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**On the numerical solution of incompressible three-dimensional
Navier-Stokes equations**

Babu, V., Ph.D.

The Ohio State University, 1991

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ON THE NUMERICAL SOLUTION OF INCOMPRESSIBLE
THREE-DIMENSIONAL NAVIER-STOKES EQUATIONS

DISSERTATION

Presented in Partial Fulfillment of the Requirements for
the Degree Doctor of Philosophy in the Graduate
School of The Ohio State University

By

V. Babu, B.S., M.S.

* * * * *

The Ohio State University

1991

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**To
My Grandparents**

ACKNOWLEDGEMENTS

I would like to express my sincere appreciation to my friend and adviser Seppo Korpela for his guidance and encouragement during this work. I would like thank my graduate committee members Prof. Th. Herbert and Prof. R. Bodonyi for their comments and suggestions and Prof. M. Foster for serving on my General Examination Committee. Prof. V. Subramaniam gave me encouragement and financial support during the past two summers. For this I am grateful. I am happy to acknowledge Prof. T. Scheick of the Mathematics Department who gave graciously his time in discussions of the methods for the fast Poisson solver. To my friend Natarajan Ramanan, I am grateful for many interesting discussions related to this work.

During the course of this work, I have sought the help of many systems people at various computer centers and they have gladly obliged me. I would like to thank all of them. Of note in this regard are Charlotte Hawley of the Laboratory for Computational and Visual Fluid Dynamics, Steve Koehl of the Ohio Supercomputer Center, and Amy Laurence of Robinson Color Graphics Laboratory. I would also like to thank Dr. George Delic of the Ohio Supercomputer Center for his help in the optimization of my code on the Cray Y-MP8/864.

During my graduate studies The Ohio State University has provided a University Fellowship and the Department of Mechanical Engineering has given me chance to teach. The many hours of computer time I have used during this work were provided by The Ohio Supercomputer Center. The simulation of the horizontal Bridgeman flow was a continuation of work carried out under The National Science Foundation grant CBT-85124042. NSF has also provided for graphics hardware acquisition through the grant CTS-8907601.

I would like to thank my teacher and mentor Shri S. Sundaresan for all that he has done for me. My sincere appreciation goes to my parents, my brother and my wife for their patience, love and support.

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TABLE OF CONTENTS

ACKNOWLEDGEMENTS	iii
VITA	iv
LIST OF TABLES	vii
LIST OF FIGURES	viii
NOMENCLATURE	xii

CHAPTER	PAGE
I. Introduction	1
1.1 Literature Survey	1
II. Three dimensional Thermocapillary Convection in a Cavity	7
2.1 Thermocapillary Convection	7
2.2 Formulation	8
2.2.1 Governing Equations	8
2.2.2 Boundary Conditions	9
2.3 Numerical Method	11
2.4 Results & Discussion	17
2.5 A Criticism of the Method of Solution	25
III. A Direct Method for solving Poisson's Equation	30
3.1 Matrix Decomposition on Uniform Grids	30
3.1.1 Dirichlet Problem	31

3.1.2 Neumann Problem	33
3.2 The Neumann Problem in Three Dimensions	37
3.3 Matrix Decomposition on Non-uniform Grids	41
3.4 Performance Analysis	45
IV. Three dimensional Flow in a Lid Driven Cavity	47
4.1 Flow in a Lid Driven Cavity	47
4.2 Formulation	50
4.2.1 Governing Equations	51
4.2.2 Boundary Conditions	51
4.3 Numerical Method	52
4.4 Results & Discussion	58
4.4.1 Flow In a Square Cavity	60
4.4.2 Flow In a Cubical Cavity	73
4.4.3 Flow in a Shallow Cavity	90
V. Natural Convection in a Shallow Cavity	101
5.1 Natural Convection in Cavities	101
5.2 Formulation	102
5.2.1 Governing Equations	102
5.2.2 Boundary Conditions	103
5.3 Numerical Method	104
5.4 Results & Discussion	109
VI. Conclusions	131
APPENDIX	133
REFERENCES	135

LIST OF TABLES

	TABLE	PAGE
5.1.	Comparison of the present results with those reported in the GAMM Workshop (Roux, Editor), 1990	112

LIST OF FIGURES

FIGURE	PAGE
2.1 Geometry and grid indices	14
2.2 Velocity vectors in three mutually orthogonal planes for shear driven flow in a cube at $Re = 100$, (a) $z = 0.5$, (b) $y = 0.5$, and (c) $x = 0.5$	18
2.3 Velocity vectors in three mutually orthogonal planes for thermocapillary convection in a cube at $Re = 100$, (a) $z = 0.5$, (b) $y = 0.5$, and (c) $x = 0.5$	21
2.4 The u-velocity on the free surface	22
2.5 The u-velocity on the free surface for the two-dimensional flow compared with its counterpart along the centerline in a three-dimensional flow	23
2.6 Temperature on the free surface for the two-dimensional flow compared with its counterpart along the centerline in a three-dimensional flow	24
2.7 Temperature distribution on the free surface at $Re = 100$	26
2.8 Free surface deflections for thermocapillary flow at $Re = 100$	27
4.1 Sketch of the flowfield in a two-dimensional lid driven cavity	48
4.2 Sketch of the flowfield in a three-dimensional lid driven cavity, (Reproduced from Iwatsu et al., 1989)	49
4.3 Grid Nomenclature	54
4.4 Evolution of the residuals of the continuity equation for explicit and semi-implicit schemes	59
4.5 Contours of static pressure coefficients at (a) $Re = 100$, (b) $Re=400$ and (c) $Re = 1000$	61
4.6 Contours of vorticity at (a) $Re = 100$, (b) $Re = 400$ and (c) $Re = 1000$	64

4.7	The u-velocity along vertical centerline of cavity at (a) $Re = 100$, (b) $Re = 400$ and (c) $Re = 1000$	67
4.8	The w-velocity along horizontal centerline of cavity at (a) $Re = 100$, (b) $Re = 400$ and (c) $Re = 1000$	70
4.9	Velocity profiles along vertical and horizontal centerlines on the symmetry plane at $Re = 100$, (a) u-velocity and (b) w- velocity	74
4.10	Velocity profiles along vertical and horizontal centerlines on the symmetry plane at $Re = 400$, (a) u-velocity and (b) w-velocity	77
4.11	Velocity profiles along vertical and horizontal centerlines on the symmetry plane at $Re = 1000$, (a) u-velocity and (b) w-velocity	79
4.12	(a) Velocity vectors on the symmetry plane for a cubical cavity, (b) downstream secondary eddy and (c) upstream secondary eddy at $Re = 1000$	81
4.13	Velocity vectors on the plane $x = 0.5$ for a cubical cavity at $Re = 1000$	84
4.14	Particle trace inside the cubical cavity at $Re = 1000$	85
4.15	Velocity vectors on the symmetry plane for a cubical cavity at $Re = 4000$	87
4.16	Velocity vectors on the plane $x = 0.57$ for a cubical cavity at $Re = 4000$	88
4.17	Velocity vectors on the plane $x = 0.57$ for a cavity with $W/H = 2$ at $Re = 4000$	89
4.18	The u-velocity along the vertical centerline for a two dimensional shallow cavity for aspect ratios 2,4,6,8,10 and 12 at $Re = 100$	92
4.19	Pressure along the horizontal centerline for a two dimensional shallow cavity for aspect ratios 2,4,6,8,10 and 12 at $Re = 100$	93
4.20	The w-velocity along the horizontal centerline for a two dimensional shallow cavity for aspect ratios 2,4,6,10 and 12 at $Re = 100$	94
4.21	The u-velocity along the vertical centerline on the symmetry plane for a three	

	dimensional shallow cavity for aspect ratios 2,4,6,8 and 10 at $Re = 100$	97
4.22	Pressure along the horizontal centerline on the symmetry plane for a three dimensional shallow cavity for aspect ratios 2,4,6,8 and 10 at $Re = 100$	98
4.23	The w-velocity along the horizontal centerline on the symmetry plane for a three dimensional shallow cavity for aspect ratios 2,4,6,8 and 10 at $Re = 100$	100
5.1	Velocity vectors for natural convection in a two dimensional shallow cavity at $Gr=80,000$	111
5.2	Transient behaviour of u_{max} and w_{max} along the vertical and horizontal centerlines for natural convection in a two dimensional shallow cavity at $Gr=102,000$	113
5.3	Transient behaviour of u_{max} and w_{max} along the vertical and horizontal centerlines for natural convection in a two dimensional shallow cavity at $Gr=120,000$	114
5.4	Velocity vectors for natural convection in a two dimensional shallow cavity at $Gr=120,000$	115
5.5	Transient behaviour of u_{max} and w_{max} along the vertical and horizontal centerlines for natural convection in a two dimensional shallow cavity at $Gr=160,000$	116
5.6	Velocity vectors for natural convection in a two dimensional shallow cavity at $Gr=160,000$	117
5.7	Transient behaviour of u_{max} and w_{max} along the vertical and horizontal centerlines for natural convection in a two dimensional shallow cavity at $Gr=160,000$ on a coarse (42x168) grid	119
5.8	Two possible solutions for natural convection in a two dimensional shallow cavity at $Gr=120,000$, steady solution (top) and oscillatory solution (bottom)	120
5.9	(a) Time traces of u-velocity at several points inside the cavity for natural convection in a three dimensional shallow cavity (4x1x1) at $Gr=500,000$ and $Pr=0$, (b) Power Spectrum	122

5.10	Time traces at two points inside the cavity for natural convection in a three dimensional shallow cavity (4x1x1) at $Gr=844,800$ and $Pr=0.026$, (a) Temperature, (b) u-velocity and (c) Power Spectrum	126
5.11	Time traces of temperature at four points inside the cavity for natural convection in a three dimensional shallow cavity (4x2x1) at $Gr=180,000$ and $Pr=0.026$	129

NOMENCLATURE

- Ca - Capillary number, $= \gamma \Delta T / \sigma_0$
g - gravitational acceleration
H - Height of cavity
L - Length of cavity
Gr - Grashof number, $= g \beta \Delta T H^3 / \nu^2$
Ma - Marangoni number, $= \text{Pr Re}_T$
p - dimensionless pressure
Pr - Prandtl number, $= \nu / \alpha$
Re - Reynolds number, $= UH / \nu$
 Re_T - Thermocapillary Reynolds number, $= U_T^* H / \nu$
T - dimensionless temperature
 ΔT - characteristic temperature difference
u,v,w - dimensionless velocity in x, y, z direction
U - Velocity of the cavity lid
 U_T^* - characteristic velocity, $= \gamma \Delta T / \mu$
W - Width (or span) of cavity
x - dimensionless x-coordinate
y - dimensionless y-coordinate
z - dimensionless z-coordinate

Greek

- α - thermal diffusivity
 β - coefficient of volumetric expansion
 γ - temperature coefficient of surface tension

ϵ - convergence criterion
 η - transformed y-coordinate
 ν - kinematic viscosity
 ρ - density
 σ - coefficient of surface tension
 ξ - transformed x-coordinate
 ζ - transformed z-coordinate

Subscripts

T - thermocapillary
 i,j,k - grid indices

Superscripts

n - time level

CHAPTER I

INTRODUCTION

The aim of this dissertation is to discuss methods for solving the incompressible, three dimensional Navier-Stokes equations numerically using finite-difference techniques. Even though numerical solutions to three dimensional Navier-Stokes equations were attempted as early as 1967 (Chorin, 1967, Aziz and Hellums, 1967), the number of solutions that have appeared in the literature is not yet very large. It is our aim to make a contribution to this kind of research area. To be sure, it is possible to calculate transient incompressible flows with commercial software (such as FIDAP, FLUENT, and NEKTON), but the investment on overheads to make these codes general, reduces their computing speeds. Thus it is not possible to get the same degree of accuracy with them, as one can from a computer code, specially tailored to a given task. We hope to show that very high accuracy and faithful representation of complicated three dimensional flows is possible with a well optimized code.

In contrast to the two dimensional situation, in which the stream function-vorticity formulation has enjoyed great success over other formulations, in three dimensional simulations, different formulations have been tried and work continues to clarify which of the various methods offer the most in regard conceptual simplicity and computational advantages. The different formulations that have been tried can be classified into two broad categories; those that use the primitive variables velocity and pressure and those that use derived variables such as the vector potential and vorticity.

1.1 LITERATURE SURVEY

The earliest work that used the primitive variable formulation was by Chorin (1967). Owing to the lack of a time derivative in the continuity equation he proposed that an artificial

steady state numerical solution is obtained. The steady state solution is independent of the artificial compressibility factor, for this factor multiplies the time derivative of density in the continuity equation, a term that must vanish at steady state. Using this algorithm, Chorin was able to study three dimensional convection patterns in a liquid layer heated from below in the neighborhood of the critical Rayleigh number.

In the same year Aziz and Hellums (1967) published a paper using derived variables. They transformed the Navier-Stokes equations into equations for the vorticity and a vector potential and defined the vector potential so that its curl is the velocity vector. They obtained an equation for vorticity transport by taking the curl of the momentum equation and a Poisson equation for the vector potential by writing the vorticity vector in terms of the vector potential and by making use of the fact that the vector potential can be chosen arbitrarily to be divergence free. The vector potential can be thought of as the three dimensional extension of the stream function. It is important to note that the continuity equation is satisfied identically by the vector potential in this formulation. By solving a parabolic equation for each component of the vorticity vector using the alternating direction implicit method (ADI), and the elliptic equation for each of the three components of the the vector potential using iterative methods, Aziz and Hellums (1967) were able to obtain solutions for three dimensional natural convection in a cavity on a $11 \times 11 \times 11$ grid using an IBM 7040 computer. The following year, Chorin (1968) proposed an algorithm (referred to as Chorin's splitting method) for solving the three dimensional equations of motion in primitive variable form, based on Helmholtz's decomposition theorem. In that method, a predicted velocity field is obtained from the momentum equations from which the pressure term has been neglected. The estimate is corrected by solving a Poisson equation for pressure in a form that assures the velocity field to be divergence free. In his paper he gave transient solutions to the three dimensional convection of a fluid layer heated from below using a $24 \times 24 \times 25$ grid.

A significant increase in accuracy was obtained by Williams (1969) whose work is also based on the primitive variable formulation. He was able to solve the three dimensional equations of motion on a staggered $60 \times 34 \times 34$ grid using a UNIVAC 1108 machine. He obtained the velocity field by time-marching the momentum equations and obtained the pressure from a Poisson equation using trigonometric expansions. The significance of this work

lies in the fact that he applied the Fast Fourier transform methods to the solution of the Poisson equation and despite the core memory limitation of UNIVAC 1108 to $14 \times 14 \times 14$ grid points, he obtained solutions on a $60 \times 34 \times 34$ grid (using limited access drums). The significant increase in the number of grid points allowed him to increase the accuracy of his solution.

Mallinson and de Vahl Davis (1973) four years later, presented solutions to three dimensional natural convection in a cavity using the vorticity vector potential formulation. In contrast to the earlier work of Aziz and Hellums (1967), they used the method of false transients, that is similar to Chorin's artificial compressibility method. The similarity to Chorin's work arises from the fact that the elliptic equation for the vector potential was converted to a parabolic equation by adding a false time derivative. In addition, the coefficients of the transient terms in the vorticity transport equation are also modified. Their first work was carried out on a $11 \times 11 \times 11$ grid using an IBM 360/50 computer. Later, they applied this method to solve the three dimensional natural convection in a box on a $15 \times 15 \times 15$ grid, again using the IBM 360/50 (Mallinson and de Vahl Davis, 1977).

About the same time the Japanese researchers Takami and Kuwahara (1974) studied the three dimensional flow in a lid driven cubic cavity using the primitive variable formulation. Their method is a variant of Chorin's splitting method and a staggered grid scheme, similar to the one proposed by Harlow and Welch (1965). They presented solutions to this problem for Reynolds number equal to 100 and 400, obtained on a $20 \times 20 \times 20$ grid, using a HITAC 8800-8700 (which had half the computing speed of an IBM 360/195). Goda (1979), four years later also studied the same problem with a method based on an ADI scheme to solve the parabolic equations, but which was otherwise similar to the one used by Takami and Kuwahara (1974). He carried out the computations on an ACOS 700 computer, which had one fourth the computing speed of a CDC 6600, and a memory size that limited his grids to no finer than $20 \times 20 \times 20$. Dennis, Ingham and Cook (1979) studied the flow in a lid driven cavity by formulating the problem in terms of the velocity and vorticity. The vorticity transport equation is obtained as usual, by taking the curl of the momentum equations. Poisson equations for the velocity components arise in this formulation from the continuity equation and the equations that define the vorticity components in terms of the velocity components.

They presented solutions for Reynolds number up to 100 with grid sizes of either $20 \times 20 \times 20$ or $25 \times 25 \times 25$. Agarwal (1981) also solved the lid driven cavity problem using the velocity-vorticity formulation. He set the time derivatives to zero in the vorticity transport equations and solved the resulting set of elliptic equations for the velocity and vorticity using an alternating direction line-iterative scheme. The special feature of his method was the third order accurate upwind differencing that he used for the convective terms in the vorticity transport equation. He carried out calculations on three different grids, namely $11 \times 11 \times 6$, $17 \times 17 \times 9$ and $21 \times 21 \times 11$ using a CYBER 175 and gave solutions for Reynolds numbers 0, 100 and 400.

The same velocity-vorticity formulation as in Dennis et al. (1979), has recently been implemented by Osswald, Ghia and Ghia (1987) to study the flow in a lid-driven cavity. They used a Gaussian elimination algorithm to solve the elliptic equations for the velocity components and a modified ADI method to solve the vorticity transport equations. This is in contrast to the previous works by Dennis et al. (1979) and Agarwal (1981) who relied on iterative methods. The calculations of Osswald et al. (1987) were performed on a $17 \times 17 \times 17$ grid at Reynolds number of 100 using a CYBER 205 supercomputer.

In looking at the primitive variable, vorticity-vector potential and the velocity-vorticity formulations one notes that all of them require the solution of three parabolic equations (in three dimensions) and the solution of one or more Poisson equations. This results in a stiff system of equations, since the variables governed by the Poisson equation, being elliptic, respond instantaneously to any changes in the flow field. As a result, if accurate transient solutions of the unsteady equations are desired, then these Poisson equations have to be solved at least up to the truncation error of the method during the intermediate time steps. This constitutes the major computational effort during the solution procedure. The primitive variable formulation involves the determination of four unknowns, namely, the three components of the velocity vector and the pressure. The continuity equation is replaced by a Poisson equation for the pressure with boundary conditions of the Neumann type, derived from the momentum equations. This leads to the so called, Neumann-Poisson problem for pressure. The formulation in terms of primitive variable allows boundary conditions, such as prescribed velocity and prescribed shear, to be imposed very easily. However, the Neumann-Poisson problem for pressure in this formulation converges poorly during the intermediate

time steps (Roache, 1972 & 1975) owing to the Neumann boundary conditions. In addition, the convergence towards a steady state solution is also slow.

In the vorticity-vector potential formulation, the three components of the vorticity vector and the three components of the vector potential are unknown and so three Poisson equations for the vector potential and three parabolic equations for the vorticity vector have to be solved. Their solution requires increased memory requirements and increased computing times. Moreover, now it is difficult to impose even simple boundary conditions for the velocity in a straight forward manner (Anderson, Tannehill and Pletcher, 1984). The velocity-vorticity formulation also requires the determination of six unknowns, namely, the three components of the velocity vector and the three components of the vorticity vector and hence the solution of three Poisson equations for vorticity and three parabolic equations for the velocity. The boundary conditions for vorticity have to be derived using the boundary conditions for velocity. This usually necessitates the evaluation of derivatives of velocity on the boundaries, preferably to second order accuracy. Roache (1975) argues in favor of the velocity-vorticity formulation since he believes it is better to study the development of vorticity than the pressure, the vorticity being more meaningful physically.

