Modeling of airflow and particle trajectories in the vicinity of the narrow head-disk interface gap

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**MODELING OF AIRFLOW AND PARTICLE
TRAJECTORIES IN THE VICINITY OF THE NARROW
HEAD-DISK INTERFACE GAP**

**BENZI JOHN
SCHOOL OF MECHANICAL & AEROSPACE ENGINEERING
2009**

**MODELING OF AIRFLOW AND PARTICLE
TRAJECTORIES IN THE VICINITY OF THE NARROW
HEAD-DISK INTERFACE GAP**

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ABSTRACT

Rarefied gas flow situations are encountered in a wide range of applications that range from hypersonic flow applications in the upper atmosphere to simulation of low speed gas flows in MEMS devices. With the advent of miniaturization, flow in MEMS devices has received considerable attention recently. In a modern hard disk drive (HDD), the head-disk interface (HDI) gap size is of the order of nanometers. Flow at micro- and nano- scales have been found to deviate from the continuum regime and hence the flow in HDI region needs to be modeled by appropriate computational models. Thus the main aim of the work in this thesis has been directed towards the development of appropriate computational models which can predict rarefied and non-equilibrium flow accurately in micro flow applications such as that in the HDI gap.

This work focuses on the modeling of air flow characteristics in the vicinity of the HDI gap. Direct Simulation Monte Carlo (DSMC) method has been chosen as the computational model for predicting flow characteristics in the HDI gap in this work. The flow outside the slider falls in the continuum regime and hence demands the use of a hybrid continuum-atomistic method to couple the DSMC model in the HDI region to the Navier-Stokes equations model in regions outside the slider. In this work various flow modeling aspects for micro flow simulations in the HDI gap have been discussed in detail both for a stand-alone DSMC computation and for the case of a hybrid continuum-atomistic simulation when Navier-Stokes equation needs to be coupled to a DSMC solver.

The DSMC method has been initially applied to micro flows such as Couette and Poiseuille flows to validate the prediction of various flow features associated with flows at a micro- and nano- scale. As DSMC is a computationally intensive method parallel DSMC codes using Message Passing Interface (MPI) have been developed to compute the flow in the HDI region. Parallel performance metrics and load balancing issues of the parallel DSMC method on various computing platforms illustrating the portability and scalability of the method have been addressed in this work. An appropriate implicit boundary treatment method has been used for implementing the pressure boundary

conditions at the inflow and outflow boundaries and has been extended for the case of a three-dimensional DSMC micro flow simulation. Various Reynolds equation gas lubrication models have also been formulated and solved using the finite difference method to compute the pressure distribution in the slider bearing region. A coupled Reynolds-DSMC model has also been proposed for coupling the Reynolds equation model solutions to the DSMC model for situations in which a detailed atomistic simulation is required in any localized region in the vicinity of the HDI gap.

A hybrid continuum-atomistic framework based on the Schwarz Alternating method has been developed for coupling the Navier-Stokes solution to the DSMC model. The Schwarz coupling has been implemented by the iterative exchange of Dirichlet boundary conditions across overlap regions which are considered in two dimensions. The Chapman-Enskog molecular velocity distribution is employed for boundary condition imposition from the continuum region to the DSMC region. The hybrid solutions have been compared with the exact solution in the entire region and the influence of the size of the overlap region on the convergence behavior of the Schwarz method has also been investigated in this work. It has been found that a finite overlap region is required for the convergence of the Schwarz method as the hybrid solutions diverge with a zero overlap.

Particle contamination in the HDI region may lead to performance degradation of the hard disk drives. In this work an attempt has also been made to compute particle trajectories in the HDI gap by incorporating a two-phase DSMC method. The two-phase model is based on a one-way coupled method, by computing the forces on a particle assuming locally free molecular flow conditions. The two-phase method has been incorporated in the parallel DSMC method and representative particle trajectories in the HDI gap have been computed for nanometer size particles of various densities that may enter the slider region both for the two-dimensional and three-dimensional cases.

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CHAPTER 1

INTRODUCTION

1.1 Background

Rarefied gas flow situations are encountered in a wide range of applications that range from hypersonic flow applications in the upper atmosphere such as reentry vehicles and orbital vehicles to simulation of low speed gas flows in MEMS devices. The Knudsen number is typically used to find the degree of rarefaction involved, based on which different flow regimes could be identified. Flow regimes can be classified depending on whether the continuity hypothesis holds or breaks down on the basis of the Knudsen number. The Knudsen number, Kn is defined as $Kn = \lambda/L$, where λ is the mean free path defined as the average distance traveled by a molecule before it collides with another molecule and L is the characteristic length involved. Accordingly flow regimes can be classified into continuum, slip, transition and free-molecular regions as described in Karniadakis and Beskok [1]. Excellent descriptions and reviews of rarefied gas flow physics and the limit of continuum theory can also be found in Shen [2] and Gad-el-hak [3]. Continuum models such as the Navier-Stokes equation model can be employed if $Kn < 0.01$ and with proper slip boundary conditions it can be extended to model the flow in the slip regime when $0.01 < Kn < 0.1$. In MEMS devices the continuum assumption breaks down and the flow falls in the transition regime if $0.1 < Kn < 10$ and when $Kn > 10$ the free molecular regime is encountered where molecular collisions are not dominant. In the case of upper atmosphere applications rarefied gas flow conditions are caused by low density conditions. Under low density conditions the mean free path is in the order of meters resulting in a high Knudsen number. MEMS applications have emerged more recently and they typically operate under standard atmospheric temperature and pressure (STP) conditions. The mean free path of air at STP is in the order of nanometers and rarefied flow conditions in such applications are caused by the

extremely small characteristic dimensions involved which are often at micro- and nano-scales. Rarefied gas flow applications could also involve regions of both continuum and rarefaction simultaneously occurring demanding the use of multi-scale methods.

A classic example for a rarefied flow at a nano-scale is in the case of the head-disk interface (HDI) gap in a modern hard disk drive (HDD). The demand for high recording density in today's HDD industry calls for a HDI gap as small as possible. In recent hard drives the HDI gap is just a few nanometers in width which is less than the mean free path of air at standard temperature (273 K) and 1 atm pressure (STP), resulting in high Knudsen number flow conditions. The HDI gap distance is expected to decrease further for the next generation drives, since smaller the flying height, the greater the recording capacity. An HDD model showing its various components and the slider-head region is shown in Fig 1.1. A very good understanding of airflow characteristics in the HDD enclosure and in the HDI region is required for accurate head positioning and to predict the particle trajectories. For instance, particle contamination may lead to performance degradation of the HDD due to processes such as erosion or scratch.

The Knudsen number demarcation in different regions in the vicinity of the HDI gap, based on the approximate interface distances as the characteristic length scale is schematically shown in Fig 1.2. The Knudsen number within the HDI region is such that it falls in the transition regime, i.e. $0.1 < Kn < 10$. In the Navier-Stokes equation model, the shear stress and the heat flux are expressed in terms of lower order macroscopic magnitudes such as velocity and temperature, such as the linear relation between stress and rate of strain, and the linear relation between heat flux and temperature gradient. This is only valid when the flow is near thermodynamic equilibrium. However under high Knudsen number flow conditions as in the HDI gap, the flow variable gradient length scales are so small that it is comparable to the molecular mean free path and the gas is no longer in thermodynamic equilibrium. Therefore the Navier-Stokes equation cannot predict the flow accurately in the HDI region. Hence there is a need to apply appropriate flow models for predicting the flow characteristics and particle trajectories within the HDI region. The flow outside the HDI region however falls in the continuum regime as

$Kn < 0.01$ and can be accurately modeled by the Navier-Stokes equation. This demands the use of an appropriate multi-scale method to couple the rarefied flow region within the HDI region to the flow outside the slider modeled by Navier-Stokes equation. The slider is attached to the suspension arm at a point about which it can move up and down and also rotate in the pitch, skew and roll directions. During the read/write operation in a HDD, the slider to which the read/write head is attached glides back and forth along the radius of the disk as shown in Fig 1.3. Depending on the orientation of the slider at a particular point in time, the flow that enters the HDI region could be either in a tangential direction or at a certain angle.

The numerical prediction of global airflow characteristics outside the HDI gap, particle trajectories and the effect of geometrical structures on airflow patterns in HDD enclosures using continuum flow models based on the Navier-Stokes equations have been reported in literature by various researchers such as Shimizu et al. [4], Kubotera et al. [5], Song et al. [6] and Ali et al. [7-9]. The global flow field inside the HDD can be typically solved using the incompressible Navier-Stokes equations which can be represented as:

$$\nabla \cdot \vec{U} = 0 \quad (1.1a)$$

$$\frac{\partial \vec{U}}{\partial t} + \vec{U} \cdot \nabla \vec{U} = -\frac{1}{\rho} \nabla P + \nu \nabla^2 \vec{U} \quad (1.1b)$$

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\vec{U}(\rho E + p)) = \nabla \cdot (K \nabla T) + \phi \quad (1.1c)$$

where $\vec{U}$ is the velocity vector, ν is the kinematic viscosity, K is the thermal conductivity and ϕ is the dissipation function which describes the effects due to viscous stresses.

The global flow field in a modern small form factor HDD enclosure computed using the Navier-Stokes equations solved in the commercial flow solver *Fluent* [10] is shown in Fig 1.4. Trajectories followed by particles released from various points near the slider computed by the discrete phase model (DPM) in *Fluent* are shown in Fig 1.5.

Figure 1.1: HDD enclosure showing the major components with the zoomed section of the slider region

Figure 1.2: Schematic showing Knudsen Number demarcation in regions in the vicinity of the HDI gap

Figure 1.3: Schematic showing slider orientation with respect to the rotating disk in a HDD enclosure

(a)

(b)

Figure 1.4: Computed flow fields of a) pressure and b) velocity vectors at a plane between slider and top disk surface. Adapted from [11]

Figure 1.5: Particle trajectories in the vicinity of the HDI. Adapted from [11]

Preliminary computations done to check if compressibility effects are significant by studying the nature of the global pressure and velocity fields in the HDD enclosure reveal that the flow field is essentially incompressible. The study has been undertaken on a HDD in which the disk spins at 5400 rpm. Compressible flow modeling is done by solving for the continuity, momentum and energy equations, along with the thermodynamic relation (ideal gas law) to close the model in *Fluent*. Figure 1.6 shows the visualization planes in the HDD enclosure used for the visualization of computed flow patterns and contours of computed flow variables. The computed density and pressure contours from the compressible flow model on visualization plane 1 are shown in Fig 1.7. The density and pressure values above the disk surface in the HDD enclosure are uniform, with no significant variations observed. This can be attributed due to the fact that in a HDD the flow is driven by the rotating disk, and hence the flow conditions can be considered as similar to that for a Couette flow. Significant variations are observed only for the velocity, while the pressure and density remains about a constant value, which implies that the compressibility effects in a HDD enclosure outside the HDI gap can be considered as negligible. A detailed comparison of the computed velocity and gauge pressure based on the compressible and incompressible flow models on visualization plane 2 is shown in Fig 1.8. A comparison of the computed particle trajectories in the HDD enclosure between the two flow models is made in Fig 1.9. The computation of particle trajectories is enabled by the discrete phase model (DPM) in *Fluent*. No significant differences could be observed between the results of the two models which prove that the global flow field can be assumed to be incompressible.

The present study focuses on the modeling and development of computational models, which can accurately predict the air flow characteristics and particle trajectories in the vicinity of the HDI gap. Flow modeling in the HDI gap is particularly challenging due to the multi-scale nature of the flow in this region. Various computational models and multi-scale methods have been surveyed with a view to select appropriate models for flow simulation in the HDI gap. The literature review on the various flow simulation models considered, scope and significance of the present study carried out in this thesis are described in the subsequent sections.

(a) Plane 1- an x - y plane 0.5 mm below the rotating disk of the HDD enclosure

(b) Plane 2 – an x - z plane across the disk of the HDD enclosure

Figure 1.6: Visualization planes used for showing comparison of various plots.

(a)

(b)

Figure 1.7: Computed (a) gauge pressure and (b) density contours on the visualization plane 1 shown in Fig 1.6(a).

(a) Velocity plot for compressible model

(b) Velocity plot for incompressible model

(c) Gauge pressure - compressible model

(d) Gauge pressure - incompressible model

Figure 1.8: Comparison of computed airflow characteristics between compressible and incompressible flow models on plane 2 shown in Fig 1.6(b).

(a) Compressible model

(b) Incompressible model

Figure 1.9: Comparison of computed particle trajectory of $0.1 \mu m$ titanium particles between (a) Compressible and (b) Incompressible flow models in the HDD enclosure.

1.2 Appropriate Flow Simulation Models in the HDI region

The flow in the HDI region falls primarily in the transition and slip regime and hence needs to be modeled by an appropriate simulation model which is valid for a wide range of Knudsen numbers. The mathematical model at a molecular level for dilute gases such as air is the Boltzmann Equation, which describes the fluid in terms of its distribution function $f(r, c, t)$ a function of its position $r(x, y, z)$, molecular velocity $c(u, v, w)$ and time t . The distribution function represents the number of particles in a six-dimensional phase space $drdc$ at time t . The Boltzmann equation is given by

$$\frac{\partial}{\partial t}(f) + c \cdot \frac{\partial}{\partial r}(f) + F \cdot \frac{\partial}{\partial c}(f) = \iiint_c \int_0^{4\pi} (f^* f_1^* - ff_1) g \sigma_1 de^* dc \quad (1.2)$$

where c is the particle velocity vector, r is the particle position vector, g is the relative velocity, σ is the differential collision cross section, de^* is the scattering angle, F is the external force field and f^* is the distribution function before collision and f_1^* is the distribution function after collision.

The first term on the left hand side of equation (1.2) represents the time variation of the distribution function of the particles while the second term gives the spatial variation of the distribution function and the third term describes the effect of a force on the particles. The contributions of these three terms are then related to the effect of collisions between the particles taken into account by the right hand side of the equation which represents the collision integral term. However the complexity of the Boltzmann equation in terms of the number of dimensions involved and the nature of the collision integral term (a non-linear integro-differential equation) makes it computationally prohibitive to solve for any practical purpose. Therefore discrete models are often used which uses either simplified forms of the Boltzmann equation or physically based simulation methods are used rather than direct numerical simulation of a complex mathematical model such as the Boltzmann equation.

Various discrete particle methods employed for flow simulations such as Molecular Dynamics (MD), Lattice Boltzmann method (LBM), Smooth Particle hydrodynamics (SPH), Dissipative Particle dynamics (DPD), Direct Simulation Monte Carlo (DSMC) method and the Reynolds equation gas lubrication methods have been surveyed to check their suitability for flow modeling in the vicinity of the HDI. A brief description on the various methods and its suitability in the HDI region is discussed. The Lattice Boltzmann method is a mesoscopic fluid model that fits between the microscopic molecular dynamics and macroscopic continuum approaches by solving a simplified Boltzmann equation on a discrete lattice. This approach initially introduced by McNamara and Zanetti [12] is based on the assumption that the macroscopic behaviour of a fluid does not depend directly on its detailed microscopic behaviour. The assumptions that go into this method make it a very computationally efficient method for handling complex geometries for continuum flows near the incompressible limit. However LBM is not a suitable model to simulate flow in the transition and free molecular regimes where in the high Knudsen number leads to large rarefaction and compressibility. SPH and DPD methods are particle based mesoscale simulation techniques. Smooth Particle hydrodynamics (SPH) is a Lagrangian, particle method introduced by Lucy and Monaghan [13] as a meshless simulation method. SPH has been an effective computational method for astrophysical fluid dynamics problems, it being grid free and being able to capture the interaction between the particles efficiently. Dissipative Particle Dynamics (DPD) introduced by Hoogerbrugge and Koelman [14] has been widely used for the simulation of complex fluids such as colloidal suspensions, emulsions, polymers, and multiphase flows. The method has been extended to various applications of continuum flow, but not a suitable model for simulation of a dilute gas at a molecular level.

Molecular dynamics (MD) is the most basic particle method wherein the trajectory of each and every molecule is calculated from Newton's equations given an empirically determined inter-particle potential as described by Allen and Tildesley [15]. A potential energy function such as the Lennard-Jones Potential for a simple fluid needs to be specified in order to describe the interaction between atoms or molecules. The force

on a molecule can be calculated as the derivative of the energy function with respect to the change in the atom's position. Newton's equations of motion are then integrated to advance the molecular positions and velocities. This method is a deterministic method where in the exact time evolution of the molecular system is modeled. However to simulate even one cubic micron of air at STP would require approximately twenty seven million molecules and evolution of the molecular system is extremely time consuming. Therefore this method is not a computationally efficient model especially for simulating a dilute gas such as air where the interaction forces between the molecules is very small and can be neglected. Molecular Dynamics is widely used for liquid flows for which the interaction forces between molecules are significant.

