(3,3,2) = diff2(3,2,3)
else
  diff2(1,2,2) = (nx(x,y+1,z)-2.d0*nx(x,y,z)+nx(x,y-1,z))/(dy*dy)
  diff2(2,2,2) = (ny(x,y+1,z)-2.d0*ny(x,y,z)+ny(x,y-1,z))/(dy*dy)
  diff2(3,2,2) = (nz(x,y+1,z)-2.d0*nz(x,y,z)+nz(x,y-1,z))/(dy*dy)
  diff2(1,2,3) = (nx(x,y+1,z+1)+nx(x,y-1,z-1)-nx(x,y+1,z-1)-
#nx(x,y-1,z+1))/(4.d0*dy*dz)
  diff2(2,2,3) = (ny(x,y+1,z+1)+ny(x,y-1,z-1)-ny(x,y+1,z-1)-
#ny(x,y-1,z+1))/(4.d0*dy*dz)
  diff2(3,2,3) = (nz(x,y+1,z+1)+nz(x,y-1,z-1)-nz(x,y+1,z-1)-
#nz(x,y-1,z+1))/(4.d0*dy*dz)
end if
else
  diff2(1,2,2) = 0.d0
  diff2(2,2,2) = 0.d0
  diff2(3,2,2) = 0.d0
  diff2(1,2,3) = 0.d0
  diff2(2,2,3) = 0.d0
  diff2(1,3,2) = diff2(1,2,3)
  diff2(2,3,2) = diff2(2,2,3)
  diff2(3,3,2) = diff2(3,2,3)
end if

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endi
if (D. eq. 3) then
  diff2(1,1,2) = (-nx(x-1,y+1,z)+nx(x-1,y-1,z)-nx(x-1,y+1,z)-
  nx(x-1,y-1,z))/(4.d0*dx*dy*#(dx*dx))
else
  diff2(1,1,2) = 0.d0
end if
endif
endif
if (y .eq. 0) then
  if (ymir .eq. 1) then
    diff2(1,1,2) = 0.d0
    diff2(1,2,1) = 0.d0
    diff2(1,2,2) = 0.d0
    diff2(1,2,3) = 0.d0
    diff2(1,3,2) = 0.d0
    if (D .eq. 3) then
      diff2(2,1,2) = (ny(x+1,y+1,z)-ny(x-1,y+1,z)-ny(x-1,y+1,z)-
      ny(x+1,y+1,z))/(4.d0*dx*dy*#(dy*dy))
    else
      diff2(2,1,2) = 0.d0
    endif
    diff2(2,2,1) = diff2(2,1,2)
    diff2(2,2,2) = (ny(x,y+1,z)-2.d0*ny(x,y,z)-ny(x,y+1,z))/(dy*dy)
    diff2(2,2,3) = (ny(x,y+1,z+1)-ny(x,y+1,z-1)-ny(x,y+1,z-1)-
    ny(x,y+1,z+1))/(4.d0*dy*dz)
  endif
endif
elif (y .eq. Numy) then
  if (ymir .eq. 1) then
    diff2(1,1,2) = 0.d0
    diff2(1,2,1) = 0.d0
    diff2(1,2,2) = 0.d0
    diff2(1,2,3) = 0.d0
    diff2(1,3,2) = 0.d0
    if (D .eq. 3) then
      diff2(2,1,2) = (ny(x+1,y+1,z)-ny(x-1,y+1,z)-ny(x-1,y+1,z)-
      ny(x+1,y+1,z))/(4.d0*dx*dy*#(dy*dy))
    else
      diff2(2,1,2) = 0.d0
    endif
    diff2(2,2,1) = diff2(2,1,2)
    diff2(2,2,2) = (ny(x,y+1,z)-2.d0*ny(x,y,z)-ny(x,y+1,z))/(dy*dy)
    diff2(2,2,3) = (ny(x,y+1,z+1)-ny(x,y+1,z-1)-ny(x,y+1,z-1)-
    ny(x,y+1,z+1))/(4.d0*dy*dz)
  endif
endif
elseif (y .eq. Numy) then
  if (ymir .eq. 1) then
    diff2(1,1,2) = 0.d0
    diff2(1,2,1) = 0.d0
    diff2(1,2,2) = 0.d0
    diff2(1,2,3) = 0.d0
    diff2(1,3,2) = 0.d0
  endif
endif
diff2(1,2,2) = 0.d0
diff2(1,2,3) = 0.d0
diff2(1,3,2) = 0.d0
if (D. eq. 3) then
diff2(2,1,2) = (-ny(x+1,y-1,z)+ny(x-1,y-1,z)+ny(x-1,y-1,z)-
  ny(x+1,y-1,z))/((4.d0*dx*dy)
diff2(2,2,2) = (-ny(x,y-1,z)-2.d0*ny(x,y,z)+ny(x,y-1,z))/
  (dy*dy)
diff2(2,2,3) = (-ny(x,y-1,z+1)+ny(x,y-1,z-1)+ny(x,y-1,z-1)-
  ny(x,y-1,z+1))/(4.d0*dy*dz)
else
  diff2(2,1,2) = 0.d0
  diff2(2,2,2) = 0.d0
  diff2(2,2,3) = 0.d0
end if
diff2(2,2,1) = diff2(2,1,2)
diff2(2,3,2) = diff2(2,2,3)
diff2(3,1,2) = 0.d0
diff2(3,2,1) = 0.d0
diff2(3,2,2) = 0.d0
diff2(3,2,3) = 0.d0
diff2(3,3,2) = 0.d0
end if