From the above qualitative considerations, it appears that the primitive variable formulation is conceptually the simplest and also the most attractive in regard to the ease with which a variety of problems can be handled. In addition, this formulation requires only one Poisson equation to be solved as opposed to three in the other two formulations. Also, considerable progress has been made by Briley (1974), Ghia et al. (1976), Ghia et al. (1977) and Abdallah (1987) in improving the convergence towards steady state of the incompressible Navier-Stokes equations in primitive variable form, which has been one of the criticisms of this formulation. Briley (1974) identified the reason for the poor convergence of the Neumann-Poisson problem for pressure. He showed that the pressure field, which should satisfy an integral constraint arising from Green's theorem, may not satisfy it in discretized form during the intermediate time steps in a time marching scheme. To fix this, he proposed that the source term of the Poisson equation be modified uniformly at all grid points in such a way as to satisfy this constraint in discretized form to machine accuracy at each time step. With this modification, Briley (1974), Ghia et al. (1976), Ghia et al. (1977) and Abdallah (1987) were

able to obtain converged steady state solutions for the incompressible, Navier-Stokes equations. The computing times reported in these works for solving two dimensional problems with the primitive variable formulation are reasonable so their use for three dimensional problems seems to be practical.

In the following chapters, efforts to develop a fast and accurate numerical method for solving the incompressible, three dimensional Navier-Stokes equations on uniform and non-uniform grids are described. The main objective was to simulate both steady and unsteady flows. Our earliest attempts towards solving these equations is described in Chapter 2, where the consistent finite-differencing scheme proposed by Abdallah (1987) is extended to three dimensions and used to analyze thermocapillary convection in a cubic cavity. This method uses an odd-even point SOR scheme to solve the Poisson equation for pressure and an explicit time differencing scheme. The main weakness of this method is the iterative method used for the solution of the Neumann-Poisson problem. The issue of developing fast and accurate methods for solving this problem is taken up in Chapter 3, where a direct method to solve Poisson equation to machine accuracy on uniform and non-uniform grids is described. The computational efficiency of this method is established through a performance analysis on the Cray Y-MP8/864, a topic that is discussed in section 3.4. Another weakness of the method given in Chapter 2 is the manner in which the pressure boundary condition is applied. This is made rigorous in the method discussed in Chapter 4, where a three dimensional flow in a lid driven cavity for increasing values of Reynolds number is considered. Difficulties with the explicit time differencing scheme used in both Chapters 2 and 4 for the time integration of the momentum equations are discussed in section 4.3 and a semi-implicit scheme which can overcome these difficulties for diffusion dominated flows is given in section 4.3. This idea is taken up further in Chapter 5, and an unconditionally stable algorithm for the time integration of these equations is proposed. Using this and the direct method for the solution of pressure, some unsteady solutions for natural convection of low Prandtl number fluids in shallow cavities are given in that chapter. For large Grashof numbers these show chaotic behaviour. Even though we were able to obtain accurate unsteady solutions with this method, it still has a disadvantage that it is only first order accurate. Development of second order time accurate schemes for time integration is left for a future study.

CHAPTER II

THREE DIMENSIONAL THERMOCAPILLARY CONVECTION IN A CAVITY

2.1 THERMOCAPILLARY CONVECTION

In this chapter, we consider three dimensional thermocapillary convection of a liquid contained in a cubic cavity. It is a continuation of the study by Ramanan and Korpela (1990), who considered the axi-symmetric thermocapillary flow in a cylindrical cavity of a liquid that is heated at its free surface by a Gaussian heat flux. Interest in these flows arises from the needs of industry to simulate realistic situations in materials processing such as welding, zone refining, and crystal growth. The strategy for generating information about these flows has been to try to discover first the physical behavior of the flow in a simplified two-dimensional situation and use the experience so gained as a guide for the three dimensional simulations.

Both in welding and in zone refining it is well known that surface tension gradients are the source of bulk fluid motion (Oreper and Szekely, 1984, Smith and Davis, 1983). Since surface tension depends on temperature (Levich, 1962), nonuniform heating of the free surface leads to surface tension gradients, which in turn give rise to shear stresses that drive the bulk flow. Surface tension gradients can also arise from nonuniformity of concentration of chemical species on the free surface, particularly surfactants (Levich, 1962). Here, this effect is ignored by assuming that the surface is of uniform composition.

Except for the finiteness of the third direction, the problem considered here is identical to that of Zebib, Homsy and Meiburg (1985). That is, we consider an open cubical cavity filled with liquid to its rim. Two of the side walls have uniform temperatures, one hotter than the other. The bottom of the cavity is insulated, as are the other two walls. If we also neglect heat transfer through the free surface at the top, then the amount of heat that is transferred at steady state through each vertical section normal to the primary flow by conduction and convection must be constant. This provides a check on how well the thermal

energy balance is satisfied. The free surface is assumed to be pinned to the rim of the cavity, as would be the case if the container were full and the free surface deflections were so small that the liquid would not spill from the container. This is assumed to be true and in addition, the stronger condition, that the surface is flat to a leading order approximation is also imposed. Flatness can be assumed if the surface tension forces that diminish surface deflections are much larger than the pressure forces that act to displace the surface. This assumption allows us to calculate the surface deflection *a posteriori*.

Since the main aim here is to examine the way in which the primitive variable formulations are to be consistently implemented in three dimensional flows and to understand the qualitative differences that the three dimensionality brings into thermocapillary convection, solutions for very large values of thermocapillary Reynolds number have not been attempted. Depending on the application, large value for Reynolds number may not be a requirement, although in the problems on welding it is invariably necessary to calculate flows that have very thin boundary layers along the free surface (Ramanan and Korpela, 1988, Babu, 1989).

2.2 FORMULATION

Consider an incompressible liquid of density ρ , kinematic viscosity ν , and thermal diffusivity α . This liquid is confined to a cubic box of length L . The top surface of the liquid is free and in contact with a gas above. The left and right sides of the box are maintained at certain fixed temperatures such that the left surface is hotter than the right one. As a result, thermocapillary stresses are induced on the free surface of the liquid which, since the surface tension increases as temperature decreases, is pulled from the hot side to the cold side and a convective motion ensues in the box.

2.2.1 GOVERNING EQUATIONS

The equations that govern the motion of the fluid are the Navier-Stokes equations and the energy equation. We write the governing equations in dimensionless form so that the

relevant parameters can be identified. Lengths are non-dimensionalized by L , velocities by a characteristic velocity U_T , time by L / U_T , pressure by ρU_T^2 , and temperature by the temperature difference ΔT between the two walls. The characteristic velocity U_T is obtained by balancing the thermocapillary stress with the shear stress on the free surface. It is given by $U_T = |\gamma| \Delta T / \mu$, where $\gamma = d\sigma/dT$ is the temperature coefficient of the surface tension σ . The governing equations in dimensionless form are,

$$\nabla \cdot \vec{u} = 0 , \quad (2.1)$$

$$\frac{\partial \vec{u}}{\partial t} + \left[\vec{u} \cdot \nabla \right] \vec{u} = -\nabla p + \frac{1}{\text{Re}} \nabla^2 \vec{u} , \quad (2.2)$$

$$\frac{\partial T}{\partial t} + \left[\vec{u} \cdot \nabla \right] T = \frac{1}{\text{PrRe}} \nabla^2 T , \quad (2.3)$$

where $\vec{u} = u \hat{i} + v \hat{j} + w \hat{k}$ is the velocity vector,

$$\nabla \equiv \hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z} , \quad \nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} ,$$

and the parameters are defined as,

$$\text{Pr} = \frac{\nu}{\alpha} , \quad \text{Re} = \frac{U_T L}{\nu} .$$

2.2.2 BOUNDARY CONDITIONS

Since all the sides of the box, except the top surface, are rigid, the fluid velocities are zero on these surfaces. Hence,

$$u = v = w = 0 , \quad x = 0, 1 , \quad (2.4a)$$

$$u = v = w = 0 , \quad y = 0, 1 , \quad (2.4b)$$

$$u = v = w = 0 , \quad z = 0 . \quad (2.4c)$$

For small capillary numbers $Ca (= \gamma \Delta T / \sigma_0)$, the free surface can be assumed to be flat (Zebib et al., 1985) to leading order when the surface deflection is expanded in a perturbation series in powers of the capillary number. The parameter σ_0 is the surface tension evaluated at a reference temperature; such as the temperature of the cold wall. Since the free surface does not deflect, the vertical velocity is zero along it. A force balance on this surface shows that along the surface the shear stresses are balanced by the thermocapillary forces. Accordingly we have, in dimensionless form,

$$\frac{\partial u}{\partial z} = -\frac{\partial T}{\partial x}, \quad \frac{\partial v}{\partial z} = -\frac{\partial T}{\partial y}, \quad w = 0, \quad z = 1. \quad (2.4d)$$

where we have made use of the fact that for pure metals, γ is negative.

Following Zebib et al. (1985) we can determine the surface deflections by expressing the perturbed free surface as $z = 1 + f(x, y)$. A stress balance in the normal direction then yields a Poisson equation for $f(x, y)$ (Milne-Thomson, 1968):

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = -Ca Re(p + p_0), \quad (2.5)$$

where we have introduced an arbitrary constant p_0 to account for the fact that the pressure field is determined only to an additive constant. This constant can be determined by requiring that the total volume of the liquid in the cavity remain fixed, which can be written as,

$$\iint f(x, y) dx dy = 0. \quad (2.6)$$

By assuming that the deflections are zero along the rim, the boundary conditions to be satisfied by f are,

$$f(0, y) = f(1, y) = f(x, 0) = f(x, 1) = 0. \quad (2.7)$$

The arbitrary constant p_0 can be eliminated from equation (2.5) by writing

$$f(x, y) = g(x, y) - Ca Re p_0 h(x, y). \quad (2.8)$$

Substituting this into equation (2.5), we get the two equations,

$$\frac{\partial^2 g}{\partial x^2} + \frac{\partial^2 g}{\partial y^2} = -\text{Ca Re } p , \quad (2.9a)$$

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = 1 . \quad (2.9b)$$

The functions $g(x,y)$ and $h(x,y)$ are made to satisfy homogeneous boundary conditions as indicated in equation (2.7). The constant p_0 can now be computed by substituting equation (2.8) into equation (2.6). This gives

$$p_0 = \frac{1}{\text{Ca Re}} \left[\iint g(x,y) dx dy \right] / \left[\iint h(x,y) dx dy \right] . \quad (2.10)$$

We now turn to the thermal boundary conditions. The left and right surfaces of the cube are maintained at fixed temperatures and all the other surfaces are insulated. These conditions can be written as,

$$T = 1/2 , \quad x = 0 , \quad (2.11a)$$

$$T = -1/2 , \quad x = 1 , \quad (2.11b)$$

$$\frac{\partial T}{\partial y} = 0 , \quad y = 0, 1 , \quad (2.11c)$$

$$\frac{\partial T}{\partial z} = 0 , \quad z = 0, 1 . \quad (2.11d)$$

2.3 NUMERICAL METHOD

We are interested in studying both the steady state and transient velocity and temperature fields. To this end we decided to use an explicit time differencing scheme for discretizing equations (2.2) and (2.3) in time. In a semi-discrete form, the momentum and energy equations can be written as

$$\frac{\vec{u}^{n+1} - \vec{u}^n}{\Delta t} + (\vec{u}^n \cdot \nabla) \vec{u}^n = -\nabla p^{n+1} + \frac{1}{\text{Re}} \nabla^2 \vec{u}^n, \quad (2.12)$$

$$\frac{T^{n+1} - T^n}{\Delta t} + (\vec{u}^n \cdot \nabla) T^n = \frac{1}{\text{PrRe}} \nabla^2 T^n, \quad (2.13)$$

where the superscripts indicate the time level. Although the pressure term is evaluated at time level $n+1$ in equation (2.12), the method remains explicit, for a Poisson equation for pressure can be obtained by taking the divergence of equation (2.1) and the pressure solved before the velocity field is advanced in time. The Poisson equation for pressure can be written as,

$$\nabla^2 p^{n+1} = -\frac{1}{\Delta t} \nabla \cdot (\vec{u}^{n+1} - \vec{u}^n) - \nabla \cdot [(\vec{u}^n \cdot \nabla) \vec{u}^n] + \frac{1}{\text{Re}} \nabla^2 (\nabla \cdot \vec{u}^n). \quad (2.14)$$

The right hand side of equation (2.14) involves a divergence term at time level level $n+1$. To eliminate this term we follow Harlow & Welch (1965) and force this dilation of the velocity field to be zero at the new time level, i.e.

$$\nabla \cdot \vec{u}^{n+1} = 0. \quad (2.15)$$

Equation (2.15) can now be used in equation (2.14) to get

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t} \nabla \cdot \vec{u}^n - \nabla \cdot [(\vec{u}^n \cdot \nabla) \vec{u}^n], \quad (2.16)$$

where the contribution from the diffusive terms can be set equal to zero according to equation (2.1) evaluated at time level n . It was found that retaining this term does not significantly affect the iterative convergence when the Poisson equation was solved by successive over-relaxation during the intermediate time steps. Retaining the unsteady dilation term in equation (2.16) is, however, essential to avoid numerical instability, as discussed by Harlow and Welch (1965) and Roache (1972). Boundary conditions for pressure can be obtained by satisfying the appropriate momentum equations (2.12) along the boundaries. Thus,

$$\frac{\partial p^{n+1}}{\partial x} = -(\vec{u}^n \cdot \nabla) u^n + \frac{1}{\text{Re}} \left[\frac{\partial^2 u^n}{\partial x^2} + \frac{\partial^2 u^n}{\partial y^2} + \frac{\partial^2 u^n}{\partial z^2} \right], \quad x = 0, 1, \quad (2.17a)$$

$$\frac{\partial p^{n+1}}{\partial y} = -(\vec{u}^n \cdot \nabla) v^n + \frac{1}{\text{Re}} \left[\frac{\partial^2 v^n}{\partial x^2} + \frac{\partial^2 v^n}{\partial y^2} + \frac{\partial^2 v^n}{\partial z^2} \right], \quad y = 0, 1, \quad (2.17b)$$

$$\frac{\partial p^{n+1}}{\partial z} = -(\vec{u}^n \cdot \nabla) w^n + \frac{1}{\text{Re}} \left[\frac{\partial^2 w^n}{\partial x^2} + \frac{\partial^2 w^n}{\partial y^2} + \frac{\partial^2 w^n}{\partial z^2} \right], \quad z = 0, 1. \quad (2.17c)$$

The coupled set of partial differential equations (2.12), (2.13), and (2.16) was solved numerically using finite difference techniques. All spatial derivatives were discretized using second order accurate central differences. The derivative boundary conditions, namely, equations (2.11c) and (2.11d) for temperature and equation (2.4d) for velocity were represented by second order accurate one-sided differences.

The Poisson equation (2.16) together with equations (2.17) lead to the well known Neumann problem for pressure (Briley, 1974, Ghia et al., 1977, Abdallah, 1987). As mentioned before, since the pressure must satisfy Neumann conditions at the boundaries, a solution is possible only if the pressure field satisfies an integral constraint given by,

$$\iiint \nabla^2 p \, dV = \iint \frac{\partial p}{\partial n} \, dS. \quad (2.18)$$

In order for the numerical scheme to converge to a steady state solution, the pressure field has to satisfy the discretized form of equation (2.18) after each time step. If the pressure field does not satisfy this constraint, then it has to be corrected in a manner described in Briley (1974) and Ghia et al. (1977), so that equation (2.18) is satisfied in discrete form. We followed Abdallah (1987), and although we used slightly different finite difference expressions for equations (2.16) and (2.17), we retained the advantage of his approach that leads to finite difference equations that faithfully represent the integral constraint (2.18) in discretized form. As a result the pressure field automatically satisfies this equation to machine accuracy during each time step. With reference to the grid indices given in Figure 2.1 the finite difference form of equation (2.16) is,

$$\frac{p_{i+1,j,k} - 2p_{i,j,k} + p_{i-1,j,k}}{(\Delta x)^2} + \frac{p_{i,j+1,k} - 2p_{i,j,k} + p_{i,j-1,k}}{(\Delta y)^2} + \frac{p_{i,j,k+1} - 2p_{i,j,k} + p_{i,j,k-1}}{(\Delta z)^2} = -c_{i,j,k}$$

Figure 2.1. Geometry and grid indices

$$-\frac{1}{\Delta t} \left[\frac{u_{i+1,j,k} - u_{i-1,j,k}}{2(\Delta x)} + \frac{v_{i,j+1,k} - v_{i,j-1,k}}{2(\Delta y)} + \frac{w_{i,j,k+1} - w_{i,j,k-1}}{2(\Delta z)} \right], \quad (2.19)$$

where $c_{i,j,k}$ is the finite difference form of the divergence of the acceleration term in equation (2.16). This is given by

$$\begin{aligned} c_{i,j,k} = & \frac{1}{\Delta x} \left[u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} \right]_{i+1/2,j,k} - \frac{1}{\Delta x} \left[u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} \right]_{i-1/2,j,k} \\ & + \frac{1}{\Delta y} \left[u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} \right]_{i,j+1/2,k} - \frac{1}{\Delta y} \left[u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} \right]_{i,j-1/2,k} \\ & + \frac{1}{\Delta z} \left[u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} \right]_{i,j,k+1/2} - \frac{1}{\Delta z} \left[u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} \right]_{i,j,k-1/2} \end{aligned} \quad (2.20a)$$

Here and in what follows the superscripts have been dropped for convenience. In the above equation the terms are evaluated in a manner described in Abdallah (1987). For example,

$$\begin{aligned} u_{i+1/2,j,k} &= \frac{u_{i,j,k} + u_{i+1,j,k}}{2}, \\ \left[\frac{\partial u}{\partial x} \right]_{i+1/2,j,k} &= \frac{u_{i+1,j,k} - u_{i,j,k}}{\Delta x}, \\ \left[\frac{\partial u}{\partial y} \right]_{i+1/2,j,k} &= \frac{u_{i+1,j+1,k} - u_{i+1,j-1,k} + u_{i,j+1,k} - u_{i,j-1,k}}{4 \Delta y}, \\ \left[\frac{\partial u}{\partial z} \right]_{i+1/2,j,k} &= \frac{u_{i+1,j,k+1} - u_{i+1,j,k-1} + u_{i,j,k+1} - u_{i,j,k-1}}{4 \Delta z}. \end{aligned}$$

The pressure boundary conditions (2.17) are applied at the mid-plane between the boundary and the grid line nearest to it. For example, equation (2.17a) is applied at $i = 1/2$, and $L+1/2$ instead of at $x = 0$ and 1. This can be written in finite difference form as,

$$\frac{p_{m,j,k} - p_{m-1,j,k}}{\Delta x} = - \frac{u_{m,j,k}^2 - u_{m-1,j,k}^2}{2(\Delta x)}$$

$$\begin{aligned}
& - (v_{m,j,k} + v_{m-1,j,k}) \frac{u_{m,j+1,k} - u_{m,j-1,k} + u_{m-1,j+1,k} - u_{m-1,j-1,k}}{8(\Delta y)} \\
& - (w_{m,j,k} + w_{m-1,j,k}) \frac{u_{m,j,k+1} - u_{m,j,k-1} + u_{m-1,j,k+1} - u_{m-1,j,k-1}}{8(\Delta z)} \\
& + \frac{u_{m,j+1,k} - 2u_{m,j,k} + u_{m,j-1,k} + u_{m-1,j+1,k} - 2u_{m-1,j,k} + u_{m-1,j-1,k}}{2 \operatorname{Re}(\Delta y)^2} \\
& - \frac{v_{m,j+1,k} - v_{m,j-1,k} - v_{m-1,j+1,k} + v_{m-1,j-1,k}}{2 \operatorname{Re}(\Delta y)(\Delta z)} \\
& - \frac{w_{m,j,k+1} - w_{m,j,k-1} - w_{m-1,j,k+1} + w_{m-1,j,k-1}}{2 \operatorname{Re}(\Delta x)(\Delta z)} \\
& + \frac{u_{m,j,k+1} - 2u_{m,j,k} + u_{m,j,k-1} + u_{m-1,j,k+1} - 2u_{m-1,j,k} + u_{m-1,j,k-1}}{2 \operatorname{Re}(\Delta z)^2}, \\
& m = 1, L+1, 1 \leq j \leq M, 1 \leq k \leq N.
\end{aligned} \tag{2.21}$$

Similar expressions can be written down for equations (2.17b) and (2.17c). In approximating $\partial^2 u / \partial x^2$ in equation (2.17a) by finite differences, equation (2.15) evaluated at time level n , can be used to write,

$$\frac{\partial^2 u}{\partial x^2} = - \left[\frac{\partial^2 v}{\partial x \partial y} + \frac{\partial^2 w}{\partial x \partial z} \right].$$

Abdallah (1987) used a similar device while working with the vorticity. Written in this manner, equation (2.20) represents the discretized form of equation (2.16).