Direct Simulation Monte Carlo (DSMC) is an efficient method introduced by Bird [16] for simulating the flow of a dilute gas such as air. DSMC method has been traditionally used for the simulation of rarefied and non-equilibrium flows in hypersonic reentry flows and for analyzing detailed shock structure as in Bird [17] and Moss and Bird [18]. Application of the DSMC method to low speed gaseous flow application in MEMS devices has been recently outlined in Oran et al. [19] and Piekos and Breuer [20]. The DSMC method is a physical model based on which the discrete molecular nature of the system is modeled, such that it essentially captures the physics of a dilute gas governed by the Boltzmann equation. This method models the macroscopic behavior of a fluid based on the discrete molecular character of gases by simulating the motion, interaction and collision of representative particles with in an array of computational cells. The evolution of molecules is determined by tracking their positions and velocities. Starting from a set of initial conditions, the flow is developed in a physically realistic manner by evaluating the collisions between the particles, boundary interactions of the particles at the wall and at inflow/outflow boundary. In contrast to the molecular dynamics method the exact trajectory of each particle is not calculated in DSMC, but a stochastic algorithm is used to evaluate collision probabilities and scattering distributions in accordance with the kinetic theory. This is valid for a dilute gas such as air since the interaction force between the molecules is very small and the energy possessed by the molecules can be assumed to be purely kinetic energy. Each particle used by DSMC

represents a large number of real gas molecules that are roughly at the same position with roughly the same velocity. As DSMC is a stochastic method it involves the generation of random numbers and flow variables such as pressure, density and temperature are computed as averages by sampling after the flow reaches a steady state. DSMC is the best particle method for the simulation of gas flows as it is valid for all flow regimes and is several orders of magnitude more computationally efficient than Molecular Dynamics. In this work DSMC has been chosen as the particle method for computing the flow characteristics in the HDI gap and also as the atomistic method for the case of the hybrid continuum-atomistic simulation and further details of this method are explained in Chapter 2.

The Reynolds gas lubrication equations have been traditionally used for modeling slider air bearing flows and this model has also been investigated in this thesis for solving the pressure distribution in the HDI gap. Reynolds equation is originally derived for continuum flows from Navier-Stokes equation. It determines the relation between the film thickness and the pressure profile between two non parallel plates which are set in a constant relative motion to each other. Different slip correction models have been introduced into the Reynolds equation when the flow deviates from the continuum regime by various researchers. A more sophisticated model for the Reynolds equation, based on a linearized Boltzmann equation has been developed by Fukui and Kaneko [21]. The Reynolds equation model has been typically used in the design of slider air bearings for HDD's. The steady state and dynamic flying attitudes for the slider air bearing are determined in such simulations by solving the lubrication equations together with the equations of motion of the slider. The CML software developed by Computer Mechanics Laboratory at University of California Berkeley [22] has been widely used in the HDD industry today for the dynamic simulation of air bearings. The details of the modified Reynolds equation with various slip correction models and the Fukui-Kaneko model are further explained in detail in Chapter 5.

Particle contamination in the vicinity of the HDI gap is a major cause of performance degradation of a HDD. In modern designs of HDD, the HDI gap distance

has been decreasing to meet the demand for high recording intensity and this extreme proximity between the slider and the disk increases the likelihood of slider-disk interactions which could result in particle generation and result in contamination particles in the HDD enclosure which can result in serious problems such as slider crash and thermal asperities. Multiphase models are required for the modeling of particle-laden flow and computation of particle trajectories that may enter the HDI region. Particle contamination studies in the HDI region have been previously conducted by Zhang and Bogy [23] by considering various forces such as drag, lift and gravity forces. For such computations they have employed the first order slip corrected Reynolds gas lubrication model to compute the air flow velocities in the HDI gap. In this work a two-phase DSMC model is employed to model particle-laden flow in the HDI gap that falls in the transition regime both for the two-dimensional and three-dimensional cases. The two-phase model is based on the one-way coupled model by Gallis et al. [24]. The particle concentration is dilute and the gas flow surrounding the particle is assumed to be locally free molecular. Under such conditions the forces on a particle from the rarefied gas flow surrounding it can be calculated by summing the contributions from all computational molecules with in the DSMC cell. The particle sizes used in this work are taken such that they are smaller than the mean free path of the gas, to satisfy the locally free molecular flow assumption. Representative particle trajectories have been computed for particles of a few nanometers size and various densities.

1.3 Hybrid Continuum-Atomistic Modeling

The flow field in the vicinity of the HDI gap spans a wide range of Knudsen numbers as shown in Fig 1.2. Although the DSMC method can be used to model the entire Knudsen number regime accurately, it is computationally prohibitive when compared to the use of continuum models to model the entire domain. The flow outside the slider falls in the continuum regime which can be modeled accurately by the incompressible Navier-Stokes equations. This demands the use of an appropriate multi-scale method to couple the rarefied flow region within the HDI region to the continuum

flow outside the slider. The majority of the multi-scale methods previously applied for gaseous flow problems have been that for hypersonic compressible flow problems as in Garcia et al. [25], Hash and Hassan [26] and Wadsworth and Erwin [27]. Hybrid formulations applicable for incompressible flow problems in MEMS devices have received attention only very recently. In high speed compressible flow applications, the characteristic time scale is comparable to the DSMC time step as a result of which the hybrid coupling can be attained explicit in time. In comparison, incompressible flows have a characteristic time scale which is much longer than the DSMC time step, which makes a hybrid coupling scheme based on explicit integration in time computationally infeasible as outlined by Wijesinghe and Hadjiconstantinou [28]. Therefore, an implicit method is needed to provide a framework for attaining hybrid coupled solutions in applications where low speed incompressible flow is encountered. The Schwarz alternating method provides an implicit framework for obtaining coupled solutions in such instances. By using the Schwarz method the coupling between the continuum and atomistic sub-domains is attained implicitly by iteration between the steady state solutions of the two sub-domains with the aid of an overlap region to facilitate the exchange of boundary conditions. Wijesinghe and Hadjiconstantinou [28] demonstrated the Schwarz hybrid coupling for a driven cavity test problem by employing overlap regions in both x and y directions (two-dimensional coupling). Applications of the Schwarz Alternating method to hybrid continuum-atomistic methods for gaseous flows in MEMS devices are however very few in the literature. The Schwarz method has been applied recently by Aktas et al. [29] to predict the flow field in microfluidic filters. They employed the Schwarz method to do a one dimensional coupling of the continuum and atomistic sub-domains using the Maxwellian distribution function. In the current work a hybrid continuum-atomistic method based on the Schwarz alternating method has been employed for coupling the DSMC model in the slider bearing region to the Navier-Stokes equation model outside the slider. The coupling has been done in two dimensions with the aid of Chapman-Enskog distribution for boundary condition imposition from the continuum domain to the DSMC domain. The formulation and various aspects of this hybrid coupling implementation will be dealt with in Chapter 6.

1.4 Scope of Work

The present work is concerned with the selection of an appropriate flow model for computing the flow in the HDI gap region. DSMC has been chosen as the flow model in this work and various flow modeling aspects of the DSMC method have been discussed in detail both for a stand-alone DSMC computation and for the case of a hybrid continuum-atomistic simulation, which is then applied to compute the flow in the vicinity of the HDI gap. The DSMC method has been first implemented for Couette flows and Poiseuille flows to identify and validate various features identified with rarefied gas flow such as slip velocity and temperature jump. Both two-dimensional and three-dimensional computer codes implementing the DSMC method have been developed and tested during the course of this research work. The DSMC computer code is then used to compute the flow characteristics in the HDI region. As DSMC is a computationally intensive method, the DSMC codes have been parallelized on a variety of local computing platforms using Message Passing Interface (MPI) [30]. Various parallelization aspects of the DSMC method and the performance of the parallel DSMC code on several modern advanced computing platforms illustrating the portability and scalability of the method have been compared and discussed in this work. Load balancing issues have also been considered and a dynamic load balancing scheme has been used to obtain further computational savings.

The impact of the number of cells, number of particles and time step size on the accuracy of a DSMC simulation of the flow in the HDI gap have been investigated in this work. An appropriate implicit boundary treatment method for modeling the inflow and outflow boundaries for micro flows is extended in this work for a three-dimensional DSMC simulation. A hybrid continuum-atomistic model based on the Schwarz Alternating method is employed for the coupling of the continuum flow outside the slider to the rarefied flow regions in the HDI gap. The Schwarz coupling has been done in two dimensions using the Chapman-Enskog distribution for boundary condition imposition from the continuum region to the DSMC region. The impact of the size of overlap region on the convergence of the Schwarz method is also discussed. A multiphase model to

compute particle trajectories is also incorporated in the DSMC method based on a one-way coupled method, by computing the forces on a particle assuming locally free molecular flow conditions. Representative particle trajectories in the HDI gap for flows in the transition regime have been computed for particles of a few nanometer diameter size and various densities.

The Reynolds equation gas lubrication model has also been formulated and solved using a finite difference method to compute the pressure distribution in the slider bearing region. The modified Reynolds equation model incorporating various slip models has been solved to obtain the pressure profile corresponding to the flow in the HDI region. Also considered is the coupled Reynolds-DSMC model to couple the Reynolds equation model solutions to the DSMC model in instances where a detailed atomistic simulation is required in localized regions near the HDI region.

A significant part of the work involved, in terms of both human and computer time has been towards writing and developing the codes for both stand-alone and hybrid continuum-atomistic parallel DSMC simulations. The codes for all the DSMC simulations, both for the two-dimensional and three-dimensional cases reported in this thesis have been developed in C++ programming language. All the DSMC codes employed for the HDI gap simulations and for the case of the hybrid continuum-atomistic modeling have been parallelized using MPI. *Fluent* software has been used to solve the Navier-Stokes equations in the continuum region for the hybrid continuum-atomistic case. The various Reynolds equation models have been solved using codes which have been written for the purpose in Matlab [31].

1.5 Significance of Work

Typically the Reynolds equation model based on the Fukui-Kaneko model is employed to obtain the pressure profile in the HDI gap. This model is computationally efficient and is widely used for the dynamic simulation of the slider flying characteristics and in the design of slider surfaces. The DSMC method although computationally

expensive, has many advantages over the Reynolds equation model in that many of the assumptions required by the lubrication theory can be relaxed and thus can capture the exact physics. The next generation HDD's require flying height of the order of a few nanometers in which case various factors such as particle-surface interaction, disk surface shape and heat generation due to slider-disk contact would play a key role in determining the accurate flow field conditions near the read/write head region. In such instances DSMC model should be employed for an accurate simulation as it can provide useful information related to the design or positioning of the read/write head. Hence the major focus of this thesis has been towards the development of appropriate DSMC models which can provide accurate and computationally efficient flow solutions pertaining to several different conditions in the HDI gap. A coupled Reynolds-DSMC model has been proposed to couple the Reynolds equation model solutions to the DSMC model, in instances where a detailed atomistic simulation is required in any localized region in the HDI gap. Flow modeling in the vicinity of the HDI gap is particularly challenging owing to the multi-scale nature of the flow in this region. Flow modeling aspects for both a stand-alone DSMC computation and for a hybrid continuum-atomistic simulation coupling the Navier-Stokes description to the DSMC method have been addressed in this work. A purely atomistic treatment using the DSMC method is computationally expensive and intractable for large regions outside the slider where continuum hypothesis is valid. Hybrid continuum-atomistic models such as the Schwarz method developed in this thesis for the flow simulation in the HDI gap can couple atomistic solutions in small localized regions to the Navier-Stokes description outside the slider, thereby achieving accurate and computationally efficient flow solutions.

1.6 Organization of the Thesis

The thesis is organized into seven chapters. Literature review for the different topics studied in this thesis is dealt with in the respective chapters that deal with them. The theory and implementation details related to the DSMC method have been dealt with in Chapter 2. Two-phase modeling using the DSMC method has also been addressed. In Chapter 3 the problem formulation for the DSMC method applied to simulate Couette

flows, Poiseuille flows and the HDI gap, and the computed flow results are described. Particle trajectories have also been computed using a two-phase DSMC model in the HDI gap both for the two-dimensional and three-dimensional cases. Chapter 4 deals with the parallelization aspects of the two-phase DSMC method and parallel performance of the three-dimensional parallel DSMC method on various computing platforms. Chapter 5 deals with the Reynolds gas lubrication model and a coupled Reynolds-DSMC model in the vicinity of the HDI region. In Chapter 6 various hybrid continuum-atomistic modeling aspects are discussed and the Schwarz Alternating method has been employed for the hybrid coupling of the Navier-Stokes equation to the DSMC model. The work is concluded in Chapter 7 which also states opportunities for future work.

CHAPTER 2

SINGLE AND TWO-PHASE DIRECT SIMULATION MONTE CARLO (DSMC) METHOD

2.1 Introduction

DSMC is a particle method introduced by Bird [16] in which the fluid is modeled at a molecular level. The molecular theory for dilute gases such as air is the kinetic theory. Since the gas is dilute, only binary collisions of molecules need to be considered. Also for a dilute gas the interaction forces between the molecules are very small and it can be assumed that the total energy possessed by molecule is only kinetic energy. The number of molecules even for very small systems is extremely large and so DSMC extensively uses statistical mechanics concepts such as probability distribution functions and random numbers based on the kinetic theory for flow simulations. The DSMC method has been proved to be consistent with the Boltzmann equation for the case of extremely small time steps and cell dimensions by Wagner [32]. Previous applications of DSMC to the slider bearing problem include that by Alexander et al. [33] and Liu and Ng [34]. Application of three-dimensional DSMC for the slider bearing application has been previously reported by Huang et al. [35]. Although DSMC is a well established method for modeling rarefied gas flow simulations, modeling of particle-laden flow using the DSMC method in rarefied flows has received considerable attention only recently with the advent of miniaturization and wide application of MEMS devices. A recent two-phase DSMC method by Gallis et al. [24] attempts to incorporate a two-phase model in the DSMC procedure by calculating the forces acting on the particle from the surrounding gas molecules under locally free molecular conditions. In this chapter the theory and implementation aspects of the DSMC method and two-phase DSMC model for computing particle trajectories are dealt with.

2.2 Basic Steps for Implementing the DSMC Method

DSMC models the macroscopic behavior of a fluid based on the discrete molecular character of gases by simulating the motion, interaction and collision of representative particles within an array of computational cells. Each particle in the DSMC method corresponds to a collection of large number of real gas molecules. The state of the system is given by the positions and velocities of particles. The particles in the simulation are considered to be hard spheres with the same diameter and the collisions between particles are assumed to be elastic. The evolution of the molecules is tracked and appropriate boundary conditions are applied to the particles that may reach a boundary interface such as the wall or outflow. For accurate simulations there are constraints that need to be followed when choosing the time step size and the linear cell dimensions. The impact of time step and cell size on transport coefficients for a DSMC simulation have been studied in recent works such as that by Alexander et al. [36], Garcia and Wagner [37] and Hadjiconstantinou [38]. The linear cell dimensions in a DSMC simulation must be smaller than the mean free path and the time step is taken to be much smaller than the mean collision time for an accurate DSMC simulation. Therefore collisions between the particles can be decoupled from the particle positional changes for every time step, i.e. the particles are moved as if they do not interact and collision is considered only after all the particles have moved for a time step. The constraints on time step, cell size, and number of particles make DSMC a computationally expensive method for the simulation of very large physical domains.

The core of any DSMC algorithm consist of the following main processes - move particles, index and sort particles, process particle-boundary interactions, simulate collisions and sampling of the flow field. Particles are initially randomly distributed with uniform density through out the system as shown schematically in Fig 2.1. Each simulated particle represents a large collection of real gas molecules which are roughly at the same place with the same velocity. In addition to its position each particle is initialized with a velocity chosen from a Maxwellian (equilibrium) distribution. After the particles are initialized the particles are evolved in two distinct steps – advection and

collision. In the advection phase the particles are moved as if they did not interact. Particles that reach an interface such as the wall, inflow or outflow boundary are treated according to appropriate boundary conditions as described in subsequent sections. After all particles have been moved and processed according to the boundary conditions imposed, particles are sorted and indexed based on the cell number. Particles in the same cell are randomly selected for collisions. After the collision process is done, the same procedure is repeated. Once the simulation reaches a steady state, sampling is done to derive the macroscopic properties. The procedures involved in a DSMC simulation are summarized in the flow chart shown in Fig 2.2.

Figure 2.1: Schematic showing the domain divided into cells and particles randomly initialized

Figure 2.2: Flowchart for the DSMC method

2.2.1 Collision Mechanism between Particles

Although molecular interactions could depend on complex quantum mechanical considerations, it can be treated through consideration of phenomenological collision models in a DSMC simulation. Various collision models such as the Hard Sphere model, Variable Hard Sphere (VHS) model and Variable Soft Sphere (VSS) models exist that can be incorporated to simulate the intermolecular collisions in a DSMC routine. The VHS model introduced by Bird [16] incorporates the hard-sphere scattering law for collision, and treats the cross-section of the molecules as a function of the relative translational energy during the collision. The VHS procedure ensures that the variation of coefficient of viscosity with temperature exactly matches that of a real gas. The VSS model by Koura and Matsumoto [39] introduces an additional parameter into the hard sphere expression for the deflection angle such that it reproduces the diffusion coefficient in a gas mixture correctly. Among other collision models include the generalized Hard Sphere (GHS) model introduced by Hash and Hassan [40] which can be used for modeling an intermolecular attractive-repulsive potential like the Lennard-Jones potential. Thus the VHS model should be employed when the flow field involves temperature gradients, while the VSS model should be used when a gas mixture is considered. Application of collision models like the GHS model may be significant only at very low temperatures. The Hard Sphere collision model has been found adequate for all the DSMC simulations reported in this work as the flow field under consideration is isothermal besides being computationally efficient and is described in detail in this section.

