University of Cincinnati

Date: 3/19/2018

I, Dilip Kalagotla, hereby submit this original work as part of the requirements for the degree of Master of Science in Aerospace Engineering.

It is entitled:

Modeling Particle Drag in Accelerating Flows with Implications for SBLI in PIV - A Numerical Analysis

Student's name: Dilip Kalagotla

This work and its defense approved by:

Committee chair: Paul Orkwis, Ph.D.

Committee member: Prashant Khare

Committee member: Mark Turner, Sc.D.

29297

Modeling Particle Drag in Accelerating Flows with Implications for SBLI in PIV - A Numerical Analysis

by

Dilip Kalagotla

B.Tech., Mechanical Engineering,

IIT(ISM), Dhanbad, 2015

A thesis submitted in partial fulfillment
of the requirements for the degree of
Master of Science,
Aerospace Engineering,
College of Engineering and Applied Science,
University of Cincinnati, Ohio
2018

Thesis Committee:

Chair: Paul D. Orkwis, PhD

Member: Mark G. Turner, ScD

Member: Prashant Khare, PhD

Abstract

Since its inception, Particle Image Velocimetry (PIV) has been increasingly used to measure the velocity of the flow field, especially in aerospace applications. One of the major assumptions of PIV is that velocity of the flow field is same as the velocity of tracers in it. The ability of PIV to measure velocity depends upon the potential of tracers to track the flow surrounding them.

Shock-Boundary Layer Interactions (SBLIs) have been studied extensively over the years using experimental and computational methods due to their importance in almost every supersonic flow. PIV has been doing a great job in analyzing SBLIs over the past few years but it has its limitations especially when there are high temporal and spatial accelerations. On the other hand, numerical simulations that better predict shock interactions have a hard time analyzing the turbulence properties of SBLIs. This implies that only by using both computational and experimental results together physics of SBLIs can be better understood.

The current study was divided into two parts. First, development and validation of a post-processing code to be able to accommodate the solid particles. For this, Visual3 has been chosen because it lets a user control even smallest of its processes. Visual3 code has been modified to track particles using accurate physics within a flow. Forces acting on a particle in a flow were analyzed and compared using data obtained from Modified-Visual3 (MV3). Based on this data, dominant forces on a particle in high-speed flow are determined. Results obtained from Modified-Visual3 are compared with Melling(1997) data to validate the code. A specific case is solved mathematically to compare with Modified-Visual3 and Melling's data. A second validation was done using an example of a generalized oblique shock to understand the behavior of the particle passing through the shock. Finally, particle relaxation times for different particle specifications were calculated to understand which particles have better traceability to use in Particle Image Velocimetry(PIV).

Second, the MV3 code was used to post-process the CFD results of the UM-PIV data. These CFD results were obtained from the numerical analyses conducted at the UC. A standard case with 2.75 Mach and 7.75° wedge angle were used in MV3 to be in compliance with the CFD analysis. Particle, fluid velocities, position at every instant were collected from MV3 and were later used for comparison. This obtained data was filtered using a Python script to compare with the experimental plane defined in Eagle's (2011) work. Different particle sizes were used to compare the obtained results. These results were then used to analyze

particle lag, velocity differences, velocity and acceleration contours. Finally, an error analysis was done to compare PIV, CFD and particle data.

Results obtained from particulate data showed remarkable improvement in agreement with experimental data. Streamwise velocity, which was previously a major drawback, has shown a considerable improvement. This implies that particle lag in PIV plays an important role in analyzing flow especially when there are high spatial accelerations as is the case in SBLIs.

© $\frac{Dilip\ Kalagotla}{All\ Rights\ Reserved}$ 2018

Sic Parvis Magna

- Sir Francis Drake

Acknowledgements

This work would not have been possible without Dr. O, my mentor. Thanks for believing in me and for your support throughout the entire process. I could not have expected better technical guidance from anyone. I am exceedingly grateful for your mentorship, especially in the face of your many competing priorities. I hope I will live up to your expectations one day.

Dr. Turner is the “backbone” of this project. Your ideas molded the project the way it is now. Thank you for treating me as one of your own and sitting with me through all the discussions we had in the lab. The best playground the university can offer is in your office and I hope we can spend more time together there.

My sincere thanks to Dr. Khare in guiding me through multi-phase analysis and for your moral support. Special thanks go to Robert Ogden for his continuous support in making this project a fun learning experience for me. Rob, without you this project would have been a hell to set up. I learned a great deal from your experience. Thanks for everything you’ve done.

I thank Robert (Bob) Haimen and other researchers from Massachusetts Institute of Technology (MIT), who have worked hard on the VISUAL3 project and made it open source. Special thanks to Bob for his help initially in setting up the code.

Thanks are also owed to my colleagues and fellow graduate students, Aatresh Karnam, Kranthi Yellugari, Justin Holder, Logan Naber, Kiran Siddappaji, Matteo Ugolotti, Nathan Wukie, Mayank Sharma, Rithangshu Giri for all their intellectual and moral support. Thanks to my roommate Harsha Jangala for all the assistance he has provided me throughout my stay here.

Finally, like Dr. O always say, “Family comes first!”. Love to my parents Nagarajakumari, Chandra Reddy Kalagotla, and sister Srividya Reddy Kalagotla. I owe all of this to you guys for pushing me to great lengths and providing encouragement when it was most needed.

Once again heartfelt thanks to everyone for making me what I am today. Let this be only a small beginning towards something great!

Contents

1	Introduction	1
1.1	VISUAL3	3
1.2	UM - Experimental Campaign	4
1.3	UC - Computational Efforts	5
1.4	Shock Waves	6
1.5	Boundary-Layer structure	8
1.6	Shock Boundary-Layer Interactions (SBLI)	9
2	Literature review	13
2.1	Particle Image Velocimetry (PIV)	13
2.2	Computational efforts	15
3	Present work	18
4	Modeling of a multi-phase flow	20
4.1	Forces acting on a particle in a flow	20
4.2	Modeling of drag on a particle	23
4.3	Mathematical formulation for numerical analysis	26
5	Modifications made to Visual3 to accommodate particle	27
6	Rudimentary code validation	34

6.1	Data setup	34
6.2	Flow visualization in Modified-Visual3	35
6.2.1	Particle-Spawn regime	36
6.2.2	Upstream regime	36
6.2.3	Downstream regime	36
6.2.4	Shock regime	36
6.3	Validation techniques	37
6.3.1	Melling data : Tracer particles response across a shock	37
6.3.2	Flowfield initialization	38
6.3.3	Validation of the code	39
6.3.4	Effect of viscosity	40
6.3.5	Exploration of other empirical drag models	41
7	Particle tracer uncertainty quantification using MV3	43
8	Analysis of forces acting on a particle using MV3	47
9	Generalized oblique shock analysis	49
10	Analysis of the UM PIV data using MV3	53
10.1	Importing data into MV3	55
11	MV3 results - Standard case	58
11.1	Single particle analysis	58

11.2 Velocity Contours	69
11.3 Acceleration contours	75
11.4 Statistical Analysis	79
12 Error metric	85
13 Conclusion	87
A Particle size variation	90
A.1 Streamwise contours	91
A.1.1 Velocity	91
A.1.2 Velocity comparison	92
A.1.3 Acceleration due to drag	94
A.1.4 Particle acceleration	95
A.1.5 Fluid acceleration	96
A.2 Transverse contours	97
A.2.1 Velocity	97
A.2.2 Velocity comparison	98
A.2.3 Acceleration due to drag	100
A.2.4 Particle acceleration	101
A.2.5 Fluid acceleration	102
B Spanwise Velocity	103

C	Range scaling for acceleration contours	104
C.1	Reference - Fluid acceleration	104
C.2	Reference - Drag acceleration	107
C.3	Reference - Particle acceleration	109
D	Error metric - Continuation	111
E	User reference	113

List of Figures

1	Structure of SBLI formed due to external disturbance (Normal Shock) coupling with boundary layer; credit: Eagle et al. [25]	2
2	Structure of SBLI formed due to internal disturbance (Corner Shock) coupling with boundary layer; credit: Eagle et al. [25]	2
3	Cursor-mapping from 2D to 3D window in visual3	4
4	Structure of a turbulent boundary layer on a flat plate; credit: Babinsky et al. [14]	9
5	Time-averaged oblique SBLI structure without flow separation, credit: Delery [16]	10
6	Wall pressure distribution in an SBLI without flow separation, credit: Delerey [16]	11
7	Time-averaged oblique SBLI structure without flow separation, credit: Lapsa [10]	11
8	Time-averaged oblique SBLI structure with flow separation, credit: Delery [16]	12
9	Wall pressure distribution in an SBLI with flow separation, credit: Delerey [16]	12
10	Different grids used in CFD analysis at University of Cincinnati.	16
11	Effect of relative Reynolds number on drag coefficient of a smooth sphere; Courtesy: Frank M. White [55]	22
12	Different types of coupling in particle-fluid flow; Crowe et al. [40]	23
13	Hexahedron cell standard convention in computational domain; Source: Haimes et al. [47] . .	28
14	Algorithm for obtaining particle path in Modified-Visual3	31
15	Time step variation	33
16	Grid transformation schematic for oblique shock	34
17	3D window of Visual3 showing streamlines	35

18	Different flow regimes in Modified-Visual3	35
19	Distance normal to shock (mm) vs Shock normal velocity (m/s) [4]	37
20	Digitized data obtained from Fig. 19	37
21	Flow data in 3-D window	39
22	Normal shock-distance (m) vs Normal velocity component (m/s)	40
23	Viscosity comparision, Shock-normal diatance (m) vs velocity (m/s)	41
24	Variation of empirical coefficient of drag	42
25	Relaxation curves for particle and fluid	45
26	Uncertainty vs Shock-normal distance	46
27	Time (s) vs Normalized velocity ($\frac{u_p - u_{f2}}{u_{f1} - u_{f2}}$)	47
28	Variation based on density	48
29	Generalized oblique shock grid data; all dimensions in mm	50
30	Grid in MV3 with density as scalar variable	50
31	Particle velocity contour in XY-plane; all dimensions in m	51
32	Fluid velocity contour in XY-plane; all dimensions in m	51
33	Velocity contour showing smearing of shock; all dimensions in m	52
34	Part of grid that was imported into MV3	53
35	Shock-normal velocity vs time	55
36	Relative shock-normal distance vs time	55
37	Relative shock-normal velocity vs time	55
38	CFD data as visualized in MV3 with density as scalar variable	56

39	Streamwise velocity data	57
40	Transverse velocity data	57
41	Path traced by particles (red) and streamlines (blue) in central plane; all dimensions are in mm	58
42	Path traced by particles (red) and streamlines (blue) in central plane near separation zone; all dimensions are in mm	60
43	Streamlines (blue) and particle paths (red) seen from different planes near separation zone; all dimensions are in mm	61
44	Velocity (m/s) vs. Streamwise distance (m) in central plane near separation zone; [Streamlines - blue, Particles - red]	62
45	Path traced by particles (red) and streamlines (blue) in central plane near mid span; all dimensions are in mm	63
46	Streamlines (blue) and particle paths (red) seen from different planes near mid span; all dimensions are in mm	64
47	Velocity (m/s) vs. Streamwise distance (m) in central plane near mid span; [Streamlines - blue, Particles - red]	65
48	Path traced by particles (red) and streamlines (blue) in central plane near wedge surface; all dimensions are in mm	66
49	Streamlines (blue) and particle paths (red) seen from different planes near wedge surface; all dimensions are in mm	67
50	Velocity (m/s) vs. Streamwise distance (m) in central plane near wedge surface; [Streamlines - blue, Particles - red]	68
51	Streamwise velocity contours linearly interpolated onto 700x700 grid	70
52	Transverse velocity contours linearly interpolated onto 700x700 grid	71
53	Streamwise velocity contours	72

54	Transverse velocity contours	73
55	Y vs U-velocity	74
56	Streamwise acceleration contours	77
57	Transverse acceleration contours	78
58	Type III-A Laskin Nozzle Aerosol Distribution @ 23 PSI Using PAO-4 Oil; Courtesy: ATI Techniques	80
59	Path traced by particles of different sizes and streamlines (blue) in central plane near mid-span; all dimensions are in mm	81
60	Path traced by particles of different sizes and streamlines (blue) seen from different planes in central plane near mid-span; all dimensions are in mm	82
61	Velocity (m/s) vs. Streamwise distance (m) in central plane near mid-span	83
62	Particle diameter: 177nm	91
63	Particle diameter: 293nm	91
64	Particle diameter: 499nm	91
65	Particle diameter: 573nm	91
66	Particle diameter: 177nm	92
67	Particle diameter: 293nm	92
68	Particle diameter: 499nm	92
69	Particle diameter: 573nm	92
70	Particle diameter: 177nm	93
71	Particle diameter: 293nm	93
72	Particle diameter: 499nm	93

73	Particle diameter: 573nm	93
74	Particle diameter: 177nm	94
75	Particle diameter: 293nm	94
76	Particle diameter: 499nm	94
77	Particle diameter: 573nm	94
78	Particle diameter: 177nm	95
79	Particle diameter: 293nm	95
80	Particle diameter: 499nm	95
81	Particle diameter: 573nm	95
82	Particle diameter: 177nm	96
83	Particle diameter: 293nm	96
84	Particle diameter: 499nm	96
85	Particle diameter: 573nm	96
86	Particle diameter: 177nm	97
87	Particle diameter: 293nm	97
88	Particle diameter: 499nm	97
89	Particle diameter: 573nm	97
90	Particle diameter: 177nm	98
91	Particle diameter: 293nm	98
92	Particle diameter: 499nm	98
93	Particle diameter: 573nm	98

94	Particle diameter: 177nm	99
95	Particle diameter: 293nm	99
96	Particle diameter: 499nm	99
97	Particle diameter: 573nm	99
98	Particle diameter: 177nm	100
99	Particle diameter: 293nm	100
100	Particle diameter: 499nm	100
101	Particle diameter: 573nm	100
102	Particle diameter: 177nm	101
103	Particle diameter: 293nm	101
104	Particle diameter: 499nm	101
105	Particle diameter: 573nm	101
106	Particle diameter: 177nm	102
107	Particle diameter: 293nm	102
108	Particle diameter: 499nm	102
109	Particle diameter: 573nm	102
110	Spawise velocity contours	103
111	Streamwise velocity contours with fluid acceleration as reference	105
112	Transverse velocity contours with fluid acceleration as reference	106
113	Streamwise velocity contours with acceleration due to drag as reference	107
114	Transverse velocity contours with acceleration due to drag as reference	108

115	Streamwise velocity contours with particle acceleration as reference	109
116	Transverse velocity contours with particle acceleration as reference	110
117	Particle diameter vs. Uncertainty	112
118	User reference chart to work with MV3 code; Red: Required input, Blue: Output, Green: Saved data, Oval: Operations	114

List of Tables

1	Error metric comparisons (From Friedlander [38])	16
2	Coefficient of drag in terms of relative Reynolds number	22
3	Flow data for plot3D format	35
4	Flow parameters for oblique shock	37
5	Particle specifications for tracer particle	38
6	Hou's PIV data	43
7	Pre and Post shock values for numerical analysis	43
8	Particle specifications from Hou's PIV analysis	43
9	MV3 output	44
10	Flow parameters for oblique shock in Michigan PIV	54
11	Particle specifications for tracer particle used in Michigan PIV	54
12	Particle distribution; all dimensions in nm	79
13	Error metric comparisons; Highlighted in red is the current model; Remaining data is from Friedlander et al. [37]	86
14	Error metric comparisons for particles of different sizes, presented as "MV3 - <i>diameter of particle</i> "	111

Nomenclature

Initializations & Acronyms

AIAA American Institute of Aeronautics and Astronautics

ARK4 Adaptive 4th order Runge Kutta

BBO Basset-Bossinesq-Ossen

CFD Computational Fluid Dynamics

CPT Critical Point Theory

GTSL Gas Turbine Simulation Laboratory

LHS Left Hand Side

MIT Massachusetts Institute of Technology

MV3 Modified Visual3

NASA National Aeronautics and Space Administration

PAO-4 4 cSt Polyalphaolefin

PIV Particle Image Velocimetry

RANS Reynolds Averaged Navier Stokes

RHS Right Hand Side

RK4 4th order Runge Kutta

SBLI Shock Boundary Layer Interaction

SPIV Stereo Particle Image Velocimetry

SST Shear Stress Turbulence

UC University of Cincinnati

UM University of Michigan

USAF United States Air Force

V3 Visual3

Greek

Δt Time step, s

δ Deflection angle

$\delta(x)$ Boundary Layer Thickness, m

∞ Free stream properties

κ Von karman constant

μ Dynamic viscosity, kg/m-s

∇ Gradient

ν Kinematic viscosity, m^2/s

ρ Density, kg/m^3

σ Shock angle

τ Characteristic time scale, s

Symbols

A Cross-section of a spherical particle, m^2

a Radius of particle, m

C_D Coefficient of drag

d Diameter, m

g Acceleration due to gravity, m/s^2

J Jacobian

K_B Boltzmann constant, $kg - m^2/K - s^2$

K_{nd} Knudsen number

l Mean Free Path, m

l_{cell} Length of cell, m

M	Mach number
m	Mass, kg
P	Pressure, Pa
R	Ideal gas constant, J/kg-K
R_{er}	Relative Reynolds number
s	Entropy, J/K
T	Temperature, K
$u(t), u$	Velocity of fluid, m/s
$V(t), V, v$	Velocity of particle, m/s
W	Coles wake parameter
y	Wall normal distance, m
$Y(t)$	Position of particle at an instant, m

Subscript

Δu	Relative velocity
$grid$	CFD grid data
$node$	Respective node
x	x-component
y	y-component
z	z-component
AM	Added Mass
B	Basset history
D	Drag
f	Fluid
G-B	Gravitational and Buoyant

max	Maximum quantity
n	Normal to the shock direction
p	Particle
PG	Pressure Gradient
t	Tangential to the shock direction

1 Introduction

Particle Image Velocimetry (PIV) has become an important step in the development process of many aerospace components. One of the major assumptions of PIV is that the velocity of a flow field is same as the velocity of the tracer particles in it. The ability of a tracer particle to follow the flow surrounding it depends on its Stokes number. Stokes number is the ratio of particle response time, τ_p to flow time scale, τ_f . PIV can predict the behavior of flows accurately in subsonic regions. The extension of PIV to supersonic regions presents a challenge regarding the flow tracking capability of tracer particles. This is because of the presence of expansion waves, compression waves, shocks, and vortices. These regions pose high local acceleration and decelerations, which cause particles to be emitted towards low-velocity regions with high initial velocities or vice-versa. Adrian [1] - [3], stated that the motion of tracer particles might not accurately represent the fluid surrounding them, especially if there are strong temporal and spatial accelerations. Works of Melling [4], Lang [5], Koike et al. [6], Ragni et al. [7] shows the importance of particle lag in PIV and provide many insights into improving them. Melling conducted a numerical analysis to calculate response time of different sized particles crossing an oblique shock wave. In that study, the author used an empirical relation to calculate the drag. This has become a common practice for many numerical investigations directed at calculating particle response time. Lang, Ragni conducted numerical and experimental analysis using the approach proposed by Melling to elucidate the particle lag effect in PIV. Koike et al. on the other hand, proposed a numerical method for the correction of PIV data. The author used Stokes drag to correct for particle lag in PIV. He concluded that the results showed improvement in the downstream velocity after implementing particle lag correction.