For each time step the velocity and temperature fields are updated using existing values of pressure. The boundary values are then updated. Using the new values of velocity, the Poisson equation for pressure is solved. This was carried out by a point SOR scheme with odd-even ordering which speeds the calculations greatly in vector computers (Press et al., 1986). For all the steady state solutions discussed below, only 20 to 30 iterations of the Poisson equation were carried out between time steps. When accurate transient solutions were sought then we iterated the pressure Poisson equation was iterated to values below the truncation error of the method. With the new values of the pressure field, the velocity and

temperature fields are updated again and the entire procedure repeated until a suitable convergence criterion was satisfied. In order to study the convergence of the numerical scheme towards a steady state, the relative change in the values of the field variables at the end of each time step was calculated via the formula

$$\varepsilon = \left| 1 - \frac{\phi^{n+1}}{\phi^n} \right|,$$

where the superscripts refer to successive time step values for a field variable. For all the results reported here, the convergence criterion was satisfied when the value of ε was less than 10^{-5} . All the calculations were carried out on the Cray X-MP/28 at the Ohio Supercomputer Center.

2.4 RESULTS & DISCUSSION

To validate the numerical method, some calculations for the driven flow in a cubical box were carried out. A detailed discussion of this problem is postponed until Chapter IV. Solutions to this problem have been published by Osswald et al. (1987) and Ku et al. (1987). The pseudo-spectral solutions obtained by Ku et al. (1987) are very accurate and the accuracy of the present numerical method can be ascertained by comparing our results with those presented by them. The computations reported below were carried out on a uniform $21 \times 21 \times 21$ grid at a Reynolds number of 100. The solutions are presented in Figure 2.2. Superimposing the plots of plane projections of the velocity vectors and contours of constant values of the third velocity component gives an effective way to view the three dimensional vector field. This has been done for three mutually orthogonal planes in the cube. To make the weak motions visible the arrows in the different views in these figures do not in general represent the same magnitudes of velocities. In the contours the solid lines depict positive values for the variables and the dashed lines represent negative values. The solutions shown correspond to conditions at the end of 1000 time steps, at which time the value of ε was less than 10^{-5} for *all* the field variables. The entire calculation took about 70 seconds of CPU

Figure 2.2. Velocity vectors in three mutually orthogonal planes for shear driven flow in a cube at $Re = 100$, (a) $z = 0.5$, (b) $y = 0.5$, and (c) $x = 0.5$

time on the Cray X-MP/28.

The velocity vector fields for the driven cavity compare very well with those of Osswald et al. (1987). The plots of the u - and v -velocities along the horizontal and vertical centerlines of the cube are also nearly identical with those given in Ku et al. (1987). The flow pattern is similar to the two-dimensional case. It consists of a vortex the center of which is shifted toward the upper right corner, as shown in Figure 2.2b. Since our results are for $Re=100$ the flow is neither a Stokes flow, nor is it one for which distinct boundary layers have developed along the walls. Nevertheless, the flow behaves more like a large Reynolds number flow than a very viscous one. In order to explain the physical mechanisms at work in the flow one would need to carry out solutions for larger values of Reynolds number from which hopefully the asymptotic structure would emerge. Some progress in explaining the mechanisms has been made by Mallinson and de Vahl Davis (1977). They elaborate on the reasoning of Davis (1967), who noted that the rotating vortex interacts with the end walls in a way that has a resemblance to Bödewadt's (1940) boundary layer solution. If Re is sufficiently large these boundary layers do exist next to the end walls, which in Figure 2.2a are the top and bottom walls and in Figure 2.2c the side walls. The core pressure distribution would cause an inward spiraling flow near these walls towards the axis of the vortex. To satisfy continuity the fluid in the wall layers has to be injected into the core. Weak ejection of fluid near the walls is visible in Figures 2.2a and c.

The results for thermocapillary flow presented here are for a fluid with Prandtl number equal to 0.01 and thermocapillary Reynolds number equal to 100 and for a fluid with $Pr=1$ and $Re=100$ and 300. The calculations were carried out on $31 \times 31 \times 21$ uniform grid for $Re=100$ and on a $41 \times 31 \times 21$ uniform grid when Re was increased to 300. These solutions took 10-20 minutes of CPU time on the Cray X-MP/28. To get an idea of the accuracy of the thermocapillary simulation we computed values for the total heat transfer across each vertical plane. They agree to within 5%, which is reasonable considering the coarseness of our grids. A check of the residual of the continuity equation shows that it is satisfied to second order accuracy for all but 1% of the total number of points when the thermocapillary Reynolds number was 100 and in all but 5% of the points when Re was 300.

The results for thermocapillary convection are in many ways quite similar to those for the lid-driven flow. The velocity vector plots in Figure 2.3 show the presence of a vortex in the $y = 0.5$ plane, with the fluid on the surface being pulled toward the cold wall near which the surface tension is largest. In Figure 2.4 the main velocity component on the free surface is seen to be largest along the centerline $y = 0.5$. As a result, convection causes the thermal field to vary in such a way that the temperature of the fluid particles along this centerline is always larger than the temperature of the neighboring ones, albeit only slightly so. Nevertheless, the variation is sufficient to cause a slight span-wise flow along the surface, as can be seen from Figure 2.3c. This lateral flow accentuates the effect caused by the main vortex on the flow along the wall layers; an effect that alone caused the injection of fluid from the wall layers in the lid-driven flow and leads to what appears in Figure 2.3c to be two small vortices along the end walls near the free surface. One would expect the end walls to have a retarding effect on the flow. This effect is best seen from Figure 2.3a. The contour plots in this figure, which is a top view of the $z = 0.5$ plane, show this well, for the velocity of the sinking fluid on the right half is larger near the center than next to the end walls. The same is true for the rising fluid on the left.

The qualitative trend of the main component of the surface velocity, as seen in Figure 2.5, is the same as in the two dimensional case investigated by Zebib et al. (1985) and Ramanan and Korpela (1990). This is to be expected since the flow is only weakly three dimensional for the thermal boundary conditions imposed. Interestingly the centerline surface velocities in the three dimensional cases are larger than for the two-dimensional flow if the Marangoni number $Ma=RePr$ is 100 or 300, but this is not so when $Ma=1$, which corresponds to $Pr=0.01$ and $Re=100$. In the low Prandtl number fluid conduction of heat dominates convection, with the result that the temperature in the bulk fluid, as well as along the top surface, drops linearly across the cavity, as seen in Figure 2.6. For larger values of Ma convection becomes more important and the hot fluid is carried closer to the cold wall along the free surface. As a result, the temperature gradients are larger near the cold wall. It is these large gradients that are responsible for the higher surface velocities in the three dimensional flows.

Figure 2.3. Velocity vectors in three mutually orthogonal planes for thermocapillary convection in a cube at $Re = 100$, (a) $z = 0.5$, (b) $y = 0.5$, and (c) $x = 0.5$

Figure 2.4. u-velocity on the free surface

Figure 2.5. u-velocity on the free surface for the two-dimensional flow compared with its counterpart along the centerline in a three-dimensional flow

Figure 2.6. Temperature on the free surface for the two-dimensional flow compared with its counterpart along the centerline in a three-dimensional flow

The surface temperature distribution for $Re=100$, $Pr=1$ is shown in Figure 2.7. Although the eye position for viewing this plot is not the best, it was thought prudent to always give a view of the surface quantities from the same eye position, even if in this figure much of the surface variation is hidden. Since the Marangoni number is relatively small, the surface temperature still is predominantly linear and shows very little variation in the y -direction. The deflection of the free surface for $Re=100$, $Pr=1$ is shown in Figure 2.8. The magnitudes of the deflections have been exaggerated to show the details clearly. Again, owing to small magnitude of the Marangoni number, these deflections show little variation in the y -direction, except near the end walls where they decrease to zero.

2.5 A CRITICISM OF THE METHOD OF SOLUTION

We now take a critical look at the solution methodology presented above with a view to identifying the shortcomings of the method and thus provide the motivation for the improvements to be presented in Chapter 4. The main criticism of this method is that it is not possible to obtain accurate transient solutions with it. There are two reasons for this. The first is that the boundary conditions for pressure from equation (2.17) are applied on the planes midway between the boundaries and the grid surfaces closest to them, instead of on the boundaries themselves. If a true transient solution is desired, this is inconsistent since the time derivative was dropped from this equation. Dropping of the time derivative would be allowed if the condition were applied on the boundaries. The time derivative had to be neglected in equation (2.17), for its discretized form requires knowing the velocity field at time level $n+1$, which is undetermined.

The second reason for the inability to obtain true transient solutions is the slow iterative convergence of the Neumann-Poisson problem between each time step. If accurate transient solutions are desired, then the Poisson equation has to be iterated until the residuals are below the truncation error of the method at the end of each time step. It is not possible to achieve this with the present method since the number of iterations increases greatly as a result of the poor iterative convergence of the Neumann-Poisson problem. The spectral radius of SOR iterations with the optimal value for the acceleration parameter is given by

Figure 2.7. Temperature distribution on the free surface at $Re = 100$

Figure 2.8. Free surface deflections for thermocapillary flow at $Re = 100$

(Young, 1962),

$$\rho_{SOR} = \left[\frac{\cos \frac{\pi}{L}}{1 + \sin \frac{\pi}{L}} \right]^2, \quad (2.22)$$

where, L is the total number of grid points in any direction. For large values of L this gives

$$\rho_{SOR} = 1.0 - \frac{2\pi}{L}. \quad (2.24)$$

Since for large L , the spectral radius is close to one, poor convergence results.

One can overcome the slowdown in convergence by either using multi-grid methods or direct methods to solve for the pressure during each time step. Multi-grid methods have been used by Ghia, Ramamurti and Ghia (1988). Direct methods for solving the Neumann-Poisson problem can yield machine accurate solutions on a given grid. A disadvantage of direct methods, however, is that they are restricted to regular domains. The linear algebraic system of equations of the Neumann-Poisson problem have a block tridiagonal structure and so direct methods can be used to solve this system. A survey of direct methods for the Poisson equation together with operation counts is given by Dorr (1970). Two of these schemes are attractive by virtue of their operation counts and vectorizability, namely, the Buneman odd-even reduction scheme (Buneman, 1969) and the method of matrix decomposition (Buzbee, Golub and Nielson, 1970). Buneman developed the original odd-even reduction method for Dirichlet problems but it has been extended to include other types of boundary conditions also (Buzbee et al., 1970). In studying the method of matrix decomposition, we saw how to extend it to the three dimensional Neumann-Poisson problem at least for uniform grids and decided to implement it.

For many problems in fluid dynamics, sharp gradients occur in the flow field close to the boundaries and these gradients have to be resolved accurately. In order to do so, fine grid spacings have to be used in regions of sharp gradients and if uniform grid spacings were to be used throughout the domain, a large number of grid points would be needed to cover the

entire flow domain. Since farther way from the boundaries the gradients in the flow field become milder and coarser grids would adequately serve to resolve the flow, it would be desirable to use non-uniform grid spacings with fine grids in regions of sharp gradients and coarse grids in all the other regions. This opens the task of extending the method of matrix decomposition for solving the Neumann-Poisson problem to non-uniform grids. We have been successful in carrying it out. In the next chapter, we review the use of the method of matrix decomposition for the solution of the two- and three-dimensional Poisson's equation on uniform grids and show how to extend it to non-uniform grids.

CHAPTER III

A DIRECT METHOD FOR SOLVING POISSON'S EQUATION

In this chapter, we consider the method of matrix decomposition (Buzbee et al, 1970) for obtaining fast, direct solutions to the Neumann-Poisson problem for pressure, that arises during the solution of the incompressible Navier-Stokes equations in primitive variable form. In an attempt to keep the discussion general, the application of this method for solving Poisson's equation subject to Dirichlet boundary conditions will also be discussed. This problem arises, for example, during the solution of two dimensional Navier-Stokes equations in streamfunction-vorticity form. In sections 3.1.1 and 3.1.2, the relationship of the method of matrix decomposition to Fourier methods (Le Bail, 1972, Pickering, 1986) is established and in section 3.2, its application to the three dimensional Neumann-Poisson problem is discussed. In section 3.3, the extension to non-uniform grids is presented. Finally, in section 3.4, an analysis of its performance on the Cray Y-MP8/864 is discussed.

3.1 MATRIX DECOMPOSITION ON UNIFORM GRIDS

Consider solving

$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} = c, \quad (3.1)$$

inside the rectangle $0 \leq x \leq 1$, $0 \leq y \leq A$ subject to either Dirichlet or Neumann boundary conditions. Equation (3.1) can be written in finite-difference form as,

$$p_{i+1,j} + p_{i-1,j} + p_{i,j+1} + p_{i,j-1} - 4p_{i,j} = \Delta x^2 c_{i,j}, \quad (3.2)$$

if we take $\Delta x = \Delta y$.

3.1.1 DIRICHLET PROBLEM

For the Dirichlet problem values for the dependent variable are specified along the boundaries, $i=0, L+1$ and $j=0, M+1$. Equation (3.2) is applied at all the interior points and the boundary points that occur in these finite-difference equations can be taken to the right hand side. The resulting system of linear algebraic equations can then be written in a block tridiagonal form as,

$$\begin{bmatrix} G & I & . & . & . \\ I & G & I & . & . \\ . & . & . & . & . \\ . & . & I & G & I \\ . & . & . & I & G \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ . \\ . \\ q_M \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ . \\ . \\ d_M \end{bmatrix}, \quad (3.3)$$

where,

$$q_j = \begin{bmatrix} p_{1,j} \\ p_{2,j} \\ . \\ . \\ p_{L,j} \end{bmatrix}, \quad d_j = \begin{bmatrix} c_{1,j} \\ c_{2,j} \\ . \\ . \\ c_{L,j} \end{bmatrix}.$$

Those elements $c_{i,j}$ on the grid lines closest to the boundaries, namely, $i=1, L$, $j=1, M$ now include the terms from the boundary conditions also. The matrix I is the identity matrix and the matrix G is the tridiagonal matrix,

$$G = \begin{bmatrix} -4 & 1 & . & . & . \\ 1 & -4 & 1 & . & . \\ . & . & . & . & . \\ . & . & 1 & -4 & 1 \\ . & . & . & 1 & -4 \end{bmatrix}.$$

The method of matrix decomposition is, in essence, the separation of variables applied to equation (3.3). The first step is to diagonalize the matrix G so that $S^T G S = \Lambda$, where, S is the matrix of eigenvectors and Λ is the diagonal matrix of eigenvalues of the eigenvalue

problem $G s_i = \lambda_i s_i$. This diagonalization results in the separation of the x-coordinate and yields a one dimensional problem on each grid line parallel to the y-axis. Equation (3.3) can now be written, for $1 \leq i \leq L$ as,

$$\begin{aligned} \lambda_i \bar{p}_{i,1} + \bar{p}_{i,2} &= \bar{c}_{i,1} , \\ \bar{p}_{i,j-1} + \lambda_i \bar{p}_{i,j} + \bar{p}_{i,j+1} &= \bar{c}_{i,j} , \quad 2 \leq j \leq M-1 , \\ \bar{p}_{i,M-1} + \lambda_i \bar{p}_{i,M} &= \bar{c}_{i,M} , \end{aligned} \quad (3.4)$$

where

$$(\bar{p}_{1,j}, \bar{p}_{2,j}, \dots, \bar{p}_{L,j})^T = S^{-1} (p_{1,j}, p_{2,j}, \dots, p_{L,j})^T ,$$

and

$$(\bar{c}_{1,j}, \bar{c}_{2,j}, \dots, \bar{c}_{L,j})^T = S^T (c_{1,j}, c_{2,j}, \dots, c_{L,j})^T .$$

These tridiagonal systems can be easily solved using the Thomas algorithm. Once all the $\bar{p}_{i,j}$'s have been obtained, we can get p from

$$\begin{bmatrix} p_{1,j} \\ p_{2,j} \\ \vdots \\ p_{L,j} \end{bmatrix} = S \begin{bmatrix} \bar{p}_{1,j} \\ \bar{p}_{2,j} \\ \vdots \\ \bar{p}_{L,j} \end{bmatrix} , \quad 1 \leq j \leq M . \quad (3.5)$$

The eigenvectors of G can be obtained analytically (Smith, 1985). The eigenvectors turn out to be sines and this makes the relationship of these methods to Fourier transform methods clear, for, if a Fourier transform method were used to solve this problem, sines would be used as the expansion functions (Le Bail, 1972). Thus, for this problem, matrix decomposition turns out to be identical to solving it with discrete Fourier transform methods.

3.1.2 NEUMANN PROBLEM

We now turn to the Neumann problem where the normal derivatives for p are prescribed on the boundaries. It is well known that a solution to this problem is unique only to an arbitrary constant and it is subject to an integral constraint of the form,

$$\iint c \, dA = \int \frac{\partial p}{\partial n} \, ds . \quad (3.6)$$

Equation (3.2) can be applied at all points including the boundaries after introducing a row of fictitious grid points outside the domain. These fictitious grid points can then be eliminated from the finite difference equations by using central differences for discretizing the boundary conditions. Alternatively, one can apply equation (3.2) at the interior points alone. The boundary points that occur in these finite difference equations can be eliminated by using second order accurate *one sided* differences for discretizing the boundary conditions.

If one uses central differences at the boundaries, the following block tridiagonal system of equations can be obtained after the fictitious grid points have been eliminated using the boundary conditions :

$$\begin{bmatrix} G/2 & A & . & . & . \\ A & G & A & . & . \\ . & . & . & . & . \\ . & . & A & G & A \\ . & . & . & A & G/2 \end{bmatrix} \begin{bmatrix} q_0 \\ q_1 \\ . \\ . \\ q_{M+1} \end{bmatrix} = \begin{bmatrix} d_0 \\ d_1 \\ . \\ . \\ d_{M+1} \end{bmatrix}, \quad (3.7)$$

where

$$G = \begin{bmatrix} -2 & 1 & . & . & . \\ 1 & -4 & 1 & . & . \\ . & . & . & . & . \\ . & . & 1 & -4 & 1 \\ . & . & . & 1 & -2 \end{bmatrix}, \quad A = \begin{bmatrix} 1/2 & . & . & . & . \\ . & 1 & . & . & . \\ . & . & . & . & . \\ . & . & . & 1 & . \\ . & . & . & . & 1/2 \end{bmatrix}.$$

Here, the q_j 's and the d_j 's are defined in the same manner as before and the $c_{i,j}$'s on the

boundaries include terms from the boundary conditions also. In going from equation (3.2) to (3.7), some of the equations have been adjusted so that G becomes symmetric. There are two reasons for doing this. The first one is that it is much easier to work with symmetric matrices since they are guaranteed to have real eigenvalues and eigenvectors. The second reason is as follows. If G is symmetric, the block tridiagonal matrix on the left hand side of equation (3.7) becomes symmetric. Now, if all the rows of this block tridiagonal matrix were added together, the resulting row would consist entirely of zeroes (Mitchell, 1969). For this system to be consistent, the sum of all the elements of the right hand side should be equal to zero as well, which can be thought of as the solvability constraint. This solvability constraint is the discretized form of the integral constraint, equation (3.6). Forcing G , and hence the block tridiagonal matrix on the left hand side of equation (3.7), to be symmetric facilitates exhibiting the solvability constraint and the linear dependency in this system of equations. Here and in the rest of this chapter it is assumed that the given right hand vector c satisfies the above solvability constraint to machine accuracy. In the next chapter, we will consider the case when this is not so. We now turn to the application of the matrix decomposition method to solving this system.