The intermolecular collisions in a hard sphere model are considered to be elastic by considering monatomic molecules wherein there is no interchange of translational and rotational energy. The intermolecular collisions are dealt with on a probabilistic rather than a deterministic basis, i.e. instead of calculating the exact trajectory of each particle, a stochastic algorithm is used to evaluate collision probabilities and scattering distributions in accordance with the kinetic theory as described by Garcia [41].

The collision frequency, η of N particles in a volume V is given by

$$\eta = \frac{N}{V} \pi d^2 \langle v_r \rangle \quad (2.1)$$

The number of candidate collision pairs that need to be selected in a cell for a time step Δt can then be represented by

$$M_{cand} = \frac{1}{2} N_c \eta \Delta t = \frac{N_c \pi d^2 v_{r,max} \Delta t}{2V_c} \quad (2.2)$$

where V_c is the cell volume, N_c is the number of particles per cell and $v_{r,max}$ is the maximum relative velocity in a cell. Only particles in the same cell are allowed to collide with each other. All pairs of particles with in a cell are considered to be candidate collision partners regardless of their positions in the cell, only the magnitude of the relative velocity between particles is used in determining their collision probability. A pair of particles is randomly selected from a cell and acceptance-rejection theorem is used to determine if the pair is to be accepted or rejected as a collision pair. For the purpose the maximum relative velocity in a cell $v_{r,max}$ is defined and a collision pair is accepted only if

$$\frac{|v_i - v_j|}{v_{r,max}} > R_f \quad (2.3)$$

where $v_i - v_j$ is the relative velocity between two particles i and j , and R_f is a uniform deviate in $(0,1)$. This procedure is repeated until the required number of candidate collision pairs in equation 2.2 are selected in each cell.

After collision is done, their post collision velocities are calculated based on the hard sphere collision model. If v_i and v_j are the pre-collision velocities of a pair of particles i and j , v'_i and v'_j the post-collision velocities, v_{cm} and v'_{cm} the velocities of the centre of mass before and after collision then from conservation of linear momentum the centre of mass velocity remains unchanged.

$$v_{cm} = \frac{1}{2}(v_i + v_j) = \frac{1}{2}(v'_i + v'_j) = v'_{cm} \quad (2.4)$$

If v_r and v'_r are the relative velocities before and after collision then from conservation of energy the relative velocity remains unchanged.

$$v_r = |v_i - v_j| = |v'_i - v'_j| = v'_r \quad (2.5)$$

The direction of the relative velocity is determined by the angles θ and ϕ which are the angular coordinates in the spherical coordinate system. For the hard sphere model these angles are uniformly distributed over the unit sphere and the post collision relative velocity is given by

$$v'_r = v_r \left[(\sin \theta \cos \phi) x + (\sin \theta \sin \phi) y + (\cos \theta) z \right] \quad (2.6)$$

The azimuthal angle ϕ is uniformly distributed between 0 and 2π and so it is selected as $\phi = 2\pi R_1$, where R_1 is a uniform deviate in $[0, 1]$. The θ angle is computed as $q = \cos \theta = 2r - 1$ and $\sin \theta = \sqrt{1 - q^2}$, where r is a random variable uniformly distributed in $(0, 1)$ and q distributed uniformly in $[-1, 1]$.

2.2.2 Particle Interactions with Boundaries

Appropriate boundary conditions must be employed if a particle comes across a wall or inflow/outflow boundary. The interaction between the particles and a wall surface can be mainly classified as fully specular, fully diffuse or a certain combination of these two. In specular reflection the collision between the wall and particle is purely elastic and the particle merely reflects off the wall. As a result the magnitude of velocity does not change in a specular reflection. The velocity component normal to the wall is reversed in sign after collision, while the tangential components remain unchanged. The angle between the particle's incident velocity v and the surface θ_i is equal to the angle made between the particle's reflected velocity v' and the surface denoted by θ_r . In diffuse reflection model however, the collision involves exchange of energy between the particle and the wall and the post collision molecular velocity is related to the temperature of the wall surface. Therefore the particle interacting with a surface is allowed to scatter randomly in all directions in the diffuse reflection model. Schematic illustrating the specular and diffuse reflection models are shown in Fig 2.3.

Figure 2.3: Schematic illustration of (a) specular and (b) diffuse reflection of a particle from a wall

For a real surface, interaction of gas molecules with respect to a wall surface may not be entirely specular or diffusive. The accommodation coefficient a is a measure of the tendency of the gas to accommodate to the wall surface, which is dependent on various factors such as surface material, roughness, temperature etc. In a DSMC simulation an accommodation coefficient of one indicates that the gas molecules have fully accommodated to the wall temperature. For real engineering surfaces however the accommodation coefficient could be less than one. Maxwell model [42] is the most popular method in literature to take into account the effect of accommodation coefficient in the gas surface scattering model in a DSMC simulation. This model assumes that the gas molecules diffusely reflect from the solid surface with complete energy accommodation with probability a and specularly reflect with probability $(1 - a)$. There are more complex models of gas surface scattering such as the Cercignani and Lampis model which takes into account two accommodation coefficients, a normal energy accommodation coefficient and a parallel momentum accommodation coefficient. The Cercignani–Lampis (CL) model [43] has been adapted and extended by Lord [44] for application in DSMC studies and has been shown to satisfy reciprocity (detailed balance) condition. For the slider bearing application it is expected that low values of accommodation coefficient could result in low pressure values and correspondingly a lower load capacity as already shown in works such as that by Alexander et al. [33]. Experimental studies have been conducted recently by Rettner [45] who used molecular beam techniques to obtain the accommodation coefficient for nitrogen (N_2) colliding

with four different surfaces representative of a Hard Disk. Their experimental results conclude that for all the four surfaces, the gas is essentially fully accommodated to the wall surface at ambient room temperature and the calculated accommodation coefficient values are in the range of 0.95 to 1. For the purpose of the DSMC simulations carried out in the present work, the particle-wall interactions follow the diffuse reflection model with full thermal accommodation, as this does not detract from the generality of the results and conclusions presented in the thesis.

When a particle strikes a diffuse (thermal) wall all three components of the velocity are reset according to a biased Maxwellian distribution as explained by Alexander and Garcia [46]. The distributions are biased because the faster particle strikes the wall more frequently. An accommodation coefficient of one indicates a perfect thermal wall. If m is particle mass, k_B the Boltzmann constant and T_w the temperature of the wall then the component normal to the wall is distributed as

$$P(v_y) = \frac{m}{kT_w} v_y e^{-mv_y^2/2k_B T_w} \quad (2.7a)$$

while each parallel components are distributed as

$$P(v_x) = \sqrt{\frac{m}{2\pi kT_w}} e^{-mv_x^2/2k_B T_w} \quad (2.7b)$$

$$P(v_z) = \sqrt{\frac{m}{2\pi kT_w}} e^{-mv_z^2/2k_B T_w} \quad (2.7c)$$

At the inflow/outflow boundaries depending on the nature of the flow under consideration, various boundary treatments such as *periodic*, *stream* or *pressure* boundary conditions can be employed. In DSMC, boundary conditions are specified by injecting particles into the system with a molecular velocity distribution corresponding to the mean flow macroscopic variables characteristic to the external flow to be imposed at the boundaries. In stand alone DSMC computations boundary conditions are often implemented with the aid of the equilibrium Maxwell-Boltzmann distribution function. In such cases particles are typically injected from the boundary surface, based on which the normal velocity components of the injected particles correspond to the biased

Maxwellian distribution function and are generated by the acceptance-rejection theorem [16]. The parallel components are obtained separately from the ordinary Maxwellian distribution function. Apart from the molecular velocity information, the mean flow parameters should also be set for the injected particles. For high speed compressible flow applications, given the density and the mean flow velocity of the external flow, the mean flow parameters of the injected particles can be directly set as the free *stream* boundary condition. In micro flow applications however the *stream* boundary conditions are not appropriate and *pressure* boundary conditions are typically employed. For hybrid continuum-atomistic applications Chapman-Enskog distribution must be employed to fix the boundary conditions. The modeling and implementation aspects of boundary condition imposition both for a stand-alone DSMC simulation and for the case of a hybrid continuum-atomistic simulation are discussed in detail in subsequent chapters.

2.2.3 Sampling

For each cell which is assumed homogeneous, sampling is done with the number of particles in each cell to get the macroscopic properties. Sampling is done after the system has reached a steady state, by taking time averaged values of the properties over the sampling period. This is necessary since the properties obtained after each time step are instantaneous and fluctuating values. The expressions for computing the macroscopic properties such as density, velocity, temperature and pressure are expressed as

$$\text{Density,} \quad \rho = \frac{N_c m}{V_c} \quad (2.8a)$$

$$\text{Velocity,} \quad U = \frac{1}{N_c} \sum_{i=1}^{N_c} v_i \quad (2.8b)$$

$$\text{Temperature,} \quad T = \frac{m}{3kN_c} \left[\sum_{i=1}^{N_c} v_i^2 - U^2 \right] \quad (2.8c)$$

$$\text{Pressure,} \quad p = nk_B T \quad (2.8d)$$

where N_c is the number of particles in a cell, k_B is the Boltzmann constant, m is the mass of the particle and n is the number density.

2.3 Two-Phase DSMC Model

Multiphase flows which involve the transport of solid particles in a gaseous medium are found in a wide variety of applications. The vast majority of numerical models for studying the particle transport have been for cases where the continuum assumption is valid and tracking of particle trajectories in such models is achieved by coupling conventional CFD techniques with a suitable particle transport model. Particle transport modeling in rarefied flows has received considerable attention very recently with the advent of miniaturization and wide application of MEMS devices such as in the HDD and semiconductor industry. Particle transport under rarefied flow conditions are also encountered in low density applications in the upper atmosphere such as rocket exhaust, spacecraft thruster etc. In these applications the continuum based CFD techniques are not valid and hence flow modeling and computation of particle trajectories should be based on an accurate flow model like DSMC.

In a HDD enclosure, particle contamination may lead to performance degradation of the HDI region due to processes such as erosion or scratch. Since the HDI gap is in the order of nanometers, larger particles either do not enter the HDI region or gets trapped near the leading edge of the slider. Smaller particles of nanometer size have a greater chance of entering the HDI region and coming to contact with the read/write head. In this work an attempt is made to model particle-laden flow in the HDI gap using the DSMC method for the case where the flow falls in the transition regime. A two-phase DSMC model has been incorporated in the DSMC method to compute particle trajectories in the HDI gap, based on a recent one-way coupled model by Gallis et al. [24]. The particle concentration is assumed to be dilute, such that there are no collisions between particles. The particles are assumed to be spherical and small with respect to the mean free path of gas molecules so that locally free molecular conditions around the particle can be assumed. Locally free molecular conditions imply that the collisions between reflected gas molecules off the particle and incident molecules are not significant and the surrounding gas flow is not affected by the presence or motion of the particle. To satisfy the locally free molecular flow conditions around the particle, the particle Knudsen

number Kn_p must be greater than one, where Kn_p is defined as $Kn_p = \lambda/R_p$, R_p being the particle radius. A one way coupling can be therefore assumed, wherein the influence of the particle phase will have a negligible effect on the gas phase. The gas molecules that collide with the particle during a given time step could deflect off the particle surface in one of the three ways: specular reflection, isothermal diffuse reflection or adiabatic diffuse reflection. Gallis derived expressions for finding the force and heat transfer Green's functions which represent the force on and heat transfer to a spherical particle from a delta-function molecular velocity distribution, from the rates of delivery and removal of momentum and energy by incident gas molecules. The net total force acting on a particle from locally free molecular flow surrounding it can then be calculated by summing the individual contributions from all computational molecules. This approach can be numerically implemented in the DSMC method, since the velocity of each gas molecule is known. This two-phase DSMC method has been recently implemented and applied for the case of free expansion flows in low density high altitude rocket exhaust applications by Burt and Boyd [47]. They considered the reflection scheme of gas molecules off the particle surface to be only due to specular and diffuse reflection with full thermal accommodation to the particle temperature, as gas-solid interactions in rarefied flow can be accurately modeled by these two types of reflection models. Based on the one-way coupled method, the rates of momentum transfer to a solid particle due to the presence of a single computational gas molecule in the same cell as the particle is given by the following expression

$$\vec{f}_p = \frac{\pi R_p^2 N_g}{V_c} \left(mc_r + \frac{\tau}{3} \sqrt{2\pi m k_B T_p} \right) \vec{u}_r \quad (2.9)$$

where R_p is the radius of the particle, V_c is the cell volume, N_g is the number of real gas molecules that a computational particle represent, m is the mass of a gas molecule, $\vec{u}_r$ is the relative velocity of the gas molecule $\vec{u}_g$ with respect to the particle velocity $\vec{u}_p$ given as $\vec{u}_r = \vec{u}_g - \vec{u}_p$, c_r is the absolute value of $\vec{u}_r$, k_B is the Boltzmann's constant, T_p is the particle temperature and τ is the thermal accommodation coefficient for the particle

surface. Both the force $\vec{f}_p$ and the relative velocity $\vec{u}_r$ are vectors, and have either two or three components depending on the number of dimensions used in the simulation. The expression for computing $\vec{f}_p$ suggests that the force per unit area will be the same for all particles for which the locally free molecular flow assumption applies. In this case the force vector is in the same direction as the relative velocity. The total net force $\vec{F}_p$ acting on the particle from all computational molecules within the same DSMC cell as the particle can be computed by summing the individual contributions from all molecules.

$$\vec{F}_p = \sum_{i=1}^N \vec{f}_p \quad (2.10)$$

In the DSMC method, the two-phase DSMC computations begin only after steady state flow has been attained. Starting from an initial location and with an initial particle velocity, particle motion is tracked at each time step based on the total net forces acting on the particles from the surrounding gas molecules. The change in the particle velocity during a small time step can be computed based on the impulse-momentum theorem which states that the impulse imparted on an object during a small time interval, Δt is equal to the change in momentum of the object. Accordingly the change in particle velocity is computed as the product of the total net force vector $\vec{F}_p$ and $\Delta t / M_p$, where Δt is the time step and M_p is the particle mass. The new position vector of the particle $\vec{X}_f$ is calculated as

$$\vec{X}_f = \vec{X}_i + \vec{V}_f \cdot \Delta t \quad (2.11a)$$

where $\vec{V}_f$ is the new particle velocity vector computed as $\vec{V}_f = \vec{V}_i + d\vec{V}$, $d\vec{V}$ is the change in particle velocity, $\vec{V}_i$ is the current particle velocity vector and $\vec{X}_i$ is the current particle position vector given as

$$\vec{X}_i = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \quad (2.11b)$$

$$\vec{V}_i = \begin{pmatrix} u_p \\ v_p \\ w_p \end{pmatrix} \quad (2.11c)$$

$$d\vec{V} = \begin{pmatrix} F_{p,x} \\ F_{p,y} \\ F_{p,z} \end{pmatrix} \times \frac{\Delta t}{M_p} \quad (2.11d)$$

Since the current two-phase DSMC model is based on the one-way coupling assumption which implies that the particle phase has no influence on the gas phase, it can be easily implemented in a DSMC code. In the current work, the two-phase computations to calculate particle trajectories are integrated in the *sampling* phase of the DSMC procedure. The modified DSMC flowchart to incorporate the two-phase DSMC computations is shown in Figure 2.4.

2.4 Implementation of Probability Distributions in DSMC

2.4.1 Uniform Deviates

Random number generators are essential for a stochastic algorithm like DSMC. Uniform probability distributions are generated using uniform deviates, which generates random numbers in the interval $[0, 1)$. Uniform deviates can be generated by the linear congruential method. By this method, given a seed (an initial integer value), a sequence of integers is generated using the mapping

$$I_{new} = (aI_{old} + c) \bmod M \quad (2.12)$$

where a , c and M are integer constants and mod represents the remainder portion.

The uniform deviate is now computed as

$$R = \frac{I_{new}}{M} \quad (2.13)$$

Thus a series of random numbers in $[0, 1)$ is generated, with each succeeding random number using the previous result as its seed.

Figure 2.4: Flowchart for the Two-phase DSMC method

2.4.2 Other Probability Distributions

For other probability distributions such as Gaussian, Exponential, Poisson distribution etc, uniform deviates is used as the basic building block for random number generation. Uniform deviates are transformed to generate random numbers from invertible distributions typically by mapping the uniform deviate R $[0, 1)$ into the required random variable. In a DSMC simulation the molecular velocities typically correspond to a normal distribution. The Box-Muller transformation procedure can be employed to generate Gaussian (Normal) distributed random numbers from uniform deviates, given the standard deviation and mean of the probability distribution as described by Garcia [41].