One of the areas of interest is Shock Boundary Layer Interactions (SBLIs). They are an important phenomenon in almost every aerospace, aeronautical applications but not limited to them. Important consequences of SBLIs include flow separation due to the adverse pressure gradient, total pressure loss, increase in drag, increase in flow unsteadiness and potential to produce intense localized heating. There are many ways SBLIs may arise, important among them are the interaction of an external shock with a boundary layer (Fig. 1), and interaction of a shock formed due to deflection in the flow field with boundary layer, see Fig. 2. For example, the formation of shocks on transonic airfoils is required to match the pressure along the trailing edge but the interaction of shocks with boundary layers causes serious performance issues due to flow separation, resulting in an increase in drag, flow unsteadiness, and buffet. In supersonic inlets, SBLIs increase the thickness of the boundary layer, affecting inlet flow to the engine. Complicated boundary layer

control mechanisms must be installed to regulate the flow into these inlets. These modifications add weight to aircraft and decrease its total efficiency. In case of hypersonic flows, SBLIs have the capability to produce high localized heating that can destroy a vehicle. Therefore, understanding SBLIs has been a major problem since they were first encountered. Despite the continuous efforts of experimentalists and computationalists, understanding of SBLIs physics is still at rudimentary stages.

Figure 1: Structure of SBLI formed due to external disturbance (Normal Shock) coupling with boundary layer; credit: Eagle et al. [25]

Figure 2: Structure of SBLI formed due to internal disturbance (Corner Shock) coupling with boundary layer; credit: Eagle et al. [25]

The current state of computational efforts provides a new approach to visualizing and analyzing SBLIs. Simultaneously, development of experimental techniques provides better validation and new insight into physics of SBLIs. This method for analyzing SBLIs was presented in a review paper by Dolling [8] in 2001. Recognizing this, many organizations including National Aeronautics and Space Administration (NASA),

and United States Air Force (USAF) put renewed interest in analyzing SBLIs. This approach of validating results simultaneously using both experimental and computational techniques can be seen in the works of Lapsa et al. [9], Friedlander et al. [37], Eagle et al. [25], and Galbraith et al. [36]. Understanding physics of SBLIs and their control enables engineers to increase the efficiency of supersonic aircraft. Most of these applications include usage of mixed compression inlets which have better pressure recovery compared to standard inlets. These inlets operate by the production of a train of oblique shock waves followed by a normal shock. Interaction of these shocks with boundary layers decreases the pressure recovery and also decreases the inlet mass flow rate, which causes a serious drop in efficiency compared to theoretical calculations.

Although many of the works mentioned above complement each other, there are still some inherent differences between PIV and CFD that are not considered in many of the works until now. One of these differences includes particle lag effects which were briefly reviewed in Friedlander et al. [38]. In that work, the author has an improved CFD model which was post-processed using a rudimentary linear model for particle lag. This model was implemented with a MATLAB code to see improved results. The motivation for the current work comes from the conclusion of Friedlander [37] who states that “the simplified particle models should be improved on in order to further understand the effects of PIV as related to post-processing CFD data for experimental data comparison”.

1.1 VISUAL3

VISUAL3 is developed as a tool to visualize volumetric data. It was developed at Massachusetts Institute of Technology (MIT) by Haimes et al. [47] for educational purposes. It is designed for better investigation and interpretation of computational results. It has the ability to be used as a flow solver debugger unlike other post-processing tools available today. One of the important and unique features of VISUAL3 is that the tool can be modified to do the bidding of the user. This is the main reason to choose VISUAL3 for current work.

Figure 3: Cursor-mapping from 2D to 3D window in visual3

Other highlights of VISUAL3 include its capability of simultaneously mapping volumetric data in multiple windows (3D, 2D, 1D) as shown in Fig. 3. This provides the user with thought continuity while visualizing certain data. Most of the terminology related to VISUAL3 can be found at [48]. The other advantages and tools available in VISUAL3 are pointed out in [50].

1.2 UM - Experimental Campaign

To date, two important experimental campaigns were performed at the University of Michigan to understand the structure and physics of SBLI in a wind tunnel. These two operations are briefly reviewed here.

The first experimental effort was conducted by Lapsa et al. around 2005. The motivation behind this work was the increasing presence of SBLIs in aerospace applications. The major drive for this work comes from the fact that with the increase in computational power, new and improved numerical methods are becoming available, which require high fidelity experimental data for validation and to extend progressively to more complex applications. This renewed interest in USAF and NASA, among other organizations.

In the first campaign, the focus was to enhance the understanding, prediction, and ability to control SBLI. This also paved a path for the provision of high fidelity results for computationalists to better develop their numerical models. In view of this, a wind tunnel facility with shock generators was specifically designed.

Stereo Particle Image Velocimetry (SPIV) was used to measure velocity fields throughout the interaction region. This technique enabled them to obtain instantaneous velocity components (u, v, w) and six of the nine gradient quantities ($\partial u_i / \partial x_j$). Ensemble averages of hundreds or thousands of statistically independent realizations were obtained, together with instantaneous measurements, the fluctuating components can be obtained. Also, all the nine components of the Reynolds stress tensor ($\overline{u'_i u'_j}$) were obtained, which in turn enabled computation of turbulence kinetic energy ($\bar{k}$) and all nine components of anisotropy tensor ($\bar{b}_{ij}$), three of the six unique components of the strain rate tensor ($\bar{S}_{ij}$), one component of vorticity vector ($\bar{\omega}$), and six of the nine components of the kinetic energy dissipation rate tensor (ϵ). All these results were first of their kind for compressible boundary layers, and provide highly resolved statistical quantities suitable for evaluation using DNS simulations.

The second experimental campaign was carried out by Eagle et al. circa 2011. This operation was mainly focused on analyzing the three-dimensional structure of SBLI in every aspect and directly measure the causes and effects of secondary interactions. However, both streamwise and spanwise planes are considered in SPIV to understand the 3D structure of SBLI. For the first time, PIV on an SBLI was conducted in a spanwise direction to contemplate the corner interactions. In the current work, results obtained from streamwise mid-plane were considered from the second campaign to evaluate the particle lag effect.

1.3 UC - Computational Efforts

University of Cincinnati's very own Gas Turbine Simulation Laboratory (GTSL) collaborated with the UM wind tunnel experiment to provide computational assistance for the development of wind tunnel. Prof. Orkwis and Prof. Turner acted as chair members for the AIAA workshop conducted in 2010 [11]. In this workshop, initial data from the wind tunnel experiment was provided to different computationalists who were kept "blind" to all experimental results. Using only this data, different solving techniques were implemented to obtain the results, which were later compared using an error metric with experimental data. The important conclusion from the workshop was that "The choice of turbulence model appears to be the dominant factor in the accuracy of the Reynolds Averaged Navier-Stokes (RANS) solutions. Large-eddy simulations had similar error levels as the RANS methods but provided superior predictions of the normal stresses. There appeared to be no dependence on computational grid type (structured or unstructured)".

Later in 2011, Galbraith et al. at UC in coordination with Eagle et al. from UM developed a robust computational grid and tested different shock generator angles to help with experimentation. A 24 million

node grid was developed to make the solver grid independent. Galbraith used the OVERFLOW v2.1z [17] flow solver which utilizes the Chimera overset mesh technique [18]. Then $k - \omega$ turbulence model was used in the flow solver for this computational study. The results showed that the corner separations in the tunnel affect the flow in the center of the wind tunnel. These results highlight the 3D structure of shocks in the wind tunnel, in turn, implying the complexity of the structure of 3D-SBLI.

Finally, in 2013, Friedlander et al. [38] tried to close the gap between experimental and computational results by improving the grid and using better solution techniques. The grid was made independent with the use of 56 million nodes and $y+$ was reduced to a maximum of 0.25 at the wall. The grid was more closely packed around walls and the oblique shock region. This grid uses a left-handed coordinate system, consistent with the workshop while experiments used a right-handed system. These details were further discussed in “Initialization of Michigan data” section. Similar to the previous case, the OVERFLOW solver was used to simulate the flow. However, the SST turbulence model was used in this case instead of $k - \omega$. Different boundary conditions were applied to replicate the real physics of wind tunnel. In his work, Friedlander did a crude linear study of particle lag by “re-post-processing” the obtained results in MATLAB and found that the effect of particle lag is considerable and cannot be ignored. This was the starting point and main motivation for the current study. The standard case model was chosen for applying particle lag effect as described in Friedlander [37].

SBLIs are a consequence of close coupling between the shock wave and boundary layer. Hence a brief introduction to shock waves, boundary layers, and SBLIs is followed.

1.4 Shock Waves

The discontinuities in fluid dynamics take many forms, slip lines between two flows with different velocities, shear layers in the case of a boundary layer, and shock waves. In this section, a brief introduction to shock waves, their governing equations and their influence on PIV analysis is presented.

To define any compressible flow, the following properties are relevant: density, pressure, velocity, temperature, entropy, internal energy and coefficient of viscosity. When the flow passes through a shock, the following changes happen to flow properties:

1. Density of the flow increases.

2. Static pressure increases, which produces strong adverse pressure gradient to thicken the boundary layer.
3. Velocity suddenly decreases, causing a discontinuity in the flow.
4. Static temperature increases, which may be very high especially in hypersonic flows in case of strong shocks. This will lead to strong localized heating which can be severe enough to destroy a vehicle.
5. Stagnation pressure decreases and entropy increases. This causes an increase in wave drag and decreases recovery pressure.

The rate of increase of entropy is given by

$$\rho T \frac{Ds}{Dt} = \Phi - \nabla \cdot q \quad (1)$$

For an adiabatic flow, the second term in Eq. 1 becomes zero. It can be shown that the dissipation function, Φ is always greater than zero for a viscous flow.

$$\rho T \frac{Ds}{Dt} = \Phi \quad (2)$$

$$\rho T \frac{Ds}{Dt} = \tau_{ij} \frac{\partial u_i}{\partial x_j} \quad (3)$$

This equation shows that in an adiabatic and non-reacting flow the only source of entropy is viscosity. This proves that in a shock wave which has a thickness of the order of mean free path of the flow, the only probable explanation for a rise in entropy is viscosity and heat conduction. Thermodynamic equilibrium does not prevail inside a shock wave. Therefore, analysis of shocks from continuum considerations at best gives approximate results. For adequate analysis, kinetic theory or even quantum mechanics should be considered as mentioned in Shaprio [13].

Drag produced by a shock wave is called wave drag. Drag in any form can be considered as a source of entropy. This relation was given by Oswatitsch as Eq. 4. Drag generated by the production of entropy in boundary layers is called friction drag. In general, friction drag is less compared to other losses in a system. In case of SBLI, especially during a separation, entropy increases which in turn increases friction drag making it comparable to wave drag. Therefore, controlling SBLIs helps in the reduction of drag on a vehicle improving its thrust.

$$D = \frac{1}{V_\infty} \iint_S T_\infty \delta s (\rho \vec{V} \vec{n} dA) \quad (4)$$

In PIV, when a particle passes through a shock wave it is injected into the post-shock flow with high velocity. This injected particle takes time to settle back to the velocity of the surrounding fluid. The time taken by the particle to settle back to $(1-1/e)$ times the fluid velocity after passing through a shock is known as particle relaxation time. This is one of the major drawbacks in PIV when analyzing a flow with high temporal and spatial accelerations.

Shockwave interaction with a boundary layer can be better understood with the help of shock-polar representations or hodograms. A detailed study on these has been deferred to Babinsky et al. [14].

1.5 Boundary-Layer structure

Turbulent boundary layer structure has been well understood for many years now. In this section, the structure of the boundary layer will be briefly discussed. In general, a boundary layer consists of three zones, namely, viscous sub-layer in contact with the wall, logarithmic layer above it and an outer wake-like region that comprises most part of the boundary layer structure. These regions are presented in Fig. 4. The importance of each of these regions depends on various factors like Reynolds number and externally imposed pressure gradient.

Velocity profile inside a turbulent boundary layer region can be analytically defined using Coles wake law combined with Van Driest correction. This is valid in logarithmic and wake region but is invalid close to the wall.

$$\frac{u_\infty^* - u^*}{u_{\tau w}} = -2.5 \ln\left(\frac{y}{\delta}\right) + \frac{\Pi}{\kappa} (2 - W) \quad (5)$$

Figure 4: Structure of a turbulent boundary layer on a flat plate; credit: Babinsky et al. [14]

Where, u^* represents Van Driest correction of velocity, $u_{\tau w}$ is friction velocity near the wall. Lapsa [10] in his analysis of SBLI used this equation to compare with experimental data. One of the important parameters of interest is the effect of pressure gradient on boundary layers. This was analyzed in White [55] with several empirical relations. The conclusion from that analysis is that adverse pressure gradients cause separation in the boundary layer and may cause recirculation. This is one of the regions where error due to light scattering might be high as particles will go in and out of the experimental plane in PIV analysis. This error is reinforced by the highly three-dimensional structure of SBLI.

1.6 Shock Boundary-Layer Interactions (SBLI)

SBLIs are highly unsteady processes. They have been studied for almost half a century because of their importance in aerospace applications. Even with this extensive research their underlying physics is not completely understood to control them. The review by Delery (2001) [15] showed important properties of SBLI and the need to study them. Until recently most experimentalists considered SBLIs as two-dimensional interactions. Only because of the recent efforts in PIV community by Humble et al. [22], and Helmer et al. [26] the structure of SBLIs is now known to be three-dimensional. This section provides a brief description of the structure of SBLI.

The structure of SBLI is assumed to be two dimensional to learn the basic physics behind them. A typical time-averaged oblique shock wave boundary interaction without flow separation was shown in Fig. 5. As illustrated in the figure, incident oblique shock C1 curls as it enters the boundary layer because of decreasing

local Mach number. Correspondingly, the magnitude of pressure rise decreases and vanishes altogether when the sonic line is reached. At the wall, the streamwise pressure rise through C_1 is experienced where the incident shock should have impacted in absence of a boundary layer. This pressure rise is experienced over a finite length, unlike the assumed inviscid solution as shown in Fig. 6. Due to this adverse pressure gradient, the subsonic region of the boundary layer thickens and causes the rotational supersonic flow to deflect. This supersonic flow region constitutes the major part of the boundary layer region if the flow is turbulent. The deflection in the supersonic flow acts like a ramp inducing compression waves, η_1 , which eventually coalesce to form the reflected shock, C_2 . Penetration of the incident shock into the supersonic region results in a succession of reflected shocks and expansion waves. This mechanism of external shock penetration into boundary layer was more detailed in Henderson [19]. The formation of compression or expansion train due to the reflection of the shock passing through rotational part of the boundary layer depends on the strength of the reflected shock (ability to deflect the flow downstream) C_2 formed. Two different cases were depicted one by Delery et al. [16], shown in Fig. 5 and the other by Lapsa [10], shown in Fig. 7.