As before, the first step of matrix decomposition is to diagonalize G . But now, the matrices G and A have to be diagonalized simultaneously such that

$$S^T G S = \Lambda, \quad S^T A S = I.$$

Here, S is the matrix of eigenvectors and Λ is the diagonal matrix of eigenvalues of the general eigenvalue problem $G s_i = \lambda_i A s_i$. Equation (3.7) can be written as,

$$\begin{aligned} \lambda_i/2 \bar{p}_{i,0} + \bar{p}_{i,1} &= \bar{c}_{i,0}, \\ \bar{p}_{i,j-1} + \lambda_i \bar{p}_{i,j} + \bar{p}_{i,j+1} &= \bar{c}_{i,j}, \quad 1 \leq j \leq M, \\ \bar{p}_{i,M} + \lambda_i/2 \bar{p}_{i,M+1} &= \bar{c}_{i,M+1}, \end{aligned} \tag{3.8}$$

where, the $\bar{p}_{i,j}$'s and the $\bar{c}_{i,j}$'s are defined in the same manner as before. Again, Thomas algorithm can be used to solve these tridiagonal systems. However, the tridiagonal matrix

corresponding to $i=L+1$ is singular owing to the system of equations being linearly dependent, as already mentioned. The procedure, then, is to set $\bar{p}_{L+1,M+1}$ arbitrarily to zero and solve for the remaining $\bar{p}_{i,j}$'s (Pickering, 1986). This is allowed since the solution to equation (3.7) can be determined only up to an arbitrary constant. Once all the $\bar{p}_{i,j}$'s have been obtained, we can get p from an equation similar to (3.5).

One can derive the eigenvectors of the problem $A^{-1}G s_i = \lambda_i s_i$ analytically as before (Pickering, 1986) and in this case they are cosines. If Fourier transform methods were used, cosines would be used as expansion functions (Le Bail, 1972), thus showing that the two methods are identical for this case also.

An alternative to using central differences for the boundary conditions is to discretize them using second order accurate one sided differences as shown below, for example along $x=0$:

$$\frac{-p_{2,j} + 4p_{1,j} - 3p_{0,j}}{2\Delta x} = \left[\frac{\partial p}{\partial x} \right]_{i=0}, \quad 1 \leq j \leq M. \quad (3.9)$$

The right hand side of equation (3.9) is prescribed as boundary condition and when equation (3.2) is applied in the interior of the domain, boundary points that occur in those finite difference equations can be eliminated using equations similar to and including (3.9) to yield

$$\begin{bmatrix} 3G/2+2A & A & . & . & . \\ A & G & A & . & . \\ . & . & . & . & . \\ . & . & A & G & A \\ . & . & . & A & 3G/2+2A \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ . \\ . \\ q_M \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ . \\ . \\ d_M \end{bmatrix}, \quad (3.10)$$

where, now,

$$G = \begin{bmatrix} -4 & 1 & . & . & . \\ 1 & -4 & 1 & . & . \\ . & . & . & . & . \\ . & . & 1 & -4 & 1 \\ . & . & . & 1 & -4 \end{bmatrix}, \quad A = \begin{bmatrix} 3/2 & . & . & . & . \\ . & 1 & . & . & . \\ . & . & . & . & . \\ . & . & . & 1 & . \\ . & . & . & . & 3/2 \end{bmatrix}.$$

As before, we have forced G and hence the block tridiagonal matrix on the left hand side of equation (3.10) to be symmetric. From this point on, the solution procedure is identical to that described for the first scheme and hence will not be repeated. Following Pickering (1986), the eigenvectors for this case also can be obtained analytically. In this case, the eigenvectors turn out to be linear combination of sines, as shown in the Appendix.

Before concluding this section, we digress a bit and consider the consistent differencing scheme of the previous chapter with a view to establishing its relationship with the two schemes described above. In the consistent differencing scheme, equation (3.2) is applied at all the interior points and the boundary points that occur in these finite-difference equations are eliminated using boundary conditions that are applied along $i = 1/2, L+1/2$ and $j = 1/2, M+1/2$. The resulting algebraic system can be written as,

$$\begin{bmatrix} G+I & I & . & . & . \\ I & G & I & . & . \\ . & . & . & . & . \\ . & . & I & G & I \\ . & . & . & I & G+I \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ . \\ . \\ q_M \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ . \\ . \\ d_M \end{bmatrix},$$

where, now,

$$G = \begin{bmatrix} -3 & 1 & . & . & . \\ 1 & -4 & 1 & . & . \\ . & . & . & . & . \\ . & . & 1 & -4 & 1 \\ . & . & . & 1 & -3 \end{bmatrix}.$$

The $c_{i,j}$'s next to the boundaries now include the terms from the boundary conditions also. Unlike in the previous two schemes, the block tridiagonal matrix on the left hand side of this system is already symmetric. It is easy to verify that the sum of all the rows on the left hand side of this system would yield a row consisting entirely of zeroes. Hence, the sum of all the right hand side elements should be equal to zero as well. With this solvability condition established, the solution to this system can now be obtained by matrix decomposition method.

3.2 THE NEUMANN PROBLEM IN THREE DIMENSIONS

Here, we consider the three dimensional Poisson equation

$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} + \frac{\partial^2 p}{\partial z^2} = c, \quad (3.11)$$

subject to prescribed values of the normal derivative of pressure on the boundaries. The method of solution for equation (3.11) is very similar to the two dimensional case and so only those details which are different will be given. Equation (3.11) is discretized using central differences as usual and the derivative boundary conditions are discretized using second order accurate one sided differences. To make things simpler, it is also assumed that $\Delta x = \Delta y = \Delta z$. The resulting set of finite-difference equations can be written in the familiar block tridiagonal form shown below, after the boundary terms have been eliminated :

$$\begin{bmatrix} 3H/2+2B & B & . & . & . \\ B & H & B & . & . \\ . & . & . & . & . \\ . & . & B & H & B \\ . & . & . & B & 3H/2+2B \end{bmatrix} \begin{bmatrix} r_1 \\ r_2 \\ . \\ . \\ r_N \end{bmatrix} = \begin{bmatrix} e_1 \\ e_2 \\ . \\ . \\ e_N \end{bmatrix}, \quad (3.12)$$

where

$$r_k = \begin{bmatrix} q_{1,k} \\ q_{2,k} \\ . \\ . \\ q_{M,k} \end{bmatrix}, \quad q_{j,k} = \begin{bmatrix} p_{1,j,k} \\ p_{2,j,k} \\ . \\ . \\ p_{L,j,k} \end{bmatrix},$$

and

$$e_k = \begin{bmatrix} d_{1,k} \\ d_{2,k} \\ . \\ . \\ d_{M,k} \end{bmatrix}, \quad d_{j,k} = \begin{bmatrix} c_{1,j,k} \\ c_{2,j,k} \\ . \\ . \\ c_{L,j,k} \end{bmatrix},$$

As before, those elements $c_{i,j,k}$ on the grid surfaces closest to the walls, namely, $i=1,L, j=1,M, k=1,N$ now include the terms from the boundary conditions also. The matrix H is a block tridiagonal matrix and the matrix B is a block diagonal matrix,

$$H = \begin{bmatrix} 3G/2+2A & A & . & . & . \\ A & G & A & . & . \\ . & . & . & . & . \\ . & . & A & G & A \\ . & . & . & A & 3G/2+2A \end{bmatrix}, \quad B = \begin{bmatrix} 3A/2 & . & . & . & . \\ . & A & . & . & . \\ . & . & . & . & . \\ . & . & . & A & . \\ . & . & . & . & 3A/2 \end{bmatrix},$$

where

$$G = \begin{bmatrix} -7 & 1 & . & . & . \\ 1 & -6 & 1 & . & . \\ . & . & . & . & . \\ . & . & 1 & -6 & 1 \\ . & . & . & 1 & -7 \end{bmatrix}, \quad A = \begin{bmatrix} 3/2 & . & . & . & . \\ . & 1 & . & . & . \\ . & . & . & . & . \\ . & . & . & 1 & . \\ . & . & . & . & 3/2 \end{bmatrix}.$$

We also define the following vectors for later use,

$$q'_{i,k} = \begin{bmatrix} p_{i,1,k} \\ p_{i,2,k} \\ . \\ . \\ p_{i,M,k} \end{bmatrix}, \quad d'_{i,k} = \begin{bmatrix} c_{i,1,k} \\ c_{i,2,k} \\ . \\ . \\ c_{i,M,k} \end{bmatrix}.$$

It can be seen that both H and G have been made symmetric and by using the same arguments as for the two dimensional problem, it follows easily that the system given by equation (3.12) is overdetermined and that the right hand side elements have to satisfy a solvability constraint. Once this has been done, the method of matrix decomposition can be used to solve equation (3.12).

As before, we start by diagonalizing simultaneously the matrices G, A so that

$$S^T G S = \Lambda, \quad S^T A S = I,$$

Here S is the matrix of eigenvectors and Λ is the diagonal matrix of eigenvalues of the general eigenvalue problem $G s_i = \lambda_i A s_i$. This diagonalization results in the separation of the x-coordinate and yields a two dimensional problem involving the y- and the z-coordinates on each grid plane normal to the x-axis. Equation (3.12) can now be written as, for $1 \leq i \leq L$,

$$\begin{aligned} (3\tilde{G}_i/2+2\tilde{A}) \bar{q}'_{i,1} + \tilde{A} \bar{q}'_{i,2} &= \bar{d}'_{i,1} , \\ \tilde{A} \bar{q}'_{i,k-1} + \tilde{G}_i \bar{q}'_{i,k} + \tilde{A} \bar{q}'_{i,k+1} &= \bar{d}'_{i,k} , \quad 2 \leq k \leq N-1 \\ \tilde{A} \bar{q}'_{i,N-1} + (3\tilde{G}_i/2+2\tilde{A}) \bar{q}'_{i,N} &= \bar{d}'_{i,N} , \end{aligned} \quad (3.13)$$

where $\bar{q}'_{i,k} = S^{-1} q'_{i,k}$ and $\bar{d}'_{i,k} = S^T d'_{i,k}$ and

$$\tilde{G}_i = \begin{bmatrix} 3\lambda_i/2+2 & 1 & . & . & . \\ 1 & \lambda_i & 1 & . & . \\ . & . & . & . & . \\ . & . & 1 & \lambda_i & 1 \\ . & . & . & 1 & 3\lambda_i/2+2 \end{bmatrix}, \quad \tilde{A} = \begin{bmatrix} 3/2 & . & . & . & . \\ . & 1 & . & . & . \\ . & . & . & . & . \\ . & . & . & 1 & . \\ . & . & . & . & 3/2 \end{bmatrix}.$$

The next step is to diagonalize simultaneously the matrices $\tilde{G}_i, \tilde{A}$ so that

$$R_i^T \tilde{G}_i R_i = \Gamma_i, \quad R_i^T \tilde{A} R_i = I,$$

Here, R_i is the matrix of eigenvectors and Γ_i is the diagonal matrix of eigenvalues of the general eigenvalue problem $\tilde{G}_i \mathfrak{s}_j = \gamma_{i,j} \tilde{A} \mathfrak{s}_j$. It is worth noting that in the case where $L=M$, $\tilde{A}=A$ and $\tilde{G}_i A^{-1} G = G A^{-1} \tilde{G}_i$ and hence the same set of eigenvectors S can be used for this diagonalization also. This diagonalization results in the separation of the y-coordinate and yields a one dimensional problem involving the z-coordinate on each grid line parallel to the z-axis. Equation (3.13) can now be written as, for $1 \leq i \leq L, 1 \leq j \leq M$,

$$\begin{aligned} (3\gamma_{i,j}/2+2) \bar{\bar{p}}_{i,j,1} + \bar{\bar{p}}_{i,j,2} &= \bar{\bar{c}}_{i,j,1} , \\ \bar{\bar{p}}_{i,j,k-1} + \gamma_{i,j} \bar{\bar{p}}_{i,j,k} + \bar{\bar{p}}_{i,j,k+1} &= \bar{\bar{c}}_{i,j,k} , \quad 2 \leq k \leq N-1 \end{aligned} \quad (3.14)$$

$$\bar{\bar{p}}_{i,j,N-1} + (3\gamma_{i,j}/2+2) \bar{\bar{p}}_{i,j,N} = \bar{\bar{c}}_{i,j,N} ,$$

where

$$(\bar{\bar{p}}_{i,1,k}, \bar{\bar{p}}_{i,2,k}, \dots, \bar{\bar{p}}_{i,M,k})^T = R_i^{-1} \bar{q}'_{i,k} ,$$

and

$$(\bar{\bar{c}}_{i,1,k}, \bar{\bar{c}}_{i,2,k}, \dots, \bar{\bar{c}}_{i,M,k})^T = R_i^T \bar{d}'_{i,k} .$$

As before, these tridiagonal systems of equations can be solved by using the Thomas algorithm. Now, in the three dimensional case, the tridiagonal matrix corresponding to $i=L, j=M$ is singular and we proceed as before and set $\bar{\bar{p}}_{L,M,N}$ arbitrarily to zero and solve for the remaining $\bar{\bar{p}}_{L,M,k}$'s. Once all the $\bar{\bar{p}}_{i,j,k}$'s have been obtained, the p can be obtained easily from the sequence,

$$\bar{q}'_{i,k} = R_i \begin{bmatrix} \bar{\bar{p}}_{i,1,k} \\ \bar{\bar{p}}_{i,2,k} \\ \vdots \\ \bar{\bar{p}}_{i,M,k} \end{bmatrix} , \quad q'_{i,k} = \begin{bmatrix} p_{i,1,k} \\ p_{i,2,k} \\ \vdots \\ p_{i,M,k} \end{bmatrix} = S \bar{q}'_{i,k} .$$

So far, we have considered the application of the method of matrix decomposition to solve Poisson's equation on uniform grids. Even though it has been assumed that $\Delta x = \Delta y = \Delta z$, the situation when they are uniform but not equal to each other can be handled without any change in the algorithm discussed above. But as mentioned in the previous chapter, in the applications that we are interested in, it is desirable to have the grid spacings change continuously throughout the domain from fine grids near the boundaries to coarse grids in the middle. The extension of this method to include non-uniform grids is discussed in the next section.

3.3 MATRIX DECOMPOSITION ON NON-UNIFORM GRIDS

We are interested in solving equation (3.1) subject to given values of the normal derivative on the boundaries on a non-uniform grid. It is sufficient here only to discuss the two-dimensional problem, for the extension to three-dimensions follows directly from it. To get equation (3.1) into a proper form when using a non-uniform grid, the grid in the physical domain is first transformed into a uniform grid in a computational domain using one dimensional transformations of the form $\xi = \xi(x)$ and $\eta = \eta(y)$. The transformations $\xi(x)$ and $\eta(y)$ have been chosen to have odd symmetry about the vertical and horizontal centerlines respectively. The transformed equation (3.1) is then

$$\left(\frac{\partial \xi}{\partial x} \right)^2 \frac{\partial^2 p}{\partial \xi^2} + \frac{\partial^2 \xi}{\partial x^2} \frac{\partial p}{\partial \xi} + \left(\frac{\partial \eta}{\partial y} \right)^2 \frac{\partial^2 p}{\partial \eta^2} + \frac{\partial^2 \eta}{\partial y^2} \frac{\partial p}{\partial \eta} = c \quad (3.15)$$

and the boundary conditions are transformed similarly.

The derivatives of p appearing in equation (3.15) are discretized using second order accurate central differences at all *interior* grid points and the transformation derivatives are evaluated either analytically or to second order accuracy using finite differences. Thus, equation (3.15) can be written in a finite difference form as,

$$\begin{aligned} & \left[\frac{1}{\Delta \xi^2} \left(\frac{\partial \xi}{\partial x} \right)^2 + \frac{1}{2 \Delta \xi} \left(\frac{\partial^2 \xi}{\partial x^2} \right) \right]_i p_{i+1,j} + \left[\frac{1}{\Delta \xi^2} \left(\frac{\partial \xi}{\partial x} \right)^2 - \frac{1}{2 \Delta \xi} \left(\frac{\partial^2 \xi}{\partial x^2} \right) \right]_i p_{i-1,j} \\ & + \left[\frac{1}{\Delta \eta^2} \left(\frac{\partial \eta}{\partial y} \right)^2 + \frac{1}{2 \Delta \eta} \left(\frac{\partial^2 \eta}{\partial y^2} \right) \right]_j p_{i,j+1} + \left[\frac{1}{\Delta \eta^2} \left(\frac{\partial \eta}{\partial y} \right)^2 - \frac{1}{2 \Delta \eta} \left(\frac{\partial^2 \eta}{\partial y^2} \right) \right]_j p_{i,j-1} \\ & - \left[\frac{2}{\Delta \xi^2} \left(\frac{\partial \xi}{\partial x} \right)^2 + \frac{2}{\Delta \eta^2} \left(\frac{\partial \eta}{\partial y} \right)^2 \right] p_{i,j} = c_{i,j}. \end{aligned} \quad (3.16)$$

As discussed in section 3.1, one can either use central differences or second order accurate one sided differences for discretizing the boundary conditions. The algorithm that is described below can be used for solving the system of linear algebraic equations resulting from either

case. Here, we follow the latter approach and apply equation (3.16) at all the interior points in the domain. The boundary points that occur in these finite difference equations can be eliminated by using second order accurate one sided differences similar to equation (3.9) for discretizing the boundary conditions. The discretized form of the boundary condition, for example, at $x=0$ is given as,

$$\left[\frac{\partial \xi}{\partial x} \right]_{i=0} \frac{-p_{2,j} + 4p_{1,j} - 3p_{0,j}}{2\Delta \xi} = \left[\frac{\partial p}{\partial x} \right]_{i=0},$$

where the right hand side is known from the boundary condition. Once the boundary terms have been eliminated, the resulting system of equations can be written in a block tridiagonal form as,

$$\begin{bmatrix} G_1 & A_1 & . & . & . \\ B_2 & G_2 & A_2 & . & . \\ . & . & . & . & . \\ . & . & B_{M-1} & G_{M-1} & A_{M-1} \\ . & . & . & B_M & G_M \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ . \\ . \\ q_M \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ . \\ . \\ d_M \end{bmatrix}, \quad (3.17)$$

where, the q_j 's and the d_j 's are defined in the same manner as in section 3.1.1 and

$$G_j = \begin{bmatrix} h_{1,j} & g_{1,j} & . & . & . \\ f_{2,j} & h_{2,j} & g_{2,j} & . & . \\ . & . & . & . & . \\ . & . & f_{L-1,j} & h_{L-1,j} & g_{L-1,j} \\ . & . & . & f_{L,j} & h_{L,j} \end{bmatrix},$$

$$B_j = \begin{bmatrix} b_{1,j} & . & . & . & . \\ . & b_{2,j} & . & . & . \\ . & . & . & . & . \\ . & . & . & b_{L-1,j} & . \\ . & . & . & . & b_{L,j} \end{bmatrix}, \quad A_j = \begin{bmatrix} a_{1,j} & . & . & . & . \\ . & a_{2,j} & . & . & . \\ . & . & . & . & . \\ . & . & . & a_{L-1,j} & . \\ . & . & . & . & a_{L,j} \end{bmatrix}.$$

The strategy that is adopted here for solving equation (3.17) is the same as before. We first put the block tridiagonal matrix Q given by

$$Q = \begin{bmatrix} G_1 & A_1 & 0 & . & . \\ B_2 & G_2 & A_2 & 0 & . \\ . & . & . & . & . \\ . & 0 & B_{N-1} & G_{N-1} & A_{N-1} \\ . & . & 0 & B_N & G_N \end{bmatrix},$$

in a symmetric form. As a consequence the matrices G_j 's, also become symmetric. The process of bringing Q into a symmetric form is best carried out by first examining the center row corresponding to $j = M/2 + 1$. It should be noted that, here, L, M are assumed to be odd. Since the transformation $\eta = \eta(y)$ is an odd function about the horizontal centerline, the second derivative of η with respect to y is zero at all points in this row and equation (3.16) shows that $B_{M/2+1} = A_{M/2+1}$. By similar arguments for $\xi(x)$ it can be seen that $f_{L/2+1,j} = g_{L/2+1,j}$, for $1 \leq j \leq M$. The matrix $G_{M/2+1}$ can now be made symmetric by starting with the middle row and working outwards while multiplying each row by the appropriate factors†. As a result of making the matrix $G_{M/2+1}$ symmetric the elements of the off-diagonal matrices $B_{M/2+1}$ and $A_{M/2+1}$ and the right hand side vector $d_{M/2+1}$ will also be altered. Proceeding away from the central block to bring the matrix Q into a symmetric form those operations that make the off-diagonal blocks symmetric also make the diagonal matrices, the G_j 's, symmetric. In addition, the matrices are such that after the symmetry operations are completed the relations,

$$G_j = \alpha_j G_{M/2+1} + \beta_j A_{M/2+1}, \quad 1 \leq j \leq N, \quad (3.18)$$

and

$$A_j = B_{j+1} = \gamma_j A_{M/2+1}, \quad 1 \leq j \leq M-1, \quad (3.19)$$

† If L is even and M is odd, then $B_{M/2+1} = A_{M/2+1}$ and $g_{L/2,j} = f_{L/2+1,j}$, for $1 \leq j \leq M$. In this case, one can leave the middle two rows of $G_{M/2+1}$ and work outwards as before.

hold. The coefficients α_j , β_j , and γ_j can easily be accumulated into vectors. The matrix Q is now symmetric and as before, if all the rows of Q were added together, the resulting row would consist entirely of zeroes. For consistency, then, the sum of all the $c_{i,j}$'s should be equal to zero as well.