c  ***Now, we have determined all of our spatial derivatives.***
c  ***At this point, we determine the derivatives of our Free energy***
c  ***with respect to the components of n (nx,ny,nz).***
c  ***These are built from our derivatives of nx wrt x,y.z.***
c  ***The code below was generated from the free energy equation by***
c  ***Maple V5 R5.***

if (m .EQ. 1) then
  ***m=1 means we wish to form Fgnx rather than Fgny or Fgnz***
c  ***Form Fgnx***
c  ***Form Fsnx (Fgnx = Fsnx-Fenx)***
c  ***Fs is the strain free energy.***
c  ***Fsnx is the derivative of Fs wrt nx***
t1 = ny(x,y,z)
t2 = K33*t1
t4 = nz(x,y,z)
t5 = diff2(3,1,2)*t4
t7 = diff1(1,3)
t8 = diff1(3,2)
t9 = t7*t8
t11 = diff1(2,2)
t12 = K33*t11
t13 = diff1(3,1)
t14 = t13*t4
t16 = nx(x,y,z)
t17 = K33*t16
t19 = diff2(3,2,2)*t4
t21 = t13*t8

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t23 = diff1(2,3)
t24 = t23*t8
t27 = diff2(2,2,3)*t4
t29 = diff1(2,1)
t30 = t29**2
t32 = diff1(1,2)
t34 = t23*t4
t36 = t4**2
t37 = K22*t36
t38 = diff2(1,2,2)
t40 = t1**2
t41 = K33*t40
t42 = diff2(2,1,2)
t45 = t32**2
t47 = K22*t16

48 = t23**2
t51 = diff2(2,3,3)*t1
t53 = t13**2
t55 = t23*t5**2+9*t12*t14-t17*t19+2.D0*t2*t21+2.D0*t17*t24+t17*t27
    #+#t17*t30-K33*t32*t34-t37*t38+t41*t42-t41*t38-t45+t2.D0*t47*t48-
    #t17*t51+t17*t53
t58 = K33*t36
t59 = diff2(3,1,3)
t62 = diff2(3,2,3)*t1
t64 = K22*t40
t65 = diff2(1,3,3)
t67 = t16**2
t68 = K33*t67
t71 = K33*t4
t72 = diff1(3,3)
t85 = K22*t23

t87 = K22*t1
t89 = 4*diff2(2,1,3)
t92 = 2.D0*K22*t8*q0+t58*t59+t17*t62-t64*t65+t68*t42+2.D0*
    #t71*t13*t72+2.D0*t2*t29+t11-t47*t62-t47*t51-2.D0*K22*t7*t23+t1-t58
    #+#t65-t68*t38+t37*t42-2.D0*t85*q0-t37*t89+t64*t59
t94 = t72*t32
t97 = t8**2
t99 = t72*t29
t101 = t4*t29
t104 = K33*t23
t121 = t87*t94+t68*t59+2.D0*t47*t97-t87*t99-2.D0*t85*t101+t2*t89+2
    #:D0*t104*t101+t2*t99+2.D0*t87*t13-K33*t8*t101-2.D0*t71*t72-
    #t2*t94-K11*diff2(1,1,1)+t104*t1*t13-K11*t59+t87*t9-K1
    #1*t42
t122 = K22*t4