2.4.3 Acceptance-Rejection Method

If we need to generate random numbers satisfying an arbitrary distribution function $f(x)$ which is difficult to invert (eg. *Chapman-Enskog distribution* or a *biased normal distribution*), the acceptance-rejection method is the best technique possible. Instead of sampling directly from the distribution $f(x)$, an envelope distribution $g(x)$ can be used by means of which sampling is made easier. The envelope distribution $g(x)$ is such that $g(x) > f(x)$ for all x . The acceptance-rejection method is based on a simple geometrical argument. Let $f(x)$ be the probability distribution that needs to be generated, so that the area under the curve in any range of x corresponds to the desired probability of generating an x in that range as shown in Fig 2.5. The basic idea behind the acceptance rejection theorem is to choose random points (x, y) with uniform probability in the area under the curve for the probability distribution $f(x)$. The x value of such random points generated will then have the required probability distribution. To do this suitable an envelope function $g(x)$ need to be employed such that $g(x) > f(x)$ for all x . Uniform deviates are then used to pick random points (x_{trial}, y_{trial}) as shown in the figure below. If the point falls below the required distribution $f(x)$, it is accepted, and if it falls above $f(x)$ it is rejected. The accepted x values will then correspond to the required probability distribution $f(x)$.

Figure 2.5: Schematic representation of the acceptance-rejection method

CHAPTER 3

APPLICATION OF DSMC TO FLOWS REPRESENTATIVE OF HEAD DISK INTERFACE FLOWS

In this Chapter the DSMC method has been applied to flows representative of that in the HDI region and the formulation is discussed. The DSMC method is initially applied to Couette flows to identify and validate flow features associated at micro- and nano- scales. The boundary condition treatment considerations for modeling the inflow/outflow boundaries for a micro flow DSMC simulation is then discussed and an appropriate implicit boundary treatment for fixing the pressure boundary condition is extended for modeling the flow in the HDI gap. The implicit boundary condition is first applied for micro Poiseuille flows. The DSMC method is then applied to model the flow conditions in the HDI region both for the two-dimensional and three-dimensional cases. The impact of the number of cells, number of particles per cell and time step size on the accuracy of DSMC results for the simulation of the HDI region have also been investigated. The impact of various parameters on the pressure profile and loading capacity has also been addressed. Particle trajectories in the HDI gap have also been computed using the two-phase DSMC method both for the two-dimensional and three-dimensional cases. Representative particle trajectories in the HDI gap for flows in the transition regime have been computed for particles of a few nanometer diameter sizes.

For all the DSMC simulations reported in this work a monatomic molecule (argon gas) with a mass $m = 6.63 \times 10^{-26} \text{ kg}$, diameter $d = 3.66 \times 10^{-10} \text{ m}$ and density $\rho = 1.78 \text{ kg/m}^3$ has been chosen as the gaseous medium. The Hard Sphere collision model is considered, while the particle-wall interactions are assumed to be inelastic and follow the diffuse reflection model with full thermal accommodation. Due to the computationally intensive nature of the DSMC method, all DSMC simulations that have

been done for the HDI gap simulation reported in this thesis are done with the aid of parallel DSMC method. The time step should be much smaller than the mean collision time and for all the DSMC simulations in this work it is taken as five times smaller than $\Delta x/c_0$, where Δx is the smallest cell dimension and c_0 is the most probable velocity.

3.1 Couette Flow Simulation

Microscale flow characteristics for the Couette flow have been previously analyzed in works such as that by Xue et al. [48], Bahukudumbi and Beskok [49] and Bahukudumbi et al. [50]. Couette flow refers to the flow between two infinitely long parallel plates in relative motion, moving with a tangential velocity $\pm U_w$ as shown in Fig 3.1. The temperature of the plates is fixed at T_w . The gas between the plates is initially at rest under STP conditions with a temperature $T_0 = T_w$ and the flow is driven by the moving plates. In the current work both one-dimensional and two-dimensional DSMC simulations have been conducted to analyze the flow conditions.

Figure 3.1: Schematic for a Couette flow

3.1.1 One-Dimensional DSMC Simulation model

A one-dimensional (1D) Couette flow simulation at micro- and nano- scales has been done first to validate the DSMC computational model. Couette flow can be analyzed by a 1D simulation as the flow properties vary significantly in only one direction (y direction here), while along other directions flow gradients are not significant. Correspondingly in a 1D DSMC simulation, particles move only along the y direction, i.e. only the y coordinate of each particle is tracked. Schematic of the computational domain for a 1D DSMC system for Couette flow is shown in Fig 3.2. The computational domain is divided into a regular array of cells with particles initialized randomly with a uniform density and the velocity of the particles initialized according to a Maxwellian velocity distribution.

3.1.2 Two-Dimensional DSMC Simulation model

In a two-dimensional (2D) simulation the particles move in both x and y directions, while the properties in the z direction are assumed to be homogeneous. Uniform rectangular cells have been taken along the xy plane. Schematic of the computational domain for a two-dimensional DSMC system for Couette flow is shown in Fig 3.3. At the entrance and exit of the Couette flow system, periodic boundary conditions have been applied which implies that a particle exiting out of either inlet or outlet reappears at the other end with the same particle velocity. By varying the distance between the two plates, the flow conditions at various Knudsen number can be simulated.

Figure 3.2: Schematic of a one-dimensional DSMC system for Couette flow

Figure 3.3: Schematic of a two-dimensional DSMC system for Couette flow

3.2 DSMC Couette Flow Results

3.2.1 One-Dimensional Flow Results

The DSMC code has been first validated with results available in Bahukudumbi and Beskok [45] for the case of Couette flow by considering rarefied gas flow between two infinite parallel plates moving with a velocity of $\pm U_w$ as shown in Fig 3.1. For validation purposes the same set of parameters as available in the literature has been employed for carrying out the DSMC simulations. The wall surfaces have been maintained at 273 K and have been assumed to be fully accommodating ($a = 1$). The simulations have been carried out using argon gas with molecular mass $m = 6.63 \times 10^{-26}\text{ kg}$ and a hard sphere diameter $d = 3.66 \times 10^{-10}\text{ m}$. For the DSMC simulations about 20 cells have been taken across the channel height with about 50 particles per cell. The sampling process has been carried out for a period of about 500,000 iterations. Couette flow simulations have been carried out at three different cases corresponding to $k = 0.1, 1.0$ and 10 , where k is the rescaled Knudsen number given as $k = (\sqrt{\pi}/2)Kn$. The wall velocity has been taken as 15.4 m/s which corresponds to a mach number $Ma = 0.05$. The complete velocity profiles for Couette flow obtained for the three different cases considered are shown in Fig 3.4. Validation of the computed velocity profiles in the upper half of the channel at the three different Knudsen numbers considered, with results available from literature is shown in Fig 3.5. A good correlation with the results from literature is observed for all the three cases considered.

Figure 3.4: Velocity profiles obtained for Couette flow in the entire channel at $k = 0.1$, 1.0 and 10.0.

Figure 3.5: Validation of velocity profiles obtained for Couette flow in the upper half of the channel.

One-dimensional DSMC simulations have also been done for the case of Couette flow for which the lower plate is stationary while the upper plate moves with a uniform velocity. The simulations have been carried out for different cases of Knudsen numbers ranging from 0.01 to 8 by varying the gap between the plates. For all the DSMC simulations the cell size is taken much lesser than a free path size with at least 100 particles per cell and sampling has been done for a period of about 300,000 iterations. Fig 3.6 shows the corresponding profiles of velocity obtained for the different cases of Knudsen numbers considered.

Figure 3.6: Velocity profiles for different Kn ranging from 0.01 to 8

3.2.2 Two-Dimensional Flow Results

For the Couette flow case, two-dimensional simulations have also been done for different cases of Knudsen numbers ranging from 0.1 to 8 similar to that carried out for the 1D simulation. The velocity, temperature and pressure profiles obtained from the two-dimensional simulations are shown in Fig 3.7.

From the velocity profiles obtained from both one-dimensional and two-dimensional simulations as shown in Fig. 3.6 and Fig. 3.7, it can be observed that there exists a velocity slip at the walls, when the flow deviates from the continuum regime. Velocity slip implies that there is a difference between the velocity of the gas on the wall, U_g and the wall velocity, U_w itself, i.e. $U_s = U_g - U_w$. Similarly from the temperature profile as shown in Fig. 3.7, it can be seen that there exists a temperature jump at the walls. A temperature jump implies that the temperature of the gas at the wall T_g is different from the temperature of the wall T_w , i.e. $T_{jump} = T_g - T_w$. The variation of velocity slip and temperature jump on both the walls with variation in Knudsen number is shown in Fig 3.8 and Fig 3.9. It can be inferred from the figures that the deviation from the continuum theory increases with increase in the Knudsen number and is maximum when the flow regime approaches the free molecular regime.

Also it can be observed from the velocity plots that the velocity profile starts to become non-linear near the walls, when the Knudsen number is greater than 0.1. For $Kn > 0.1$, a slight bending in the velocity profiles near the walls can be observed. This is due to the effect of Knudsen layer which is a very thin layer about one mean free path next to the wall. With increase in Knudsen number, the thickness of the Knudsen layer becomes comparable to the distance between the plates. The velocity profile becomes linear after Kn exceeds 1. The pressure profile is almost uniform with a pressure gradient near the wall identified due to the effect of the Knudsen layer. These phenomenon predicted by the DSMC code are consistent with that expected for flows at micro- and nano- scales.

(a) Velocity profile

(b) Temperature profile

Figure 3.7: Profiles for (a) velocity (b) temperature and (c) pressure for Kn from 0.1 to 8

(c) Pressure profile

Figure 3.7: Profiles for (a) velocity (b) temperature and (c) pressure for Kn from 0.1 to 8
(Continued)

Figure 3.8: Variation of velocity slip with Kn from 0.1 to 8

Figure 3.9: Variation of temperature jump with Kn from 0.1 to 8

3.3 Boundary Condition Treatment Considerations for Micro flows

The inflow/outflow boundary conditions in a DSMC simulation are implemented by injecting particles into the system corresponding to the external flow conditions. The number of particles to be injected is derived from the density information while the molecular velocity distribution of the injected particles must correspond to the mean flow macroscopic variables characteristic to the external flow as have been outlined in works such as that by Bird [16], Lilley and Macrossan [51], and Tysanner and Garcia [52]. For hybrid continuum-atomistic methods which couple the continuum solutions to the DSMC region, a reservoir region upstream and downstream of the inflow/outflow boundaries are incorporated to impose the boundary conditions. Particles must fill the reservoir region with a molecular velocity distribution corresponding to the flow velocity and velocity gradients in the continuum solutions. The equilibrium Maxwellian distribution function representation of the continuum equations is adequate for Euler equations, but in the case of the Navier-Stokes equations and when finite velocity gradients exist in the solution, the Chapman-Enskog distribution must be used as given in Chapman and Cowling [53].

For stand-alone DSMC computations, boundary conditions are often based on the equilibrium Maxwell-Boltzmann distribution function. In such cases particles are typically injected from the inflow/outflow boundary face, such that the velocity component of the injected particles u which is normal to the inflow/outflow boundary corresponds to the biased Maxwellian distribution function. The other two molecular velocity components v and w are obtained separately from the ordinary Maxwellian distribution function. Besides the molecular velocity information, mean flow parameters such as density, temperature and velocity also need to be known to correctly set for the properties of the incoming molecules at the inflow and the outflow boundaries. For high speed compressible flow applications, given the density and the mean flow velocity of the external flow, the mean flow parameters of the injected particles can be directly set as corresponding to the free stream boundary condition. In micro flow applications, as the flow conditions near the inflow and outflow boundaries are not uniform owing to the influence from the presence of walls, free stream boundary conditions are not appropriate. Typically, in MEMS applications only the pressure information at the inflow and outflow boundaries is known *a priori*. Therefore in such applications pressure boundary conditions are employed such that given the pressure information, other flow variables such as velocity etc. are derived adaptively as the flow simulation progresses to fix the boundary conditions.

3.3.1 Pressure Boundary Conditions

Various methods for implementing the implicit boundary treatment for the inflow and outflow boundaries for micro- and nano- scale flows modeled by the DSMC method have been proposed in literature such as that by Ikegawa and Kobayashi [54], Nance et al. [55] and Wu and Tseng [56]. One approach is the particle flux conservation concept in which the information on the number of particles crossing the boundaries is used to update the inflow velocity. The method of computing the inflow velocity at each time step using the particle flux conservation concept could result in errors under low speed flow conditions, since the number of particles crossing the inflow boundary at low speed is very small and result in fluctuations in the imposed flow variables at the boundary. These fluctuations can be minimized by deriving the inflow velocity from the average

number of particles entering the system over several time steps. Fang and Liou [57] had proposed a simple scheme by which a first-order extrapolation is used to determine the inflow mean velocity from the computed values at the cells inside the computational domain at the inflow boundary. However the inflow velocity left uncorrected may not embody the pressure information and could be problematic if the wall temperature is different from the gas temperature. To overcome these difficulties, Wang and Li [58] had proposed a pressure correction scheme for both the inflow and outflow pressure boundaries based on the theory of characteristics and implemented the same for a two-dimensional simulation of Poiseuille flow, orifice flow and corner flow in micro geometries. The advantage of the pressure boundary condition is that it does a feedback correction to fix the desired pressure conditions at the boundaries, by deriving the local mean flow parameters such as the inflow and outflow velocity in an implicit manner as the simulation progresses. This approach has been extended in this work for the three-dimensional flow modeling in the slider bearing region.

Figure 3.10 shows a schematic of a typical three-dimensional slider bearing geometry representative of HDI gap between the slider and the hard disk and the computational domain of length L and width W in which the flow has been simulated using the DSMC method. The lower wall represents the spinning disk region moving with a tangential velocity U_w relative to the upper wall, which represents the slider surface. The channel height h varies along the length of the slider as the slider is inclined at a pitch angle α relative to the lower wall. The channel height at the inflow boundary has been denoted by H_1 while that at the outflow boundary which represents the flying height has been denoted by H_0 . For the three-dimensional slider shown in Fig 3.10, the inflow boundary has been represented by the $y-z$ plane at the entrance, while all the other three sides of the slider have been treated as outflows. At the inflow and outflow boundaries of the slider bearing, ambient conditions of pressure $P_0 = 1 \text{ atm}$ and temperature $T_0 = 273 \text{ K}$ have been imposed by injecting particles with appropriate molecular velocity distribution from the inflow/outflow boundaries. The inflow and outflow boundary conditions for micro flows are discussed next.

Figure 3.10: Schematic of three-dimensional slider geometry and computational domain

The details of the treatment of boundary conditions at the inflow and outflow sections of the HDI gap at the entrance and exit given by the $y-z$ plane as shown in Fig 3.10 is explained in this section. The number of particles, N entering the computational domain from either the inflow boundary or outflow boundary is determined from the Maxwellian distribution function.

$$N = \Delta t A n \frac{1}{2\beta\sqrt{\pi}} \left\{ e^{-\beta^2 U_j^2} + \beta\sqrt{\pi} U_j [1 + \text{erf}(\beta U_j)] \right\} \quad (3.1)$$

where n is the number density at the inflow/outflow face, U_j represents the normal local mean flow velocity component at the boundary, A the cross-sectional area of the inflow/outflow face and $\beta = 1/\sqrt{2RT}$ where R is the universal gas constant.

The velocity component distribution of the injected particles has been determined as follows. The velocity component, u of the particles entering the computational domain which is normal to the inflow or outflow boundary is generated using the acceptance-rejection procedure since it corresponds to the biased Maxwell-Boltzmann distribution. The molecular velocity components v and w parallel to y and z axes of the $y-z$ plane are obtained independently by sampling from the velocity distribution characteristic of the external flow as

$$v = \left(\sqrt{-\ln(R_f)} / \beta \right) \cos(2\pi R_f) + V_j \quad (3.2)$$

$$w = \left(\sqrt{-\ln(R_f)} / \beta \right) \sin(2\pi R_f) + W_j \quad (3.3)$$

where V_j, W_j represents the local mean flow velocity components in the y and z directions, j is the cell at the inflow or outflow boundary and R_f is a random fraction which ranges from 0 to 1.

The mean flow parameters have been determined as follows. At the inflow boundary the known flow variables are pressure, P_{in} and temperature, T_{in} . The number density, n_{in} can be then obtained from the equation of state as

$$(n_{in}) = \frac{P_{in}}{kT_{in}} \quad (3.4)$$

The inflow velocity is then changed adaptively during the course of the flow simulation to enforce the pressure boundary conditions. The mean inflow velocity is obtained implicitly from the pressure information based on the theory of characteristics as follows:

$$(U_{in})_j = U_j + (P_{in} - P_j) / \rho_j a_j \quad (3.5)$$

where the subscript j denotes the cell at the boundary, ρ is the density and a is the local velocity of sound.

Similarly at the subsonic outflow boundary the only known flow parameter is the exit pressure P_e . The other flow variables such as density and mean flow velocity have been determined implicitly as the simulation progresses as

$$(\rho_e)_j = \rho_j + (P_e - P_j) / (a_j)^2 \quad (3.6)$$

$$(U_e)_j = U_j + (P_j - P_e) / \rho_j a_j \quad (3.7)$$

3.4 Poiseuille Flows

Poiseuille flows refer to the flow between two stationary parallel plates under the influence of a pressure gradient. A schematic for a Poiseuille flow is shown in Fig 3.11. The pressure P_{in} , temperature T_{in} at the inflow boundary and the pressure at the outflow boundary P_e is known and a temperature T_w is specified at the walls. A two-dimensional DSMC simulation to model the Poiseuille flow at micro- and nano- scales has been developed and the implicit boundary treatment method has been applied to fix the pressure boundary conditions at the inflow and outflow.