The method of matrix decomposition can now be applied to solve this system of equations. As before, the first step is to diagonalize the matrices $G_{N/2+1}$, $A_{N/2+1}$ simultaneously so that

$$S^T G_{N/2+1} S = \Lambda, \quad S^T A_{N/2+1} S = I,$$

The matrix S is the matrix of eigenvectors and Λ is the diagonal matrix of eigenvalues of the generalized eigenvalue problem $G_{N/2+1} s_i = \lambda A_{N/2+1} s_i$. Since the matrices G_j , A_j , and B_j involve a linear combination of matrices $G_{N/2+1}$ and $A_{N/2+1}$, the same eigenbasis can be used for diagonalizing all the other blocks of Q . This diagonalization results in the separation of the i index and yields a scalar tridiagonal system on each $j = \text{constant}$ line. As a result the system of equations given by equation (3.17) can be written, for $1 \leq i \leq L$ as,

$$\begin{aligned} (\alpha_1 \lambda_i + \beta_1) \bar{p}_{i,1} + \gamma_1 \bar{p}_{i,2} &= \bar{c}_{i,1}, \\ \gamma_{j-1} \bar{p}_{i,j-1} + (\alpha_j \lambda_i + \beta_j) \bar{p}_{i,j} + \gamma_j \bar{p}_{i,j+1} &= \bar{c}_{i,j}, \quad 2 \leq j \leq M-1, \\ \gamma_{M-1} \bar{p}_{i,M-1} + (\alpha_M \lambda_i + \beta_M) \bar{p}_{i,M} &= \bar{c}_{i,M}, \end{aligned} \quad (3.20)$$

where, the $\bar{p}_{i,j}$'s and the $\bar{c}_{i,j}$'s are defined in the same manner as in section (3.1). As before, these tridiagonal equations can be solved by Thomas algorithm after setting $\bar{p}_{L,M}$ to zero. Once all the $\bar{p}_{i,j}$'s have been obtained, we can get p from equation (3.5).

We now turn to an analysis of the performance of the method of matrix decomposition. Since our ultimate goal is to solve the incompressible, three dimensional Navier-Stokes equations, a task that is best done on a supercomputer, the performance of this method on the Cray is considered in the next section. At the time this part of the analysis was carried out, the Ohio Supercomputer Center had replaced its Cray X-MP/28 with a Cray Y-MP8/864.

3.4 PERFORMANCE ANALYSIS

The major steps of the matrix decomposition method for solving a symmetric block tri-diagonal system of equations can be summarized as follows :

- (i) Compute the matrix of eigenvalues and eigenvectors.
- (ii) Obtain $\bar{c}$ (or $\bar{\bar{c}}$, as the case may be) from a given right hand side vector c by transforming once (or twice) to the eigenspace.
- (iii) Solve the tridiagonal systems for $\bar{p}$ (or $\bar{\bar{p}}$).
- (iv) Compute p from $\bar{p}$ (or $\bar{\bar{p}}$) by transforming once (or twice) back to the physical space.

Firstly, it can be seen that the matrix of eigenvalues and eigenvectors required in step (i) need to be computed only once and they can be stored and used for any given right hand side vector. Secondly, the matrix multiplications required in steps (ii) and (iv) to transform to and from the eigenspace, which require the major effort, can be performed very efficiently on the Cray by using Cray Assembly Language (CAL) routines. These matrix operations can be performed at speeds around 310 Mflops on the Y-MP. Thirdly, the tridiagonal systems in step (iii) can be solved very efficiently using a fully vectorized Thomas algorithm. As a result of the latter two considerations, the overall computing speed of the method of matrix decomposition comes out to be around 300 Mflops. The best feature of this method is that this computing speed is retained even on non-uniform grids, which makes it very attractive for solving the Poisson's equation.

Another desirable feature of this method is that it easily lends itself to parallel processing (Buzbee, 1973). This can be seen clearly in the case of three dimensional problems, where the matrix decomposition method decomposes the problem into a set of two dimensional problems, each of which can be solved independently. With regard to operation counts, the matrix multiplication involved in steps (ii) and (iv) require $2LM^2$ multiplications (in the two dimensional case). The Thomas algorithm in step (iii) requires $O(LM)$ multiplications. Hence, the method of matrix decomposition requires $2LM^2$ multiplications on the whole. This is more than the operation count for the Buneman odd-even reduction scheme, which is $O(LM \log L)$ (Buzbee, 1970, Part II). A detailed timing study of these two methods together

with ADI and the point SOR methods for the solution of Poisson's equation is presented in that reference. Even though the operation count favors the Buneman's method, we agree with Buzbee et al. (1970, Part II) that the method of matrix decomposition is certainly competitive because of its generality and especially in view of our success of implementing it for non-uniform grids. The fast computing speeds mentioned above for this method lend weight to this opinion.

CHAPTER IV

THREE DIMENSIONAL FLOW IN A LID DRIVEN CAVITY

In Chapter 2 some results for a three dimensional flow in a lid driven cavity were given. In this chapter we give its formulation and implement improved methods for solving the equations that govern the flow. In Chapter 2 some results for a three dimensional flow in a lid driven cavity were given. In this chapter we give its formulation and implement improved methods for solving the equations that govern the flow.

4.1 FLOW IN A LID DRIVEN CAVITY

Consider an incompressible fluid of density ρ and kinematic viscosity ν that is confined to a rectangular box of length L , height H and span W . The coordinate axes are placed such that x -direction is along the length, y -direction is along the span and z -direction is vertical and opposed to gravity so as to form a right handed coordinate system. The top surface of the box moves in the positive x -direction with a velocity U . All the other surfaces are fixed and rigid. We wish to study the resulting fluid motion in the box. The two dimensional version of this problem was first proposed and solved by Burggraf (1966). A sketch of the major features of the flow in two- and three-dimensions is given in Figures 4.1 and 4.2. The two dimensional flow shows the presence of a primary eddy occupying the core of the flow and two secondary eddies in the downstream and upstream corners on the bottom surface, all of which can be seen at Reynolds number (based on cavity height and lid velocity) as low as 100. At larger Reynolds number (around 3200), a tertiary eddy develops in the upstream corner of the upper (moving) surface. As the Reynolds number is increased even further, additional counter-rotating eddies appear near the downstream corners on the bottom surface. It has been possible to observe these high Reynolds number features only in very accurate

Figure 4.1. Sketch of the flow field in a two-dimensional lid driven cavity

Figure 4.2. Sketch of the flow field in a three-dimensional lid driven cavity (Reproduced from Iwatsu et al., 1989)

simulations such as those of Ghia et al. (1982) and Schreiber and Keller (1983). No evidence of hydrodynamic instabilities for this two dimensional flow have been reported in these two studies for Reynolds number up to 10000.

The three dimensional flow shown in Figure 4.2 exhibits the same features on planes parallel to the end walls in the interior of the cavity. The flow in the spanwise direction exhibits symmetry about the central plane. In addition, corner vortices have appeared where the top and the end walls meet. Similar vortices exist at the junction of the bottom and the end walls also. Experimental investigations by Koseff and Street (1984a,b,c) reveal the presence of weak longitudinal vortices along the floor of the cavity at higher Reynolds numbers. In contrast to the two dimensional situation, accurate numerical solutions for the three dimensional problem are almost non-existent, except for those presented by Ku et al. (1987) and Iwatsu et al. (1989) for the flow in a cubical cavity. The latter work shows that the flow is unsteady for Reynolds number greater than 3000 and as Figure 4.2 (taken from that paper) shows, it confirms the experimental observation regarding the presence of the longitudinal floor vortices at Reynolds number 4000. In this chapter, we first consider the flow in a cubical cavity in order to try to capture the qualitative features of this flow as presented in the above works and then we investigate the flow in a shallow cavity for which the length of the box L is much larger than its height H .

4.2 FORMULATION

The formulation of this problem follows very closely to that presented in the previous chapter. Here, we have one less equation to solve, namely, the energy equation and so, except for the differences brought in by the absence of this equation, one can expect the equations and boundary conditions to be similar to those given before.

4.2.1 GOVERNING EQUATIONS

The equations that govern the motion of the fluid are the incompressible, three dimensional Navier-Stokes equations. These are written in dimensionless form, with lengths non-dimensionalized by the height of the box H , the velocities by the velocity U of the moving lid, time by H/U and pressure by ρU^2 . The governing equations in dimensionless form are,

$$\nabla \cdot \vec{u} = 0 , \quad (4.1)$$

$$\frac{\partial \vec{u}}{\partial t} + \left[\vec{u} \cdot \nabla \right] \vec{u} = -\nabla p + \frac{1}{\text{Re}} \nabla^2 \vec{u} , \quad (4.2)$$

where $\text{Re} = U H / \nu$ is the Reynolds number.

4.2.2 BOUNDARY CONDITIONS

Since all the sides of the box, except the top surface, are rigid, the fluid velocities are zero on these surfaces. On the top surface, the x-component of the velocity is equal to unity while the other two components are zero. Also, the flow exhibits symmetry about the $y = W/2H$ plane and so symmetry conditions can be used on this surface. Accordingly, we have,

$$u = v = w = 0 , \quad x = 0, L/H , \quad (4.3a)$$

$$u = v = w = 0 , \quad y = 0 , \quad (4.3b)$$

$$\frac{\partial u}{\partial y} = \frac{\partial w}{\partial y} = v = 0 , \quad y = W/2H , \quad (4.3c)$$

$$u = v = w = 0 , \quad z = 0 , \quad (4.3d)$$

$$u = 1 , v = 0 , w = 0 , \quad z = 1 . \quad (4.3e)$$

4.3 NUMERICAL METHOD

Equation (4.2) is discretized in time by using first order accurate explicit time differencing as before and this gives,

$$\frac{\vec{u}^{n+1} - \vec{u}^n}{\Delta t} + (\vec{u}^n \cdot \nabla) \vec{u}^n = -\nabla p^{n+1} + \frac{1}{\text{Re}} \nabla^2 \vec{u}^n . \quad (4.4)$$

The governing equation for pressure can be obtained in the same manner as equation (2.16) and is given as,

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t} D^n - \nabla \cdot [(\vec{u}^n \cdot \nabla) \vec{u}^n] + \frac{1}{\text{Re}} \nabla^2 D^n , \quad (4.5)$$

where, $D \equiv \nabla \cdot \vec{u}$. The only difference between equation (4.5) and (2.16) is that the diffusion terms have been retained in equation (4.5) since they were found to be essential for steady state convergence of the numerical method when the Reynolds number is small. Boundary conditions for pressure can be obtained by satisfying the appropriate momentum equations (4.4) along the boundaries. These can be written, after using equation (4.3), as,

$$\frac{\partial p^{n+1}}{\partial x} = \frac{1}{\text{Re}} \frac{\partial^2 u^n}{\partial x^2} , \quad x = 0, L/H \quad (4.6a)$$

$$\frac{\partial p^{n+1}}{\partial y} = \frac{1}{\text{Re}} \frac{\partial^2 v^n}{\partial y^2} , \quad y = 0 \quad (4.7b)$$

$$\frac{\partial p^{n+1}}{\partial y} = 0 , \quad y = W/2H , \quad (4.7c)$$

$$\frac{\partial p^{n+1}}{\partial z} = \frac{1}{\text{Re}} \frac{\partial^2 w^n}{\partial z^2} , \quad z = 0, 1 . \quad (4.7d)$$

As mentioned in Chapter 3, we wish to solve equations (4.4) and (4.5) on a suitable non-uniform grid with fine grids near the boundaries and coarse grids in the interior. This can be accomplished in two ways; using second order accurate finite difference expressions for discretizing these equations on non-uniform grids (Blottner, 1974) or transforming the non-

uniform grid in the physical domain to a uniform grid in a computational domain and solving the transformed equations there. We chose the latter course and generated an appropriate non-uniform grid in the physical domain using the Roberts transformation (Anderson, Tannehill and Pletcher, 1984),

$$z = \beta \tanh \left[\frac{1}{2} \log \left(\frac{1+\beta}{1-\beta} \right) \zeta \right].$$

Here, ζ is the computational coordinate corresponding to the z -coordinate in the physical domain and β is a stretching parameter. The grid in the physical domain together with the notation for the grid indices is shown in Figure 4.3. Similar expressions can be written for the other two coordinates. The governing equations and boundary conditions are transformed using one-dimensional transformations of the form $\xi = \xi(x)$, $\eta = \eta(y)$ and $\zeta = \zeta(z)$ to the computational domain, where they are solved on a uniform grid. These transformations have an odd symmetry about the mid-planes $x = L/2H$, $y = W/2H$ and $z = 1/2$ respectively. Equations (4.4) and (4.5) can be transformed as,

$$\frac{\bar{u}^{n+1} - \bar{u}^n}{\Delta t} + (\bar{u}^n \cdot \nabla) \bar{u}^n = -\nabla p^{n+1} + \frac{1}{\text{Re}} \nabla^2 \bar{u}^n, \quad (4.8)$$

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t} D^n - \nabla \cdot [(\bar{u}^n \cdot \nabla) \bar{u}^n] + \frac{1}{\text{Re}} \nabla^2 D^n, \quad (4.9)$$

where, now,

$$\nabla \equiv \hat{i} \left[\frac{\partial \xi}{\partial x} \right] \frac{\partial}{\partial \xi} + \hat{j} \left[\frac{\partial \eta}{\partial y} \right] \frac{\partial}{\partial \eta} + \hat{k} \left[\frac{\partial \zeta}{\partial z} \right] \frac{\partial}{\partial \zeta},$$

and

$$\begin{aligned} \nabla^2 \equiv & \left[\frac{\partial \xi}{\partial x} \right]^2 \frac{\partial^2}{\partial \xi^2} + \frac{\partial^2 \xi}{\partial x^2} \frac{\partial}{\partial \xi} + \left[\frac{\partial \eta}{\partial y} \right]^2 \frac{\partial^2}{\partial \eta^2} + \frac{\partial^2 \eta}{\partial y^2} \frac{\partial}{\partial \eta} \\ & + \left[\frac{\partial \zeta}{\partial z} \right]^2 \frac{\partial^2}{\partial \zeta^2} + \frac{\partial^2 \zeta}{\partial z^2} \frac{\partial}{\partial \zeta}. \end{aligned}$$

The boundary conditions for pressure can be transformed as,

Figure 4.3. Grid Nomenclature

$$\frac{\partial p^{n+1}}{\partial \xi} = \frac{1}{\text{Re}} \left[\frac{\partial \xi}{\partial x} \right] \frac{\partial^2 u^n}{\partial \xi^2} , \quad \xi = 0, L/H , \quad (4.10a)$$

$$\frac{\partial p^{n+1}}{\partial \eta} = \frac{1}{\text{Re}} \left[\frac{\partial \eta}{\partial y} \right] \frac{\partial^2 v^n}{\partial \eta^2} , \quad \eta = 0 , \quad (4.10b)$$

$$\frac{\partial p^{n+1}}{\partial \eta} = 0 , \quad \eta = W/2H , \quad (4.10c)$$

$$\frac{\partial p^{n+1}}{\partial \zeta} = \frac{1}{\text{Re}} \left[\frac{\partial \zeta}{\partial z} \right] \frac{\partial^2 w^n}{\partial \zeta^2} , \quad \zeta = 0, 1 . \quad (4.10d)$$

In the above equation, the first derivatives of the normal velocity that appear as a result of the transformation of the second derivative have been set equal to zero by invoking the continuity equation on the boundaries.

All the derivatives of the velocities and pressure appearing in equations (4.8) and (4.9) were discretized using second order accurate central differences. The transformation derivatives were evaluated analytically since the expressions for $\xi(x)$, $\eta(y)$ and $\zeta(z)$ are known. In evaluating the source term for the pressure Poisson equation, the divergence of the velocity field, D , has to be evaluated to fourth order accuracy so that second order accuracy can be maintained when computing $\nabla^2 D$. This requires the normal components of the velocities to be available on a fictitious row of grid points just outside the boundaries. These velocities were evaluated using a fourth order accurate discretization of the continuity equation on the boundaries. This was done, for example, at $x=0$ as

$$u_{-1,j,k}^n = \frac{-10 u_{0,j,k}^n + 18 u_{1,j,k}^n - 6 u_{2,j,k}^n + u_{3,j,k}^n}{3} , \quad 1 \leq j \leq M , \quad 1 \leq k \leq N .$$

The derivatives for pressure on all solid boundaries that appear in equation (4.10a,b,d) were discretized using second order accurate one-sided differences. The second derivatives of the velocities on these boundaries were evaluated using second order accurate central differences. The velocities at points outside the domain that appear in the resulting finite difference expressions were eliminated by using a third order accurate discretization of the

continuity equation on the boundaries in a manner described in Anderson, Tannehill and Pletcher (1984). The advantage of this procedure is that it retains second order accuracy while evaluating the right hand sides of equations (4.10a,b,d). Thus, we can write equation (4.10a), for example, at $x=0$ as,

$$\frac{-3p_{0,j,k}^{n+1} + 4p_{1,j,k}^{n+1} - p_{2,j,k}^{n+1}}{2\Delta\xi} = \frac{1}{\text{Re}} \left[\frac{\partial \xi}{\partial x} \right] \frac{8u_{1,j,k}^n - u_{2,j,k}^n}{2\Delta\xi^2}, \quad 1 \leq j \leq M, 1 \leq k \leq N. \quad (4.11a)$$

Similar expressions can be derived for the boundary conditions on all the other solid boundaries. On the symmetry plane, the x- and z-momentum equations and the pressure Poisson equation were solved. The points outside the computational domain that appear in these equations were eliminated using central differencing for discretizing the symmetry condition for the velocities and pressure on this plane. The system of equations (4.8) and (4.9) together with boundary conditions can now be solved.