t127 = K22*t11
t130 = t7**2
t140 = t7**4
t145 = diff2(1,2,3)*t4

t149 = -2.D0*t122*t32*8-2.D0*t2*t32+11-t127*t14-t87*t5-t17*t130+
    #K22*t32*t34-87*t21-t47*t27-t97-4.D0*t47*t24+3.D0*t122*t29*t8+
    #t127*t140+t47*t19-t12*t140+2.D0*t87*t145-2.D0*t2*t145-t17*t48

\text{Fsnx} = t55+92+t121+t149
**Form Fenx** (\(F_{\text{Fnx}} = F_{\text{snx}} - F_{\text{enx}}\))

**Fe** is the electric free energy.

**Fenx** is the derivative of **Fe** with respect to **nx**

\[
t_1 = V_{00} - V_{100}
\]

\[
t_2 = t_1^2
\]

\[
t_3 = dx^2
\]

\[
t_11 = t_1/dx*De
\]

\[
F_{\text{enx}} = e_0*(t_2/t_3*De*nx(x,y,z)/2.D0+t_11*ny(x,y,z)*(V_{010}-V_{0_10})/dy/2.D0+t_11*nz(x,y,z)*(V_{001}-V_{00_1})/dz/2.D0)/2.D0
\]

**Form Fgnx**

**FinAns** = **Fsnx** - **Fenx**

else if (m .EQ. 2) then

*** m=2 means we wish to form Fgny rather than Fgnx or Fgnz***

**Form Fgny**

**Form Fsny** (\(F_{\text{gny}} = F_{\text{sny}} - F_{\text{eny}}\))

**Fs** is the strain free energy.

**Fsny** is the derivative of **Fs** with respect to **ny**

\[
t_1 = nz(x,y,z)
\]

\[
t_2 = t_1^2
\]

\[
t_3 = K_{33}*t_2
\]

\[
t_4 = \text{diff2}(3,2,3)
\]

\[
t_6 = ny(x,y,z)
\]

\[
t_7 = K_{22}*t_6
\]

\[
t_8 = \text{diff1}(3,1)
\]

\[
t_9 = t_8^2
\]

\[
t_11 = K_{33}*t_6
\]

\[
t_12 = \text{diff1}(1,2)
\]

\[
t_13 = t_12^2
\]

\[
t_15 = \text{diff1}(1,3)
\]

\[
t_16 = K_{22}*t_15
\]

\[
t_18 = t_6^2
\]

\[
t_19 = K_{33}*t_18
\]

\[
t_21 = t_15^2
\]

\[
t_24 = nx(x,y,z)
\]

\[
t_25 = t_24^2
\]

\[
t_26 = K_{33}*t_25
\]

\[
t_27 = \text{diff2}(2,1,1)
\]

\[
t_31 = \text{diff2}(2,3,3)
\]

\[
t_34 = \text{diff1}(3,2)
\]

\[
t_35 = t_34^2
\]

\[
t_39 = K_{22}*t_25
\]

\[
t_41 = K_{22}*t_2
\]

\[
t_44 = K_{33}*t_24
\]

\[
t_46 = \text{diff2}(3,1,2)*t_1
\]

\[
t_48 = t_3**4+2.D0*t_7**2+11+t_11^3+2.D0*t_16*q_0+t_19^4+2.D0*K_{22}*t_24^3*t_6
\]

\[
#t_26**4*K_{33}*t_21+t_6+t_19^3+t_3**3+t_3**21+t_11^3+2.D0*K_{22}*t_18^3*q_0+t_3**3+t_4**3+2.D0*K_{22}*t_44*t_46
\]

\[
t_49 = \text{diff1}(2,3)
\]

\[
t_50 = t_49^2
\]

\[
t_53 = \text{diff2}(3,1,1)*t_1
\]