Figure 3.11: Schematic for Poiseuille flow

The dimensions of the channel for modeling Poiseuille flow are taken as $L = 2\mu m$ and $H = 300nm$. The inflow temperature is taken as $T_{in} = 300K$ and the wall temperature $T_w = 320K$. The pressure ratio P_{in}/P_e considered is 2 where $P_{in} = 2 atm$ and $P_e = 1 atm$. 60×20 uniform rectangular cells are considered for the simulation, with about 30 particles per cell considered.

3.4.1 Computed Flow Results

Fig. 3.12 shows the contour of the stream-wise flow velocity across the two-dimensional plane. The flow velocity obtained is parabolic with a higher velocity at the centerline as expected for Poiseuille flows. Due to the pressure gradient the flow velocity

increases as it develops downstream. It can be observed from the velocity contours that there exists a velocity slip at the walls as expected in the case of micro flows. The variations of the gas slip velocity along both the bottom and top walls are shown in Fig 3.13. The slip velocity is defined as $U_s = U_g - U_w$, where U_g represents the gas velocity on a wall and U_w the wall velocity. As can be observed the slip velocity increases towards the downstream section where the flow velocities are higher.

Fig. 3.14 shows the contours of the temperature distribution across the two-dimensional plane. The temperature decreases towards the downstream and the lowest values of temperature are noticed at the exit where flow expansion takes place. The variations of temperature jump along the both the bottom and top walls are shown in Fig. 3.15. The temperature jump is defined as the difference between the wall temperature and gas temperature at the wall $T_g - T_w$, where T_g represents the gas temperature on the wall and T_w the wall temperature. As can be observed the temperature jump is higher near the inflow and outflow boundary of the channel.

Shear stresses in a DSMC simulation can be calculated from the drag forces acting on the wall. The tangential forces acting on a wall (the drag force) could be calculated as the time-averaged change in the momentum of the particles striking the wall. The shear stress acting on the wall can be calculated as

$$\tau = \frac{\xi}{A\Delta t} \sum (mv_x - mv'_x) \quad (3.8)$$

where ξ is the number of molecules that a particle represent, m is the mass of the particle, v_x is the velocity of the particles before hitting the wall, v'_x is the velocity of the particles after hitting the wall, A denotes the slider surface area and Δt is the time period for sampling. The distribution of the shear stress on the wall across the top and bottom plates is shown in Fig. 3.16. Shear stress has been found to be higher in regions where slip velocity is higher.

Figure 3.12: Streamwise velocity contours

Figure 3.13: Slip velocity along the wall

Figure 3.14: Temperature contours

Figure 3.15: Temperature jump along the wall

Figure 3.16: Wall shear stress distribution along the wall

3.5 Head-Disk Interface Gap DSMC Simulations

The formulation and results of the DSMC simulations for the HDI gap is discussed in this section. Implicit boundary treatments have been employed to fix the pressure boundary condition at the inflow and outflow sections as described in section 3.3. The problem setup of the HDI gap geometry and the computational domain of interest are shown in Fig 3.10. A slider air bearing is formed by the air flow between the slider and the rotating disk which provides sufficient lift force for the slider to fly above the rotating disk. Both two-dimensional and three-dimensional DSMC models have been developed to simulate the flow conditions in the HDI gap, a brief discussion of which is made here. Parallelization and performance aspects of the DSMC models will be dealt with in detail in Chapter 4.

3.5.1 Two-Dimensional DSMC Model

A two-dimensional DSMC model has been developed first to simulate the flow conditions in the HDI gap. In the case of a slider bearing, the channel height across any section is very small compared to the width of the domain and therefore the flow can be

reasonably assumed to be two-dimensional. A sketch of the two-dimensional DSMC system for a slider bearing is shown in Fig 3.17. Uniform rectangular cells have been considered for the collision cells. The use of such Cartesian rectangular cells makes it easier to sort particles and implement collisions. Since the slider wall is inclined at a certain pitch angle, it cuts through some of the cells within the computational domain resulting in partial cells as shown in the figure. The partial cells have been accounted for by considering only the part of the cell volume that lies within in the simulation domain, which has been obtained by subtracting the cell volume that lies outside the computational domain from the total cell volume. When a partial cell is very small and the number of particles in it is small, statistical calculation in that cell may not be reliable, which has been taken care of by combining the smallest incomplete cells with their lower adjacent cells. The cut-cell approach has been previously employed for the DSMC simulation of the slider bearing such as that in Huang et al [35]. The cut cell approach is a very convenient and efficient approach for the DSMC simulation of the slider bearing application especially when H_0 is very small and H_1/H_0 is very large.

Figure 3.17: Schematic of a two-dimensional DSMC computational domain

At the inflow and outflow of the computational domain ambient pressure conditions exist. The pressure boundary conditions have been fixed by injecting particles at the inflow and outflow based on the implicit boundary treatment method. At the start of the simulation, the flow velocity at the inflow and outflow boundary has been initially set to U_w , the disk speed. The flow properties of the cells at the inflow and outflow

boundary are monitored at every time step. Particles are injected from the inflow and outflow boundaries with the mean flow parameters such as velocity, temperature and density adaptively changed to fix the ambient pressure conditions for further iterations. Particles accumulate in the control volume with every time step as new particles are injected from the inflow and outflow boundary. Particles that exit the simulation domain from either the inflow or outflow boundary are discarded from the simulation. The total number of particles in the system increases with every iteration and after a certain number of time steps the system attains steady state, at which the number of particles fluctuates about a constant value. Once steady state has been attained, the sampling procedure is done to derive the macroscopic properties such as pressure, temperature and velocity.

3.5.2 Three-Dimensional DSMC Model

A three-dimensional DSMC model has also been developed to simulate the flow conditions in the HDI gap. A schematic of the three-dimensional computational domain for the slider geometry is shown in Fig 3.18. In the three-dimensional case the x , y and z coordinates of the particles have to be tracked and cells need to be taken in all the coordinate directions. Similar to the two-dimensional case, uniform rectangular cells have been employed and partial cells are taken into account by considering only the cell volume within the computational domain. Particles in a three-dimensional simulation can exit from all the four boundary interfaces with every time step. The particles that exit the computation domain are discarded from the simulation.

Figure 3.18: Schematic of a three-dimensional DSMC computational domain

Ambient pressure conditions have to be imposed at all the four boundary interfaces. The pressure boundary conditions are fixed by injecting particles from all the four boundary interfaces with mean flow parameters that are determined implicitly as described in section 3.3. Particles thus accumulate in the control volume for every time step and fluctuate around a constant number after a certain number of time steps, at which steady state has been attained. Once the steady state has been attained, sampling process is done to derive the macroscopic properties similar to that for the two-dimensional case.

3.6 Computed Flow Results in the HDI Region

Computed flow results obtained using the DSMC method and the impact of various parameters such as the number of cells, number of particles and time step size on the accuracy of a DSMC simulation for the slider bearing application have been addressed in this section. For an accurate DSMC simulation there are several guidelines to be followed involving the number of particles, number of cells and the time step size. The general rule is that the cell dimensions must be less than a mean free path long and the time step no longer than a mean free time with an average of at least 20-25 particles per cell. However these constraints are problem specific and could be relaxed depending on the flow velocity and gradients of the specific problem under consideration. Since DSMC is a computationally intensive method, it is important to have guidelines regarding the minimum number of cells and number of particles per cell required without compromising the accuracy, especially for a three-dimensional simulation. The impact of the number of cells, number of particles per cell and time step size on the accuracy of the DSMC results for the simulation of the slider bearing problem have been investigated in this report. This study serves as a guideline for selecting the parameters for all the DSMC simulations of the HDI gap. Based on the results of this study, adequate care has been taken to ensure the accuracy of the results for all DSMC simulations in the vicinity of the HDI gap reported in this thesis.

3.6.1 Accuracy Considerations

The effect of the number of simulated particles per cell on the accuracy of the DSMC solutions for a two-dimensional simulation has been investigated. The investigation has been done for a slider configuration shown in Fig 3.10 with $L = 4\mu m$, flying height $H_0 = 25nm$ and a tangential velocity $U_w = 25m/s$. Five DSMC simulations have been carried out using a total of 100×5 cells with an average of about 10, 20, 25, 35 and 50 particles per cell. For all the cases considered, a constant sampling period of about 150,000 iterations has been employed. Fig 3.19 shows the effect of the number of particles per cell on the accuracy of the solutions of pressure and flow velocity along the extent of the slider length on the lower wall or disk surface. It can be inferred that for cases using 20 or more particles per cell, the variation between the computed flow solutions is not significant and hence is adequate for an accurate DSMC simulation. The variations between the solutions for pressure and velocity are plotted in Fig 3.20 in terms of the mean variance with respect to the highest fidelity solution considered, i.e. 50 particles per cell. The variance is calculated as $\sum (x - \bar{x})^2 / N$, where $\bar{x}$ is the mean solution taken for the present study as the case corresponding to 50 particles per cell and N is the number of data points. For all the DSMC simulations carried out in this work for the HDI gap at least 35 particles per cell have been employed.

The effect of the number of cells on the computed flow field have been assessed by using 40×5 , 60×5 , 80×5 , 100×5 , 120×5 and 150×5 cells, which correspond respectively to cell dimensions of about 1.6, 1.07, 0.8, 0.64, 0.53 and 0.43 times the mean free path in the flow direction. All the cases considered are based on an average of about 35 particles per cell. Fig 3.21 shows the effect of the cell size on the variation of the computed pressure profile and flow velocity distribution along the bottom wall. It is seen that by increasing the total number of cells along the flow direction, the variation between the computed flow solutions is negligible and the accuracy of the solution is not improved further. This suggests that since the velocity gradients in the flow direction are negligible in the case of a slider bearing, cell dimensions in the flow direction can be even greater than a mean free path.

Another important parameter that affects the accuracy of the DSMC solutions is the choice of the time step size. The time step should be such that it is smaller than the mean collision time and must be small enough so that particles take several iterations before it crosses over to the next cell. A sensitivity study has been done in the current work to investigate the impact of the time step size on the accuracy of the DSMC results by using various time step sizes. The time steps have been taken in the range 3.8×10^{-12} sec to 30.8×10^{-12} sec by considering five cases i.e. $0.1 \times (\Delta x/c_0)$, $0.2 \times (\Delta x/c_0)$, $0.333 \times (\Delta x/c_0)$, $0.5 \times (\Delta x/c_0)$ and $0.8 \times (\Delta x/c_0)$, where Δx is the smallest cell dimension and c_0 is the most probable velocity. Fig 3.22 shows the effect of time step size on the variation of the computed pressure profile and flow velocity distribution along the extent of the bottom wall. It has been observed that the pressure solutions obtained using larger time steps are not accurate. No significant variation between the flow solutions has been observed for time steps smaller than $0.333 \times (\Delta x/c_0)$. The variations between the solutions for both pressure and velocity in terms of the mean variance with respect to the highest fidelity solution considered i.e. $\Delta t = 3.8 \times 10^{-12}$ sec are plotted in Fig 3.23. To ensure accurate solutions for all the DSMC computations of the HDI gap carried out in this work, the time step has been chosen as five times smaller than $\Delta x/c_0$, i.e. $\Delta t = 0.2 \times (\Delta x/c_0)$.

(a)

(b)

Figure 3.19: Effect of the number of particles on the accuracy of a) pressure b) velocity

Figure 3.20: Error in terms of the mean variance for solutions of pressure and velocity as a function of number of particles per cell

(a)

(b)

Figure 3.21: Effect of the number of cells on the accuracy of a) pressure b) velocity

Figure 3.22: Effect of the time step size on the accuracy of a) pressure b) velocity

Figure 3.23: Error in terms of the mean variance for pressure and velocity solutions as a function of time step size

3.6.2 Two-dimensional Slider Air Bearing Results

The DSMC code has been first validated with results available in the literature. The validation of the DSMC code for the slider bearing simulation has been shown for three different cases corresponding to two different slider geometry configurations and different cases of wall velocity and Knudsen number. The three cases considered correspond to slider configurations; $L = 5\mu m, H_1 = 100nm, H_0 = 50nm, U_w = 25m/s, Kn_0 = 1.250$, $L = 5\mu m, H_1 = 100nm, H_0 = 50nm, U_w = 307.8m/s, Kn_0 = 1.250$ and $L = 1.5\mu m, H_1 = 30nm, H_0 = 15nm, U_w = 153.9m/s, Kn_0 = 4.167$. For the DSMC simulations, a temperature of $273K$ has been fixed at both the walls. A total of 100×5 cells have been taken for all the cases and the simulations have been carried out for 300,000 time steps, with sampling done for over a period of about 200,000 time steps. The pressure plots obtained from the DSMC code are compared with results reported by Alexander et al [33] for the same slider configurations and the validation is shown in Fig 3.24. In the plots the pressure is non-dimensionalized with respect to the ambient pressure P_0 and the length in the x direction is normalized with respect to the length L of the slider. There is a good correlation between the pressure profiles for all the three cases.

(a) Case 1: $L = 5\mu m, H_1 = 100nm, H_0 = 50nm, U_w = 25m/s, Kn_0 = 1.250$

(b) Case 2: $L = 5\mu m$, $H_1 = 100nm$, $H_0 = 50nm$, $U_w = 307.8 m/s$, $Kn_0 = 1.250$

(c) Case 3: $L = 1.5\mu m$, $H_1 = 30nm$, $H_0 = 15nm$, $U_w = 153.9 m/s$, $Kn_0 = 4.167$

Figure 3.24: Validation of the DSMC code for slider air bearing with available results from literature for three different cases

During the read/write operation in a HDD, the slider could operate under various conditions of flying height and disk speeds. The operating conditions under which the slider functions could also vary between different HDD models. The effect of various parameters such as flying height, disk velocity and pitch angle on the flow field in the HDI is investigated in this section. A slider bearing with dimensions of $L = 5\mu m$, $H_1 = 65nm$, $H_0 = 15nm$ and $U_w = 25m/s$ is taken as the baseline case for the study. For the DSMC simulations, ambient pressure conditions of $P_0 = 1atm$ and a temperature of $T_0 = 273K$ have been fixed at the boundaries and at the walls $T_{wall} = T_0$. A total of 100×5 cells have been taken, and the simulations have been carried out for 300,000 time steps with sampling done for over a period of about 200,000 time steps, to minimize the scatter associated with the DSMC method.

The computed flow conditions for the baseline slider geometry are shown in Fig 3.25. The pressure profile is shown in Fig 3.25 (a). The velocity profile along the extent of the slider length on the disk surface is shown in Fig 3.25 (b). Velocity slip along the disk surface can be observed from the velocity profile as expected for flow at high Knudsen numbers. A higher velocity is observed towards the trailing edge of the HDI region with the maximum velocity observed at the exit. This is consistent with the lower cross sectional area towards the exit to have the same mass flow rate. The plot of density along the x direction is shown in Fig 3.25 (c). The temperature distribution being almost uniform across the system, the density variation is much similar to the variation in the pressure solutions.

Shear stress distribution along the slider and the disk surface has also computed and the results are shown in Fig 3.26. For the slider, shear stress value increases towards the trailing edge which is due to the higher velocities at the exit. For the disk surface negative shear stress values are observed because of the moving disk, while a positive value is observed near the outflow boundary due to the higher flow velocity at the exit compared to the tangential velocity of the disk.

(a)

(b)

(c)

Figure 3.25: Computed flow conditions for (a) pressure (b) density (c) velocity in the HDI region

(a)

(b)

Figure 3.26: Wall shear stress along (a) slider surface (b) disk surface

3.6.3 Effect of Variation of Flying Height on the Pressure Profile

The effect of variation of flying height on the pressure profile has been investigated for four different slider configurations of $L = 5\mu m$ with a flying height H_0 of $3nm$, $5nm$, $15nm$ and $25nm$. For all the cases the disk velocity has been fixed at $U_w = 25 m/s$ and the pitch angle considered is $\alpha = 0.01 rad$. Fig 3.27 shows the variation of particle accumulation in the simulation domain as a function of iteration number for the various cases considered. It is seen from the particle accumulation plot that for the cases of slider geometry considered, steady state is attained relatively faster for those with a larger flying height. For the cases with a large value of H_0 , the computational domain is larger and hence needs a greater number of real gas molecules to fill. However since the effective number i.e. the number of real gas molecules that each particle represents, is also larger for the case with a large value of H_0 , it accumulates fewer particles as compared to the cases with very small values of H_0 .

The computed pressure profiles for the different cases considered are shown in Fig 3.28. Higher values of peak pressure are obtained for the cases with small values of H_0 . The location of the peak pressure point moves further towards the trailing point of the slider with reduction in flying height. The load-carrying capacity, F of the slider bearing which represents the bearing force to support the slider over the spinning disk can be calculated as the integration of the pressure distribution over the length of the slider and is given by

$$F = \int_0^L (p - P_0) W dx \quad 3.9$$

where W is the width of the slider and L is the length of the slider. The variation in the load capacity for the different flying heights is plotted in Fig 3.29. As can be observed from the plots, with a reduction in flying height the loading capacity of the slider bearing is significantly increased. This is consistent with the higher values of pressure obtained for the cases with small values of H_0 .