The pressure Poisson equation (4.9) can be written in matrix form as $Q \mathbf{p} = \mathbf{c}$, where Q is a block tridiagonal matrix as shown in the previous chapter. After the boundary points and points outside the computational domain have been eliminated using boundary conditions (4.11), the matrix Q can be put in a symmetric form. Putting Q into a symmetrical form leads to an altered constraint for the elements of $\mathbf{c}$. Now, their properly weighted sum is equal to zero. Since the right hand sides of equations (4.9) and (4.11) are being evaluated using finite difference expressions, this sum usually is different from zero owing to truncation errors. We follow Briley (1977) and distribute this difference equally amongst the elements of $\mathbf{c}$ so that their sum is equal to zero to machine accuracy. This has to be done every time step so that the pressure field satisfies the discretized form of the integral constraint at all intermediate times. This is especially important when using non-uniform grids since the truncation errors tend to be large in regions where the stretching of the grids is severe (Vinokur, 1982).

With the velocity field at time level n known, the pressure Poisson equation (4.9) with boundary conditions given by equations similar to and including (4.11a) can be solved by the method of matrix decomposition described in the previous chapter. The momentum equations (4.9) can now be solved with this pressure field at time level $n+1$ and the velocity field

advanced to the next time level at $n+1$. The boundary conditions can then be updated. For obtaining steady state solutions the whole procedure is repeated until a suitable steady state convergence criterion is satisfied. By calculating the residuals of the steady state momentum equations, the time iterations were stopped once the maximum of the absolute value of these residuals were of $O(10^{-5})$.

The stability of the above numerical procedure with explicit time differencing for the momentum equations is governed by two criteria, namely, the diffusion criterion and the Courant condition (Anderson, Tannehill and Pletcher, 1984, Roache, 1972). Each of these require the size of the time step, Δt , to be below some value. For overall stability of the numerical scheme, the actual time step has to be a certain combination of these two time steps. For low values of Reynolds numbers the diffusion time step becomes very small and so the computing time needed to reach a converged steady state solution in such cases becomes very large. As a first step towards solving this difficulty, the diffusion terms in the momentum equations were treated implicitly during each time step as,

$$\frac{\vec{u}^{n+1} - \vec{u}^n}{\Delta t} + (\vec{u}^n \cdot \nabla) \vec{u}^n = -\nabla p^{n+1} + \frac{1}{\text{Re}} \nabla^2 \vec{u}^{n+1} . \quad (4.12)$$

As before, all the spatial derivatives of the field variables in this equation were discretized using second order accurate central differences. The method of matrix decomposition described in the previous chapter for Poisson's equation can then be used to solve the Helmholtz equation (4.12) as well. This can be thought of as an extension of the matrix decomposition technique to solve parabolic equations also. Further details of such techniques are given by Shintani (1969). With the diffusion terms treated implicitly, the stability of the numerical scheme for solving equation (4.12) is governed only by the Courant condition which is much less restrictive. The stability and convergence towards steady state can be improved further by using implicit schemes such as the Douglas-Gunn ADI scheme. The implementation of the Douglas-Gunn method was carried out after the results discussed in this chapter were completed. Thus its discussion is deferred until the next chapter.

The equations governing the pressure, however, remain the same as before, for, if these equations were derived from equation (4.12), they would require the velocity field at time level $n+1$ to be known for evaluating the diffusion terms. These velocities are not known at the time of solving for p^{n+1} . So, these terms have to be evaluated at time level n , thus forcing us to use equations (4.9) and (4.10) for the pressure. One might guess then, that this procedure would give rise to larger errors for the divergence of the velocity field at steady state than the explicit scheme. The graph in Figure 4.4 of the maximum absolute value of the residual of the continuity equation against time for both the explicit and this semi-implicit scheme for the two dimensional lid driven cavity problem at $Re=1000$ shows that this is so. The residuals of the divergence of the steady state velocity field tend to different values but are of the same order of magnitude. These values for the maximum residuals of the continuity equation at steady state might seem high, but they are at the grid points closest to the singular corners where the moving lid meets the stationary walls. The average value for these residuals are $o(10^{-3})$, which is reasonable since the discretized form of the continuity equation cannot be satisfied to machine accuracy in such a non-staggered grid system for the velocities and the pressure (Roache, 1975, Sotiropoulos & Abdallah, 1991). This is because in a non-staggered grid system the central difference operator for the first derivative operating on itself does not give the central difference operator for the second derivative.

With the velocity field obtained at each time step using this semi-implicit scheme, one can march forward in time the same way as before until a steady state solution is reached. The semi-implicit scheme requires more operations per time step than does the explicit scheme and so is clearly not advantageous in cases where the diffusion and the Courant time steps are of the same order. The solutions presented in the next section have been obtained with either the explicit scheme or the semi-implicit scheme based on the considerations given above.

4.4 RESULTS & DISCUSSION

Numerical solutions for the flow in both the two dimensional and three dimensional lid driven cavity for several Reynolds number are presented first. The motivation here in

Figure 4.4. Evolution of the residuals of the continuity equation for explicit and semi-implicit schemes

presenting two dimensional solutions is to compare them with the solutions reported by Ghia et al. (1982) to check the accuracy of the present calculations. This has been done for the three dimensional case also by comparing with the solutions presented by Ku et al. (1987) for flow in a cubical cavity.

4.4.1 FLOW IN A SQUARE CAVITY

Flow in a two dimensional square cavity for three different Reynolds numbers, namely, 100, 400 and 1000 was considered. A 128x128 grid was used for all three Reynolds numbers. For all the results reported for these cases, calculations were carried out until the residuals of the momentum equations were $O(10^{-5})$ or lower. The maximum residual of the pressure Poisson equation was $O(10^{-13})$ or lower.

The contours of static pressure coefficients in the cavity are plotted in Figure 4.5 and show excellent agreement with the plots presented by Sotiropoulos and Abdallah (1990). Here, the static pressure coefficient is taken to be $(p - p_{ref})$, as a result of the non-dimensionalization employed, where p_{ref} is chosen to be equal to the pressure at the mid-point of the bottom surface of the cavity (Burggraf, 1966). The contours of vorticity plotted in Figure 4.6 also show good agreement with those given in previous works (Ghia et al., 1982, Sotiropoulos & Abdallah, 1990). The values used for the contour levels in Figures 4.5 and 4.6 are the same as those used in the latter reference. Plots of u - and v -velocities along the horizontal and vertical centerlines of the cavity are shown in Figures 4.7 and 4.8. The values given by Ghia et al. (1982) are also plotted in these figures for comparison and, as can be seen the two values agree well. The maximum percentage error between the two sets of values being 5%. In order to estimate the accuracy of our values better, we tried to compute the order of the truncation error in our steady state solutions in a manner discussed in Smith (1985). Solutions to the driven cavity problem at a Reynolds number equal to 100 were also computed on three different grids, namely, 64x64, 128x128 and 256x256. From these, a 64x64 matrix of solution values at points common to the three grids can be formed. Letting subscripts I, II and III denote solutions at these points from the first, second and the third grid respectively, the order of the truncation error q at any of these points can be obtained as,

Figure 4.5. Contours of static pressure coefficients at (a) $Re = 100$

Figure 4.5. (continued)

(b) $Re = 400$

Figure 4.5. (continued)

(c) $Re = 1000$

Figure 4.6. Contours of vorticity at (a) $Re = 100$

Figure 4.6. (continued)

(b) $Re = 400$

Figure 4.6. (continued)

(c) $Re = 1000$

Figure 4.7. The u-velocity along vertical centerline of cavity at (a) $Re = 100$

Figure 4.7. (continued)

(b) $Re = 400$

Figure 4.7. (continued)

(c) $Re = 1000$

Figure 4.8. The w-velocity along horizontal centerline of cavity at (a) $Re = 100$

Figure 4.8. (continued)

(b) $Re = 400$

Figure 4.8. (continued)

(c) $Re = 1000$

$$2^q = \frac{\phi_{II} - \phi_I}{\phi_{III} - \phi_{II}}.$$

Here, ϕ represents either the u- or the v-velocity component (the order of the pressure field cannot be computed by this method owing to the presence of an arbitrary constant in the Neumann problem). Even though second order accuracy had been maintained formally while discretizing both the governing equations and boundary conditions, the values of q from above did not indicate second order accuracy at all the points. In fact, the distribution of q 's on the common set of points did not seem to fit any obvious pattern except that the values for q were smaller in the interior of the cavity than near the boundaries. This was puzzling especially in view of the fact that the solution on the coarsest grid considered, namely, 64x64, is acceptable based on the values available in the literature for this value of Reynolds number. It may be that since the method used above for computing the order of the truncation error is valid only in the limit of vanishingly small grid spacings, still finer grids should be used. These observations generally seem to agree with those of Schreiber & Keller (1983).

4.4.2 FLOW IN A CUBICAL CAVITY

We now turn to the three dimensional flow in a cubical cavity. Solutions corresponding to Reynolds numbers 100, 400 and 1000 will be presented. Accurate numerical solutions for these three cases using pseudo-spectral methods have been given by Ku et al. (1987) and our intention here is to make a quantitative comparison of our results with theirs. We used a 33x33x33 uniform grid for $Re = 100$. Since the flow is symmetric about the $y = 1/2$ plane, calculations were performed only on 33x17x33 points. With this in mind, in what follows, we give only the number of points used for calculations unless otherwise mentioned. A plot of the u- and v-velocities along the vertical and horizontal centerlines on the symmetry plane similar to the two dimensional case is given in Figure 4.9. Also included in these plots are the corresponding two dimensional solutions, in order to bring out the differences brought about by the three dimensionality of the problem and the solutions of Ku et al. (1987), for comparison. It can be seen from these plots that the results from our finite-difference

Figure 4.9. Velocity profiles along vertical and horizontal centerlines
on the symmetry plane at $Re = 100$, (a) u-velocity

Figure 4.9. (continued)

(b) w-velocity

calculations agree very well with the pseudo-spectral results. Also, the velocity profiles from the three dimensional and two dimensional cases lie close to each other, indicating only a weak three dimensionality in the flow for this Reynolds number. However, when the Reynolds number is increased to 400, there is considerable departure from the corresponding two dimensional solutions, as can be seen from Figure 4.10. The calculations for $Re = 400$ were performed on a $63 \times 33 \times 63$ uniform grid. Again, the velocities from our finite-difference calculations seem to agree reasonable well with those of Ku et al. (1987), who kindly provided us with the data used to plot their graphs to Figures 4.9 and 4.10.

For $Re = 1000$, a $81 \times 41 \times 81$ *non-uniform* grid was used for this case and the finest grid spacing was $1/128$ and the coarsest spacing was $1/64$. The total CPU time required in this case to reach steady state came out to be around 4 hours of computing time on the Cray Y-MP. The u - and v -velocity profiles on the symmetry plane are plotted in Figure 4.11. Strong three dimensionality is indicated in these figures, for the three dimensional profiles deviate significantly from the two dimensional ones. The velocities in the former case are smaller than the corresponding two dimensional values. It is apparent that with increasing Reynolds number, the confining effect of the end walls becomes stronger, thus bringing in more spanwise variations in the flow. Also, the increasing values for the shear stress on these walls have the overall effect of slowing down the flow and this is seen in the diminishing velocities on the symmetry plane. The velocity vectors in the symmetry plane are shown in Figure 4.12 together with a close-up view of the downstream and upstream secondary eddies. The velocity vectors on the $x = 1/2$ plane are shown in Figure 4.13. In this view, strong corner vortices can be seen, which is another indication of the three dimensionality of the flow field. In these figures, only one-fourth of the total number of points have been used in order to illustrate the features clearly. These figures agree qualitatively well with the pictures presented by Iwatsu et al. (1989). The strong three dimensionality of the flow can also be seen from the particle trace shown in Figure 4.14. A particle introduced into the flow field from the downstream secondary eddy exhibits a spiraling motion towards the end walls where it turns around and is injected into the corner vortices. The particle then drifts towards the interior of the cavity due to the negative spanwise velocities in that region of the flow. This agrees quite well with the conceptualization of Koseff & Street (1984a). Based on the discussion

Figure 4.10. Velocity profiles along vertical and horizontal centerlines
on the symmetry plane at $Re = 400$, (a) u-velocity

Figure 4.10. (continued)

(b) w-velocity

Figure 4.11. Velocity profiles along vertical and horizontal centerlines on the symmetry plane at $Re = 1000$, (a) u-velocity

Figure 4.11. (continued)

(b) w-velocity

Figure 4.12. (a) Velocity vectors on the symmetry plane for a cubical cavity

Figure 4.12. (continued)

(b) downstream secondary eddy

Figure 4.12. (continued)

(c) upstream secondary eddy at $Re = 1000$

Figure 4.13. Velocity vectors on the plane $x = 0.5$ for a cubical cavity at $Re = 1000$

Figure 4.14. Particle trace inside the cubical cavity at $Re = 1000$

presented, we concluded that the accuracy of the steady state solutions obtained using methods described in the previous section, is quite good. We now turn to a discussion of other solutions.

We considered the case $Re = 4000$ next, in order to see if we could capture the weak, longitudinal floor vortices that have been seen previously in both experimental and numerical simulations. Since it had been reported that these floor vortices meander in the spanwise direction (Koseff & Street, 1987), symmetry conditions on the $y = 1/2$ plane were not applied in these simulations. The equations were solved on a $81 \times 81 \times 81$ grid with the solution at $Re = 1000$ given as starting conditions. The results of these calculations are shown in Figures 4.15 and 4.16. They required approximately 90 minutes of CPU time to obtain. Longer runs showed drift which finally led to divergence of the solution. The velocity vectors in the $y = 1/2$ plane for this Reynolds number are shown in Figure 4.15. They are very similar to those for $Re = 1000$ but now there is also a weak tertiary eddy present in the downstream corner of the moving lid. The velocity vectors on the $x = 0.57$ plane are shown in Figure 4.16. The corner vortices have become stronger now and in addition two pairs of TGL vortices can be seen near the bottom surface of the cavity. A pair of small vortices can also be seen near the top surface. The flow field still remains symmetric in this figure.

We obtained solutions for a cavity with an aspect ratio of 2 (i.e., $W/H = 2$) in the spanwise direction using the same $80 \times 80 \times 80$ grid at Reynolds number 4000 also. The velocity vectors on the plane $x = 0.57$ for this case are given in Figure 4.17. The presence of the strong corner vortices and a pair of floor vortices can be seen clearly in this case also. The results presented for $Re = 4000$ for aspect ratio equal to 2, required about 2 hours of CPU time on the Y-MP to generate. As mentioned earlier, smaller time steps could help advance the solution further in time but it seems likely to us, after observing the rapid divergence of the solution subsequent to the appearance of the floor vortices, that, such divergence might be unavoidable in a numerical scheme that is only first order accurate in time.

Figure 4.15. Velocity vectors on the symmetry plane for a cubical cavity at $Re = 4000$

Figure 4.16. Velocity vectors on the plane $x = 0.57$ for a cubical cavity at $Re = 4000$

Figure 4.17. Velocity vectors on the plane $x = 0.57$ for a cavity with $W/H = 2$ at $Re = 4000$

4.4.3 FLOW IN A SHALLOW CAVITY

We now consider the flow in a shallow cavity for which $W/H = 1$ and $L/H \gg 1$. Two very closely related problems in two dimensions, namely, natural convection and thermocapillary convection in a shallow cavity have been considered in detail elsewhere (Cornack et al., 1974, Sen & Davis, 1982). Similar to these two situations, the present problem also exhibits a flow field that consists of two regions; a core flow region in the middle of the cavity and a region near the end walls, where the flow turns around. The main difference, however, is that now the flow field has a preferred direction and hence there is no centro-symmetry. If the end effects are neglected, analytical solutions can be obtained for the core flow, in the limit $L/H \rightarrow \infty$. Our aim here was to study the effect of finite values for the aspect ratio L/H on the overall flow field. This was done by deriving the analytical solutions first and then solving the full governing equations numerically for increasing values of aspect ratios. This was done for both the two- and three-dimensional cases.

The equations that govern the core flow in the two dimensional case can be written in dimensionless form as,

$$\frac{1}{\text{Re}} \frac{d^2 u}{dz^2} = \frac{dp}{dx} = \text{constant} , \quad (4.13)$$

subject to

$$u = 0, \quad z = 0, \quad u = 1, \quad z = 1, \quad \int_0^1 u \, dz = 0, \quad (4.14)$$

where, the last condition arises as a result of mass conservation in every cross-sectional plane. Here, the core flow can be assumed to be fully developed and so the w -velocity is equal to zero. The solution to this system is the classical Couette-Poiseuille flow with the pressure gradient such that the mass flow across every vertical plane is zero. Thus

$$u = z - 3z(1-z), \quad \frac{dp}{dx} = \frac{6}{\text{Re}} .$$

Alternatively, one could recover the above solution for the core flow as the leading order solution of a formal matched asymptotic expansions using the aspect ratio $A (= L/H)$ as a perturbation parameter.

By using a stretched coordinate of the form $\hat{x} = x/A$ in the end region, Cormack et al. (1974) showed that only the viscous terms were important in that region. In the work of Sen & Davis (1982) also, only the viscous terms were retained in the end region after the inertial terms were neglected on account of a lubrication type approximation. Since the inertial terms are absent in both of these cases, the resulting equations and boundary conditions for the flow in the end regions exhibit centro-symmetry about the vertical center plane. In the present problem, however, the inertial terms are not negligible for reasons mentioned before and so the full Navier-Stokes equations have to be solved in the end regions.

The governing equations for the flow in finite aspect ratio cavities are the two dimensional, incompressible Navier-Stokes equations. These were solved numerically for aspect ratios increasing from 2 to 12 in increments of 2. The Reynolds number was kept at 100. The u -velocity profile along the vertical centerline of the cavity is shown in Figure 4.18. As expected, the profile for this aspect ratio shows the maximum deviation from the asymptotic profile ($W/H = \infty$) and all the other profiles lie in between. The velocities change only in the third decimal place when going from an aspect ratio of 10 to 12 and they are within 5% of the asymptotic values. Pressure profiles along the horizontal centerline of the cavity for the various aspect ratios, with the aspect ratio increasing in the direction of the arrow are shown in Figure 4.19. The linear portions that can be seen in the curves from aspect ratio 6 onwards represent the core flow region and this is seen to occupy about 70% of the cavity width for an aspect ratio 12. The slope of these linear portions also agree with the asymptotic value given above to within 5%. A plot of the w -velocity along the horizontal centerline for different aspect ratios is shown in Figure 4.20. As expected, the w -velocity is very small in the core region. In the end regions, the flow behaves like a wall jet as can be seen from the w -velocity profiles. Also, the wall jets are very strong in the downstream (right) end but relatively weak in the upstream (left) end of the cavity as a result of the preferred direction from left to right. Grid spacings equal to $1/32$ were found to be sufficient to resolve these gradients. These observations were qualitatively confirmed by full Navier-Stokes calculations in

Figure 4.18. The u -velocity along the vertical centerline for a two dimensional shallow cavity for aspect ratios 2,4,6,8,10 and 12 at $Re = 100$

Figure 4.19. Pressure along the horizontal centerline for a two dimensional shallow cavity for aspect ratios 2,4,6,8,10 and 12 at $Re = 100$

Figure 4.20. The w-velocity along the horizontal centerline for a two dimensional shallow cavity for aspect ratios 2,4,6,8,10 and 12 at $Re = 100$

the end region with matching to the core flow solution. In looking at the pressure profiles in Figure 4.19 near the downstream end region, it can be concluded that the pressure decreases initially owing to the high velocity of the fluid in the wall jet. The pressure increases again as we get closer to the right wall, since the fluid slows down rapidly, to satisfy the zero velocity condition on the wall. The same effect can be seen near the upstream end also, but here the changes in pressure are small due to the fact that the increase in the w -velocity of the fluid is smaller here than in the other end.