Figure 5: Time-averaged oblique SBLI structure without flow separation, credit: Delery [16]

A boundary layer is a flow within which the stagnation pressure decreases when approaching the wall and where - at least, for short distances, it can be considered constant along the length of a streamline. Since the stagnation pressure is low in the inner boundary layer, a small change in static pressure will decrease the velocity. When the incident shock becomes strong enough, the adverse pressure gradient in the subsonic region can cause the flow to locally reverse. The structure of this flow is illustrated in the Fig. 8. The compression waves formed due to the thickening of the subsonic region are more concentrated

Figure 6: Wall pressure distribution in an SBLI without flow separation, credit: Delerey [16]

Figure 7: Time-averaged oblique SBLI structure without flow separation, credit: Lapsa [10]

and are coalesced to form separation shock, C_2 , upstream of the incident shock C_1 . This separation shock interacts with the incident shock at I . At this point, both incident shock and separation shock undergoes deflection (refraction) to form shocks transmitted shock, C_4 and reflected shock, C_3 respectively. C_4 curls as it passes through the rotational supersonic region of the boundary layer as observed in the previous case. The penetration of C_4 into boundary layer produces an expansion fan, ϵ . Finally, flow velocity is returned parallel to the wall by the production of a train of compression waves which coalesce to form reattachment shock in the outer stream at the downstream of reattachment point, R . Downstream of separation point, S is a recirculating bubble flow bounded by a dividing streamline (S), which separates the recirculating flow from flow above. Unlike other streamlines in the flow, dividing streamline originates at separation point S and ends at reattachment point R . As shown in Fig. 9, the wall pressure distribution through interaction is now divided into three regions, first is pressure rise produced by the upstream of compression waves, the second is almost constant pressure region typical of separated flows and the third is pressure rise produced by the downstream system of compression waves. The upstream portion of the interaction is

essentially a free interaction process, leading to the major consequences that, provided separation exists, the upstream pressure rise is independent of downstream conditions; namely incident shock strength. Therefore, for increasing shock strengths the pressure rise downstream of compression fan becomes increasingly large. This was explained in more detail using shock-polar representations, inviscid flow relations in Babinsky et al. [14].

Figure 8: Time-averaged oblique SBLI structure with flow separation, credit: Delery [16]

Figure 9: Wall pressure distribution in an SBLI with flow separation, credit: Delery [16]

Analysis of 3D-SBLI structure is still in its early stages of development. Eagle [25] considered critical point theory (CPT) proposed by Legendre [15] to understand the three-dimensional structure. Further study on 3D-SBLI is deferred to Eagle's dissertation (2012) [25].

2 Literature review

In this section, previous works done to understand the particle lag effect in PIV are briefly reviewed. Also, the literature on the understanding of SBLI using PIV is presented. Finally, computational efforts trying to compliment the PIV analysis of SBLIs are recalled.

2.1 Particle Image Velocimetry (PIV)

The term Particle Image Velocimetry (PIV) was coined almost 35 years ago. With the help of PIV, experimentalists are able to infer the velocity of complex flow fields. PIV is capable of predicting velocities even at the smallest scales, as shown recently by experimentalists like Lapsa (2009) [10], Humble et al. (2009) [23], Helmer (2011) [24], Eagle (2012) [25]. PIV rely on scattered particles suspended in the flow to predict velocities. The ability of PIV to obtain these velocities depends on the potential of scattered particles tracking the flow. In general, the smaller the particle size, the better it is at tracking with respect to the continuous field. Problem with small particles lies with the inherent diminishing of their light scattering ability which is important for particle imaging. Therefore, a compromise has to be made between particle size and it's light scattering ability while selecting seeds for PIV.

Neither computational analysis nor PIV has predicted exact flow behavior of supersonic flows to date. PIV can be applied to study a measurement plane that includes most relevant part of a turbulent flow whereas computational efforts require the simulation of whole flow field to study even a small plane. In a review article, by Adrian [3], the author states that “Unique opportunities are provided to elucidate the nature of turbulence when combining the strengths of experimental and numerical approaches”. PIV approach is limited when there are high temporal and spacial accelerations, which is the case when there are shocks and vortices. SBLIs are highly unsteady turbulent processes. So, PIV cannot predict flow behavior if the seeds selected do not have a good particle response time. Works of Melling [4], Lang [5], Kokie et al. [6], Ragni et al. [7] shows the importance of particle lag in PIV and provides many insights into improving them. Melling conducted a numerical analysis in his study to calculate particle response time of different sized particles crossing an oblique shock wave. In that study, the author used an empirical drag relation to calculate drag. This has become a common practice for many numerical investigations to calculate particle response time. Lang, Ragni conducted numerical and experimental analysis using the approach proposed by Melling to elucidate the particle lag effect in PIV. Kokie et al. on the other hand, proposed a numerical

method for correction of PIV data. Kokie used Stokes drag to correct for particle lag in his study. The author concluded that the results seem to be promising in terms of improvement in velocity downstream but there is no other evidence in supporting that argument. This is one of the reasons recent efforts towards the study of supersonic flows using PIV needs to be validated with a corresponding study of CFD or numerical analysis.

The accuracy of particle image velocimetry (PIV) with respect to particles/seeds to estimate flow field data depends on the following parameters;

1. Thickness of light sheet. This should be as small as possible to capture particles in the reference plane.
2. Interframe time, between pulses, determines the time between two frames captured in PIV. This is an important factor in determining if PIV is able to calculate smallest possible scales in turbulence.
3. Stokes number, the ratio of time scales of particle and fluid. This determines the ability of the particle to track fluid.

All these properties are interdependent on one another. For example, if Stokes number is high and interframe time is low, the analysis still cannot predict small-scale eddies of turbulence.

Use of PIV to study SBLI can be dated back to 1999 [20]. This shows that PIV is still relatively new when it comes to analysis of supersonic flows. Thanks to an extensive literature review of Eagle [25], most of SBLI analyses using PIV have been documented in one place. Beresh et al. [20] used aluminum oxide as tracer particles for his PIV analysis to study the structure of SBLI. The manufacturer specified a diameter of $0.3\mu m$ for the particles but it was found to be $1.0\mu m$ from a scanning electron microscope. This yielded a particle response time of $54\mu s$. Flow relaxation time was calculated to be $25\mu s$, which produces a Stokes number, $S_t = 2$. This is very high for an analysis to understand the structure of SBLI. This will grossly misrepresent the flow features, according to Samimy and Lele's [56] predictions.

Hou's [21] PIV analysis was one of the best when it comes to particle lag error. Hou used Titanium oxide as tracer particles for his analysis. The manufacturer specified particle diameter was $0.021\mu m$ but experimentally obtained diameter by passing the particle through a shock was calculated to be $0.26\mu m$. This is a ten-fold increase, which will increase the error. However, Stokes number for this particle was calculated as 0.1, which is considered suitable for PIV analysis. More analysis of this data is presented in further sections.

According to Mie scattering theory particle diameter should be around one micron if the flow field being analyzed is air, [3]. Haertig et al. [28] used $0.4\mu m$ (manufacturer quoted) TiO_2 particles as tracers for supersonic nozzle flow experiment. At TU-Delft [29], tracer particles were heated for 40 minutes at $120^\circ C$ before usage to make sure of proper dehydration. The particle (TiO_2) size was quoted to be $0.03\mu m$ which has a response time of $2.48\mu s$.

2.2 Computational efforts

CFD has overcome many milestones since its inception but it has yet to solve the problem of turbulence. This has been a major issue in analyzing SBLIs. In 2010, an AIAA workshop [11] was conducted comparing results obtained from different CFD codes with experimental data available. One of the conclusions from the workshop was that most of the results from CFD agreed with each other but they are not in agreement with experimental data. This data was then analyzed by Galbraith et al. [36] at UC in coordination with the UM glass inlet wind tunnel experiment which was conducted by Lapsa et al. [9] and Eagle et al. [25]. One of the main tasks of the UM wind tunnel experiment was to provide the CFD community with high-fidelity experimental data of the quantities on which most of the CFD models are based, including velocity, higher-order fluctuations, and gradient quantities.

In 2011, Galbraith [36] explored the geometry of the UM wind tunnel to understand different configurations. This combined effort between CFD and experimental approaches led to a better final design of the tunnel. CFD solutions were obtained with the OVERFLOW code and the study included a $k - \omega$ model for the computational study. This study also explored cases for starting of the wind tunnel based on Mach number, tunnel width, wedge length and wedge angle. Finally, 3D-SBLI structure was investigated which showed a close resemblance to the skin-friction oil case results presented in Eagle et al. [25].

In 2013, a CFD study was done at UC on the UM PIV trying to close the gap between experimental and computational results. In this study, Friedlander [37] increased an already existing grid (Galbraith et al. [36]) to 56 million grid points as shown in Fig. 34. Upgrading the grid was done in the experimental plane region to better improve both streamwise and spanwise results. OVERFLOW [17] a RANS solver was used to solve for the required data. The analysis was done utilizing SST turbulence model with all zones considered turbulent. Different boundary conditions, geometries and boundary layer structures (transition from laminar to turbulent) were explored to compare results with each other and with the UM results. Finally, the standard case (as tabulated in Table. 1) results were re-post-processed with linear particle drag

(a) Grid used by Galbraith et al. [36]

(b) Modified grid from Friedlander et al. [37]

Figure 10: Different grids used in CFD analysis at University of Cincinnati.

equations using a MATLAB script. The error metric that was defined in the AIAA workshop, Eqs. 6, 7 was used to justify the founding. The improvement in error compared with experiment was found to be considerable.

These efforts emphasized the importance of particle lag consideration when comparing PIV data with CFD results. In this study, this particle lag effect will be applied to flow field obtained from CFD based on the physics of the particle in a flow. From the data obtained, these results will be post-processed to compare with PIV.

U Error		V Error	
0.02676	Standard (Long Lag)	0.01158	Standard (Medium Lag)
0.02747	Standard (Medium Lag)	0.01185	Standard (Long Lag)
0.02853	Standard (Short Lag)	0.01224	Standard (Short Lag)
0.02964	Standard	0.01377	Standard
0.03020	Standard (SST-GY)	0.01950	Standard (SST-GY)
0.03115	Standard (BSL)	0.02227	Standard (BSL)

Table 1: Error metric comparisons (From Friedlander [38])

$$e(f)_n = |(f_{cfd})_n - (f_{exp})_n| \quad (6)$$

$$E(f) = \frac{1}{N} \sum e(f)_n \tag{7}$$

3 Present work

The current study is designed to develop a particle drag model to post-process CFD results and compare them with experimental/PIV results. A new algorithm was developed to spawn a particle in an already existing flowfield. Results obtained not only helped in reducing the error between CFD and PIV but also provided a new way to understand the structure of SBFI presented in Lapsa et al. [9].

Modeling of a particle in multi-phase flow is discussed in section 4. All the forces acting on a particle were considered and how to model each of them on a solid particle in a numerical analysis is elucidated. The mathematical formulation for all the forces acting on the particle is presented. Of all these forces, drag acting on the particle was considered in detail. The coefficient of drag for a spherical body based on relative Reynolds number is studied. Different types of coupling between the particle and fluid medium are described. Based on the requirement for a particle analysis in supersonic flows, the assumptions for numerical analysis are detailed.

Section 5 describes the previous setup of the Visual3 code and presents the changes made to accommodate particles in a flow field. A brief description of the algorithm used for plotting streamlines is discussed. The changes made to the algorithm to track particles with mass is presented. A procedure to introduce particles with mass in an existing flow field is explained.

The initial validation techniques used for analyzing particles in the flow field are discussed in section 6. Here the data setup to be used in MV3 code has been discussed. Flow visualization as seen in MV3 with directions for a user is presented. A first validation of the code was done by comparing the results obtained with Melling's [4] data. This analysis provided insight into the importance of empiricism of drag coefficient. Viscosity variation is also considered and was shown to be a very important parameter in analyzing particulate data.

Section 7 discusses a few uncertainties caused by tracers in PIV analysis and their quantification in numerical analysis. For the purpose of quantification, the PIV investigated conducted by Hou et al. [21] was chosen. This particular PIV was chosen because of Titanium oxide tracer particle used for analysis. TiO_2 is considered as one of the best tracers available for PIV, because of its high density and almost constant diameter compared to any other tracers. The analysis presented in this section not only tries to quantify uncertainties due to the usage of tracers in PIV but also shows that there will be uncertainty even with the

usage of Titanium oxide as a tracer.

Different forces acting on a particle in a flow field and their effect on particle relaxation time is discussed in Section 8 of this study. This study shows the importance of using particles with a small diameter and high density in PIV. The assumption of “Only drag” consideration in numerical analysis is explained here.

In section 9, generalized oblique shock data was introduced into MV3 code for analyzing particle effects. For this, a two-dimensional oblique shock was constructed in three-dimensions. This section highlights the velocity contour analysis and shock smearing effect due to particle size variation in PIV.

Section 10 discusses the method for importing CFD data into MV3 code. This section highlights the nuances of CFD and experimental data in terms of grid coordinate transformation. Initial data used for importing the UM data into both CFD and MV3 are presented. An oblique shock analysis with uncertainty quantification was done based on the particles used in the UM PIV analysis. This shows the importance of the particle lag analysis presented in later sections.

The different results obtained from particle data using the MV3 code are presented in section 11. Single particle analysis was done to show the non-linearity of particulate data with respect to fluid data. Velocity contours are presented to compare the differences between CFD, PIV, and MV3 data. For the first time ever, acceleration contours were presented for the UM PIV analysis. The importance of these contours and their analysis is presented. Finally, a statistical analysis is presented based on the data obtained from the nozzle manufacturer. This analysis shows the importance of the averaging technique used in PIV.

Section 12 presents the error metric to quantify the results obtained. This error analysis was done to be in compliance with the AIAA SBLI workshop [11]. The results obtained from the particle lag model were presented alongside the data obtained by Friedlander et al. [38] to show the importance of particle lag in PIV.

Section 13 provides a summary of the major conclusions.

4 Modeling of a multi-phase flow

In this section, the forces acting on a spherical solid particle convecting in a flow based on its specifications are discussed. Also, the dominant forces acting on a particle used as a tracer in PIV are deduced. Finally, the modeling of the particle in a numerical analysis based on the acting dominant forces in a flow is detailed.

4.1 Forces acting on a particle in a flow

At any instant of time, there are several forces acting on a particle in a flow. The particle is assumed to be perfectly spherical for the purposes of numerical analysis. However, in PIV the shape of the particles may differ but since the tracers size is almost negligible they are assumed to be spherical even in the post-processing of PIV data. New methods are being developed for non-spherical particle assessments in multi-phase flow [30] but are beyond the scope of this study.

The different forces acting on a particle in a flow are:

1. Drag force
2. Force due to pressure-gradient
3. Body forces
4. Added-mass force
5. Basset-history force

The equation of motion for a spherical particle in a flow field is given by Eq. 8. This equation is known as Basset-Bossinesq-Ossen (BBO) equation. This is the form presented in Maxey et al. [46] and Mei [41] without the correction for the added mass term.

$$\begin{aligned}
m_p \frac{dV_i}{dt} &= (m_p - m_f)g_i + m_f \frac{Du_i}{Dt} \Big|_{Y(t)} - \frac{1}{2}m_f \frac{d}{dt} \{V_i(t) - u_i[Y(t), t] - \frac{1}{10}a^2 \nabla^2 u_i|_{Y(t)}\} \\
&\quad - 6\pi a \mu \{V_i(t) - u_i[Y(t), t] - \frac{1}{6}a^2 \nabla^2 u_i|_{Y(t)}\} \\
&\quad - 6\pi a^2 \mu \int_0^t d\tau \left(\frac{d/d\tau \{V_i(\tau) - u_i[Y(\tau), \tau] - \frac{1}{6}a^2 \nabla^2 u_i|_{Y(\tau)}\}}{[\pi \nu(t - \tau)]^{\frac{1}{2}}} \right) \\
&= F_{G-B} + F_{PG} + F_{AM} + F_D + F_B \quad (8)
\end{aligned}$$

Drag computes resultant pressure and viscous shear forces acting on the surface of a particle. Any pressure, velocity, shear distributions around a particle can be determined by solving the Navier-Stokes equation. Solving this mathematically is very difficult and no general case has been obtained. These can only be solved for certain specialized cases (Eg.: Stokes drag derivation). Drag force varies with relative Reynolds number ($R_{er} = \frac{|v_p - u_f|d_p}{\nu}$) along with other parameters which are discussed later. The first mathematical equation for drag force is given by Stokes (1851) in a flow with very low relative Reynolds number ($R_{er} \ll 1$), Eq. 9. Stokes assumed the surface of the sphere to be smooth and neglected the change in velocity due to the curvature of the sphere.

$$F_d = -6\pi R_{er} \mu (v_p - u_f) \quad (9)$$

In later years, a generalized equation for drag force was derived empirically considering the assumptions made by Stokes. Eq. 24 is proved to be dimensionally correct and is in good agreement with experimental results.

$$F_d = -\frac{1}{2}C_D \rho_f A (v_p - u_f) |v_p - u_f| \quad (10)$$

The drag coefficient is a function of relative Reynolds number and is determined empirically from experimental results. The following are some of the empirical relations for C_D based on the range of relative Reynolds number, table 2. The equations in the table were obtained empirically [40]. The plot in Fig. 15 justifies these equations.

Relative Reynolds Number	Coefficient of Drag
$R_{er} \ll 1$	$\frac{24}{R_{er}}$
$R_{er} < 0.45$	$\frac{24}{R_{er}}(1 + \frac{3}{16}R_{er})$
$1 < R_{er} < 800$	$\frac{24}{R_{er}}(1 + \frac{1}{6}R_{er}^{\frac{2}{3}})$
$10^3 < R_{er} < 3 \times 10^5$	0.44 (Almost constant)
$R_{er} = 4 \times 10^5$	0.07 (Boundary layer becomes turbulent)

Table 2: Coefficient of drag in terms of relative Reynolds number

Figure 11: Effect of relative Reynolds number on drag coefficient of a smooth sphere; Courtesy: Frank M. White [55]

Force due to pressure gradient is the result of a difference in pressure along the fluid flow direction. The second term in the BBO-equation represents this force. This is independent of particle density but depends on fluid density. In general, this force is negligible compared to drag force acting on a particle. In case of high temporal or spacial accelerations, the pressure-gradient force might be considered but it highly depends on particle size.

The forces acting throughout the volume of the body are called body forces. Body forces include forces due to gravity and buoyancy in the case of a particle in a flow field. The first term in Eq. 8 represent body forces. Added-mass force is produced due to fluid kinetic energy gain from the work done by accelerating the particle. This force is applied to a certain amount of fluid, called added-mass. The third term in the Eq. 8 represents this force. It is dependent on the relative velocity of a particle in the flow and is independent of the density of the particle. The force that appears due to the lagging boundary layer development with changing relative velocity is known as Basset-history force [40]. The last term on the RHS of Eq. 8 represents this force.