Figure 3.27: Variation in particle accumulation in the simulation domain for different cases of H_0

Figure 3.28: Variation in the pressure profile for different cases of H_0

Figure 3.29: Variation in the load capacity as a function of flying height

3.6.4 Effect of Variation of Tangential Disk Velocity on the Pressure Profile

To study the effect of the variation of the tangential disk velocity on the pressure profile, a slider bearing with dimensions $L = 5\mu m$, $H_1 = 65nm$, $H_0 = 15nm$ has been considered. Four different cases of tangential disk velocity have been considered viz. $U_w = 10, 25, 50$ and $75 m/s$. Fig 3.30 shows the particle accumulation in the control volume as a function of iteration number. Particles get accumulated in the computational domain with each iteration, and after a certain stage fluctuates about a certain number, at which steady state has been attained. A higher velocity induces a larger number of particles into the system. Fig 3.31 shows the variation of pressure profile for different cases of tangential disk velocity. With decrease in the disk velocity, the peak pressure drops significantly and a shift in the peak pressure point to the left is observed. The variation in the load capacity for the different cases of tangential disk velocities considered is plotted in Fig 3.32. For the cases with small values of disk velocity, the loading capacity of the slider bearing is significantly reduced.

Figure 3.30: Variation in particle accumulation in the simulation domain for different cases of tangential disk velocity

Figure 3.31: Variation in the pressure profile as a function of disk velocity

Figure 3.32: Variation in the load capacity of the slider bearing with change in disk velocity

3.6.5 Effect of Variation of Pitch Angle on the Pressure Profile

Simulations have also been done to study the effect of pitch angle α on the computed pressure profile, for a slider air bearing configuration with $L = 5\mu\text{m}$, $H_1 = 65\text{nm}$, $H_0 = 15\text{nm}$ and $U_w = 25\text{m/s}$. Four cases of pitch angle have been considered, viz. $\alpha = 0.007, 0.01, 0.012$ and 0.015rad . Fig 3.33 shows the variation in the particle accumulation plot for the different cases of pitch angle considered. As can be observed from the plots, particle accumulation is greater for larger values of pitch angle because of a larger control volume in this case. Fig 3.34 shows the variation of pressure profile as a function of pitch angle. As the pitch angle increases, the peak pressures obtained are higher and the peak pressure point moves towards the trailing edge where the head is located. Correspondingly higher values of load capacity are obtained as shown in Fig 3.35.

Figure 3.33: Variation in the particle accumulation for different cases of pitch angle

Figure 3.34: Variation in the pressure profile for different cases of pitch angle

Figure 3.35: Variation in the load capacity for different cases of pitch angle

3.6.6 Effect of Accommodation Coefficient on the Flow Distribution

The effect of the accommodation coefficient a on the flow distribution in the HDI gap has been investigated by considering four different cases, i.e. $a = 1.0, 0.9, 0.8$ and 0.7 . The Maxwell model [42] has been incorporated in the DSMC code to investigate the effect of incomplete accommodation. The baseline slider bearing geometry with dimensions of $L = 5\mu m$, $H_1 = 65nm$, $H_0 = 15nm$ and $U_w = 25 m/s$ is taken for the study. Fig 3.36 shows the effect of the accommodation coefficient on the flow velocity solutions along the extent of the slider length on the lower wall or disk surface. Incomplete accommodation significantly increases the velocity along the disk surface as can be observed from the velocity plot. The variation of the pressure profile and load capacity as a function of the accommodation coefficient is plotted in Fig 3.37. From the plots it is observed that reduction in the accommodation coefficients results in lower values of pressure and correspondingly lower values of load capacity.

Figure 3.36: Variation in the flow velocity distribution along the disk surface for different cases of accommodation coefficient

Figure 3.37: Variation of a) pressure and b) load capacity for different cases of accommodation coefficient

3.7 Three-dimensional DSMC Results

3.7.1 Accuracy Considerations

The impact of the number of particles per cell, number of cells and time step size have also been investigated for a three-dimensional DSMC simulation of a slider configuration shown in Fig 3.10 using $L = 3\mu m$, $W = 3.3\mu m$, $H_0 = 25nm$ and $U_w = 25m/s$. To study the effect of number of particles, four DSMC simulations using an average of about 13, 25, 38 and 50 particles per cell have been carried out. For all the cases considered, a constant sampling period of about 200,000 iterations has been employed. The computed flow solutions for the different cases, across a section along the disk surface located at $z/W = 0.5$ are shown in Fig 3.38. It can be observed that for the case with 13 particles per cell, the solutions are not accurate. For the case corresponding to 25 particles per cell, the solution converges and further increase in the number of particles per cell reduces the statistical fluctuations. The variation between the solutions of pressure and velocity are plotted in Fig 3.39, in terms of the mean variance with respect to the highest fidelity solution case considered i.e. 50 particles per cell. The variance is calculated as $\sum (x - \bar{x})^2 / N$, where $\bar{x}$ is the mean solution taken for the present study as the case corresponding to 50 particles per cell and N is the number of data points. Based on this study at least 30 particles per cell have been used for all three-dimensional DSMC flow simulations carried out in this work.

The effect of the number of cells in the z direction on the accuracy of a three-dimensional DSMC flow simulation has also been investigated for varying cell sizes, viz. $64 \times 4 \times 20$, $64 \times 4 \times 30$, $64 \times 4 \times 40$, $64 \times 4 \times 50$ and $64 \times 4 \times 60$ cells, which corresponds to a cell dimension of about 2.64, 1.76, 1.32, 1.06 and 0.88 times the mean free path, in the z direction respectively. Fig 3.40 shows the variation of the computed pressure profile along the disk surface corresponding to the various cell sizes. It can be seen that increase in the number of cells in the z direction does not result in any observable increase in the accuracy. This suggests that cell dimensions can be much greater than the mean free path in the z direction where the velocity gradients are small.

(a)

(b)

Figure 3.38: Effect of the number of particles on the accuracy of a) pressure and b) velocity solutions for three-dimensional DSMC

Figure 3.39: Error in terms of the mean variance for pressure and velocity solutions as a function of number of particles per cell

Figure 3.40: Effect of the number of cells in the z direction on the accuracy of pressure

A sensitivity study has also been done to investigate the impact of the time step size on the accuracy of the DSMC results by using various time step sizes. The time steps are taken in the range of 3.2×10^{-12} sec to 8.1×10^{-12} sec by considering four cases i.e. $0.1 \times (\Delta x / c_0)$, $0.15 \times (\Delta x / c_0)$, $0.2 \times (\Delta x / c_0)$ and $0.25 \times (\Delta x / c_0)$, where Δx is the smallest cell dimension and c_0 is the most probable velocity. Fig 3.41 shows the effect of the time step size on the variation of the computed pressure profile and flow velocity distribution, along the extent of the bottom wall. No significant variations between the flow solutions are observed for all the cases, as the time steps considered are much smaller than the mean free time due to the small cell dimensions involved. The variations between the solutions for both pressure and velocity in terms of the mean variance with respect to the highest fidelity solution case considered i.e. $\Delta t = 3.2 \times 10^{-12}$ sec, are plotted in Fig 3.42. To ensure accurate solutions for all the three dimensional DSMC computations of the HDI gap carried out in this work, the time step has been chosen as five times smaller than $\Delta x / c_0$, i.e. $\Delta t = 0.2 \times (\Delta x / c_0)$.

(a)

(b)

Figure 3.41: Effect of the time step size on accuracy of a) pressure and b) velocity

Figure 3.42: Error in terms of the mean variance for pressure and velocity solutions as a function of time step size

3.7.2 Computed Flow Results

Three-dimensional DSMC simulations of the HDI gap have been done for a slider geometry of configuration $L = 3\mu m$, $W = 3.3\mu m$ and $U_w = 25m/s$. For the DSMC simulations, ambient pressure conditions of $P_0 = 1atm$ and a temperature of $T_0 = 273K$ have been fixed at the boundaries and at the walls $T_w = T_0$. For the three-dimensional DSMC simulation, particles enter the computational domain from all the four boundary interfaces with each iteration and upon attainment of a steady state the total number of particles in the simulation domain fluctuates about a constant value. Fig 3.43 shows the particle accumulation plot for the case of a three-dimensional slider bearing geometry of configuration $L = 3\mu m$, $W = 3.3\mu m$, $H_0 = 15nm$ and $U_w = 25m/s$. A total of about $64 \times 4 \times 50$ cells have been taken and the simulations have been carried out for 250,000 time steps, with the sampling process done for over a period of about 100,000 time steps. The computed flow fields for the slider bearing geometry considered is shown in Fig 3.44. The computed three-dimensional pressure profiles are shown in Fig 3.44 (a). The contours of pressure and velocity on the bottom wall which represents the disk surface are shown in Fig 3.44 (b) and Fig 3.44 (c) respectively.

Figure 3.43: Particle Accumulation in the simulation domain as a function of iteration number

(a) Three-dimensional pressure profile

(b) Pressure Contours on the disk surface

(c) Velocity Contours on the disk surface

Figure 3.44: Computed flow fields for $H_0 = 15 \text{ nm}$

The velocity profiles across three selected sections along the disk surface at $z/W = 0.125, 0.5$ and 0.875 are shown in Fig 3.45. The velocity profiles along the different sections considered are similar, with a peak velocity observed towards the exit which corresponds to the sudden pressure drop towards the trailing edge of the slider. Along the midsection, i.e. at $z/W = 0.5$ peak values of pressure and correspondingly peak values of flow velocity are observed.

Figure 3.45: Computed velocity profiles along the extent of disk surface

The three-dimensional pressure profile and pressure contours on the disk surface obtained for the same slider geometry of $L = 3\mu m$, $W = 3.3\mu m$ and $U_w = 25 m/s$, but with different cases of flying height such as $H_0 = 6, 10$ and $25 nm$ are shown in Fig 3.46. A constant pitch angle of $\alpha = 0.01 rad$ is considered for all the cases. As expected, the peak values of pressure are obtained for the cases with a smaller value of H_0 , with the peak pressure values located towards the trailing edge of the slider. The pressure profiles at the midsection at $z/W = 0.5$ along the length of the slider for all the cases considered are summarized in Fig 3.47.

(a) Three-dimensional pressure profile

(b) Pressure Contours on the disk surface

(i)

(a) Three-dimensional pressure profile

(b) Pressure Contours on the disk surface

(ii)

(a) Three-dimensional pressure profile

(b) Pressure Contours on the disk surface

(iii)

Figure 3.46: Computed pressure profiles for (i) $H_0 = 6\text{ nm}$, (ii) $H_0 = 10\text{ nm}$ and (iii) $H_0 = 25\text{ nm}$

Figure 3.47: Computed pressure profiles along the extent of the disk surface at $z/W = 0.5$

3.8 Computed Two-Phase DSMC Results

In a HDD enclosure, particle contamination may lead to performance degradation of the HDI region due to processes such as erosion or scratch. Since the HDI gap is in the order of nanometers, larger particles either do not enter the HDI region or gets trapped near the leading edge of the slider. Smaller particles of nanometer size have a greater chance of entering the HDI region and coming to contact with the read/write head. Investigation of particle trajectories in the HDD enclosure based on continuum flow models have been previously examined by Song et al. [6] and Ali et al. [7-9]. Such models have investigated the trajectories of particles released from various locations inside the HDD and provides useful guidelines for design and filter location. Particle motion and contamination on the slider walls in the HDI region have been previously studied in works such as that by Zhang and Bogoy [23] and Shen and Bogoy [59] based on a Lagrangean approach by considering various forces such as drag, lift and gravity forces. For the computation of particle trajectories in the HDI gap, they have employed the first order slip corrected Reynolds gas lubrication model to compute the air flow velocities. In this work an attempt is made to model particle-laden flow in the HDI gap using the DSMC method for the case where the flow falls in the transition regime. The two-phase DSMC model is based on a recent one-way coupled model by Gallis et al. [24] as explained in section 2.3. Representative particle trajectories have been computed for extremely small particles of a few nanometer sizes and for various cases of densities, both for the two-dimensional and three-dimensional cases.

3.8.1 Limitations of the Two-Phase DSMC Approach for HDI Simulations

The current two-phase DSMC approach is based on a one-way coupled model by Gallis et al. which assumes locally free molecular flow conditions around the particle. This implies that the particle Knudsen number Kn_p must be greater than one, where Kn_p is defined as $Kn_p = \lambda/R_p$, R_p being the particle radius. The study of particle motion in the HDI gap carried out in this work has been done for a particular range of nanometer sized particles in a simple slider bearing geometry. The largest particle radius considered

for the two-phase calculations in this work is 15 nm for which $Kn_p > 4$ and the smallest particle considered is of $R_p = 5\text{ nm}$ for which $Kn_p > 12$. Hence it is assumed that around the particle, locally free molecular flow conditions exist in which case the particle can be considered sufficiently small such that it has no effect on the molecular distribution function of the surrounding gas. However due to the small gap size in the case of the HDI which is in the order of nanometers, this assumption may not be completely valid as there could be gradients in the flow properties on length scales comparable to the particle dimensions. In such cases the finite volume of particles cannot be completely neglected and particles may not be assumed as point sources. Besides since the flying height of the slider H_0 is in the order of nanometers, the relatively large size of the particle compared to the minimum channel height may cause blockage of flow around that region. It is to be noted however that for a real HDD, the slider length L and width W are about 1 mm , the channel height at the leading edge H_1 is in the order of microns, while the channel height at the trailing edge H_0 where the read/write head is located, is in the order of nanometers. Moreover real slider surfaces are more complex with cavities or recessed regions in the major part of its domain with dimensions in the order of microns, which makes the channel heights in these regions even larger. For the motion of nanometer size particles in recessed regions of such sliders the assumptions of locally free molecular flow could be completely valid. The two-phase DSMC models developed in the current work can provide the basis for investigating the motion of nanometer sized particles in complex slider geometries such as for the case of a step slider with cavities. In such computations if the particle comes near the read/write head region it can assumed that the particle sticks to the wall surface. Taking these factors into account the computed particle trajectories using the two-phase method for the case of a simple slider geometry considered in this thesis and shown in sections 3.8.2 and 3.8.3 should be seen only as representative results.

3.8.2 Two-Dimensional Computed Particle Trajectories

In the present work, representative particle trajectories are computed for nanometer size particles in a slider bearing geometry for which the flow falls entirely in the transition regime. The particle sizes have been taken such that it is much smaller than

the mean free path of the gas, to satisfy the locally free molecular flow assumption. This implies that the particle Knudsen number Kn_p must be greater than one, where Kn_p is defined as $Kn_p = \lambda / R_p$, R_p being the particle radius. The largest particle radius considered for the two-dimensional case is 15 nm for which $Kn_p > 4$. The particle motion is investigated for various particle sizes and densities. For the study particle sizes of radius $R_p = 5, 10, 15\text{ nm}$ and varying densities of $\rho = 2000, 4000, 8000\text{ kg/m}^3$ is considered. The computational domain of interest and the HDI region is shown in Fig 3.48. The dimensions of the slider considered are $L = 5\mu\text{m}$, $H_1 = 120\text{ nm}$, $H_0 = 50\text{ nm}$ and $U_w = 25\text{ m/s}$. The gas temperature and the wall temperatures have been taken to be the same i.e. $T_0 = T_w = 273\text{ K}$. As the flow field in the slider bearing can be assumed to be isothermal, the particle temperature T_p is assumed to be the same as that of the surrounding gas i.e. $T_p = T_g$, which implies that there is no net heat transfer to the particle. The simulation region is divided into a total of about 100×6 cells with about 50 particles per cell. The particles are initially located near the inflow of the slider with an initial particle velocity corresponding to the disk velocity. The particles are assumed to stick to the wall surface if they come into contact with a wall.

Figure 3.48: Schematic of the HDI region and the computational domain of interest

Particle motion along the HDI gap has been investigated first for a particle of radius $R_p = 5\text{ nm}$ and density $\rho = 2000\text{ kg/m}^3$. Fig 3.49 shows the magnitude of the total average momentum transfer (total net force) acting on the particles along the extent of the HDI gap. The corresponding particle velocity along the extent of the HDI gap and the particle trajectory plot is also shown. It can be observed that towards the exit of the HDI gap, there is an increase in the total net force acting on the particle and in the corresponding particle velocity. Otherwise no significant variations are observed in the total net force and the particle velocity along the extent of the HDI gap. It can be observed from the particle trajectory plot that particle is initially lifted from its initial position slightly after which the particle motion is largely planar.

The impact of particle size on the motion of the particle has been investigated by plotting the trajectory of particles with different sizes but same material density. The study has been done for three different cases of density $\rho = 2000, 4000$ and 8000 kg/m^3 . Fig 3.50 shows the particle trajectory plots for the different cases. It can be observed that for all the cases, particles are initially lifted from its initial position after which the particle motion remains parallel to the disk surface. It appears that for the range of particle sizes considered here, the lift forces acting on the particle are very small. This result is consistent with that observed by Zhang and Bogy [23] for the case of very small particles in which they report that the motion of particles of diameter less than 100 nm is essentially planar. The effect of material density on the trajectory followed by the particle has also been investigated and the particle trajectory plot is shown in Fig 3.51. No significant differences are observed between the trajectories followed by the particles as for all the cases the particle motion remains parallel to the disk surface.

(a)

(b)

(c)

Figure 3.49: Plots of (a) magnitude of total net force (b) particle velocity and (c) particle trajectory along the extent of the HDI gap

Figure 3.50: Trajectory followed by particles with different sizes in the HDI region.

Figure 3.51: Trajectory followed by particles with different material density in the HDI region.