\[
t_55 = K_{22}*t_24
\]
t57 = diff2(2,1,3)*t1
t60 = diff2(1,1,2)
t63 = diff1(2,1)
t64 = K22*t63
t67 = diff1(1,1)
t68 = K33*t67
t69 = t49*t1
t71 = t15*t8
t76 = diff2(1,1,3)*t1
t79 = t15*t1
t87 = -444*t50+t7*t53+2*D0*t55*t57+t55*t50-K11*t60-2*D0*t44*t57-2.*
#D0*t64*t8*t1-t68*t69-2.D0*t7*t76+2*D0*t11*
#t71+t64*t79-K11*diff2(2,2,2)-K33*t63*t79+t11*t76-t11*
#t53
t93 = K22*t67
t95 = t34*t8
t99 = t6*diff2(1,3,3)
t102 = t6*diff2(3,1,3)
t104 = t34*t1
t106 = diff1(3,3)
t107 = t106*t12
t110 = t1*t12
t113 = t1*diff2(1,2,3)
t116 = t106*t63
t119 = K33*t1
t125 = 3*D0*K22*t1*t12*t8-K11*t4+t93*t69+2*D0*t44*t95-2*D0*t55*t95
#-444*t99+t44*t102+68*t104+44*t107+2*D0*K33*t115*t110+t44*t113-t55
#+t102+t55*t116-t44*t116+2*D0*t119*t34*t106-2*D0*t55*t49*t15-t55*t1
#t13

t130 = t34*t15
t141 = t49**2
t146 = t63**2
t149 = -t55*t107+t55*t99-2*D0*t119*t49*t106+3*D0*t55*t130-2*D0*t16
#+t110*K33*t8*t110+t55*t46-t44*t130-2*D0*t44*t63*t67-t93*t104+t19*t
#60-t1141+t26*t60+t41*t60+t19*t271146-t1149*t9

Fsny = t48+t87+t125+t149

c
*** Form Feny (Fgny = Fsny-Feny) ***
c *** Fe is the electric free energy. ***
c *** Feny is the derivative of Fe wrt ny ***
c

t6 = V010-V0_10
t8 = 1.D0/dy
t11 = t6**2
t12 = dy**2

Feny = e0*((V100-V_100)/dx*De*nx(x,y,z)*t6*t8/2.D0+t11/t12*De*ny(x #,y,z)/2.0*t6+t8*De*nx(x,y,z)*(V001-V00_1)/dz/2.D0/2.D0

c
*** Form Fgny ***

FinAns = Fsny-Feny
c

else
***m=3 means we wish to form Fgnz rather than Fgny***
c
*** Form Fgnz ***
c *** Form Fsnz (Fgnz = Fsnz-Fenz) ***
Fs is the strain free energy.

Fsnz is the derivative of Fs wrt nz

t1 = diff1(2,1)
t2 = t1**2
t4 = nz(x,y,z)
t6 = nx(x,y,z)
t7 = t6**2
t8 = K22*t7
t9 = diff2(3,2,2)
t11 = t4**2
t12 = K33*t11
t13 = diff2(3,1,1)
t15 = K33*t7
t17 = K33*t4
t18 = diff1(2,3)
t19 = t18**2
t21 = diff1(1,2)
t22 = K22*t21
t24 = ny(x,y,z)
t25 = t24**2
t26 = K33*t25
t28 = diff2(2,2,3)
t30 = diff2(1,1,3)
t32 = K22*t1
t34 = diff1(1,3)
t35 = t34**2
t42 = K33*t6
t43 = t18*t21
t45 = K33*t24
t46 = diff1(2,2)
t49 = -K33*t24+t4*diff2(2,1,1)
t50 = K22*t24
t51 = diff1(3,1)
t54 = diff1(1,1)
t59 = t34*t1
t63 = K22*t25
t65 = K22*t6
t72 = t21**2
t76 = t4*diff2(2,1,1)
t79 = t18*t1