4.2 Modeling of drag on a particle

The domain under observation is assumed to be compressible gas-solid two-phase flow. Depending on the type of interaction between phases, various forces will act on the particle. In numerical analysis, four different couplings between gas-solid mediums can be assumed. If the flow of a gas affects the solid particles and there is no reverse effect then the multiphase flow is said to be one-way coupled. All forces mentioned in the BBO-equation can be considered in this case. If there is a mutual effect between two mediums, the flow is said to be two-way coupled. The three-way coupling includes the effect of gas wakes and other disturbances on solid particles. Four-way coupling addresses all the interactions mentioned in three-way coupling and includes the effect of particle-particle interactions. These can be easily understood from Fig. 12. For a detailed study on different types of coupling refer to [39], [40].

Figure 12: Different types of coupling in particle-fluid flow; Crowe et al. [40]

One-way coupling is assumed to track particles, which takes into account the effect of the carrier medium on discrete/solid particles and neglects particle-particle interactions and the effect of the discrete field on the continuous field. Forces that act on a particle in one-way coupling are body forces - gravitational force and buoyant force; force due to pressure-gradient; drag force; added mass force, which is purely inertial; and Basset force or history force, which is due to diffusion of the vorticity from particle surface to bulk fluid flow [41].

The formulation of these forces depends on the mathematical or numerical model one chooses. To help decide this, the type of flow field must be established as continuum or rarefied. This depends on the

Knudsen number, $K_n = \frac{\lambda}{L}$, a characteristic parameter used to classify different flow regimes for their degree of rarefaction (where λ is mean free path and L is characteristic length). For a spherical particle where boundary layer thickness is negligible, characteristic length is of the order of its diameter in high-speed flows [42]. Flow is considered rarefied when $K_n \geq 10$ and continuum when $K_n \leq 0.01$. Since the particle diameter is on the order of micrometers and λ is on the order of nanometers for the analysis considered, the flow field can be safely assumed to be in the continuum flow regime. Hence the use of the Eulerian formulation for the gas can be justified. Particles are dealt by using the Lagrangian formulation to study the behavior of each separately. Eulerian-Lagrangian methods have many advantages over other numerical methods in multiphase flow simulations, [43].

For fluid medium, the Eulerian formulation was used. Hence continuum flow equations are implemented, Eq. 11 - 13. These equations are in conservation form as established in [44]. All other thermodynamic properties of fluid and particle are neglected. Also, an ideal gas assumption was employed for numerical simulation purposes. If the two-way coupling is used, there will be additional interaction terms in the momentum and energy equations. These terms can be eliminated by writing both solid-gas medium equations together as demonstrated in Maxwell et al.[45].

$$\frac{\partial \rho_f}{\partial t} + \nabla \cdot (\rho_f V_f) = 0 \quad (11)$$

$$\frac{\partial(\rho_f V)}{\partial t} + (\nabla \rho_f V) \cdot V = -\nabla p + \nabla \tau + \rho_f f \quad (12)$$

$$\begin{aligned} \frac{\partial}{\partial t} \left[\rho_f \left(e + \frac{V^2}{2} \right) \right] + \nabla \cdot \left[\rho_f \left(e + \frac{V^2}{2} \right) V \right] &= \rho_f \dot{q} + \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) \\ &+ \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) - \frac{\partial(wp)}{\partial x} - \frac{\partial(vp)}{\partial y} - \frac{\partial(wp)}{\partial z} + \tau : \nabla V_f + \rho_f f \cdot V \end{aligned} \quad (13)$$

Where, ρ_f is fluid density, $V_f = u\hat{i} + v\hat{j} + w\hat{k}$ is flow velocity, p is pressure, τ is stress tensor of order 3x3, f is body force per unit mass of fluid.

The drag term in Eq. 8 can be rewritten as Eq. 14. The third term is the drag in Eq. 8 and occurs because of a change in velocity curvature around the sphere. In the current study, it can be safely neglected because the particles under consideration are on the order of micrometers or less.

$$F_D = -6\pi a\mu\phi[v_p - u_f] = -\frac{1}{2}\rho C_D(A\hat{\mathbf{n}})(\vec{v}_p - \vec{u}_f) \cdot (\vec{v}_p - \vec{u}_f) \quad (14)$$

$$C_D = \frac{24}{R_{er}}\phi \quad (15)$$

In equation 15, ϕ accounts for deviation from Stokes drag. It depends on different parameters and varies based on experimental conditions. Hence it is expressed in an empirical form for different experimental environments. For high speed flows, different empirical relations are considered in [4], [53], [54] which are presented in Eq. 16. Other relations and their analysis in high-speed flows can be found in [5].

$$\phi_{melling} = \frac{1}{(1 + K_{nd})}, \phi_{ossen} = (1 + \frac{3}{16}R_{er}), \phi_{scarano} = \frac{1}{(1 + 2.4K_{nd})} \quad (16)$$

$$R_{er} = \frac{|v_p - u_f|d_p}{\nu} \quad (17)$$

$$K_{nd} = \frac{l}{d_p}; K_{nd} = 1.26\sqrt{\gamma\left(\frac{M_{\Delta u}}{R_{er}}\right)} \quad (18)$$

$$l = \frac{K_B T}{\sqrt{2}\pi d_p^2 P} = \frac{K_B}{\sqrt{2}\pi d_p^2 \rho_f R} \quad (19)$$

Pressure-gradient and body forces are used without any modifications from Eq. 8. In added-mass, the third term is neglected for the same reason presented for drag force. Finally, the Basset force history term is neglected because its effect can only be observed if the particle size is not negligible. The cases under consideration have particles of order micrometers or less. Hence the Basset force history term is neglected.

Understanding how to analyze the drag in three dimensions is a crucial part of developing any multiphase numerical analysis. In numerical analysis, the fluid velocity is calculated in three dimensions, which makes it easier to evaluate the drag in three dimensions and subsequently obtain the particle position. This approach leads to the calculation of a drag coefficient that varies in three dimensions. However, the drag coefficient is an empirical relation (for flows with high Reynolds number) dependent on Reynolds number of the flow

which in turn is constant for the flow irrespective of dimension under consideration. So, it is illogical to discuss the drag coefficient in 3-dimensions separately. Instead, the drag force is calculated based on the magnitude of the relative velocity of the particle using the empirical drag relation and is then resolved in three dimensions. This drag force is in the direction of the normal to the projected area of the particle. The normal to the projected area is dependent on the direction of relative velocity, making drag force indirectly dependent on the relative velocity of the particle to the fluid.

4.3 Mathematical formulation for numerical analysis

A mathematical model was developed to compliment the results obtained from MV3. Based on the assumptions mentioned above, and considering that particles pass through the shock wave with near pre-shock velocity, the following equations were obtained.

From Eq. 14,

$$m_p \frac{d\vec{v}_p}{dt} = -\frac{1}{2}\rho C_D (A\hat{n})(\vec{v}_p - \vec{u}_f) \cdot (\vec{v}_p - \vec{u}_f) \quad (20)$$

Considering only the normal direction to the shock

$$\frac{dv_{pn}}{dt} = -\frac{18\mu\phi}{\rho_p d_p^2} (v_{pn} - u_{fn}) \quad (21)$$

Let, $k = \frac{18\mu\phi}{\rho_p d_p^2}$.

Integrating with respect to time and applying boundary conditions gives

$$v_{pn} = (u_{f1} - u_{f2})e^{-kt} + u_{f2} \quad (22)$$

Where, u_{f1} is pre-shock flow velocity and u_{f2} is post-shock velocity.

Integrating Eq. 22 with time gives Eq. 23, the distance of particle from shock front in the normal direction.

$$x_{pn} = \frac{(u_{f1} - u_{f2})}{k} (1 - e^{-kt}) + u_{f2}t \quad (23)$$

5 Modifications made to Visual3 to accommodate particle

The base Visual3 code can accommodate only fluid phase. It can visualize any continuous volumetric data but it does not have the ability to track individual particles. Particles introduced in a flow have six constraints that require tracking, position (x, y, z) and velocity (v_x, v_y, v_z) . Visual3 is operated by both internal and user-supplied sub-routines. Internal sub-routines operate the code from initialization to rendering the supplied data. These sub-routines also have the ability to change visualization based on the input from the user. User-supplied subroutines are mainly to control the way the data is visualized. For example, creating cutting planes or inputting required scalar and vector data is done with the help of user-supplied subroutines.

Streamlines in Visual3 are plotted using an internal subroutine. With the help of this subroutine, a user can plot a curved line parallel to a vector field which represents a streamline of the flow field. They are obtained by numerical integration of the vector field along a line starting at the user-chosen location. The starting point is determined by use of a surface plotted in the 2D window. A point selected in the 2D window can be mapped back to a surface 3D window and will be used as the starting point for a streamline. This subroutine can only accommodate mass-less particles. The challenge was to introduce a particle with certain mass and size into the flow field. This will modify the streamline subroutine to track solid particles, in turn, providing the particle path and velocity at every time instant.

This approach to study particle lag data was chosen because the user has control over every single aspect of particle modeling such as particle size, density and boundary conditions applied to the particle. Also, as mentioned earlier the particle phase is being solved with rarefied flow physics, hence every particle introduced in the flow field will be solved separately for particle lag data. This provides a major advantage over using other solvers, which consider continuum mechanics if certain conditions are satisfied.

The algorithm for plotting streamlines in Visual3 is presented in Haines et al. [47]. It can be broken into two parts, the top-level part which performs the time-integration of the vector functions, and a low-level part which is responsible for evaluating the interpolated velocity at an arbitrary point in space.

The low-level task is to calculate $\vec{u}$ for an arbitrary $\vec{x}$ on an unstructured grid. For each node of a cell on physical domain (x_1, x_2, x_3) there is a mapping from some standard cell of same type in computational

space (ξ_1, ξ_2, ξ_3) . This mapping is given by Eq. 24.

$$\vec{x}(\vec{\xi}) = \sum_j f_j(\vec{\xi}) \vec{x}_j \quad (24)$$

Where, the sum is over the nodes of the cell, $\vec{x}_j$ is the coordinate vector of the j^{th} node, and f_j is a function which is equal to 1 at node j and 0 at all other nodes. This equation shows that if an arbitrary physical domain has “n” cells for numerical purposes it will be mapped on to a computational domain with “n” cells of the same type. However, this mapping is not stored in memory.

Consider a hexahedral cell, the standard structure of a mapped cell which is shown in Fig. 13. The functions f_j for this cell type are shown in Eq. 25.

Figure 13: Hexahedron cell standard convention in computational domain; Source: Haines et al. [47]

$$\begin{aligned}
f_1 &= \frac{1}{8}(1 - \xi_1)(1 - \xi_2)(1 - \xi_3) \\
f_2 &= \frac{1}{8}(1 + \xi_1)(1 - \xi_2)(1 - \xi_3) \\
f_3 &= \frac{1}{8}(1 + \xi_1)(1 + \xi_2)(1 - \xi_3) \\
f_4 &= \frac{1}{8}(1 - \xi_1)(1 + \xi_2)(1 - \xi_3) \\
f_5 &= \frac{1}{8}(1 - \xi_1)(1 - \xi_2)(1 + \xi_3) \\
f_6 &= \frac{1}{8}(1 - \xi_1)(1 - \xi_2)(1 + \xi_3) \\
f_7 &= \frac{1}{8}(1 + \xi_1)(1 + \xi_2)(1 + \xi_3) \\
f_8 &= \frac{1}{8}(1 - \xi_1)(1 + \xi_2)(1 + \xi_3)
\end{aligned} \tag{25}$$

If a function exists in physical domain for which $g = g(\vec{x})$ then the equation for mapping this onto logical space is given by Eq. 26.

$$g(\vec{\xi}) = \sum_j f_j(\vec{\xi}) g_j \tag{26}$$

Its important to note for any differential function $g(\vec{x})$ in physical domain there exists $g(\vec{\xi})$ in computational domain. This can be written in differential form as

$$\frac{\partial g}{\partial \xi_i} = \frac{\partial g}{\partial x_j} \frac{\partial x_j}{\partial \xi_i} = J_{ji} \frac{\partial g}{\partial x_j} \tag{27}$$

$$J_{ji} = \frac{\partial x_j}{\partial \xi_i} \tag{28}$$

The term “J” is called the Jacobian of the mapping. J is the ratio of the length of physical space to length in the logical domain.

Mapping Algoritm:

1. Input physical domain using Plot3D format into Visual3

2. Read and store grid data and flow data
3. Map grid data onto logical (computational) domain using Eq. 24
4. Map corresponding flow data using Eq. 26

When a user inputs a point $\vec{x}$ as the starting point of a streamline, an internal subroutine is invoked that computes the cell number in which the point is located. The Newton-Raphson method is then used to compute the corresponding $\vec{\xi}$. The initial guess $\vec{\xi}^{(0)}$ is taken to be center of the cell. The improved value is given by Eq. 29. The residual to calculate the improved value is taken as 1e-3 in the base code.

$$\xi_i^{(n+1)} = \xi_i^{(n)} + J^{-1}(x_i - x_i^{(n)}) \quad (29)$$

Later during integration, the low-level task is invoked every time step to estimate the velocity. During this process, the initial cell number is taken as the current cell. If this cell does not contain the point, the search will switch to the next cell in the $\vec{\xi}^{(n+1)}$ direction. This search method will converge quadratically to the correct point in the cell. Once correct $\vec{\xi}$ is obtained the velocity $\vec{u}$ at the point is obtained from Eq. 26.

Algorithm for low-level task:

1. User inputs $\vec{x}$ as starting point for a streamline
2. Newton-Raphson method is used and corresponding $\vec{\xi}$ is calculated
3. Eq. 26 is used to computed velocity at that point

Top-level part of the algorithm for plotting streamlines is straightforward. It uses the obtained velocity $\vec{u}(\vec{x})$ from the low-level task and integrates Eq. 30 using adaptive 4th order Runge-Kutta (RK4) method to obtain a new particle position. The adaptivity of the method depends on the amount of change in the velocity direction. If the velocity direction changes too much over one-time step, the time-step will be halved and the result will not be saved. If it changes too little, the time-step is doubled and the result is saved.

$$\frac{d\vec{x}}{dt} = \vec{u}(\vec{x}) \quad (30)$$

Algorithm for the top-level task:

Figure 14: Algorithm for obtaining particle path in Modified-Visual3

1. Velocity is obtained initially from the low-level task
2. Adaptive RK4 method is used to integrate new position

The adaptive RK4 method has a low-level task in every step of each iteration. The low-level task obtains cell number and exact velocity once the point crosses current cell. No changes have been made to low-level task in the streamline internal subroutine. The adaptive RK4 method has been changed to accommodate particles with mass. The algorithm for this modified code is presented in Fig. 14. The minimum time step for the integration depends on the size of the smallest cell in the grid and the maximum velocity of the flow field. To ensure there are at least two simulation steps in a shock-cell (A cell in the grid that has pre-shock properties at one end and post-shock on the other), time step should be calculated using Eq. 31 so that particle transitions smoothly onto the post-shock region. This has to be done to accurately depict particle motion, especially when there are regions of high accelerations.

$$\Delta t = \frac{l_{cell}}{10(V_{max})} \quad (31)$$

The effect of time step variation can be observed in Fig. 15. The data used here is in accordance with $2.0\mu m$ particle used in section 6. The minimum cell size used for this analysis is 0.1mm, which gives an

estimated time step of $1e-7s$ from the Eq. 31. From Fig. 15a, it can be observed that a fluid packet passes through the shock and does not settle to the post-shock velocity instantaneously when a time step of $1e-5s$ is used. This has a significant impact on the settling length of the particle as shown in Fig. 15b. It is to be noted that when a time step of $1e-6s$ is used, fluid packet only has one simulation step in the shock cell (shock-normal distance zero). A linear variation from pre-shock to post-shock can be seen in the plot with one simulation step in the shock cell. This affects the particle settling distance slightly at shock location, which can be observed in Fig. 15b. Finally, a time step of $1e-7s$ produces two simulation steps inside the shock cell as seen in Fig. 15a which effectively brings fluid to the post-shock velocity after passing through the shock cell.

Fluid - Time step variation

(a) Fluid packet

Particle - Time step variation

(b) Particle

Figure 15: Time step variation

6 Rudimentary code validation

In this section, data with high localized accelerations is setup for post-processing in the modified code (MV3), along with initial validation techniques for a particle passing through shock wave.

6.1 Data setup

A two-dimensional oblique shock system was created to be analyzed in the MV3. The solution for the oblique shock was obtained from the Rankine-Hugoniot relations. The grid created was aligned with shock angle for ease in numerical analysis. Mathematical equations for a three-dimensional grid inclined with respect to the shock angle are presented in Eq. 32. Here, the x-direction is parallel to the shock and the z-direction is normal whilst the y-direction has no velocity making the whole system effectively two-dimensional. The schematic of the grid transformation is shown in Fig. 16. This transformation makes it easy to input pre and post-shock velocities using plot3D format. This data is tabulated in table 3.

Figure 16: Grid transformation schematic for oblique shock

$$\begin{aligned}
 x_{node} &= [i + (k - 1)\tan(\frac{\pi}{2} - \sigma)] \\
 y_{node} &= j \\
 z_{node} &= [k - (i - 1)\tan(\frac{\pi}{2} - \sigma)]
 \end{aligned} \tag{32}$$

where, i, j, k are integers and σ is the shock angle.