3.8.3 Three-Dimensional Computed Particle Trajectories

The two-phase DSMC method has also been incorporated for the three-dimensional DSMC case and representative particle trajectories are computed in the HDI gap for which the flow falls entirely in the transition regime. The dimensions of the slider considered for the three-dimensional case are $L = 3\mu m$, $W = 3\mu m$, $H_1 = 100nm$, $H_0 = 50nm$ and $U_w = 25m/s$. Similar to the two-dimensional case the gas temperature and the wall temperatures are taken to be the same and fixed i.e. $T_0 = T_w = 273K$ and the particle temperature is taken to be the same as that of the surrounding gas i.e. $T_p = T_g$. The simulation region is divided into a total of about $60 \times 5 \times 50$ collision cells with about 40 particles per cell. The particle motion has been investigated for various sizes of particle and densities. For the study particle sizes of radius $R_p = 5, 10, 15nm$ and different material densities such as $\rho = 2000, 4000, 8000 kg/m^3$ is considered. The largest particle radius considered is $15nm$ for which the particle Knudsen number $Kn_p > 4$, so as to fully satisfy the assumption of locally free molecular flow around the particle. The three-dimensional computational domain of interest and the HDI region is as shown in Fig 3.10. The particles are initially located near the inflow of the slider with an initial particle velocity corresponding to the disk velocity.

Particle motion along the HDI gap is investigated first for particles of radius $R_p = 5nm$ and density $\rho = 2000 kg/m^3$. Two particles are considered which are released from two different locations along the z direction viz. $z_i/W = 0.5$ and $z_i/W = 0.67$. The initial position of the two particles are given by $x_i = 0.2\mu m$, $y_i = 20nm$, $z_i = 2\mu m$ and $x_i = 0.2\mu m$, $y_i = 20nm$, $z_i = 1.5\mu m$. Fig 3.52 shows the magnitude of the total average momentum transfer (total net force) acting on the particles and the corresponding particle velocity along the HDI gap. No major variations are observed in the total net force and the particle velocity along the extent of the HDI gap, with a slight increase in particle velocity observed towards the exit of the slider. Fig 3.53 shows the three-

dimensional trajectory followed by the two particles. The corresponding particle trajectory plots which show the motion of the particles along the HDI gap in the y direction and span-wise direction (along the width of the slider) is shown in Fig 3.54. The trajectory followed by both the particles is very similar, with the particle released from the central location of $z_i/W = 0.5$ being lifted higher due to higher particle velocities. Both the particles are lifted from its initial position after which the particle motion becomes planar, i.e. parallel to the disk surface. Along the span-wise direction however, there appears to be no significant changes in position along the HDI region as both the particles follow almost a straight line path. This can be attributed due to the fact that there are no significant flow gradients along the span-wise direction.

Figure 3.52: Plots of (a) magnitude of the average momentum transfer (total net force) acting on the particle and (b) particle velocity along the extent of the HDI gap

Figure 3.53: Three-dimensional computed trajectories of two particles released from two different locations along the z direction

(a)

(b)

Figure 3.54: Trajectory followed by the particles along (a) y direction and (b) z direction

The impact of material density on the motion of the particle has been investigated by plotting the trajectory of particles of radius $R_p = 5\text{ nm}$ but with different cases of material density $\rho = 2000, 4000$ and 8000 kg/m^3 . The computed trajectories followed by particles released from an initial location of $x_i = 0.2\text{ }\mu\text{m}$, $y_i = 20\text{ nm}$ and $z_i = 2\text{ }\mu\text{m}$ are shown in Fig 3.55. It can be observed from the particle trajectory plot that for all the cases the particle motion is predominantly parallel to the disk surface with no significant differences and leaves the HDI region without slider contact. Along the span-wise direction, no significant changes in position are observed as both the particles almost follow a straight line path.

The impact of particle size on the trajectory followed by a nanometer size particle has also been investigated and Fig 3.56 shows the corresponding particle trajectory plot. For all the cases particles are initially lifted slightly from its initial position after which the particle motion is largely planar. For the range of nanometer sized particles considered here, the lift forces acting on the particle are very small. The results and trends of the particle motion obtained from the three-dimensional DSMC simulations are very similar to that obtained from a two-dimensional simulation, because of insignificant flow gradients in the z direction. It is to be noted that the study of particle motion in the HDI gap in this work has been done for a particular range of nanometer sized particles in a simple slider bearing geometry. The motion of larger sized particles could not be studied by this 2-phase DSMC method due to the locally free molecular flow constraint. This study can however provide the basis for detailed investigation of particle motion of nanometer sized particles in more complex slider bearing geometries.

(a)

(b)

Figure 3.55: Trajectory followed by particles of size $R_p = 5 \text{ nm}$ with different material density in the HDI region along (a) y direction and (b) z direction

(a)

(b)

Figure 3.56: Trajectory followed by particles with different particle sizes of density $\rho = 4000 \text{ kg/m}^3$ in the HDI region along (a) y direction and (b) z direction

CHAPTER 4

IMPLEMENTATION AND PERFORMANCE METRICS OF A PARALLEL TWO-PHASE DSMC METHOD

4.1 Introduction

Although the Direct Simulation Monte Carlo (DSMC) method is widely considered as the most accurate method for rarefied gas flow simulations, the application of DSMC is a computationally intensive method for realistic problems and hence motivates the usage of parallel computers to reduce the computational time. The constraints associated with the DSMC method in terms of cell size, time step size and number of particles in each cell makes DSMC computationally intensive in terms of both computer memory and time. This is especially so for the three-dimensional case which is several times more computationally intensive than an equivalent two-dimensional problem and is best done with a parallel DSMC method. Parallel implementation of the DSMC method has been widely reported in literature especially for high speed rarefied gas dynamics such as Dietrich and Boyd [60] and LeBeau [61]. Parallel DSMC software using various static and dynamic load balancing schemes have been developed by Boyd's group MONACO [60] and by Ivanov's group SMILE [62]. A general parallel DSMC method using unstructured mesh and dynamic load balancing techniques has been reported by Wu and Tseng [63]. However applications of parallel DSMC method to low speed micro flow simulations and comparisons of the parallel performance on various modern advanced computing platforms are relatively few in literature. Parallel DSMC aspects for micro flow simulations for the two-dimensional case have been reported such as Fang and Liou [64] and Aktas et al. [65]. In this study, a parallel three-dimensional DSMC method for micro flow simulation has been developed and applied for simulating the flow in the narrow HDI gap. A two-phase model has also been incorporated in the three-dimensional DSMC model based on a one-way coupled method as detailed in section 2.4. Parallelization aspects of this two-phase three-dimensional DSMC model applied for

micro flow simulation are discussed in this work. Parallel performance aspects of the DSMC code are dealt with in detail by doing a performance comparison on different advanced supercomputing platforms and a PC cluster. The performance results illustrate the portability and scalability of the method as been discussed in Benzi and Damodaran [66]. Super-linear speedup is obtained for the parallel case on all the computing platforms considered, implying a drastic reduction in the computational time. Load balancing aspects have also been dealt with and a dynamic load balancing scheme is implemented which results in further performance improvements.

4.2 Parallel Implementation of Two-phase DSMC Method

The parallel 2-phase DSMC program is implemented using Message Passing Interface (MPI) [30] library routines. The DSMC program has been implemented in C++ programming language and various programming features such as *classes* and dynamic allocation of memory have been used in this work. As three-dimensional DSMC flow simulations require massive computing resources especially in terms of the computer memory resources, the use of *classes* and dynamic allocation and deletion of memory leads to an elegant approach for memory intensive applications.

The parallel DSMC approach is summarized in the flow chart shown in Fig 4.1. In the parallel implementation the domain has been partitioned into several sub-domains and assigned to different processors. Each processor performs the computational steps for the list of gas molecules for the sub-domain it is associated with. In a DSMC simulation, data communication is associated with the transport of molecules between adjacent sub-domains at any time step. The information pertaining to a molecule crossing from its sub-domain to another sub-domain must be communicated at every time step. To account for any parallel inefficiency arising from a load imbalance owing to a disparity in the number of particles held between different processors, the domain is repartitioned once the system starts to attain a steady state, such that each processor has approximately the same number of particles. Once steady state has been achieved, each processor does sampling for its own sub-domain.

Figure 4.1: Flow chart for the parallel DSMC method

The computation of the particle trajectories in the 2 phase DSMC method starts only once the system has reached steady state as shown in Fig. 4.1. The processor, in which the particle resides currently, performs all the computational steps associated with the computation of particle trajectory. When the particle crosses over to the next sub-domain, the index number of particle and the rank number of the processor has to be communicated such that the new processor now does the computations involved for the particle trajectory. The results for both the flow variables such as number density, velocity, temperature and the particle trajectory information from the two-phase model from each processor are sent to the host processor after the sampling phase. The host processor then gathers all the separate results into one single output file. The salient features of the parallelization process based on this approach are described in detail below.

4.2.1 Domain Decomposition Approach

The computational domain is partitioned uniformly along the x direction into several sub-domains as shown in Fig 4.2 and the sub-domains mapped onto different processors. Uniform rectangular cells are considered for the collision cells. The use of such Cartesian rectangular cells avoids any cell overlaps between different processors and makes it easier to sort particles and implement collisions. Since the slider wall is inclined at a certain pitch angle, it cuts through some of the cells within the computational domain resulting in partial cells which are accounted for by considering only the part of volume of the cell within in the simulation domain. The partitioning of the domain is based on load balancing considerations as discussed later in section 4.3.3.

Figure 4.2: Schematic representation of the partitioning of the computational domain

4.2.2 Data Communication

In a parallel DSMC simulation, data communication between the processors occurs at each time step after the *move* phase in which gas molecules are allowed to move. If at any time step a molecule leaves its sub-domain and enters another sub-domain, then the particle has to be deleted from the current sub-domain and added to the existing list of particles in the new sub-domain. All the information pertaining to that gas molecule such as its spatial coordinates and velocity components needs to be communicated to the new host processor. Instead of sending separate *MPI_Send* commands and corresponding *MPI_Recv* commands for passing each of these information, MPI provides a set of packing and unpacking subroutines using *MPI_Pack* and *MPI_Unpack*, respectively by which all the non-contiguous pieces of information related to a particle are packed into a contiguous section of memory and transferred as a single message rather than sending separate messages for each information.

For the 2-phase DSMC calculations, communication needs arise if a particle crosses over to the next sub-domain after a certain number of time steps. In that case the index number of particle, the current particle co-ordinates and the current particle velocity has to be communicated so that the new processor now does the computations involved for the particle trajectory. The rank number information of the new processor is send across to all the processors using the *MPI_Bcast* command, so that that the correct processor does the particle trajectory operations.

4.2.3 Parallel Platforms Considered

To assess the portability of the parallel DSMC code, the implementation of the code on four different supercomputing platforms, namely, *AlphaServer (SC45)*, *Sun Fire 15000*, *SGI Onyx 3800* and *SGI Origin 2000* has been considered. The *AlphaServer Supercomputer (SC45)* is a distributed memory parallel super computer having 44 nodes each of which is an SMP with four 1GHz processors having 1 GB memory and 8 MB cache. The *Sun Fire* and *SGI* systems considered are shared memory computing

platforms. The *Sun Fire 15000* system comprises of 32 CPUs with 64 GB onboard memory, each utilizing 900MHz processors and 8 MB cache. The *SGI Onyx 3800* system comprises of 32 CPUs with 32 GB onboard memory, each having processors of 400MHz and 8 MB cache while the *SGI Origin 2000* system has 32 CPUs with 16 GB onboard memory, each utilizing processors of 250MHz and 4 MB cache. Besides the supercomputing platforms considered, performance study has also been done on a distributed memory Xeon Linux PC Cluster with 9 nodes each having 4 GB memory and two dual core Xeon processors of CPU speed 2.33 GHz and 4 MB cache.

4.3 Results and Discussions

In this section the parallel performance results of the parallel DSMC method on various supercomputing platforms and a PC cluster is discussed. All the performance studies reported in this work have been undertaken for single phase-DSMC, i.e two-phase computations are not considered for the performance study. Load Balancing considerations are also discussed to further improve the parallel performance.

4.3.1 Supercomputing Platforms

The performance parameters, Speedup is defined as $S = T_s/T_p$, where T_s and T_p are the serial and parallel simulation times respectively and Efficiency is defined as $E = S/p$, where p is the number of processors. To study the performance aspects of the parallel DSMC code, all performance studies have been undertaken for a slider bearing geometry of length 3 microns, width 3.3 microns and flying height 25nm consisting of $64 \times 4 \times 50$ cells and 400,000 particles.

The performance of a parallel three-dimensional DSMC method is compared to an equivalent two-dimensional DSMC simulation first on the *AlphaServer Supercomputer* (SC45) in Fig 4.3. The two-dimensional DSMC simulation has been conducted on the same geometry in two-dimensions, consisting of 64×4 cells and about

8000 particles. Approximate linear speedups are observed for up to 4 processors for the two-dimensional case after which the speedup curve drops. For the three-dimensional case super linear speedup is observed, wherein the speedup is greater than the theoretical speed up implying drastic reduction in the computational time. The super linear speedup can be attributed to cache effects. By using multiple processors the size of sub-problem is reduced such that the data easily fits into caches resulting in significant reduction in memory access time for the parallel case as compared to the serial problem where the domain is large and the potential for cache reuse is reduced. The reduction in memory access time results in additional speedup apart from that obtained due to reduction in computation time. The better performance for the three-dimensional case can be attributed to the fact that there are much more computations per time step when compared to an equivalent two-dimensional case.

Figure 4.3: Speedup plot on *Alphaserver -SC 45*

The scaling characteristics of the parallel three-dimensional DSMC method has also been investigated by considering three test cases on the same geometry but with different number of particles i.e., 200,000, 400,000 and 800,000 particles. The performance curves for the three cases are shown in Fig 4.4. The performance curves

show good scaling characteristics with super linear speedups for all the three test cases. Correspondingly efficiency greater than 100 % is obtained. For a fixed load the problem scales up well till a higher number of processors and with increase in computational load an improved performance is obtained. The best performance is observed for the case with 800,000 particles wherein super-linear speed is observed consistently till 64 processors. For the case with 400,000 particles super-linear speedup is observed up to 32 processors, while for 200,000 particles super-linear speedup is observed only up to 8 processors. With further increase in the number of processors, although the problem size reduces resulting in a higher potential for cache based performance, the speedup curve drops and subsequently falls below the theoretical speedup as the problem becomes communication bound. This shows that for large three-dimensional DSMC problems, an increased reduction in CPU time can be obtained as the parallel program scales up well up to a higher number of processors.

The performance level of the parallel program on different computers has been studied to check the portability of the DSMC program. The parallel DSMC code has been successfully run on other computational platforms such as *Sun Fire 15000*, *SGI Onyx 3800* and *SGI origin 2000*. Fig 4.5 compares the parallel performance curves obtained on these platforms, namely *SunFire* and *SGI systems*, with those obtained for *Alphaserver*. The test case with 400,000 particles has been considered for the purpose. Superlinear speedups are obtained on all the computers considered. Sustained speedups are obtained for up to 32 processors for the *Alphaserver* and *Sun Fire systems* resulting in significant reduction in computational time. The nodes of both these machines have a significantly higher processor speed and a much higher node memory. The *SGI systems* show super-linear speedup for up to only 16 processors after which the speedup curve drops. The variation of CPU time taken for the case with 400,000 particles for 2000 iterations on different supercomputing platforms considered is shown in Fig 4.6.

(a)

(b)

Figure 4.4: Performance curves on *Alphaserver -SC 45* (a) Speedup (b) Efficiency

(a)

(b)

Figure 4.5: Comparison of Parallel performance of the DSMC code between different computational platforms (a) Speedup (b) Efficiency

Figure 4.6: Variation of CPU time taken on between different computational platforms considered

4.3.2 PC Cluster

The parallel performance study has also been done on a distributed memory Linux PC Cluster with 9 nodes each having 4 GB memory and two dual core Xeon processors of CPU speed 2.33 GHz and 4 MB cache. The nodes are connected by *Linksys Gigabit Ethernet* switch. The advantage of a PC cluster is that it has a higher performance to cost ratio when compared to the supercomputing platforms considered. The performance of the parallel program is shown in Fig 4.7. The same test case with 400,000 particles is considered for this purpose. Super-linear speedup has been observed for up to 8 processors, after which the parallel efficiency drops as communications begin to dominate. Since the processors have a significantly higher memory and processor speed, drastic reductions in computational time can be achieved using a fewer number of processors, as compared to the supercomputing platforms considered. In addition with the dual core technology associated with the current processors, computational resources can be efficiently utilized. By this a parallel program in a node having two dual core processors as in the PC cluster considered currently, can be run as four MPI processes. For example in the current study the parallel DSMC code showed a 55% reduction in CPU time while going from 2 MPI processes per node to 4 MPI processes per node.