Now, we consider the shallow cavity problem in three dimensions with $L/H \gg 1$ and the spanwise aspect ratio $W/H = 1$. The core flow solution in the limit $L/H \rightarrow \infty$ was sought by assuming it to be fully developed in the x -direction as before. Here, in addition, either the v - or the w -velocity had to be assumed to be equal to zero and it follows from the continuity equation that the other component is equal to zero as well. The governing equations for the core flow reduce, in dimensionless form, to

$$\frac{1}{\text{Re}} \left[\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right] = \frac{dp}{dx} = \text{constant}, \quad (4.15)$$

$$u = 0, \quad y = 0, 1$$

$$u = 0, \quad z = 0, \quad u = 1, \quad z = 1,$$

$$\int_0^1 \int_0^1 u \, dy \, dz = 0. \quad (4.16)$$

Here, again, the last equation comes from the fact that the container is closed. Equations (4.15) can be solved analytically by using superposition of a Couette flow with zero pressure gradient (Sherman, 1990) and a Poiseuille flow with constant pressure gradient (Langlois, 1964). This can be written as,

$$u(y, z) = \left[z + 2 \sum_{n=1}^{\infty} \frac{(-1)^n}{n \pi} \frac{\cosh n \pi (y - 1/2)}{\cosh n \pi / 2} \sin n \pi z \right] + \frac{\text{Re}}{2} \frac{dp}{dx} \left[z(z-1) - 8 \sum_{n=1,3,5}^{\infty} \frac{(-1)^{(n+1)/2}}{n^3 \pi^3} \frac{\cosh n \pi (y - 1/2)}{\cosh n \pi / 2} \cos n \pi (z - 1/2) \right] \quad (4.17)$$

The pressure gradient dp/dx can be obtained by substituting the velocity profile from equation (4.17) into (4.16). This gives,

$$\frac{dp}{dx} = \frac{6}{Re} \left[\frac{1 - 12 \sum_{n=1,3,5}^{\infty} \frac{\tanh n \pi/2}{n^3 \pi^3}}{1 - 192 \sum_{n=1,3,5}^{\infty} \frac{\tanh n \pi/2}{n^5 \pi^5}} \right] \quad (4.18)$$

The value for dp/dx in the three dimensional case comes out to be higher than its value $6/Re$, in the two dimensional case. This can be explained by the presence of the walls in the spanwise direction, which exert an additional shear force on the fluid. A force balance then indicates that the pressure gradient in the three dimensional flow has to be larger in order to balance the side wall shear.

Numerical solutions of the full Navier-Stokes equations in cavities with spanwise aspect ratio W/H equal to unity and increasing values of lengthwise aspect ratio L/H from 2 upto 10 were attempted. Uniform grid spacings of $1/44$, $1/48$ and $1/52$ were used for the different cases depending upon the lengthwise aspect ratio. Symmetry conditions were used on the $y = 1/2$ plane. The CPU times required for these cases on the Y-MP were anywhere between 5 and 10 minutes. These modest CPU times are due to the fact that the Douglas-Gunn ADI scheme (discussed in the next chapter) was used to integrate the momentum equations in time. The flow field on the symmetry plane is very similar to the corresponding two dimensional one. Figure 4.21 shows the u -velocity profiles along the vertical centerline on the symmetry plane and as before, the case for which L/H is equal to 2 shows the greatest deviation from the profile corresponding to $L/H \rightarrow \infty$, obtained from above. A plot of the pressure profiles along the horizontal centerline on the symmetry plane is given in Figure 4.22. These profiles also show the presence of a core flow region from lengthwise aspect ratio 4 onwards, similar to the two dimensional ones in Figure 4.19. Both the velocity and pressure profiles asymptote for aspect ratios beyond 6, but now in the three dimensional case, these asymptotic values show a greater discrepancy from the values obtained from the solution of equations (4.15) and (4.16). This can be traced to the fact that the integral in equation (4.16) came out to be around 0.02 for the numerical solutions. This is high, despite the fact that the grid

Figure 4.21. The u -velocity along the vertical centerline on the symmetry plane for a three dimensional shallow cavity for aspect ratios 2,4,6,8 and 10 at $Re = 100$

Figure 4.22. Pressure along the horizontal centerline on the symmetry plane for a three dimensional shallow cavity for aspect ratios 2,4,6,8 and 10 at $Re = 100$

spacings used here would be considered to be adequate for $Re = 100$. Refinement of the grids beyond a spacing of $1/54$ was not attempted as this does not bring in any new structures into the flow field. The w -velocity profiles along the horizontal centerline on the symmetry plane are plotted in Figure 4.23. These profiles also show the presence of strong wall jets near the downstream end of the cavity similar to the two dimensional case, but their magnitudes are lesser now as a result of the extra degree of freedom offered by the y -coordinate.

In summary, solutions to the incompressible, three dimensional Navier-Stokes equations on uniform and non-uniform grids have been obtained using an explicit and a semi-implicit scheme for the time integration of the momentum equations with the Neumann-Poisson problem for pressure solved using a direct method. In the next chapter, we discuss the final improvement of our algorithm. There an implicit method with unconditional stability for the time integration of the Boussinesq equations for natural convection is given.

Figure 4.23. The w-velocity along the horizontal centerline on the symmetry plane for a three dimensional shallow cavity for aspect ratios 2,4,6,8 and 10 at $Re = 100$

CHAPTER V

NATURAL CONVECTION IN A SHALLOW CAVITY

In this chapter the Douglas-Gunn ADI method is implemented for solving the problem of natural convection in shallow cavities that is heated from one end and cooled from the other. This problem in both two- and three-dimensions was studied in a recent GAMM workshop (Roux, 1990) and has some importance in growing of semi-conductor crystals by the, so called, horizontal Bridgeman method.

5.1 NATURAL CONVECTION IN CAVITIES

Consider the natural convection of a fluid contained in a rectangular box of length L , height H and span or width W . The fluid has a density ρ , kinematic viscosity ν and thermal diffusivity α . It is assumed here that α is much larger than ν , so that the Prandtl number of the fluid, which is equal to ν/α is small. The coordinate axes are placed the same way as before. That is, the x -axis is along the length, the y -axis along the span and the z -axis vertically upwards along the height opposed to gravity, so as to form a right handed coordinate system. The left and right surfaces of the box are maintained at constant temperatures such that the left side is hotter than the right. All the other surfaces are assumed to be insulated. The fluid near the left side, being hotter, is lighter and rises to the top while the cooler, denser fluid near the right side sinks to the bottom. This sets up a convection pattern in the box and it is this convection that we wish to study.

5.2 FORMULATION

The formulation of this problem proceeds in essentially the same way as in Chapter 4. The main difference now, is the addition of the energy equation and the presence of a buoyancy term in the z-momentum equation. This term arises from the variation of density with temperature and accounts for the mechanism that drives the flow. The density is assumed to vary linearly with temperature while the variation of all the other properties of the fluid with temperature is neglected. This leads to the so-called Boussinesq form of the governing equations and they are outlined below.

5.2.1 GOVERNING EQUATIONS

The Boussinesq equations are written in dimensionless form with lengths scaled by the height of the box, H , time by H^2/ν , velocities by the characteristic velocity, $U = \nu/H$ and the pressure by ρU^2 . The dimensionless temperature is defined to be the difference between the actual temperature and the average of the temperatures of the left and right wall, divided by ΔT , which is the temperature difference between them. The parameters that appear in these equations are the Prandtl number $Pr = \nu/\alpha$ and the Grashof number $Gr = g\beta\Delta TH^3/\nu^2$, where β is the coefficient of volumetric expansion. The governing equations can now be written as,

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0, \quad (5.1)$$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = -\frac{\partial p}{\partial x} + \left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right], \quad (5.2a)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} = -\frac{\partial p}{\partial y} + \left[\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right], \quad (5.2b)$$

$$\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} = -\frac{\partial p}{\partial z} + \left[\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right] + Gr T, \quad (5.2c)$$

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial z} = \frac{1}{Pr} \left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right]. \quad (5.3)$$

The momentum equation has been presented in its component form to make the discussion of the numerical method in the next section clear.

5.2.2 BOUNDARY CONDITIONS

Since all the sides of the box are rigid, the normal and tangential components of velocity are equal to zero on these surfaces. Accordingly we have

$$u = v = w = 0, \quad x = 0, L/H, \quad (5.4a)$$

$$u = v = w = 0, \quad y = 0, W/H, \quad (5.4b)$$

$$u = v = w = 0, \quad z = 0, 1. \quad (5.4c)$$

As mentioned before, since all the surfaces of the box except the left and right sides are insulated, the boundary conditions for temperature can be written in dimensionless form as,

$$\frac{\partial T}{\partial y} = 0, \quad y = 0, W/H, \quad (5.5a)$$

$$\frac{\partial T}{\partial z} = 0, \quad z = 0, 1, \quad (5.5b)$$

$$T = 1/2, \quad x = 0; \quad T = -1/2, \quad x = L. \quad (5.5c)$$

We note in passing, that, the solution to equation (5.3) for $Pr = 0$ subject to (5.5a), (5.5b) and (5.5c) can be obtained as,

$$T = 1/2 - x/L, \quad 0 \leq x \leq L/H, \quad 0 \leq y \leq W/H, \quad 0 \leq z \leq 1. \quad (5.6)$$

5.3 NUMERICAL METHOD

In contrast to Chapters 2 and 4, here we consider the governing equation and boundary conditions for the pressure first and take up the issue of time discretization of the momentum and energy equations later. The reason for doing so is based on the observation that in our methodology the pressure problem remains the same irrespective of the time discretization scheme used. This is so because of the fact that the source terms in both the governing equation for the pressure and the boundary conditions have to be evaluated using the known values of velocities (and temperature), as was done for the semi-implicit method in the previous chapter. So we can use the same equations and boundary conditions for pressure from the previous chapter, after accounting for buoyancy effects. Accordingly, we have,

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t} \nabla \cdot \vec{u}^n - \nabla \cdot [(\vec{u}^n \cdot \nabla) \vec{u}^n] + \nabla^2 (\nabla \cdot \vec{u}^n) + \text{Gr} \frac{\partial T}{\partial z}. \quad (5.7)$$

The boundary conditions for pressure are obtained from the momentum equations (5.2) as,

$$\frac{\partial p^{n+1}}{\partial x} = \frac{\partial^2 u^n}{\partial x^2}, \quad x = 0, L/H, \quad (5.8a)$$

$$\frac{\partial p^{n+1}}{\partial y} = \frac{\partial^2 v^n}{\partial y^2}, \quad y = 0, W/H, \quad (5.8b)$$

$$\frac{\partial p^{n+1}}{\partial z} = \frac{\partial^2 w^n}{\partial z^2} + \text{Gr} T^n, \quad z = 0, 1. \quad (5.8c)$$

Here, n denotes time level as before. The discretization and solution of the pressure problem from this point onwards is identical to that described in Chapter 4 and so will not be discussed here. We now turn to the time integration of equations (5.2) and (5.3).

In the last chapter, the use of both an explicit and a semi-implicit method to integrate the momentum equations in time were considered. As discussed before, the advantage of the latter method is that it eliminates the diffusion time step restriction. But both the methods have the common disadvantage that the convective terms are treated explicitly. For problems

in which convection plays a dominant role, treating these terms explicitly leaves the Courant condition as a restriction on the time step for a given mesh spacing for overall stability of the numerical scheme. For fine mesh spacings, this condition becomes restrictive and if one is seeking steady state solutions the computing time required to reach steady state could be large. It can thus be seen that the semi-implicit scheme is only partially beneficial and a fully implicit scheme with unconditional stability is desirable for performing the long time integration of the momentum and energy equations. The alternating direction implicit (ADI) method for solving parabolic and elliptic equations (Peaceman, 1955, Varga, 1962) is such a method. The use of ADI methods for solving fluid dynamics problems was considered as early as 1967 by Aziz & Hellums and many papers cited by Roache (1972) concern with applications of these methods. The ADI belongs to a class of methods known as the operator splitting methods. The basic idea behind these methods is to take a block tridiagonal operator, such as the discretized form of the Laplacian and split it into a series of one dimensional operators in each of the coordinate directions, such that the split operator represents the original one to within a certain error. This splitting error is usually of the same order as the discretization error that arises as a result of discretizing the original governing equations. The advantage in splitting the operator is that the split operators are much easier to invert than the original one. In the case of the Laplacian, for example, one solves scalar tridiagonal systems instead of block tridiagonal systems as a result of operator splitting. Different variations of the ADI scheme have been proposed by Peaceman & Rachford (1955), Douglas & Rachford (1956) and Douglas & Gunn (1964). It has been shown by Douglas & Gunn (1964) that these and other variations proposed earlier can be recovered as special cases of their general formulation of the ADI method. We chose the Douglas-Gunn ADI method for solving equations (5.2) and (5.3) numerically (Briley, 1974). This method is easily extendable to three dimensions and is unconditionally stable in both two- and three-dimensions in contrast to the Peaceman-Rachford method, which loses its unconditional stability in going from two to three dimensions.

To solve equations (5.2) and (5.3) using the Douglas-Gunn ADI method, they were first linearized in a manner suggested by Briley (1974), that is, by lagging the coefficients u , v and w of the non-linear terms on the left hand side of these equations one time level and

evaluating them at time level n . All the spatial derivatives were discretized using second order accurate central differences. The equations were then discretized in time using the Crank-Nicolson scheme. The discretized forms of these equations, in the notation of Briley (1974), are given as

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = (D_x + D_y + D_z) \left[\frac{\phi^{n+1} + \phi^n}{2} \right] + S_\phi^{n+1}, \quad (5.9)$$

where,

$$D_x \equiv -u^n \delta_x + \Gamma_\phi \delta_x^2,$$

$$D_y \equiv -v^n \delta_y + \Gamma_\phi \delta_y^2,$$

$$D_z \equiv -w^n \delta_z + \Gamma_\phi \delta_z^2,$$

and δ and δ^2 are the usual central difference discretization operators for the first and second order derivatives respectively and ϕ represents any one of u , v , w or T . Also, $(\Gamma_u, \Gamma_v, \Gamma_w, \Gamma_T) = (1, 1, 1, 1/\text{Pr})$, as a result of the non-dimensionalization employed. If the Prandtl number is equal to zero, the temperature field is given by equation (5.6) and so the energy equation need not be included in equation (5.9). Its inclusion here is to make the numerical method more general. In the above equation, S_ϕ^{n+1} represents a source term that is *known* at the time of solving for ϕ . When solving the momentum equations, this source term is equal to the pressure gradient term and in the case of the z-momentum equation it includes the buoyancy term also. It is set to zero during the solution of the energy equation. The pressure gradient terms are evaluated from the known pressure field at $n+1$ after the solution of equation (5.7). By solving the energy equation using the velocity field at n before the momentum equations, the buoyancy term can also be evaluated at time level $n+1$. Thus,

$$\begin{bmatrix} S_u^{n+1} \\ S_v^{n+1} \\ S_w^{n+1} \\ S_T^{n+1} \end{bmatrix} = \begin{bmatrix} -\delta_x p^{n+1} \\ -\delta_y p^{n+1} \\ -\delta_z p^{n+1} + \text{Gr} T^{n+1} \\ 0 \end{bmatrix}.$$

The difference operators D_x , D_y , and D_z should have a superscript n on them to indicate their time dependence but these have been dropped here as there is no danger of ambiguity. Even though the Crank-Nicolson scheme used in equation (5.8) is second order accurate in time, the linearization process that led to the above form for these operators destroys the second order accuracy and so the temporal accuracy of equation (5.9) is formally only first order. Second order accuracy in time can be achieved by using the linearization procedure suggested by McDonald and Briley (1975). They give further details on the number of levels of storage required and the operation count. The application of the Douglas-Gunn ADI scheme to equation (5.8) essentially reduces to treating each of the coordinate directions implicitly in turn. This can be written as (Briley and McDonald, 1980),

$$\frac{\phi^* - \phi^n}{\Delta t} = D_x \frac{\phi^* + \phi^n}{2} + D_y \phi^n + D_z \phi^n + S_\phi^{n+1}, \quad (5.10a)$$

$$\frac{\phi^{**} - \phi^n}{\Delta t} = D_x \frac{\phi^* + \phi^n}{2} + D_y \frac{\phi^{**} + \phi^n}{2} + D_z \phi^n + S_\phi^{n+1}, \quad (5.10b)$$

$$\frac{\phi^{***} - \phi^n}{\Delta t} = D_x \frac{\phi^* + \phi^n}{2} + D_y \frac{\phi^{**} + \phi^n}{2} + D_z \frac{\phi^{n+1} + \phi^n}{2} + S_\phi^{n+1}, \quad (5.10c)$$

$$\phi^{n+1} = \phi^{***} + O(\Delta t^2). \quad (5.10d)$$

For programming purposes, equations (5.10b) and (5.10c) can be simplified by subtracting (5.10a) from (5.10b) and (5.10b) from (5.10c). This gives,

$$\frac{\phi^{**} - \phi^*}{\Delta t} = D_y \frac{\phi^{**} - \phi^*}{2}, \quad (5.11b)$$

$$\frac{\phi^{***} - \phi^{**}}{\Delta t} = D_z \frac{\phi^{***} - \phi^{**}}{2}. \quad (5.11c)$$

Equations (5.10a), (5.11b) and (5.11c) are scalar tridiagonal equations and can be solved easily using the Thomas algorithm. However, boundary conditions are now needed for the intermediate quantities ϕ^* and ϕ^{**} when solving equations (5.10a) and (5.11b). The advantage of using the Douglas-Gunn method is that these intermediate quantities are consistent representations of the solution ϕ^{n+1} and so the boundary conditions for ϕ^{n+1} can be used for

these quantities also without any loss of accuracy for time independent boundary conditions (Briley & McDonald, 1980). In case of time dependent boundary conditions, this would introduce errors in $\partial\phi/\partial t$ on the boundary of the same order as the temporal discretization error. Briley and McDonald (1980) give a detailed discussion of this issue for other ADI schemes.

In the development above, it was assumed that the grid was uniform. As mentioned in the previous chapters, problems in fluid mechanics often call for the use of non-uniform grids and hence it is essential for the numerical method to be able to handle non-uniform grids also. Our strategy for doing this is to generate a suitable non-uniform grid in the physical domain, and map it into a uniform grid in a computational domain through some transformation, analytical or numerical. The governing equations and boundary conditions are then transformed to the computational domain, where they are solved. As already shown in Chapter 3, the matrix decomposition method for solving the pressure Poisson problem can be used to solve the transformed problem also. The Douglas-Gunn ADI method that we discussed above for time integration of the momentum and energy equations can be used to solve the transformed forms of the equations that arise from the use of transformations such as the one discussed in the previous chapter (Briley & McDonald, 1977) as well. However, a subtle difficulty arises now owing to the presence of first order derivatives arising from the transformation of the diffusion terms. The discretized forms of these first derivatives contribute to the off-diagonal terms in the tridiagonal systems in equations (5.10a), (5.11b) and (5.11c). Since these first derivatives themselves are multiplied by the second derivatives of the transformation, severe stretching of the grids in the physical domain would lead to large values for these coefficients. This results in a loss of diagonal dominance of the tridiagonal systems (Ghia et al., 1977).