The minimum cell size of $(0.1mm)^3$ was created within a grid with 100x100x100 dimensions. The initial import of this data into Visual3 with streamlines plotted by the original code is presented in Fig. 17. The

Parameter	Pre-shock	Post-shock
X-velocity; v_x	792.5	792.5 m/s
Y-velocity; v_y	0	0
Z-velocity; v_z	614	254 m/s
Density; ρ	1.273	3.08 Kg/m^3
Temperature; T	278	433.58 K

Table 3: Flow data for plot3D format

left side of Fig. 17 shows, xz-view in the 3D window while the right side shows an isometric view in the 3D window.

Figure 17: 3D window of Visual3 showing streamlines

6.2 Flow visualization in Modified-Visual3

Visualization of flow in the Modified-Visual3 (MV3) has been divided into four regimes to accommodate particles. These regimes were created for user understanding of the model in MV3 and are not part of the model. All these regions are represented in Fig. 18. As shown in the figure, a particle can be spawned at any location in the particle-spawn regime, and it exits after passing through the flow field boundary.

Figure 18: Different flow regimes in Modified-Visual3

6.2.1 Particle-Spawn regime

The Particle-Spawn region is where a particle with mass will be spawned with an assumption that its velocity being same as that of the flow. This was designed to avoid all complicated boundary conditions that a particle may experience when introduced at a different velocity than the surrounding flow. Since the current design is for modeling PIV numerically, this is a safe assumption as the particle reaches flow velocity before imaging starts in PIV. It is generally located upstream of the shock. In future work, a seeding velocity can be added to better mimic specific experiments.

6.2.2 Upstream regime

Upstream region is located between the shock and particle-spawn regime. Here, the flow may be uniform or non-uniform depending on the input. In this regime, the code computes the force acting on a particle and then integrates it to compute the position, taking flow conditions in the particle-spawn region as initial.

6.2.3 Downstream regime

Similar to the upstream regime, the downstream region can be either uniform or non-uniform depending on the flow. Since the solution is obtained analytically, the conditions in this region are obtained from the post-shock quantities of the flow.

6.2.4 Shock regime

A shock is a discontinuity with negligible thickness where properties are different on either side. But [51], [52] have shown shock thickness can be measured and is in the order of nanometers or less. In the present study, the thickness of the shock depends on the minimum mesh size used in the flow solver from which the flow data was obtained. Current solvers use techniques like adaptive meshing to decrease the thickness of the shock front. In the MV3 code, the shock regime was considered to be a non-uniform steady flow region, the input for which is obtained from the end conditions of the upstream regime.

6.3 Validation techniques

In this sub-section, initial validation methods for MV3 code were presented. The results from MV3 were compared with Melling's [4] data to validate the code.

6.3.1 Melling data : Tracer particles response across a shock

In [4], Melling conducted a numerical analysis on particles of different sizes passing through an oblique shock wave and plotted normal shock distance versus shock normal velocity as shown in Fig 19. This data has been carefully digitized using WebPlotDigitizer [33] for particles of diameter 0.2, 0.4, 0.6, 0.8, 1.0, 1.2, 1.4, 1.6, 1.8 and 2.0 μm . The digitizer reproduces Melling's data with discrete points which was later converted to continuous form as shown in Fig 20 using a scatter plot tool [34]. This digitized data has been used in further sections to compare with the results obtained from Modified-Visual3 code. Table 4 has flow data and Table 5 has particle parameters as used in Melling et al. [4].

Figure 19: Distance normal to shock (mm) vs Shock normal velocity (m/s) [4]

Figure 20: Digitized data obtained from Fig. 19

Parameter	Input	Output
Mach No.	1.5	1.152
Temperature(K)	300	343.77
Pressure(atm)	1.09	1.75
Density(kg/m^3)	1.273	1.77
Velocity(m/s)	521	428
Deflection angle	9.25°	
Shock angle	55°	
Dynamic Viscosity($kg/m - s$)	1.5e-5	

Table 4: Flow parameters for oblique shock

Consider a particle with diameter d_p and density ρ_p , which is spawned in a flowfield moving with velocity u_{f1} in the upstream regime. The velocity of the particle is assumed to be the same as the flow surrounding it.

Parameter	Value
Density(kg/m ³)	1000
Diameter(μ m)	Variable(0.2-2.0)

Table 5: Particle specifications for tracer particle

This eliminates the complicated boundary conditions on the particle if it is introduced at a velocity different from the surrounding flow field. At $t=0$, the velocity of the fluid is changed from u_{f1} to u_{f2} . If the only force acting on the particle is the drag, then Melling proposed eq. 33 to estimate the particle relaxation time.

$$\frac{(u_p - u_{f2})}{(u_{f1} - u_{f2})} = e^{-\frac{t}{\tau_p}} \quad (33)$$

Where, τ_p is particle time constant [4]

$$\tau_p = \frac{d_p^2 \rho_p}{18\mu\phi_{melling}} \quad (34)$$

The ability of a particle to track the flow depends on its relaxation time and flow response time, $\tau_f = \delta/\Delta U$, where δ is the outer length scale of the flow and U is the local outer velocity. The ratio of particle relaxation time to characteristic time scale of the flow is called the Stokes number, $S_t = \tau_p/\tau_f$. Clemens et al. [31] showed that the Stokes number should be less than 0.5 in incompressible flows. Samimy et al. [56] computationally presented that for a particle to track the smallest scales in the flow $S_t < 0.05$ inside compressible free shear layer. The particles with $S_t > 0.05$ grossly misrepresented flow features starting with the location of vortices. Urban et al. [32] showed experimentally that $S_t < 0.1$ for a flow to neglect particle slip in supersonic flows.

6.3.2 Flowfield initialization

A 50x50x500 (i x j x k) grid inclined to match shock angle was created with the constant grid size of 0.1mm. The analytical data from Table 4 is imported into MV3. Figure 21 shows the imported data with the density as scalar quantity. In the figure, the blue region is pre-shock, and the green is post-shock. Each node location is determined from equations 35, 36, 37. Normal to shock is in the z-direction with maximum span. The relaxation length available for the particles in this direction is 23.28mm.

Figure 21: Flow data in 3-D window

$$x_{node} = \frac{[i + (k - 1)\tan(\frac{\pi}{2} - \sigma)]}{10000} \quad (35)$$

$$y_{node} = \frac{j}{10000} \quad (36)$$

$$z_{node} = \frac{[k - (i - 1)\tan(\frac{\pi}{2} - \sigma)]}{10000} \quad (37)$$

Where i,j,k are integers.

6.3.3 Validation of the code

In the above-mentioned flow field, particles of different sizes were introduced with only drag as the force acting on the particle. Shock-normal distance vs. normal-velocity in comparison with Melling's data was plotted as shown in Fig. 22a. For this calculation, a drag coefficient with factor $\phi = 1$ was used. From Fig. 22a, it can be seen that MV3 code is not in agreement with Melling's data. Here dynamic viscosity of $\mu = 1.5\text{e-}5 \frac{kg}{m-s}$ was used for calculation.

Figure 22: Normal shock-distance (m) vs Normal velocity component (m/s)

Finally, based on the mathematical formulation the following data was obtained. The distance traveled by $2.0 \mu\text{m}$ particle was computed from Eq. 23 with dynamic viscosity of $1.5 \times 10^{-5} \frac{\text{kg}}{\text{m-s}}$. From Eq. 22, the time taken by the particle to reach 380m/s was found to be $7.36\mu\text{s}$ and from Eq. 23 the distance traveled was calculated as 1.77mm . This is shown in Fig. 22b. This shows that with the parameters used for the analysis, MV3 code produced better results compared to Melling's numerical analysis. This difference can be attributed to ϕ . Once drag coefficient factor of $\phi_{melling}$ was used for analysis, the results are nearly in agreement with each other as shown in Fig. 22c. This shows the importance of empiricism in the choice of drag coefficient.

6.3.4 Effect of viscosity

Viscosity is an important factor in determining the particle response time. A study was conducted with different coefficients of viscosity: Constant viscosity (pre-shock value) throughout the flow field and variable viscosity using Sutherland's law (Eq. 38) [55]. Results obtained are presented in Fig. 23. In the figure, data is compared with the mathematical case solved above. It was observed that Sutherland's viscosity case agrees better with the mathematical data. Hence Sutherland's law for viscosity has been implemented in the modified code for particle lag calculation.

$$\mu = \mu_{ref} \left(\frac{T}{T_{ref}} \right)^{\frac{3}{2}} \frac{T_{ref} + S}{T + S} \quad (38)$$

Figure 23: Viscosity comparison, Shock-normal distance (m) vs velocity (m/s)

6.3.5 Exploration of other empirical drag models

In this section, empirical drag coefficients presented in some of the previous works are studied using MV3. Variation of shock-normal velocity based on empirical drag coefficient is shown in Fig. 24. From the figure, it can be seen that the drag coefficients used in the works of Melling [4] and Humble [22] predicted high drag force on the particle compared to Stokes drag. The empirical formula provided by Ossen predicted low drag compared to the other three. The results obtained by MV3 are in agreement with those obtained by Lang [5].

Figure 24: Variation of empirical coefficient of drag

7 Particle tracer uncertainty quantification using MV3

In this section, a PIV analysis conducted by Hou et al. [21] is considered as a way to quantify uncertainty. Titanium oxide (TiO_2) is used for tracer particles in the experiment. Among all the PIV analyses [20]-[27] to study the structure of SBLI considered, Hou’s experiment produced less particle lag uncertainty with a calculated Stokes number of 0.1, which is well within the range mentioned in Urban et al. [32] work. The modeling mentioned in the section 6 was followed to replicate this analysis in MV3. Table 6 shows the initial data from [21]. Table 7 shows the data used in the numerical analysis. The velocity is kept constant in turn varying other properties of the fluid. Particle specifications for the analysis are provided in table 8.

Parameter	Experimental data
Mach no.	2.0
Temperature (K)	150
Pressure (MPa)	0.262
Free stream velocity (m/s)	491
Deflection angle	14°

Table 6: Hou’s PIV data

Parameter	Pre-shock	Post-shock
Mach no.	2.0	1.49
Temperature (K)	150	187
Pressure (MPa)	0.262	0.55
Free stream velocity (m/s)	491	407.7
Shock normal velocity (m/s)	341.25	204.05
Shock tangential velocity (m/s)	353.02	353.02
Shock angle	44°	

Table 7: Pre and Post shock values for numerical analysis

Parameter	Value
Density (Kg/m^3)	4230
Size; Manufacturer specified (μm)	0.021
Size; Experimentally obtained (μm)	0.26

Table 8: Particle specifications from Hou’s PIV analysis

Experimentalists estimate the particle diameter in PIV by calculating the shock-normal velocity of a particle after passing through a shock and curve fitting with the drag equation as suggested in Melling [4]. Using this approach, Hou estimated the particle size to be $0.26 \mu m$. Based on this value a numerical analysis is performed using MV3 to estimate the particle settling time. The output of this analysis is presented in Table 9. The shock-normal velocity is solely responsible for the particle to shoot past the shock with pre-shock velocity. It can be observed from Fig. 25 that there is uncertainty between the particle and fluid velocity behind the shock. This uncertainty is termed as “particle-lag” in this work.

Parameter	99% settling velocity	99.99% settling velocity
Normal velocity, v_n (m/s)	206.09	204.07
Particle relaxation time, t_p (μ s)	6.0	16.8
Particle settling length, x_p (mm)	1.50	2.87
Exp. fluid characteristic time, τ_f (μ s)	26.0	
Time ratio, ($\frac{t_p}{\tau_f}$)	0.231	0.646
% uncertainty in location	6.22	11.91

Table 9: MV3 output

Two different uncertainties can be defined in PIV due to the particle lag. One based on the velocity and is caused because of the assumption that the velocity of the particle is same as the fluid surrounding it which is known as *slip velocity* or *velocity uncertainty*. The other can be defined as the difference between the distance traveled by the particle to distance traveled by fluid in the same amount of time, which is called *particle dispersion* or *location uncertainty*. The velocity and location uncertainties of the particle are inversely proportional to each other. This can be seen in Fig. 25, which shows the exponential decay of the velocity with respect to the shock-normal distance. In the current case, 1% uncertainty in the velocity gives 6.22% location uncertainty whereas, 0.01% uncertainty in velocity produces 11.91% uncertainty in location. Velocity uncertainty against the shock-normal distance is shown in Fig. 26a. From the figure, it can be deduced that particle velocity is maximum right after passing through the shock as expected. Fig. 26b shows the location uncertainty plotted against shock-normal distance. Unlike velocity uncertainty, the maximum error in particle dispersion occurs as the particle moves through the flow field after passing through the shock. This analysis is in accordance with the experimental study by Ragni et al. [7] and demonstrates that PIV cannot predict exact velocities in regions with high temporal and spatial accelerations.

Two points are to be noted here. First, in the current analysis shock-cell is being considered to estimate the uncertainties. This can be observed in Fig. 25 in which, fluid velocity is not equal to the post-shock velocity at $x=0$. This provides accurate uncertainty estimation between experimental and numerical techniques. However, with the improved meshing techniques like adaptive meshing and with the computational capabilities available today, this error can be reduced to less than a nanometer. Second, PIV is a gradient based technique that does not consider any of these uncertainties. The emphasis of this analysis is that these uncertainties can be used to apply a correction for the data obtained from experiments to compare with the data from numerical analysis.

Figure 25: Relaxation curves for particle and fluid

(a) Velocity Uncertainty

(b) Location Uncertainty

Figure 26: Uncertainty vs Shock-normal distance

8 Analysis of forces acting on a particle using MV3

The different forces from the BBO-equation, Eq. 8 were analyzed separately in this section. Particles of different sizes and densities were introduced in the flow field described above to check for the dominant forces acting on a particle. This helps in determining the best particles to be used in PIV. Based on Eq. 31, acceptable time step for the analysis was determined to be $1\mu s$. For all of the following cases, particles are assumed to be introduced at $t=0$

A $2.0\mu m$ particle with a density of $1000kg/m^3$ was introduced into the flow described above with the drag, pressure-gradient and added-mass forces acting separately. The results obtained are shown in Fig. 27. It can be seen from the figure that the drag force is the major factor in bringing the particles to post-shock velocity. A particle diameter study was already presented in the section 6 which shows that the particles with smaller diameters are best tracers.

Figure 27: Time (s) vs Normalized velocity $\left(\frac{u_p - u_{f2}}{u_{f1} - u_{f2}} \right)$

Now, keeping the particle diameter constant, particle density is varied. These results are presented in Fig. 28. From Fig. 28a it can be seen that the particles with low density take less time to settle. However, the low-density particles have a major effect on velocity when pressure gradient and added mass forces are considered together as seen in Fig. 28b. Hence the particles with a small diameter and high density are best

tracers for PIV analysis.

Figure 28: Variation based on density

A dimensional analysis was done to compare the effect of body forces and the drag force. It was found that a $0.2 \mu\text{m}$ particle with 1000 kg/m^3 moved on the order of 10^{-7} m when only body forces were acting and approximately 1 m when the drag is acting as a positive force. Based on the above-proposed reasons, only the drag force is considered for the analysis in MV3 when there are high spatial and temporal accelerations. Hence MV3 would be ideal for analyzing any PIV analysis which was done by selecting optimal tracers (small diameter and high density).

9 Generalized oblique shock analysis

A 200x100x100 grid with a maximum cell side length of 0.1mm was created as shown in Fig. 29 to verify the integrity of MV3. The pre-shock grid was defined using Eq. 39 and the post-shock was defined using Eq. 40. This grid was then imported into the MV3 and its 3D window with density as scalar quantity is shown in Fig. 30. The flow data was obtained using Rankine-Hugoniot relations.

$$\begin{aligned}
 x &= (i - 1) + \frac{(j - 1)}{\tan(\frac{p^i}{2} - nd\theta)} \\
 y &= j \\
 z &= k
 \end{aligned}
 \tag{39}$$

$$\begin{aligned}
 x &= (i + n - 1) + \frac{(j - 1)}{\tan(\frac{p^i}{2} + nd\theta)} \\
 y &= j \\
 z &= k
 \end{aligned}
 \tag{40}$$

Where, i, j, k are integers, n is a variable at which angle changes and θ is the shock angle.

U-velocity contours of both particle and fluid were obtained in the XY-plane to understand the particle response across an oblique shock wave. These contours help determine the particle settling length when a particle with mass has been used in PIV. Since the solution obtained for flow data is accurate, these contours should ideally represent the error between the particle and fluid data. All contours in this section are obtained for a particle of size 0.2 μm diameter and 1000 kg/m^3 density.

Figure 29: Generalized oblique shock grid data; all dimensions in mm

Figure 30: Grid in MV3 with density as scalar variable

Both particle velocity contour and fluid velocity contours are shown in Fig. 31, 32. These contours were plotted by coordinate transformation as discussed in the section 6 to understand the particle settling distance. From figure 31, the particle settling distance can be observed. It was calculated to be 0.128 mm. This implies that the shock position would be off by $128\mu m$ if this particle was used in a PIV measurement to study the physics of an oblique shock mentioned in Table 4. This may not seem to be a huge error, but in practical cases, the ideal particle used here will not be available, and there will be many uncertainties to be considered. For example, the variation of particle sizes leads to the smearing of shock as expressed in DeBonis et al. [12]. This issue was analyzed here by passing a particle through the upper half of the flow and fluid through the bottom half. This contour is shown in Fig. 33. From the figure, it can be observed that the shock appears to be bent at particle-fluid interface region shown in a white line across the contour. This implies that if there is inconsistency in particle diameter used in PIV, there will be smearing of the

shock front. This is being corrected in PIV using time-averaging techniques which might relatively reduce the error but the exact location of the shock becomes hard to predict.