t81 = -2.D0*t50*t51*t1+2.D0*t42*t34*t54-K11*t28-K11*t30+45*t59-t1 #+t28+t12*t42+t63*t30+3.D0*t65*t43+t13+3.D0*t50*t59+t12*t28-2.D0 #+t42*t51*t54-K33*t72+t4*t50+t76+45*t76+2.D0*t42*t79
t84 = diff2(2,1,3)*t24
t86 = K33*t54
t87 = t18*t24
t89 = diff1(3,2)
t90 = t89*t1
t93 = diff2(3,1,2)*t24
t95 = t89*t24
t98 = t4*diff2(1,1,2)
t100 = t51*t21
t103 = t4*t21
t106 = K22*t54
  t110 = t51**2
  t116 = t42*t84+t86*t87-t42*t90-2.D0*t42*t93-t86*t95+t45*t98-t45*t1
  #00+2.D0*K33*t1*t103-t65*t84-t106*t87-t50*t98+t50*t100-t17*t110-4.D
  #0*t32*t103+t65*t90+2.D0*t65*t93-2.D0*t65*t79
  t119 = t4*diff2(1,2,2)
  t121 = t46*t51
  t124 = t4*diff2(2,1,2)
  t127 = t24*diff2(1,2,3)
  t129 = t46*t34
  t132 = t24*t34
  t139 = t89**2
  t148 = t106*t95-t42*t119+t65*t121+t42*t124+t42*t127+t42*t129+2.D0*#K33*t21*t132-t42*t121-2.D0*t22*t132-t65*t124-t65*t127-t65*t129-t17
  #*t139-2.D0*t45*t89*t46+2.D0*K22*t72*t4-2.D0*t65*t89*t21+2.D6*t65*t119
  Fsnz = t49+81+t116+t148

  c
  c          *** Form Fenz     (Fgnz = Fsnz-Fenz)  ***
  c   *** Fe is the electric free energy.   ***
  c   *** Fenz is the derivative of Fe wrt nz  ***
  c
  t6 = V001-V00_1
  t8 = 1.D0/dz
  t19 = t6**2
  t20 = dz**2
  Fenz = e0*((V100-V_100)/dx*De*nx(x,y,z)*t6*t8/2.D0+(V010-V0_1)/dy
  #*De*ny(x,y,z)*t6*t8/2.D0+t19/t20*De*nz(x,y,z)/2.D0)/2.D0

c
  c        *** Form Fgnz ***
  FinAns = Fsnz-Fenz

c
  end if

c
  return

end Subroutine Fgni

c
  c *** The storeoldn subroutine puts what is in nx, ny, and nz
  c *** into nxo, nyo, nzo.  This subroutine is used first to
  c *** store the old values before trying the next iteration.
  c *** It is next used if the iteration was unstable to go
  c *** back to the previous time step and try again.
  c
  subroutine storeoldn(nx,ny,nz,nxo,nyo,nzo,Numx,Numy,Numz)
    integer sizex,sizey,sizez
    parameter (sizex =500,sizey = 1,sizez =100)
    real*8 nx(0:sizex,0:sizey,0:sizez),ny(0:sizex,0:sizey,0:sizez)
    real*8 nz(0:sizex,0:sizey,0:sizez),nxo(0:sizex,0:sizey,0:sizez)
    real*8 nyo(0:sizex,0:sizey,0:sizez),nzo(0:sizex,0:sizey,0:sizez)
    integer i,j,k

c
  do i = 0,Numx
    do j = 0,Numy
      do k = 0,Numz
        nxo(i,j,k) = nx(i,j,k)
        nyo(i,j,k) = ny(i,j,k)
        nzo(i,j,k) = nz(i,j,k)
  enddo
  enddo
  enddo
end subroutine storeoldn
end do
end do
end subroutine storeoldn

*** The storeoldtens subroutine is the same as storeoldn, except that instead of storing a vector, it stores a tensor. It is used here to store the dielectric tensor. It is used at the same time as storeoldn. ***

subroutine storeoldtens(tens,tensold,Numx,Numy,Numz)
integer sizex,sizey,sizez
parameter (sizex =500,sizey = 1,sizez =100)
real*8 tens(1:3,1:3,0:sizex,0:sizey,0:sizez)
real*8 tensold(1:3,1:3,0:sizex,0:sizey,0:sizez)
integer x,y,z,i,j

do x = 0,Numx
   do y = 0,Numy
      do z = 0,Numz
         do i = 1,3
            do j = 1,3
               tensold(i,j,x,y,z) = tens(i,j,x,y,z)
            end do
         end do
      end do
   end do
end subroutine storeoldtens