With the velocity field at time level n , the pressure field at $n+1$ can be obtained by solving equation (5.7). This was done using the method of matrix decomposition. The boundary pressures were then updated. The temperature field at $n+1$ can be obtained next, by solving the energy equation through the sequence of equations (5.10a), (5.11b) and (5.11c). The source terms S_u^{n+1} , S_v^{n+1} and S_w^{n+1} in the momentum equations can now be evaluated and the velocity field at level $n+1$ solved for using the Douglas-Gunn ADI sequence. By repeating the whole procedure, the equations can be marched forward in time. In case of

steady state solution, the convergence criterion used was the same as before, namely, that the residuals of the steady state momentum and energy equations be $O(10^{-5})$. In case of oscillatory solutions, however, time integration was continued until enough cycles of the oscillations have been captured. This allowed us to obtain a good estimate of the dominant frequencies of the flow field through a power spectrum analysis. This in itself does not reflect on the temporal accuracy of the solution, for, the latter is dependent on the order of the temporal truncation error of the numerical method, which in the present case is only first order and on the smallness of the time step used. It becomes apparent that time resolution of flows using a numerical method that is first order accurate in time can be achieved only through the use of small time steps. This is still a weakness, for the number of time steps required to reach a certain value of time increases, thereby increasing the required amount of computing time. This provides the motivation for the development of numerical methods that are second order accurate in time. Nevertheless, the high computing speed of the present numerical method made the first order accuracy tolerable for the problems investigated and allowed the use of time step values as small as 2.5×10^{-6} for the three dimensional simulations.

5.4 RESULTS & DISCUSSION

We now present the results for natural convection in two- and three-dimensional cavities with a lengthwise aspect ratio $L/H = 4$ and a spanwise aspect ratio W/H equal to 1 or 2. Here, specifically we consider some unsteady solutions for this problem that were reported in the GAMM workshop (Roux, 1990) and present a quantitative comparison of our results with those reported there. The main objective in doing so is to establish the feasibility of using the above numerical method, not only for obtaining steady state solutions, but for obtaining accurate unsteady solutions through long time integration of the governing equations. The required computing times are reasonable as will be seen from the discussion in the following paragraphs.

The Prandtl number of the fluid was kept equal to zero for all the two dimensional simulations and it was either zero or 0.027 (corresponding to mercury) for the three dimensional simulations. We discuss the two dimensional simulations first, for which the Grashof

number was varied between 80,000 and 160,000. A 82x328 uniform grid was used for all the cases and the time step was set equal to 10^{-5} . The computing time per time step on this grid was 0.05377 seconds in multi-processor mode on the Cray Y-MP8/864. Whenever possible, the solution corresponding to a lower value for the Grashof number was used as initial condition for simulations at higher values of this parameter. All these cases required about 100,000 to 150,000 time steps and computing times between 75 and 120 minutes. The first case that we studied was $Gr = 80,000$ for which a steady state solution was obtained. This is shown in Figure 5.1. There is a strong cell in the middle of the cavity and the entire flow field is centro-symmetric. Our results for the maximum u - and v -velocities on the vertical and the horizontal centerlines for this case compare well with the values obtained by Behnia & de Vahl Davis (1990) as shown in Table 5.1. When the Grashof number is increased to 102,000, the solution becomes oscillatory. The oscillations shown in Figure 5.2 are quasi-periodic in the beginning but they settle down after a few cycles to a periodic state with dimensionless frequency 16.105. This compares well with the value of 16.34 obtained by Ben Hadid & Roux (1990). When the Grashof number is further increased to 120,000, the oscillations of the flow field shown in Figure 5.3 become periodic with frequency equal to 17.86. This frequency value is within 0.03% of the value reported by Behnia & de Vahl Davis (1990). A plot of the velocity vectors at the extremes of these oscillations in Figure 5.4 indicate that the flow field oscillates between a single- and a three-cell structure. Our results for the minimum and maximum values of the velocities on the centerlines during a period compare very well with those of Behnia & de Vahl Davis (1990). Ben Hadid & Roux (1990) showed that if one goes further enough in time, these oscillations eventually become quasi-periodic accompanied by a loss of the centro-symmetry of the flow field. At $Gr=160,000$, the transient behavior for the first 20 cycles or so is the same as that for a Grashof number of 120,000, but then at approximately $t=1$ (dimensionless), the oscillations, as shown in Figure 5.5, suddenly become aperiodic and are quickly damped so that the flow settles down to a steady state. The steady state flow field is shown in Figure 5.6, where a two cell structure can be seen. Sufficiently long time integrations do not indicate any new transitions from this state. It has been speculated by Behnia & de Vahl Davis (1990) that the accumulation of truncation errors cause a perturbation of the unsteady oscillatory flow field, thus forcing it into a more stable state.

Figure 5.1. Velocity vectors for natural convection in a two dimensional shallow cavity at $Gr=80,000$

Table 5.1. Comparison of the present results with those reported in
the GAMM Workshop (Roux, Editor), 1990.

	Gr	Frequency			Max(u(1,y))			Max(w(x,0.5))		
		Present	Literature	%diff	Present	Literature	%diff	Present	Literature	%diff
Steady	80,000	-	-	-	95.31	95.26	0.04	73.73	73.50	0.3
Q.periodic	102,000	16.105	16.34	1.43	-	-	-	-	-	-
Periodic	120,000	17.8635	17.87	0.03	86.5	84.59	2.25	89.05	87.95	1.25
					162.0	162.6	0.3	157.72	158.53	0.5
Steady	160,000	-	-	-	239.7	240.4	0.28	169.35	169.44	0.04

Figure 5.2. Transient behaviour of $u_{\max}$ (top) and $w_{\max}$ (bottom) along the vertical and horizontal centerlines for natural convection in a two dimensional shallow cavity at $Gr=102,000$

Figure 5.3. Transient behaviour of $u_{\max}$ (top) and $w_{\max}$ (bottom) along the vertical and horizontal centerlines for natural convection in a two dimensional shallow cavity at $Gr=120,000$

Figure 5.4. Velocity vectors for natural convection in a two dimensional shallow cavity at $Gr=120,000$

Figure 5.5. Transient behaviour of $u_{\max}$ (top) and $w_{\max}$ (bottom) along the vertical and horizontal centerlines for natural convection in a two dimensional shallow cavity at $Gr=160,000$

Figure 5.6. Velocity vectors for natural convection in a two dimensional shallow cavity at $Gr=160,000$

They predict that the finer the grid size, the later the transition to steady state would be on account of the smaller truncation errors. Expressed another way, this would mean that the coarser the grid, the earlier the transition to steady state would be. In order to check this, we first solved this problem for the $Gr=120,000$ on a 42×168 grid. This solution was then given as a initial condition for the case $Gr=160,000$ as was done for the fine grid simulation. The results for this case are shown in Figure 5.7, where it can be seen that the transition to steady state occurs at approximately the same value of time as before for the finer grid. In fact, the transition was actually delayed somewhat with the coarse grid. This does not rule out the possibility that the reverse transition to steady state is caused by truncation errors, but merely shows that rigorous tests of the kind performed by Le Quéré (1990) are necessary to determine if this is indeed so.

An interesting feature of this problem is that the solutions in this range of Grashof number are dependent on the initial conditions. This is illustrated in Figure 5.8, where two possible solutions to the problem at $Gr=120,000$ are shown. If the solution corresponding to $Gr=160,000$ is used as the initial condition, then a steady two cell structure as shown in the top half of Figure 5.8 is obtained. On the other hand, as already mentioned, oscillatory solutions are also possible when the solution corresponding to $Gr=102,000$ is used as the initial condition, as shown in Figure 5.3 and in the bottom half of Figure 5.8. This shows the existence of a hysteresis cycle in the solution for this range of Grashof numbers. Detailed phase plane analysis of the hysteresis cycle is presented in the various papers in Randriamampianina et al. (1990). Since our main aim here was to validate our results, the topic was not pursued further. We now turn to the three dimensional simulations.

Natural convection of a zero Prandtl number fluid in a three dimensional shallow cavity with both rigid and free upper surfaces was considered by Afriid & Zebib (1990). They obtained numerical solutions to that problem using the SIMPLER algorithm of Patankar (1980). Experimental investigations of this problem using mercury, a low Prandtl number fluid ($Pr=0.026$), were conducted by Pratte & Hart (1990) and Hung & Andereck (1990). In all of these works the lengthwise aspect ratio of the cavity was kept fixed at 4, while the spanwise ratio was equal to 1, 2 or 8. Earlier, experiments using even shallower cavities with aspect ratio 16 in both the lengthwise and spanwise directions were performed by Hung &

Figure 5.7. Transient behaviour of $u_{\max}$ (top) and $w_{\max}$ (bottom) along the vertical and horizontal centerlines for natural convection in a two dimensional shallow cavity at $Gr=160,000$ on a coarse (42x168) grid

Figure 5.8. Two possible solutions for natural convection in a two dimensional shallow cavity at $Gr=120,000$, steady solution (top) and oscillatory solution (bottom)

Andereck (1988). Pseudo-spectral calculations of the flow in a shallow cavity with infinite aspect ratios along the length and span were done by Wang & Korpela (1989, 1991). Here, we consider only cavities with lengthwise aspect ratio 4 and spanwise aspect ratio 1 or 2 and with rigid surfaces on all sides. The first problem studied was the $4 \times 1 \times 1$ cavity at a Grashof number equal to 500,000 and Prandtl number zero. A uniform $120 \times 60 \times 60$ grid was used for this calculation. Following Afrid & Zebib (1990), symmetry conditions were imposed on the $y=1/2$ plane, and so actual computations were performed only on a $120 \times 30 \times 60$ grid. In comparison, Afrid & Zebib (1990) used a non-uniform $62 \times 17 \times 32$ grid with finest grid spacing $1/33$ for their calculations. The time step was set equal to 2.5×10^{-6} , the same as that used by Afrid & Zebib (1990). The time development of the flow field was studied by sampling the u -velocity at approximately the same points inside the cavity as they did. For these particular values of Grashof and Prandtl numbers, the flow field becomes oscillatory after a certain time as shown in Figure 5.9a. Once a long enough time series (about 2^{16} points) was available, a power spectrum analysis was carried out. This is shown in Figure 5.9b, where a peak in the spectrum at a dimensionless frequency of 36 ± 3 can be seen. This value for the dominant frequency compares well with a value of 39 obtained by Afrid & Zebib (1990). Two smaller peaks at $f/3$ and $11f/6$ can also be seen in the power spectrum, where f is the fundamental frequency. These calculations took roughly about 22 hours of CPU time on the Cray Y-MP8/864. It is worth noting, that it took Afrid & Zebib (1990) between 30 and 40 hours of CPU time on an ETA-10 which is comparable to a Cray Y-MP8/864, to carry out a calculation with a factor of 8 fewer points. Thus our numerical method appears to have substantial advantage in regard its computing speed.

We now turn to the study of natural convection of a fluid with Prandtl number 0.026 in the same $4 \times 1 \times 1$ cavity. No slip conditions are now imposed on all sides of the box. The Grashof number was first set to 844,800 for which an oscillatory flow field was seen in the experiments of Pratte & Hart (1990). They give time traces and power spectra of these oscillations by measuring the temperature at certain locations within the cavity. Our objective was to capture these oscillations through a numerical simulation. To this end, a uniform $120 \times 50 \times 50$ grid and a time step value of 5×10^{-5} were used for the simulation. We monitored both the temperature and the u -velocity at selected locations within the cavity, that were

Figure 5.9. (a) Time traces of u -velocity at several points inside the cavity for natural convection in a three dimensional shallow cavity ($4 \times 1 \times 1$) at $Gr=500,000$ and $Pr=0$

Figure 5.9. (continued)

Figure 5.9. (continued)

(b) Power Spectrum

different from those used by Pratte & Hart (1990). A time trace of these oscillations together with the power spectrum is given in Figure 5.10. A total of 2^{15} points was used for obtaining the power spectrum and the computing time required to collect this many points came out to be around 10 hours on the Cray. It can be seen that the amplitudes of the oscillations for the velocities are much larger than those for temperature. An exponential fall-off of the energy with frequency can be seen in the power spectrum, where a curve of the form $10^{-\kappa f}$ with $\kappa=1.448$ is also shown. This type of an exponential fall-off has been seen before by Hung & Andereck (1988) in their earlier experiments on large aspect ratio shallow cavities and is indicative of low-dimensional chaos. This does not agree with the results of Pratte & Hart (1990) who found the flow to be oscillatory with a frequency of 1/19 Hz for this value of Gr. An explanation of this might lie in the fact that slight asymmetries in the experimental setup could favor some oscillatory modes, the so-called 'non-robust' modes. This was indeed observed in their experiments for lower values of Grashof number.

Next, we studied the flow in a 4x2x1 cavity, i.e. spanwise aspect ratio 2, for a Grashof number of 180,000. Pratte & Hart (1990) found that for Gr=158,400, which is slightly supercritical for this value of the spanwise aspect ratio, the flow oscillates with a dominant frequency around 0.015 Hz. We used a 120x50x60 uniform grid for this case and a time step value of 10^{-5} . A plot of the temperature at five locations inside the cavity (the same as those used by Pratte & Hart) is given in Figure 5.11. The temperature values at these points do show the kind of small amplitude oscillations seen by Pratte & Hart (1990) but they eventually die out after about 40000 time steps. This could be an indication of damping of some kind in our numerical method. The computing time required for this case was around 13 hours on the Cray. We concluded from the above results that the numerical method proposed in the previous section can adequately perform long time integrations of the incompressible Navier-Stokes equations and yield accurate transient solutions for this problem. The advantage of using an unconditionally stable scheme such as the Douglas-Gunn ADI method for time marching can be seen from the fact that the numerical method does not show divergence in the presence of hydrodynamic instabilities as was the case with the explicit method of the previous chapter.

Figure 5.10. Time traces at two points inside the cavity for natural convection in a three dimensional shallow cavity ($4 \times 1 \times 1$) at $Gr=180,000$ and $Pr=0.026$, (a) Temperature

Figure 5.10. (continued)

(b) u-velocity

Figure 5.10. (continued)

(c) Power Spectrum

Figure 5.11. Time traces of temperature at four points inside the cavity for natural convection in a three dimensional shallow cavity (4x2x1) at $Gr=180,000$ and $Pr=0.026$

Figure 5.11. (continued)

CHAPTER VI

CONCLUSIONS

Numerical methods for obtaining steady and transient solutions of the incompressible, three dimensional Navier-Stokes equations were considered in this dissertation. These equations were solved in their primitive variable form on non-staggered, uniform and non-uniform grids. This required the solution of three parabolic equations, one for each component of velocity and a Poisson equation for pressure subject to Neumann boundary conditions. Any solution to this Neumann-Poisson problem is arbitrary to a constant and in addition, it has to satisfy an integral constraint that arises from Green's theorem. The consistent finite-differencing method of Abdallah (1987) allows this integral constraint to be satisfied automatically. This method was used to solve the three dimensional thermocapillary convection in a cubical cavity. Even though it was possible to obtain steady state solutions, the extension of Abdallah's method could not be used to obtain accurate, transient solutions. The reasons for the lack of accuracy were identified as the poor iterative convergence during the intermediate time steps of the point SOR scheme used to solve for the pressure and dropping of the time derivative terms when the normal component of momentum is used to supply the pressure boundary conditions; this being applied, not at the boundary, but a half grid point into the fluid. The remedy for the latter weakness is to apply second order accurate one-sided differences to discretize the normal derivatives of pressure on the boundaries. The difficulty with poor iterative convergence was overcome by use of the matrix decomposition method of Buzbee et al. (1970) for solving the Neumann-Poisson problem to machine accuracy. This method was extended to non-uniform grids and second order accurate one-sided differencing for the derivative boundary conditions was also implemented. The computing

speed of the method was improved by using Cray Assembly Language routines for carrying out the required matrix multiplications. With this method used for resolving the pressure and an explicit time differencing scheme for handling the momentum equations, solutions to the three dimensional flow in a lid driven cavity were obtained for Reynolds number up to 4000. The solution at Reynolds number 4000 showed the presence of weak longitudinal vortices along the floor of the cavity. These were seen in the experiments of Koseff & Street (1984) and the numerical solutions reported by Iwatsu et al. (1989). Stability considerations of the above first order accurate explicit scheme necessitate the use of small time steps when using fine grids. Since this increases the number of time steps and hence the computing time required to reach steady state, a semi-implicit scheme that eliminates this difficulty for diffusion dominated flows was implemented. Despite the improved stability properties, this method is still only conditionally stable. Unconditional stability was achieved through the use of the Douglas-Gunn ADI method in a manner described by Briley (1974). This was used to study natural convection in a shallow cavity in two- and three-dimensions. The convective flow exhibits low dimensional chaos for high values of Grashof numbers. Unsteady oscillatory solutions were obtained and compared with the solutions presented in Roux (1990). The linearization of the convective terms in the parabolic equations during their time integration lowered the formal second order accuracy of the Douglas-Gunn method to first order. Hence, small time steps had to be used to obtain accurate transient solutions. Consequently, computing times up to 25 hours on the Cray Y-MP8/864 were required for some cases, but these computing times were less than those reported by other researchers for same calculations. Nevertheless, second order accuracy in time is desirable and worth pursuing. Also, the use of this numerical method to study other flows such as three-dimensional thermocapillary convection in cavities and its extension to other geometries such as the cylindrical geometry are left for the future.

APPENDIX

The generalized eigenvalue problem $G e_i = \lambda A e_i$ can be written as,

$$\begin{bmatrix} -4 & 1 & 0 & . & . \\ 1 & -4 & 1 & 0 & . \\ . & . & . & . & . \\ . & 0 & 1 & -4 & 1 \\ . & . & 0 & 1 & -4 \end{bmatrix} e_l = \lambda_l \begin{bmatrix} 3/2 & 0 & . & . & . \\ 0 & 1 & 0 & . & . \\ . & . & . & . & . \\ . & . & 0 & 1 & 0 \\ . & . & . & 0 & 3/2 \end{bmatrix} e_l, \quad (A1)$$

where, $e_l = (\phi_{1,l}, \phi_{2,l}, \dots, \phi_{L,l})^T$. By multiplying both sides of equation (A1) by A^{-1} , we get

$$\begin{bmatrix} -8/3 & 2/3 & 0 & . & . \\ 1 & -4 & 1 & 0 & . \\ . & . & . & . & . \\ . & 0 & 1 & -4 & 1 \\ . & . & 0 & 2/3 & -8/3 \end{bmatrix} e_l = \lambda_l e_l. \quad (A2)$$

The system (A2) can also be written as,

$$\phi_{i-1,l} - (4 + \lambda_l) \phi_{i,l} + \phi_{i+1,l} = 0, \quad 1 \leq i \leq L, \quad (A3)$$

subject to the boundary conditions

$$3\phi_{0,l} - 4\phi_{1,l} + \phi_{2,l} = 0, \quad (A4)$$

$$3\phi_{L+1,l} - 4\phi_{L,l} + \phi_{L-1,l} = 0. \quad (A5)$$

The solution to the above system is, after substituting $\lambda_l = -4 + 2 \cos \theta_l$,

$$\phi_{i,l} = a \cos i \theta_l + b \sin i \theta_l, \quad (A6)$$

where, a and b are arbitrary constants. Elimination of b by using equation (A4) leads to the following equation for the eigenvectors ;

$$\phi_{i,l} = a (-3 \sin i \theta_l + 4 \sin (i-1) \theta_l - \sin (i-2) \theta_l), \quad (\text{A7})$$

where the constant a can be fixed by proper normalization that does not need to concern us here. Substituting the eigenvectors of equation (A7) into (A5) leads to the equation

$$9 \sin (L+1) \theta_l - 24 \sin L \theta_l + 22 \sin (L-1) \theta_l - 8 \sin (L-2) \theta_l + \sin (L-3) \theta_l = 0, \quad (\text{A8})$$

for the eigenvalues λ_l (or θ_l).

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