Figure 31: Particle velocity contour in XY-plane; all dimensions in m

Figure 32: Fluid velocity contour in XY-plane; all dimensions in m

Figure 33: Velocity contour showing smearing of shock; all dimensions in m

10 Analysis of the UM PIV data using MV3

The standard case model developed at UC (2013) based on the UM wind tunnel experiment consists of 56 million grid points. This model used the SST turbulence model and adiabatic boundary conditions to solve for the flow parameters. The grid coordinate system is left-handed and is non-dimensionalized by tunnel height of 2.75 in. To compare obtained results with experimental results, the following transformation equations are used:

$$x = 25.4(2.75x_{grid} - 38.265) \quad (41)$$

$$y = (25.4 \times 2.75)z_{grid} \quad (42)$$

$$z = 25.4(2.75y_{grid} - 1.125) \quad (43)$$

Figure 34: Part of grid that was imported into MV3

Figure 34 a 2D section (highlighted in black rectangle) of the wind tunnel that was imported into MV3 for post-processing. MV3 spawns particles at any required location with boundary conditions matching the surrounding flow. This matches the experiment, where particles have been seeded upstream and are assumed to be entering the experimental plane with the velocity of the surrounding fluid. Hence spawning particles in the chosen part of the wind tunnel should be a reasonable assumption. A 7.75° wedge is used for generating a shock in the standard case. Adiabatic shock results are presented in Table 10, and specifications of the particles used in the experiment are in Table 11

Based on the above data, a numerical analysis of a particle passing through an oblique shock was con-

Parameter	Input	Output
Mach No.	2.75	2.39
Temperature(K)	114.32	133.52
Pressure(Pa)	4035.5	6846.13
Density(kg/m ³)	0.123	0.177
Velocity(m/s)	589.38	555.68
Deflection angle	7.75°	
Shock angle	27.36°	
Ref Dynamic Viscosity(kg/m-s)	1.716x10 ⁻⁵	

Table 10: Flow parameters for oblique shock in Michigan PIV

Parameter	Value
Density(kg/m ³)	819.0
Diameter(μm)	0.281

Table 11: Particle specifications for tracer particle used in Michigan PIV

ducted to calculate particle response time and Stokes number. This analysis was done similar to the experimental analysis done in Lapsa (2009) [10]. Shock-normal particle velocity was obtained from the MV3, and this was exponentially fitted to get the particle response time. Shock-normal velocity vs. time is shown in Fig. 35. The particle response time was calculated from the numerical analysis to be 1.93 μs compared to 5.5 μs as estimated by the experimental analysis. Flow timescale was calculated in Lapsa using Eq. 44 as 17 μs . This gives a Stokes number of 0.112 which is not suitable for analysis in supersonic flows. According to Samimy et al. [56], Stokes number should be less than 0.05 for a particle to track the flow without misrepresenting flow features in PIV.

$$\tau_f = \frac{\delta(x)}{u_\infty} \quad (44)$$

Figure 36 shows the relative distance traveled by particles compared to a corresponding fluid element. This shows the actual measure of maximum error that will be obtained when 0.281 μm particle is used for analysis of the conditions mentioned in table 10. In the figure, shock occurs at approximately 48.7 μs . The maximum error in estimation of shock location would be 33.6 μm . However, this is not an estimate of maximum error happening in the UM-PIV data. The error, in that case, will undoubtedly increase because of the presence of more than one discontinuity. Figure 37 shows the difference between the velocity of the particle to its corresponding fluid element. It shows that the particle slip will be maximum at the instant when it passes through the shock and then gradually settles back to the local fluid velocity, although the particle is much farther ahead than the corresponding fluid element.

Figure 35: Shock-normal velocity vs time

Figure 36: Relative shock-normal distance vs time

Figure 37: Relative shock-normal velocity vs time

10.1 Importing data into MV3

For the reasons mentioned in above only a part of the wind tunnel is imported into MV3 code. The section that was imported as visualized in the 3D window with density as the scalar variable is shown in Fig. 38. This figure also highlights the experimental plane that was used in the PIV. The plane presented in the 2D window consists of the experimental plane, which varies from 18.2mm to 61.9mm in the horizontal direction and 0.257mm to 17.7mm in the vertical direction as shown in Friedlander [38]. All the further analysis has

been done in experimental coordinate system.

Figure 38: CFD data as visualized in MV3 with density as scalar variable

The minimum time step for the analysis was determined by Eq. 31. Minimum grid size in the experimental plane was found to be approximately $2.607 \times 10^{-4} m$ reference velocity was $603 m/s$. This gives minimum a Δt of 34ns. Hence a time step of 1ns was chosen for the analysis. The empirical drag coefficient used in the work of Humble et al. [22] was used for the current numerical analysis because of the reason that the flowfields in both analyses are similar.

Particles were then introduced into the central plane at a span of $3.5 \mu m$ between each particle in the transverse direction. A total of 180 particles were introduced from bottom to top in the transverse direction. Results obtained are written to a file and were post-processed using Python scripts and Tecplot [57].

The data obtained from MV3 was scattered as shown in Figs. 39a, 40a. Each point on the scatter plot corresponds to a particle in the flow. This data was later post-processed in later sections using Python scripts and Tecplot [57]. Velocity contours of the respective areas were presented in Fig. 39b and 40b for the comparison. It has to be noted that particles are not covering the total span in Z-direction. The MV3 code returns *NONE* once particle hits the domain boundary. Hence particles were spawned only in the region of interest i.e., experimental plane region.

Figure 39: Streamwise velocity data

Figure 40: Transverse velocity data

11 MV3 results - Standard case

The data obtained from MV3 are the position, velocity, and acceleration of both particle and its corresponding fluid packet at every instant. First, a discrete analysis was done to elucidate the particle behavior in 3D-SBLI. Figure 41 shows the path traced by particles (red) and streamlines (blue) coupled together. It can be observed from the figure that streamlines move in and out of the plane which causes uncertainty during imaging phase of PIV analysis. Particles in the experimental plane can be seen to deviate from the streamlines path only after crossing the incident shock wave. The data presented from here on has been converted using Eq. 41, 42, 43 to be in accordance with Friedlander's [38] data.

Figure 41: Path traced by particles (red) and streamlines (blue) in central plane; all dimensions are in mm

11.1 Single particle analysis

Particle deviation, the location of shock, compression, expansion waves and the effect of wedge interaction can be studied using the Single particle analysis. Red lines represent particle data while blue represents fluid data unless specified. Particles were introduced at three different locations; near separation zone, at

mid-span, and near wedge surface. Each particle and its corresponding fluid packet is studied separately for this study. The study of a particle close to the separation zone helps in understanding the effect of compression and expansion fans on the particle-lag. The study close to the mid-span zone gives an idea of particle behavior when interacting with the shock waves and the study close to wedge surface helps in understanding the effect of expansion fan and its impact on the velocity in the midsection. The terminology used below is in accordance with the SBLI structure described in “Introduction” section.

The path traced by a particle and its respective fluid packet when introduced close to the separation zone is shown in Fig. 42. The initial coordinates of the spawned particle are (13.3, 0.0035, 0.409091). It can be deduced from the figure that the fluid and particle diverge from each other. The reason for the deviation of the particle from fluid in this region was further investigated by plotting the path traced in 2D planes. These are shown in 43a, 43b, 43c. The velocities in three directions are plotted against the streamwise distance in Fig. 44. The xy-plot shows that the streamline deflects in the opposite direction to the rest of the flow because the separation occurred due to the shock interaction with the boundary layer. The flow deflection indicates that the particle is spawned inside the boundary layer. It is known that speed of sound in the flow is 219.27 m/s. From Fig. 44a it can be understood that the particle is introduced above the sonic line. This implies that the dip in the velocity in streamwise direction is due to the formation of the separation shock from compression fan. However, it is to be observed that the deviation between the particle and fluid is not considerable because of the gradual change in the velocity in compression fan. The rise in the velocity after 30mm in the streamwise velocity plot is due to the formation of the expansion fan. The error caused in this region is almost negligible when compared to other regimes in the structure of SBLI. From xz-plot, it can be seen that both the fluid and the particle move out of the experimental plane. This implies that there are external interactions due to particles moving in and out of the plane in this region, which is one of the reasons for the experimental uncertainty. This fact can be attributed to the small magnitude of spanwise velocity which is sufficient to move particles out of the plane. This suggests that particle is not tracking fluid closely. However, it is important to note that the deviation is on the order of micrometers in the z-direction. Although spanwise velocity plot, Fig. 44c does not give away much information, it shows the fluctuation in velocity between 100 and 125mm, which might be because of the vortex formation in boundary layers as seen in Galbraith’s [36] work.

The SBLI structure with the incident and reflected shocks are present in the mid-span region. Particle paths and streamlines of this region are presented in Fig. 45. From the figure, it can be noted that there is a definite deviation between the particle path and streamlines. This deviation increases as the particle move

Figure 42: Path traced by particles (red) and streamlines (blue) in central plane near separation zone; all dimensions are in mm

through the discontinuities present in SBLI structure. The coordinates of spawning the particle are (13.3, 0.35, 0.409091). The reason for the particle deviation from the fluid was further investigated by plotting particle paths and streamlines in separate 2D planes. The XY-plot is presented in Fig. 46a. It can be deduced from the plot that the particle follows the deflection caused by the wedge and an initial deviation from the fluid path can be seen where the incident shock occurs. This particle lag is decreased after the particle passes through an expansion fan present after 75mm streamwise length. From Fig. 46c, a definite difference between the particle path and the fluid streamline can be seen. The movement out of the plane is because of the velocity change in the spanwise direction as shown in Fig. 47c. So if the PIV experimental plane was in this region, the particle movement out of the plane causes a major uncertainty. This is one of the reasons that PIV is not suitable to study the post-shock regions in this case. In the Michigan PIV data, the experimental plane region is between 18-62mm, where particle deflection from central plane is zero. The streamwise velocity plot is shown in Fig. 47a is helpful in understanding the structure of SBLI. The first depression in the velocity plot is due to the incident shock, the second dip is due to the reflected shock. The sudden rise in velocity is due to the formation of expansion waves. The last dip in streamwise velocity is due to the formation of reattachment shock. This plot emphasizes that the particle velocity doesn't match fluid velocity and can be seen to differ by an amount of 10m/s at certain instances. This explanation of SBLI structure can be supported from the transverse velocity plot shown in Fig. 47b. From Fig. 47c, in

Figure 43: Streamlines (blue) and particle paths (red) seen from different planes near separation zone; all dimensions are in mm

the region between 18-62mm the velocity fluctuation is negligible, which is the desired result considering the symmetry of wind tunnel. This is however not the case when PIV is considered, the results are shown in Appendix B to support this argument.

Surface interactions are very important to consider when analyzing a flow using PIV. These were studied experimentally by Eagle [25] and computationally by Galbraith [36]. Most of the experimental setups cannot obtain data in this area. The following data presented here helps in understanding the effect of surface interaction in analyzing the structure of SBLI. The wedge is designed in the wind tunnel to produce a shock. The flow close to the surface of this wedge experiences the effect of shock the least. A representative streamline and its respective particle path in three-dimensional view are presented in Fig. 48. It is clear from the figure that the particle and fluid do not deviate from each other throughout the initial inclination of the wedge. This is elucidated in Fig. 49a. In the current analysis, there is no interaction between the particle and wedge surface. Instead, all the deviations observed are from the flow itself. So, the deflection was from the inertia of particle which has higher streamwise velocity than the fluid at any instant in this

Figure 44: Velocity (m/s) vs. Streamwise distance (m) in central plane near separation zone; [Streamlines - blue, Particles - red]

region. This can be seen in Fig. 50a. The increase in the velocity at 25mm streamwise distance is due to the presence of an expansion fan which later on interacts with the reflected shock from the SBLI. This is the reason that there is a small spike in velocity between the incident and reflected shocks in the midspan region. This can be seen in Fig. 47a. The change in velocity in the spanwise direction in all the above-mentioned cases can be attributed to the complicated interactions happening out of the experimental plane region that are caused by the shape of the wedge.

Figure 45: Path traced by particles (red) and streamlines (blue) in central plane near mid span; all dimensions are in mm

(a) XY-Plane

(b) YZ-Plane

(c) XZ-Plane

Figure 46: Streamlines (blue) and particle paths (red) seen from different planes near mid span; all dimensions are in mm

(a) Streamwise Velocity

(b) Transverse Velocity

(c) Spanwise Velocity

Figure 47: Velocity (m/s) vs. Streamwise distance (m) in central plane near mid span; [Streamlines - blue, Particles - red]

Figure 48: Path traced by particles (red) and streamlines (blue) in central plane near wedge surface; all dimensions are in mm

(a) XY-Plane

(b) YZ-Plane

(c) XZ-Plane

Figure 49: Streamlines (blue) and particle paths (red) seen from different planes near wedge surface; all dimensions are in mm

(a) Streamwise Velocity

(b) Transverse Velocity

(c) Spanwise Velocity

Figure 50: Velocity (m/s) vs. Streamwise distance (m) in central plane near wedge surface; [Streamlines - blue, Particles - red]

11.2 Velocity Contours

Results obtained from MV3 are now filtered using a Python script to separate particle results in the experimental plane. This data was then linearly interpolated on to a 700x700 grid. Streamwise and transverse contours obtained from this interpolation are shown in Fig. 51a and Fig. 52a respectively. Since the discrete data available was over 100,000 points, linear interpolation onto a fine grid should not produce a significant error. Similarly, experimental data was also interpolated from a 35x86 grid onto a 700x700 grid and these results are presented in Fig. 51b and 52b respectively. CFD data for the same quantities is shown in Fig. 51c and 52c. All of this data is normalized by the test section velocity of 603.0 m/s to be in comparison with Friedlander and the AIAA workshop. The presence of incident and reflected shocks can be identified in the CFD data but it is hard to do the same in either the PIV or particle data, due to the inertia of the particles which shoot out of the shock with pre-shock velocity. This causes an increase in the shock thickness when imaging in PIV. For similar reasons, in the transverse velocity contours, the region with the negative velocity between the incident and reflected shocks is small compared with the PIV and particle data.

That said the PIV and particle results appear to agree with each other in general comportment. More of the error analysis on this data is discussed in later sections. Fig. 53 and 54 shows comparison between CFD, PIV and MV3 model results. From these figures, it can be seen that PIV and MV3 agree with each other better compared with the other cases. The error was calculated to be 0.0128 in the u-direction and 0.0147 in v-direction when CFD results were compared with streamwise experimental plane MV3 results. In this study, the majority of this error was considered to be because of the particle lag. Particle lag is attributed to change in the velocity across the shock, the higher the velocity change across the shock the higher the particle lag. For example, consider an oblique shock, in which v_1 is the pre-shock velocity (no velocity in the transverse direction) of the fluid and v_2 is post-shock velocity. Let the deflection angle be δ . The change in velocity in the horizontal direction is $\Delta u = |v_1 - v_2 \cos \delta|$ and in the vertical direction is $\Delta v = |v_2 \sin \delta|$. As understood from the previous section, the majority of error, in this case, is associated in the regions with shocks. It is evident from Table 10 that ($\Delta u < \Delta v$) in the current case. The same is true for reflected shock as well. This implies that the change in velocity in the vertical direction is greater compared to the horizontal direction. Hence, the particle lag in the transverse direction is more resulting in high error.

From Figs. 53a and 53b it can be seen that MV3 data agrees with PIV better compared to CFD. This implies that the particle lag plays an important role in analyzing SBLIs in PIV. The difference between CFD and Particle-lag model/PIV contours can be clearly observed close to the recirculation zone in the

Figure 51: Streamwise velocity contours linearly interpolated onto 700x700 grid

experimental plane. It is to be noted that the difference between particle-lag model and PIV contours might be due to the particle size variation in PIV. The particle size variation is not considered in the current work and is an important factor to be analyzed. Also, from V-contour plots it can be observed that the MV3 data is overestimating PIV data, but this estimation has lower error compared to CFD case. To better estimate, this error, Y vs. velocity plots at different X locations were made as shown in Fig. 55. In far upstream location, at $X = 26.76\text{mm}$ it can be observed that CFD is always underpredicting PIV while MV3 data is very similar to PIV data. As we move downstream, both particle and CFD data overpredicts for the bottom half and underpredicts for the top half region. Also, from these plots, it was observed that the particle

(a) Particle lag model

(b) PIV

(c) CFD

Figure 52: Transverse velocity contours linearly interpolated onto 700x700 grid

velocity seems to be always greater than CFD/fluid velocity except for a few downstream locations. In Figs. 55e and 55f, the particle velocity is less than the fluid velocity in the bottom half. This can be attributed to the presence of expansion waves closer to the boundary layer. The top half of this region still observes positive particle lag because of the presence of shock waves in that region. One more important observation that can be made is that at the far downstream location, $X = 53.76\text{mm}$, MV3 data is overestimating the PIV data. This is happening because of the presence of a compression train which accounts for the gradual decrease in velocity of the flow field, which in turn increases the negative acceleration of particle leading to increment in its velocity.

(a) Particle lag model vs PIV

(b) Particle lag model vs CFD

(c) CFD vs PIV

Figure 53: Streamwise velocity contours

(a) Particle lag model vs PIV

(b) Particle lag model vs CFD

(c) CFD vs PIV

Figure 54: Transverse velocity contours

(a) $X = 26.76\text{mm}$

(b) $X = 30.76\text{mm}$

(c) $X = 34.76\text{mm}$

(d) $X = 38.76\text{mm}$

(e) $X = 41.76\text{mm}$

(f) $X = 53.76\text{mm}$

Figure 55: Y vs U-velocity

11.3 Acceleration contours

Acceleration contours are the best way to show regions with high drag on tracers in PIV. These contours provide insight into the exact location of regions with high accelerations or decelerations, which gives the estimation of the location of discontinuities present in a flow. These can be useful in understanding the structure of SBLIs, especially to get the location of all the shocks, compression and expansion waves. However, the location of recirculation zones is hard to estimate even with the acceleration contours. The best way to understand recirculation zones is to look at streamline plots as presented in Galbraith [36]. Two different acceleration contours can be obtained from the data obtained through MV3: Particle acceleration contours, and fluid acceleration contours.

The particle acceleration contour is obtained from the acceleration of particles introduced in the flow. It is equal and opposite in direction to the acceleration due to drag. The equation for particle acceleration is given in Eq. 45. The drag force acting on a particle increases abruptly when it passes through a shock wave which should provide a location estimate for the shock wave. On the other hand, it becomes positive as it passes through an expansion fan but it may be hard to notice on a particle acceleration contour because the change in velocity of the fluid is more gradual in the expansion zone. Therefore, making it less useful for feature detection. The particle acceleration contours do not predict the correct shock location because of their dependency on particle velocity.

$$A_p = -A_d = \frac{d\vec{v}_p}{dt} \propto -(\vec{v}_p - \vec{u}_f) \cdot (\vec{v}_p - \vec{u}_f) \quad (45)$$

The fluid acceleration contour is obtained from the acceleration of the fluid packet corresponding to each particle spawned in the flow. It neither depends on the drag nor on the particle acceleration. This contour is more robust and can estimate the location of discontinuities better than its counterparts. The equation for fluid acceleration is given in Eq. 46.

$$A_f = \frac{d\vec{u}_f}{dt} \quad (46)$$

All acceleration contours obtained for UM PIV data are normalized by $1e8$. Fig. 56 shows the streamwise acceleration contours in the experimental plane region of the wind tunnel data. From Fig. 56a it is evident

that the region with the highest drag is in the SBLI interaction zone. From this, the basic structure of incident, separation, and reflected shocks can be understood. It is important to note that the thickness of these discontinuities resembles the settling length of the tracers present in the flow. The location of expansion fan can also be pointed out from the contour. From the fluid contour shown in Fig. 56b, all the discontinuities mentioned above can be pointed out. However, the thickness of these discontinuities is not so noticeable compared to the particle acceleration contour but their location can be clearly pointed out in the fluid acceleration contours. This is the major difference to be remembered when studying acceleration contours which are obtained from the PIV data and the CFD data. In the shock region, the particle has high acceleration compared to the fluid, which can be clearly seen from Fig. 56a and 56b. Similarly in the expansion fan region particle has low acceleration compared to the fluid. This is also evident in the streamwise contours presented here.

Fig. 57 shows the transverse acceleration contours in the experimental plane region of the UM PIV data. The study of the transverse acceleration contours is a bit tricky because of its dependency on the directionality of the velocity which changes from $0 - 180^\circ$ in the transverse direction. Let us consider the fluid acceleration contour shown in Fig. 57b. It is to be remembered that the initial velocity is zero in the transverse direction. The incident shock changes this velocity to the negative y-direction. Hence the acceleration around this shock wave is negative. The separation shock changes the velocity to positive y-direction which implies that the acceleration is positive in this region. The transmitted shock has similar behavior to the incident and the reflected shock has properties similar to the separation shock in terms of the acceleration in the transverse direction. The important property of these contours is that it is easy to identify the expansion zone since it has a low thickness in the y-direction. The scale has to be adjusted to identify this region as presented in Appendix C.1. The properties of the particle acceleration contour still hold true in the transverse direction. However, it is important to apply analysis similar to the transverse fluid acceleration contour to understand them. The shift in the incident shock location in y-direction between particle and fluid data can be clearly observed in Figs. 57a and 57b respectively.

(a) Particle acceleration

(b) Fluid acceleration

Figure 56: Streamwise acceleration contours

(a) Particle acceleration

(b) Fluid acceleration

Figure 57: Transverse acceleration contours

11.4 Statistical Analysis

In any PIV analysis, the diameter of the particles is not constant. This has not been considered in the analysis presented up to this point. The particle distribution is one of the significant parameters in the production of the shock smearing in instantaneous data other than turbulence. This can be verified by introducing differently sized particles in the flow at different y-locations of the central plane. One of the significant interests in doing the particle distribution analysis is that this brings numerical analysis one step closer to actual PIV analysis and hence it should produce less error compared to the constant particle diameter case. In this section, based on the statistics of diameter distribution the analysis presented above is repeated and the data required to calculate the error between MV3 data and PIV was obtained.

A TDA-4B portable Laskin nozzle aerosol generator from ATI Techniques was used as tracer generator in the PIV analysis conducted at UM. Particles diameter produced by this nozzle is not constant. The generator consists of an array of six Laskin nozzles that create polydispersed sub-micron particles. This distribution depends upon the operating conditions of the nozzle such as nozzle pressure, the chosen aerosol reagent and the volume of air used to dilute the raw aerosol produced. A sample dispersion is shown in Fig. 58 for operating conditions of 23 PSI using PAO-4 oil. Details of this distribution are presented in Table 12. This data was provided by the manufacturer, and the following conditions were quoted to support the distribution:

1. The stated count mean diameter varies dependent primarily upon nozzle manufacturing variation.
2. Applied pressure has a lesser effect provided normal operating pressures are maintained within +/- 10%.
3. A shift from 281 nm to 263 nm is well within the typical variance limits.
4. The averages for count and mass were obtained using 37 separate particle size distributions performed between June 2008 and December 2013 operating at 20 psi using 4 cSt polyalphaolefin.

Sample size = 37	Count		Mass	
	Mean	Median	Mean	Median
Range				
Average	265	227	552	536
Min	213	177	523	499
Max	293	256	573	560

Table 12: Particle distribution; all dimensions in nm

Figure 58: Type III-A Laskin Nozzle Aerosol Distribution @ 23 PSI Using PAO-4 Oil; Courtesy: ATI Techniques

From the data provided by the manufacturer [61], a single particle analysis was presented below. Particles of extreme sizes were chosen for this analysis. The data was obtained from MV3 and the results were presented in Figs. 59, 61, 60. From Fig. 59, it can be seen that large particles deviate from streamlines more. It is important to note that the minimum size of 177nm and maximum of 573nm are quoted by the manufacturer. Also, the particle diameter estimated by Lapsa [9] is 570nm. This shows that the current analysis is well within the variance limits. The xy-plot (Fig. 60a) shows that the deviation between the particle and fluid increases during the first inclination of wedge surface and decreases as it passes through the rest of the flow. Figures 60b and 60c show that larger particle deviates less into z-plane which is a preferred feature for PIV analysis. However, if the PIV analysis is conducted using this particle size, it would give an illusion that the SBLI interaction is highly two dimensional, which produces a major error in velocity estimation. It can be seen from the streamwise velocity plot (Fig. 61a) that the heavy particle shoots past the shock and does not settle down to the fluid velocity. It is also evident in the transverse velocity plot, shown in Fig. 61b. From Fig. 61c, it is very clear that spanwise velocity fluctuation is very low with the heavy particle compared to the fluid or any other particles presented.

Figure 59: Path traced by particles of different sizes and streamlines (blue) in central plane near mid-span; all dimensions are in mm

(a) XY-Plane

(b) YZ-Plane

(c) XZ-Plane

Figure 60: Path traced by particles of different sizes and streamlines (blue) seen from different planes in central plane near mid-span; all dimensions are in mm

(a) Streamwise velocity

(b) Transverse velocity

(c) Spanwise velocity

Figure 61: Velocity (m/s) vs. Streamwise distance (m) in central plane near mid-span

The presence of different sized particles in the flow causes effects like shock smearing, which can be observed in instantaneous data. The ensemble average of this data produces an incorrect location of discontinuities present in the flow. This error can be avoided by using constant diameter particles, which might be possible with solid tracers like titanium oxide. The emphasis of this study is to understand the non-linearity of the particle path traced with the use of different sized particles in the PIV analysis and to suggest that the PIV result uncertainty increases with increase in scattered particle diameter distribution.

12 Error metric

An error analysis was employed similar to what was used in the AIAA workshop [11] to be able to compare with those results. Following equations were used to compare velocities:

$$e(f)_n = |(f_{cfd})_n - (f_{exp})_n| \quad (47)$$

$$E(f) = \frac{1}{N} \sum e(f)_n \quad (48)$$

Eq. 48 is the weighted average of Eq. 47 in the streamwise plane. The error metric was presented in Table 13. It can be seen from the table that the MV3 model when applied to the standard case CFD produced less error compared to any other models. Especially the error in the streamwise velocity improved considerably because of the effect of shock-normal velocity on the horizontal direction. This shows the importance of particle drag models in developing CFD models, especially when trying to validate these models with their respective experimental results. Experimental uncertainty was determined to be 0.008947 in the spanwise direction, which shows that particle lag model results obtained were almost same as experimental results. The error metric presented in the table is for a 281nm particle case.

U Error		V Error	
0.02193	Standard (Particle Lag Model)	0.008947	Expt.
0.02373	Q	0.009995	Standard (Particle Lag Model)
0.02633	B	0.01158	Standard (Medium Lag)
0.02669	P	0.01185	Standard (Long Lag)
0.02676	Standard (Long Lag)	0.01224	Standard (Short Lag)
0.02747	Standard (Medium Lag)	0.01377	Standard
0.02759	G	0.01449	B
0.02840	F	0.01682	P
0.02853	Standard (Short Lag)	0.01716	G
0.02899	M	0.01729	F
0.02957	I	0.01771	M
0.02964	Standard	0.01828	Q
0.02999	K	0.01867	K
0.03035	N	0.01917	N
0.03129	O	0.01961	O
0.03473	Expt.	0.02344	J
0.03571	H	0.02721	H
0.03980	L	0.03883	L
0.03995	J	0.04002	I

Table 13: Error metric comparisons; Highlighted in red is the current model; Remaining data is from Friedlander et al. [37]

13 Conclusion

A particle drag model has been successfully implemented to post-process CFD results using one-way coupling between particles and fluid. Modeling of the particle in a flow field with an oblique shock has been demonstrated. A new algorithm has been implemented to track solid particles spawned in a flow field. The code was validated using Melling's data. Results showed a deviation from actual data presented by Melling. An investigation was done using a mathematical formulation that showed MV3 produced better results. For example, Melling suggested after one relaxation time $\tau = 14.8\mu s$ a $2.0\mu m$ particle attains a velocity of 387 m/s but from both mathematical data and MV3 it was found to be 351 m/s. This deviation from Melling's data has been attributed to the drag coefficient factor. This study showed the importance of the empirical drag coefficient in numerical analysis. Different forces acting on a particle in a decelerating flow were studied. This study concluded that the drag is the only important force to consider when analyzing a particle in a flow field with high spatial accelerations. This also showed that the particles with a small diameter and high densities have better traceability in PIV. This was verified by calculating different uncertainties caused by tracers using the developed MV3 code. A 3D oblique shock model was used to verify the code convergence in generalized cases. This study helped in understanding the shock smearing effects produced in PIV.

Finally, CFD data complementing the University of Michigan PIV analysis was imported into MV3 for further post-processing based on the developed particle drag model. This data was analyzed in the streamwise plane as it was shown to produce more accurate results as compared to spanwise data. Final results obtained from MV3 showed remarkable improvement in both streamwise and transverse velocities. This was presented in the contour comparison plots. From these plots, it can be seen that streamwise velocity is still underpredicted after accounting for particle lag while transverse velocity was overpredicted. It is an important observation which shows that the particle lag effect is neither linear nor the same in both directions.

Single particle analysis provided insight into where error due to particle lag will be high or low. It helped in understanding the effect of particle lag in different regions of a wind tunnel facility. It shows that the velocity of the particle varies non-linearly to the velocity of its corresponding fluid packet. The highest velocity lag can be observed in the mid-span section of the experimental plane while the lowest can be observed near the separation zone. This implies that most of the error observed due to the particle lag is due to particles passing through discontinuities. A maximum difference of about 20 m/s in streamwise velocity is observed at the mid-span section after the particle passes through the shock. These plots are direct evidence

to show that the particle lag effect should be considered before comparing CFD with PIV results.

For the first time ever acceleration contours were plotted for the data obtained from the UM PIV analysis. Three different contours were plotted; Drag contour, Particle acceleration contour and Fluid acceleration contour. It was shown that drag and particle contours are inversely proportional to each other. These would be similar to the contours obtained from PIV data. A distinct difference can be seen between these and fluid contours. The thickness and location of discontinuities are not consistent in drag and particle contours. This is because of the drag acting on the particle when passing through a discontinuity in a flow field.

A statistical analysis was also conducted based on the specifications provided by the manufacturer of the nozzle used in PIV analysis. This analysis showed the non-linearity in the variation of particle velocity when a single particle analysis is done. This implies that instantaneous velocity cannot be averaged without considering the effect of particle size in PIV. However, if solid particles of constant diameter can be used (TiO_2), this error can be reduced. The error caused due to the effect of particle size variation is quantified and further analysis of this is presented in the Appendix D. Respective contours of different sized particles are presented in Appendix A.

An error analysis has been done by calculating the weighted average of the difference between numerical and experimental results. This analysis showed the particle lag model, when applied to CFD, produced an error of 0.02193 in streamwise direction compared to 0.02964 predicted by standard case. Even though the standard case itself predicted lower error compared to experimental uncertainty, the application of particle lag has outdone all the analyses that were done to date. On the other hand, the error in the transverse direction was calculated to be 0.009995, which for the first time was calculated to be almost equal to the experimental uncertainty (0.008947). In this case, the particle lag model has over-predicted the experimental result, but the overall error is still less than any other model. This shows the importance of particle lag when analyzing CFD results in contrast to PIV.

Appendices

Appendix A Particle size variation

In this section, the contours of different particle sizes specified by the manufacturer are presented. This helps in giving a perspective on the location of discontinuities and the error produced due to particle size variation in the PIV analysis.

In appendices, the acceleration due to drag contour is also presented alongside particle and fluid acceleration contours. The drag force is a direct result from the modified code and is not calculated separately. The drag contour is obtained from the drag force acting on the particle. It depends on the relative velocity of the tracer in the flow. The exact proportionality relation is provided in the Equation 49. The acceleration due to drag contours should be similar to the particle acceleration contours but should have deceleration regions instead of acceleration regions and vice-versa.

$$A_d \propto (\vec{v}_p - \vec{u}_f) \cdot (\vec{v}_p - \vec{u}_f) \quad (49)$$

A.1 Streamwise contours

A.1.1 Velocity

Figure 62: Particle diameter: 177nm

Figure 63: Particle diameter: 293nm

Figure 64: Particle diameter: 499nm

Figure 65: Particle diameter: 573nm

A.1.2 Velocity comparison

Figure 66: Particle diameter: 177nm

Figure 67: Particle diameter: 293nm

Figure 68: Particle diameter: 499nm

Figure 69: Particle diameter: 573nm

Figure 70: Particle diameter: 177nm

Figure 71: Particle diameter: 293nm

Figure 72: Particle diameter: 499nm

Figure 73: Particle diameter: 573nm

A.1.3 Acceleration due to drag

A.1.4 Particle acceleration

Figure 78: Particle diameter: 177nm

Figure 79: Particle diameter: 293nm

Figure 80: Particle diameter: 499nm

Figure 81: Particle diameter: 573nm

A.1.5 Fluid acceleration

Figure 82: Particle diameter: 177nm

Figure 83: Particle diameter: 293nm

Figure 84: Particle diameter: 499nm

Figure 85: Particle diameter: 573nm

The difference in fluid acceleration contours is due to the fact that these plots were obtained from a fluid packet associated with the particle. Hence the data, especially in the regions of high accelerations and decelerations is spread out.

A.2 Transverse contours

A.2.1 Velocity

Figure 86: Particle diameter: 177nm

Figure 87: Particle diameter: 293nm

Figure 88: Particle diameter: 499nm

Figure 89: Particle diameter: 573nm

A.2.2 Velocity comparison

Figure 90: Particle diameter: 177nm

Figure 91: Particle diameter: 293nm

Figure 92: Particle diameter: 499nm

Figure 93: Particle diameter: 573nm

Figure 94: Particle diameter: 177nm

Figure 95: Particle diameter: 293nm

Figure 96: Particle diameter: 499nm

Figure 97: Particle diameter: 573nm

A.2.3 Acceleration due to drag

Figure 98: Particle diameter: 177nm

Figure 99: Particle diameter: 293nm

Figure 100: Particle diameter: 499nm

Figure 101: Particle diameter: 573nm

A.2.4 Particle acceleration

Figure 102: Particle diameter: 177nm

Figure 103: Particle diameter: 293nm

Figure 104: Particle diameter: 499nm

Figure 105: Particle diameter: 573nm

A.2.5 Fluid acceleration

Figure 106: Particle diameter: 177nm

Figure 107: Particle diameter: 293nm

Figure 108: Particle diameter: 499nm

Figure 109: Particle diameter: 573nm

Appendix B Spanwise Velocity

In CFD due to the symmetry of the wind tunnel the spanwise velocity is calculated to be zero. However, this is not the case in PIV where almost a maximum of 6 m/s velocity can be observed. This deviation in spanwise direction is beyond the limits of the current study because it cannot be quantified in CFD. Spanwise velocity from CFD is shown in Fig. 110a and from PIV is shown in Fig. 110b.

(a) CFD

(b) PIV

Figure 110: Spawise velocity contours

Appendix C Range scaling for acceleration contours

Range scaling is an important factor in estimating the location of discontinuities in SBLI structure. In this section, different acceleration contours are presented to estimate the shock, compression and expansion waves location in SBLI structure. These contours were shown for 281nm particle.

C.1 Reference - Fluid acceleration

Fluid acceleration contour is used as reference and the other two are varied to match the range of the fluid acceleration.

(a) Drag acceleration

(b) Particle acceleration

(c) Fluid acceleration

Figure 111: Streamwise velocity contours with fluid acceleration as reference

(a) Drag acceleration

(b) Particle acceleration

(c) Fluid acceleration

Figure 112: Transverse velocity contours with fluid acceleration as reference

C.2 Reference - Drag acceleration

Drag acceleration contour is used as reference and the other two are varied to match the range of the drag acceleration.

(a) Drag acceleration

(b) Particle acceleration

(c) Fluid acceleration

Figure 113: Streamwise velocity contours with acceleration due to drag as reference

(a) Drag acceleration

(b) Particle acceleration

(c) Fluid acceleration

Figure 114: Transverse velocity contours with acceleration due to drag as reference

C.3 Reference - Particle acceleration

Particle acceleration contour is used as reference and the other two are varied to match the range of the particle acceleration.

(a) Drag acceleration

(b) Particle acceleration

(c) Fluid acceleration

Figure 115: Streamwise velocity contours with particle acceleration as reference

(a) Drag acceleration

(b) Particle acceleration

(c) Fluid acceleration

Figure 116: Transverse velocity contours with particle acceleration as reference

Appendix D Error metric - Continuation

The error metric for the remaining particle sizes is presented in this section. For the purpose of comparison, the standard case and the experiment error metrics are also presented.

U Error		V Error	
0.02193	MV3 - 281nm	0.008947	Experiment
0.02240	MV3 - 263nm	0.00944	MV3 - 254nm
0.02263	MV3 - 254nm	0.00957	MV3 - 263nm
0.02325	MV3 - 499nm	0.009995	MV3 - 281nm
0.02515	MV3 - 177nm	0.01016	MV3 - 177nm
0.02628	MV3 - 573nm	0.01377	Standard
0.02964	Standard	0.02068	MV3 - 499nm
0.03473	Experiment	0.02344	MV3 - 573nm

Table 14: Error metric comparisons for particles of different sizes, presented as “MV3 - *diameter of particle*”

A closer look at the error metric Table 14 shows that the MV3 code has been underpredicting streamwise velocity between 177-281nm whereas particles with diameter 499nm and 573nm are overpredicting the flow features. This can be observed in the velocity comparison contours presented in the Appendix A.1.2. This implies that the optimal seed to predict correct flow features is present somewhere between 281nm and 499nm. However, the optimal diameter has not been calculated in this study.

Similarly, in the transverse direction the MV3 code underpredicted for 177nm, 254nm and overpredicted for the diameters in range 263nm to 573nm. Refer to Appendix A.2.2 for the comparison contours. So, the optimal diameter for predicting the flow features should be between 254nm and 263nm. This shows that a compromise has to be made in predicting flow features between the streamwise and transverse directions to choose the optimal particle for PIV analysis.

U-error and V-error are pictorially represented in Fig. 117a and Fig. 117b respectively. The optimal particle diameter size can be estimated by finding the minima of those curves. The findings are in accordance with the crude particle estimations of Friedlander [37] in which, the author estimated “Long lag” to perform better in streamwise direction and “Medium lag” to perform better in transverse direction.

(a) Streamwise velocity

(b) Transverse velocity

Figure 117: Particle diameter vs. Uncertainty

Appendix E User reference

To work with Modified-Visual3 code, the user should have an understanding of Visual3. To start with Visual3 refer to [48] and [49]. In this section, brief notes are presented on how to use MV3 code to obtain required data and directions are provided to analyze it.

Figure 118 shows the working process with MV3 code. It is divided into two sub-processes, the first sub-process plots single particle plots and the second sub-script reduces the large data and plots contours on the experimental plane.

In the current version of MV3, most of the processes are manual. This helps in understanding how the data is being handled. First, the Plot3D format of CFD data needs to be imported into MV3 code. MV3 code reads these in using a Fortran script (Main Program) similar to Visual3. The main program contains the data related to the grid, flow variables, and user-defined functions. Later, a modified form of internal subroutine - *Streamlines.f* that accommodate particles along with streamlines is converted into a static library (*libVisual3.a*) that will be read by Visual3. MV3 is the Visual3 running on this modified library. The internal subroutine can be modified by the user to change particle specifications and to input the spawn location of particle/s. Once the particles are spawned in the flow, MV3 outputs the particle data in *Rich Text Format (rtf)*. This is the data that will be used for further post-processing to obtain desired results.

The obtained particle data contains variables such as “Particle position, particle velocity, particle acceleration, fluid velocity, fluid acceleration, time step, cell number” at every time step that can be used by the user in post-processing. If required gradient-data can also be obtained. This data can be written in formatted or unformatted file based on the post-processing script. For the ease of use between Fortran and Python, current data is written into a “.rtf” file.

If the data is obtained for n-particles, there will be n-files available for post-processing. For the purpose of this material, two different post-processing methods were employed. One for single particle - In this approach, the data from each file is used separately to analyze each particle separately. For the current analysis, Matplotlib library from python was used to obtain all of the single particle plots mentioned in the main work.

The second analysis consists of dealing with a large data when all the files are merged together to form a “.txt” file. The data from this file can be used to obtain scatter plots presented in the main work. This

Figure 118: User reference chart to work with MV3 code; Red: Required input, Blue: Output, Green: Saved data, Oval: Operations

merged data is then used to separate particle data on to experimental grid to be able to compare with PIV or CFD data. Scipy library from Python is used to interpolate grids. The current analysis used linear interpolation, however different techniques such as near or cubic interpolations can be used to separate and interpolate data onto the experimental plane. The interpolated data is saved in Plot3D format. This data can then be used to plot contours using Tecplot or can be used to calculate error metric.

As of this writing, the code has not been made available to the public. Contact the author for requests.

References

- [1] Ronald J. Adrian *Particle-imaging techniques for experimental fluid mechanics*. Annu. Rev. Fluid Mech. 1991.23: 261-304.
- [2] Adrian R.J. (2005). *Twenty years of particle image velocimetry*. Exp. Fluids, 39, pp. 159–169.
- [3] Jerry Westerweel, Gerrit E. Elsinga, and Ronald J. Adrian. *Particle Image Velocimetry for Complex and Turbulent Flows*. Annu. Rev. Fluid Mech. 2013. 45:409–36.
- [4] Melling A., *Tracer particles and seeding for particle image velocimetry*. Meas. Sci. Technol., 1997.
- [5] Lang N., *Investigation of the flow tracking capabilities of tracer particles for the application of PIV to supersonic flow fields*. Proceedings of the 10th international symposium on applications of laser techniques to fluid mechanics, Lisbon, PT, 2000.
- [6] Koike S, Hidemi T, Koichi T, Mitsutomo H, Kenichi T, Goro M (2007), *Correction method for particle velocimetry data based on the Stokes Drag Law*. AIAA J 45:11.
- [7] D. Ragni, F. F. J. Schrijer, B.W. van Oudheusden, and F. Scarano., *Particle tracer response across shocks measured by PIV*. Experiments in Fluids, 50(1):53–64, May 2010.
- [8] Dolling, D., 2001. *Fifty years of shock-wave/boundary-layer interaction research: what’s next?* AIAA Journal 39 (8), 1517–1531.
- [9] Andrew P. Lapsa, 2009, *Experimental Study of Passive Ramps for Control of Shock – Boundary Layer Interactions*. Ph.D. Dissertation, University of Michigan, Ann Arbor, MI.
- [10] Andrew P. Lapsa, Werner J. A. Dahm. *Stereo particle image velocimetry of nonequilibrium turbulence relaxation in a supersonic boundary layer*. Exp Fluids (2011) 50:89–108.
- [11] DeBonis, J. R., Oberkampf, W. L., Wolf, R. T., Orkwis, P. D., Turner, M. G., Babinsky, H., and Benek, J. A., *Assessment of CFD Models for Shock Boundary-Layer Interaction*, Applied Aerodynamics Conference, AIAA Paper 2010-4823, 2010.
- [12] DeBonis, J. R., Oberkampf, W. L., Wolf, R.T., Orkwis, P. D., Turner, M. G., Babinsky, H., and Benek, J. A., *Assessment of Computational Fluid Dynamics and Experimental Data for Shock Boundary-Layer Interactions*. AIAA Journal, Vol. 50, No. 4, 2012, pp. 891–903. doi:10.2514/1.J051341
- [13] Ascher, H., Shapiro., *The Dynamics and Thermodynamics of Compressible Fluid Flow*, Vol. 1, 1954.

- [14] Holger, Babinsky, John, K. Harvey, *Shock Wave-Boundary-Layer Interactions*, Cambridge University Press, 2011, Hardback (ISBN-13: 9780521848527)
- [15] Jean, M. Delery, *Robert Legendre and Henri Werle: Toward the Elucidation of Three-Dimensional Separation*, Annu. Rev. Fluid Mech. 2001. 33:129–54
- [16] Délery Jean, Dussauge Jean-Paul, *Some physical aspects of shock wave/boundary layer interactions*, ShockWaves (2009) 19:453–468
- [17] NASA Langley Research Centre, *OVERFLOW Flow Solver, Version 2.2e*, 2012, Hampton, VA.
- [18] Nichols, R. H., Buning, P. G., *Users manual for OVERFLOW 2.1, Version 2.1t*, NASA Langley Research Center, Hampton, VA, 2008.
- [19] Henderson. L. F., *The reflexion of a shock wave at a rigid wall in the presence of a boundary layer*, J. Fluid Mech. (1967), vol. 30, part 4, pp. 699–722
- [20] Beresh S. J., 1999, *The Effect of Incoming Boundary Layer on a Shock-Induced Separated Flow Using Particle Image Velocimetry*. Ph.D. Dissertation, University of Texas, Austin, TX.
- [21] Hou Y., 2003, *Particle Image Velocimetry Study of Shock-Induced Turbulent Boundary Layer Separation*. Ph.D. Dissertation, University of Texas, Austin, Tx.
- [22] Humble, R. A., Scarano, F., Van Oudheusden, B. W., *Particle image velocimetry measurements of a shock wave/turbulent boundary layer interaction*. Exp. Fluids 43 (2–3), 2007, 173–183.
- [23] Humble R. A., Elsinga G. E., Scarano F., Van Oudhudsden B. W., *Three-dimensional instantaneous structure of a shock wave/turbulent boundary layer interaction*. J. Fluid Mech. (2009), vol. 622, pp. 33–62.
- [24] Helmer D. B., 2011, *Measurements of a three-dimensional shock-boundary layer interaction*, Ph. D. Dissertation, Stanford University, CA.
- [25] Eagle E., 2012, *An Experimental Study of Three-Dimensional Inlet Shock-Boundary Layer Interactions*. Ph.D. Dissertation, University of Michigan, Ann Arbor, MI.
- [26] Helmer, D. B., Campo, L. M., Eaton, J. K., *Three-dimensional features of a Mach 2.1 shock/boundary layer interaction*. Exp. Fluids 53 (5), 2012, 1347–1368.
- [27] Eagle, E., W., Driscoll J., F., *Shock wave–boundary layer interactions in rectangular inlets: three-dimensional separation topology and critical points*. J. Fluid Mech. (2014), vol. 756, pp. 328–353.

- [28] Haertig J., Havermann M., Rey C., George F., *PIV Measurements in Mach 3.5 and 4.5 Shock Tunnel Flow*, AIAA-2001-0699, 8-11 January 2001, Reno, Nevada, 39th Aerospace Sciences Meeting & Exhibit.
- [29] Giepmans R.H.M., Schrijer F.F.J., van Oudheusden B. W., *High-resolution PIV measurements of a transitional shock wave-boundary layer interaction*, AIAA AVIATION Forum, 16-20 June 2014, Atlanta, GA, 44th AIAA Fluid Dynamics Conference.
- [30] Frohlich K., Schneiders L., Meinke M., Schröder W., *Assessment of Non-Spherical Point-Particle Models in LES using Direct Particle-Fluid Simulations*, Institute of Aerodynamics, RWTH Aachen University, Willnerstr. 5a, 52062, Aachen, Germany. “Unpublished work”.
- [31] Clemens N. T., Mungal M. G., *A planar Mie scattering technique for visualizing supersonic mixing flows*, Experiments in Fluids 17, 175-185 (1991).
- [32] Urban W. D., Mungal M. G., *Planar velocity measurements in compressible mixing layers*, J Fluid Mech, 431:189-222.
- [33] *Data digitization*, available at <https://github.com/ankitrohatgi/WebPlotDigitizer>
- [34] *Microsoft Excel*, 2017, Microsoft Corporation, Redmond, WA.
- [35] *Python programming language*, Python software foundation, version 2.x and 3.x, available at <http://www.python.org>
- [36] Galbraith, D. S., 2011, *Computational fluid dynamics investigation into shock boundary layer interactions in the glass inlet wind tunnel*. Master’s thesis, University of Cincinnati, Cincinnati, OH.
- [37] Friedlander D. J., 2013, *Understanding the Flow Physics of Shock Boundary-Layer Interactions Using CFD and Numerical Analyses*. Master’s thesis, University of Cincinnati, Cincinnati, OH.
- [38] Friedlander D. J., Georgiadis N. J., Turner M. G., Orkwis P. D., *Numerical Simulations of the University of Michigan Shock Boundary-Layer Interaction Experiments*. AIAA Journal, Vol. 53, No. 5, May 2015, pp. 1134-1145. DOI: 10.2514/1.J053040
- [39] Prashant Khare, Shanwu Wang, Vigor Yang. *Modeling of finite-size droplets and particles in multiphase flow*. Chinese Journal of Aeronautics, (2015), 28(4): 974–982.
- [40] Crowe CT. *Multiphase flow handbook*. Boca Raton, FL: Taylor and Francis; 2005. p. 13–36.
- [41] Mei R, 1996. *Velocity fidelity of flow tracer particles*. Exp Fluids 22:1–13.

- [42] Tedeschi G, Gouin H, Elena M (1999). *Motion of tracer particles in supersonic flows*. Exp Fluids 26:288–296
- [43] Subramaniam S. *Lagrangian-Eulerian methods for multiphase flows*. Prog Energy Combust Sci 2013;39(2–3):215–45.
- [44] John D. Anderson, Jr. *Computational Fluid Dynamics - The Basics with Applications*. McGraw-Hill series in mechanical engineering-McGraw-Hill series in aeronautical and aerospace engineering; p. 49-78. ISBN 0-07-001685-2.
- [45] Barry R. Maxwell and Richard G. Seasholtz. *Velocity lag of solid particles in oscillating gases and in gases passing through normal shock waves*. National Aeronautics and Space Administration, (1974), Report No. NASA TN D-7490.
- [46] Maxey M, Patel B. *Localized force representations for particles sedimenting in stokes flow*. Int J Multiphase Flow 2001;27(9): 1603–26.
- [47] Haimes R., Giles M., Darmofal. D. *Visual3 - A Software Environment for Flow Visualization*. Computer Graphics and Flow Visualization in Computational Fluid Dynamics VKI Lecture Series 10, Brussels, 16-20 September 1991.
- [48] Bob Haimes. *VISUAL3 User's & Programmer's Manual*. Massachusetts Institute of Technology, 2006.
- [49] Haimes, R. *Advanced Programmer's Guide*. Massachusetts Institute of Technology, 2006.
- [50] Haimes R., Darmofal, D. *Visualization in Computational Fluid Dynamics: A Case Study*. Computational Fluid Dynamics Laboratory, Dep. of Aeronautics and Astronautics, Massachusetts Institute of Technology.
- [51] A. B. Medvedev. *Shock-Wave Front Thickness in a Liquid Estimated on the Basis of the Navier–Stokes Equations Using a Modified Van der Waals Model*. Combustion, Explosion, and Shock Waves, Vol. 48, No. 4, pp. 475–482, 2012.
- [52] Granger, R. A. *Fluid Mechanics*. New York: Courier Dover Publications, p. 845-846, 1995.
- [53] Ossen, C. W., 1910. Ark.f. Mat. Astr. og Fys. 6, no. 29.
- [54] Scarano, F., 2008. *Particle Image Velocimetry: New Developments and Recent Applications*. Springer-Verlag.
- [55] White, F. M., *Fluid Mechanics*, 5th ed. Boston, Mass: WCB/McGraw-Hill.

- [56] Samimy, M., Lele, S., 1991. *Motion of particles with inertial in a compressible free shear layer*. Physics of Fluids 3, 1915-1923.
- [57] Tecplot, Inc., *Tecplot 360*, 2016, Bellevue, WA.
- [58] Garmann, D. J., Visbal, M. R., and Orkwis, P.D., *Three-Dimensional Flow structure and Aerodynamic Loading on a Low Aspect Ratio, Revolving Wing* Tech. Rep. AIAA 2012-3277, Air Force Research Laboratory, June 2012.
- [59] Abu-Ghannam, B. J., and Shaw, R., *Natural Transition of Boundary Layers - The Effects of Turbulence, Pressure Gradient, and Flow History*, Journal of Mechanical Engineering Science, Vol. 22, No. 5, 1980, pp.213-228.
- [60] Youhei Shinohara, Kazuyuki Toda, and Makoto Yamamoto. *Numerical Error Estimation in Particle Tracking Measurement behind a Shock Wave*. Dept. of Mech. Eng., Tokyo University of Science.
- [61] *Particle data provider*, ATI Techniques, 11403 Cronridge Drive, Owings Mills, Maryland USA 21117-2247.