Figure 4.7: Parallel performance on the PC cluster

The comparison of speedup obtained on all the different computers considered is summarized in Table 1.

nproc	<i>Alphaserver SC-45</i>	<i>Sun Fire 15000</i>	<i>SGI Onyx 3800</i>	<i>SGI Origin 2000</i>	<i>PC cluster (Einstein)</i>
2	3.21	2.61	3.0	3.01	3.17
4	7.17	5.94	6.75	7.21	7.34
8	14.8	12.6	13.3	15.9	8.15
16	28.1	26.8	25.9	30.6	10.79
32	33.6	29.5	19.9	24.8	
64	32.2				

Table 1: Summary of Speedup on different computing platforms

4.3.3 Load Balancing Considerations

There is no single domain partitioning technique that ensures an optimum load balancing through out the simulation based on the DSMC method. Rather it is problem dependent and is influenced by various factors such as flow gradients, number of particles on each processor etc. The distribution of particles in the computational domain could vary remarkably as the simulation progresses, thereby leading to a load imbalance between the processors. Various load balancing schemes based on repartitioning the domain, when there is a load imbalance between the processors have been reported in literature. Among such schemes include repartitioning of the domain at fixed intervals or based on a decision policy based on the *Stop-At-Rise (SAR)* method which has been described in Nance et al. [67], LeBeau [61] and Wu and Tseng [63].

A simple re-partitioning scheme is outlined in this work for enabling load balancing. In the HDI gap air flows between the slider and the rotating disk and providing sufficient lift force to fly the slider above the rotating disk. To enable this there is a larger particle accumulation and correspondingly higher pressure which occurs in the vicinity of the trailing edge of the slider. Hence the domain decomposition scheme in which the domain is uniformly partitioned along the x direction (referred to as *no load balancing*) as shown in Fig. 4.2 results in an unequal distribution in the number of cells and particles between the processors. Therefore a good load balancing may not be achieved especially for cases when the slider pitching angles are high. To do a detailed load balance study, a slider bearing geometry in which $L = 3\mu m$ and $H_1/H_0 = 4$ is considered. The particle accumulation plot obtained for a parallel DSMC simulation using eight processors with *no load balancing* is shown in Fig 4.8 (a) from which it can be seen that the particle keeps accumulating in the domain with each iteration and once the simulation reaches a steady state the number of particles in each processor fluctuates about a constant number. The wide disparity in the number of particles between each processors, result in load imbalance and leads to computational inefficiency. The corresponding plot for the case with domain decomposition based on approximately *equal number of cells* in each processor is shown in Fig 4.8 (b). The scheme with equal number of cells has

approximately equal number of particles in each processor initially, but as the simulation proceeds there is clearly a load imbalance based on number of particles.

To account for the load imbalance, a dynamic load balancing scheme has been implemented by which at the start of the simulation the computational domain is partitioned, such that each processor has approximately equal number of cells. Equal number of cells in each domain ensures that each processor is loaded with about the same number of particles during the initial phase of the simulation. The simulation is monitored for attainment of steady state upon which the number of particles in each processor remains about the same. Once the system starts to attain a steady state, the domain is repartitioned among the processors so that each processor has approximately equal number of particles. To illustrate the computational savings obtained by this approach, the comparison of performance based on elapsed time taken at an interval of every 100 iterations between the different domain decomposition schemes considered corresponding to *no load balancing*, *equal number of cells* and *dynamic load balancing* cases is shown in Fig 4.9.

It can be clearly seen from the figure that the domain decomposition based on *equal number of cells* performs better initially compared to that with *no load balancing*, but further down as particle accumulates the performance degrades. The best performance is observed for the *dynamic load balancing* case as a reasonably good load balance is attained through out the simulation, with computational savings of about 12 % attained for the entire simulation.

(a)

(b)

Figure 4.8: Particle accumulation plot in different processors with domain decomposition based on (a) no load balancing (b) equal number of cells

Figure 4.9: Comparison of elapsed time between different domain decomposition schemes

CHAPTER 5

THE REYNOLDS GAS LUBRICATION EQUATION AND A COUPLED REYNOLDS-DSMC MODEL

5.1 Introduction

Traditionally flow characteristics in slider air bearings have been modeled by the Reynolds gas lubrication equation. Reynolds equation is derived from the Navier-Stokes equation to approximate gas lubrication flows in slider bearings. It is a continuum model. However for gas lubrication in small form factor sliders when significant deviations from continuum hypothesis manifest, various slip correction models have been incorporated into the Reynolds equation by various researchers. A first order slip correction has been introduced by Burgdorfer [68] and a second order slip correction has been introduced later by Hsia and Domoto [69]. Implementation of the first order slip model has been shown to overestimate the pressure solution while the second order model tends to underestimate the pressure solution in the transition regime. To resolve these shortcomings, Mitsuya [70] proposed a 1.5-order slip model for solving the Reynolds equation as an attempt to mediate the estimation of the pressure. Beskok [71] proposed a velocity slip boundary condition of second order accuracy which relied on empirical coefficients for accurate predictions in the transition regime. An improved stress-density ratio slip corrected Reynolds equation model proposed by Ng et al. [72] seem to provide a more accurate solution in transition regime. A modified slip model using molecular dynamics introduced by Sun et. al. [73] attempts to account for the impact of molecular collisions. This model incorporates the variable hard sphere (VHS) and variable soft sphere (VSS) molecular effects to provide a more accurate solution. However these models do not result in accurate predictions when the flow approaches the free molecular regime. Later Sun and Chan [74] introduced an improved analytical model based on the kinetic theory of gases, which provides accurate solution in most non-continuum regimes.

Fukui and Kaneko [21] developed a more sophisticated model for the Reynolds equation, based on the Boltzmann equation, where the Poiseuille flow rate is calculated on the basis of a linearized Boltzmann equation. The Fukui and Kaneko model provides a generalized lubrication equation for any arbitrary Knudsen number and has been shown to give accurate solutions even in the free molecular regime. A phenomenological lubrication model in the entire Knudsen number regimes based on the flow rate data base by Fukui and Kaneko has been introduced by Bahukudumbi and Beskok [75] in which analytical expressions for computing the velocity profile in the entire slider bearing region were developed.

In this chapter the Reynolds equation model using the various slip correction models has been analyzed and compared for computing the pressure profile. The Fukui-Kaneko Reynolds model has been selected as it provides a generalized lubrication model and has been employed to compute the pressure profile in the slider bearing region. A coupled Reynolds-DSMC method is then proposed to couple the solutions of the Reynolds equation model to regions modeled by the DSMC method both for two-dimensional and three-dimensional cases. This method can be employed when a detailed atomistic simulation is required to obtain accurate flow conditions in any localized region such as near the read/write head region. The next generation HDD's require flying height of the order of a few nanometers. In such scenarios, various factors such as particle-surface interaction, disk surface shape, heat generation due to slider-disk contact etc would play a key role in determining the accurate flow field conditions near the read/write head region. DSMC can be employed for a detailed investigation in any such small selected region of interest to capture the true physics, while the rest of the slider bearing region can be modeled by the Reynolds equation. The coupling approach provides a frame work for coupling the Reynolds equation model to the region modeled by DSMC.

5.2 The Reynolds Equation Model

At the continuum level Navier-Stokes equations are the fundamental equations which govern the fluid flow. The thickness of the air bearing formed is extremely small in comparison to the length of the bearing and also the Reynolds number is very small due to the small characteristic dimensions involved. Hence for the slider air bearing problem the Navier-Stokes equation can be highly simplified to derive the Reynolds equation as outlined in Gross [76].

A schematic of the three-dimensional slider bearing geometry and the computational domain of interest is shown in Fig. 5.1. The bottom wall represents the spinning disk region moving with a tangential velocity U relative to the upper wall which is inclined at a pitch angle of α and represents the slider. The channel length is L and the computational domain boundaries of the region are assumed to be at a constant temperature T_0 . At the inflow and outflow ambient pressure P_0 is assumed. The visualization plane along which flow results are plotted is also shown in the figure, which is perpendicular to the yz plane and passes through the centre line of the slider.

Figure 5.1: Schematic of the three-dimensional slider geometry and computational domain

The generalized three-dimensional Reynolds equations in three dimensions for a slider bearing is expressed as

$$\frac{\partial}{\partial x}(ph^3Q\frac{\partial p}{\partial x}) + \frac{\partial}{\partial z}(ph^3Q\frac{\partial p}{\partial z}) - \left\{ \frac{\partial}{\partial x}(6\mu U_x ph) + \frac{\partial}{\partial z}(6\mu U_z ph) \right\} = 12\mu \frac{\partial(ph)}{\partial t} \quad (5.1)$$

In non-dimensional form equation 5.1 can be written as

$$\frac{\partial}{\partial X}(QPH^3\frac{\partial P}{\partial X} - \Lambda_x PH) + \frac{\partial}{\partial Z}(QPH^3\frac{\partial P}{\partial Z} - \Lambda_z PH) = \sigma \frac{\partial}{\partial T}(PH) \quad (5.2)$$

where P , H and T are the dimensionless pressure, distance and time

$$H = \frac{h}{h_{\min}}, \quad P = \frac{p}{p_a}, \quad T = \frac{t}{\omega}, \quad X = \frac{x}{L}, \quad Y = \frac{y}{L}$$

$$\Lambda_x = \frac{6\mu UL}{p_a h_m^2} \text{ and } \Lambda_z = \frac{6\mu VL}{p_a h_m^2} \text{ are the bearing numbers in the x and y direction and}$$

$$\sigma = \frac{12\mu\omega L^2}{p_a h_m^2} \text{ is the squeeze number.}$$

The term μ is the dynamic viscosity of the gas, ω is the angular disk velocity and Q is the flow factor which depends upon the slip correction. The flow factor Q for the various slip models can be expressed as:

$$Q = \frac{Q_p(D, a)}{Q_{con}(D)} \quad (5.3)$$

where Q_p is the Poiseuille flow coefficient and Q_{con} is the coefficient for a continuum flow, D is the inverse Knudsen number defined as $D = 0.5\sqrt{\pi}/Kn$ and a is the accommodation coefficient.

$$Q_{con} = \frac{D}{6} \quad (5.4)$$

The Poiseuille flow rates for the various models of Reynolds equation can be calculated as

$$\text{Continuum model} \quad Q_p = \frac{D}{6} \quad (5.5)$$

$$\text{First Order slip model} \quad Q_p = \frac{D}{6} + \frac{\sqrt{\pi}}{2} \quad (5.6)$$

$$\text{Second Order slip model} \quad Q_p = \frac{D}{6} + \frac{\sqrt{\pi}}{2} + \frac{\pi}{4D} \quad (5.7)$$

$$\text{1.5 order slip model} \quad Q_p = \frac{D}{6} + \frac{\sqrt{\pi}}{2} + \frac{\pi}{9D} \quad (5.8)$$

$$\text{Stress-density ratio model} \quad Q_p = \frac{D}{6} + \frac{\sqrt{\pi}}{2} \left(\frac{2}{\sigma} - 1 \right) \frac{\sqrt{\pi}}{2} \psi \quad (5.9)$$

$$\text{VHS and VSS slip model} \quad Q_p = \frac{D}{6} + \xi \frac{\sqrt{\pi}}{2} + \xi^2 \frac{\pi}{4D} \quad (5.10)$$

In equation 5.10, $\xi = \frac{\alpha \Gamma\left(\frac{9}{2} - \omega\right)}{(\alpha + 1)(\alpha + 2)} \pi^{0.5 - \omega}$; α and ω are the constants of the VHS and VSS models.

In equation 5.9 $\psi = C_s \mu \frac{\sqrt{2} \pi d^2}{m}$, slip coefficient, $C_s = \left(\frac{2}{\sigma} - 1 \right) \frac{1}{\sqrt{2RT/\pi}}$, σ is the accommodation coefficient and R is the gas constant

The Poiseuille flow rates for the Fukui and Kaneko's model can be calculated from the power series expressions provided by Fukui and Kaneko [77] as

$$\left\{ \begin{array}{ll} Q_p = D/6 + 1.0162 + 1.0653/D - 2.1354/D^2 & ; 5 \leq D \\ Q_p = 0.13852D + 1.25087 + 0.15653/D - 0.00969/D^2 & ; 0.15 \leq D < 5 \\ Q_p = -2.22919D + 2.10673 + 0.01653/D - 0.0000694/D^2 & ; 0.01 \leq D < 0.15 \end{array} \right\} \quad (5.11)$$

5.2.1 Problem Formulation

The generalized Reynolds equation for the steady case can be written from equation 5.2 as

$$\frac{\partial}{\partial X}(QPH^3 \frac{\partial P}{\partial X}) + \frac{\partial}{\partial Y}(QPH^3 \frac{\partial P}{\partial Y}) - \left(\frac{\partial}{\partial Y}(\Lambda_y PH) + \frac{\partial}{\partial X}(\Lambda_x PH) \right) = 0 \quad (5.12)$$

The terms in equation 5.12 needs to be expanded before it can be solved. The derivation of all the terms in the equation 5.12 is done as follows.

The first term can be written as

$$\frac{\partial}{\partial X}(PH^3 Q \frac{\partial P}{\partial X}) = PH^3 Q \frac{\partial^2 P}{\partial X^2} + 3PH^2 Q \frac{\partial H}{\partial X} \frac{\partial P}{\partial X} + H^3 Q \left(\frac{\partial P}{\partial X} \right)^2 + PH^3 \frac{\partial Q}{\partial X} \frac{\partial P}{\partial X} \quad (5.13)$$

Since Q is a function of both P and H we can write the last term in equation 4.8 as

$$PH^3 \frac{\partial Q}{\partial X} \frac{\partial P}{\partial X} = PH^3 \left(\frac{\partial Q}{\partial H} \frac{\partial H}{\partial X} \right) \frac{\partial P}{\partial X} + PH^3 \left(\frac{\partial Q}{\partial P} \right) \left(\frac{\partial P}{\partial X} \right)^2 \quad (5.14)$$

Substituting equation 5.14 in equation 5.13 we get,

$$\begin{aligned} \frac{\partial}{\partial X}(PH^3 Q \frac{\partial P}{\partial X}) = & PH^3 Q \frac{\partial^2 P}{\partial X^2} + 3PH^2 Q \frac{\partial H}{\partial X} \frac{\partial P}{\partial X} + H^3 Q \left(\frac{\partial P}{\partial X} \right)^2 \\ & + PH^3 \left\{ \frac{\partial Q}{\partial H} \frac{\partial H}{\partial X} \frac{\partial P}{\partial X} + \frac{\partial Q}{\partial P} \left(\frac{\partial P}{\partial X} \right)^2 \right\} \end{aligned} \quad (5.15)$$

Similarly the second term can be written as

$$\begin{aligned} \frac{\partial}{\partial Y}(PH^3 Q \frac{\partial P}{\partial Y}) = & PH^3 Q \frac{\partial^2 P}{\partial Y^2} + 3PH^2 Q \frac{\partial H}{\partial Y} \frac{\partial P}{\partial Y} + H^3 Q \left(\frac{\partial P}{\partial Y} \right)^2 \\ & + PH^3 \left\{ \frac{\partial Q}{\partial H} \frac{\partial H}{\partial Y} \frac{\partial P}{\partial Y} + \frac{\partial Q}{\partial P} \left(\frac{\partial P}{\partial Y} \right)^2 \right\} \end{aligned} \quad (5.16)$$

The third term in equation 5.12 can be derived as

$$\Lambda_x \frac{\partial}{\partial X} (PH) + \Lambda_y \frac{\partial}{\partial Y} (PH) = \Lambda_x \left[P \left(\frac{\partial H}{\partial X} \right) + H \left(\frac{\partial P}{\partial X} \right) \right] + \Lambda_y \left[P \left(\frac{\partial H}{\partial Y} \right) + H \left(\frac{\partial P}{\partial Y} \right) \right] \quad (5.17)$$

On substituting all the terms, equation 5.12 can be expressed as

$$\begin{aligned} & PH^3 Q \left\{ \frac{\partial^2 P}{\partial X^2} + \frac{\partial^2 P}{\partial Y^2} \right\} + 3PH^2 Q \left\{ \frac{\partial H}{\partial X} \frac{\partial P}{\partial X} + \frac{\partial H}{\partial Y} \frac{\partial P}{\partial Y} \right\} + H^3 Q \left\{ \left(\frac{\partial P}{\partial X} \right)^2 + \left(\frac{\partial P}{\partial Y} \right)^2 \right\} \\ & + PH^3 \left\{ \frac{\partial Q}{\partial H} \left[\frac{\partial H}{\partial X} \frac{\partial P}{\partial X} + \frac{\partial H}{\partial Y} \frac{\partial P}{\partial Y} \right] + \frac{\partial Q}{\partial P} \left[\left(\frac{\partial P}{\partial X} \right)^2 + \left(\frac{\partial P}{\partial Y} \right)^2 \right] \right\} \\ & - \Lambda_x \left\{ \left[P \left(\frac{\partial H}{\partial X} \right) + H \left(\frac{\partial P}{\partial X} \right) \right] + \Lambda_y \left[P \left(\frac{\partial H}{\partial Y} \right) + H \left(\frac{\partial P}{\partial Y} \right) \right] \right\} = 0 \end{aligned} \quad (5.18)$$

5.2.2 Numerical Solution

To solve the Reynolds equation numerically, finite difference method has been employed. The domain is first divided into a rectangular grid of $m \times n$ elements, where along the X direction there are $i = 0, 1, \dots, m-1$ nodes and along the Y direction there are $j = 0, 1, \dots, n-1$ nodes. The pressure at any discrete node point can be then expressed as $P_{i,j}$. The derivatives in equation 5.18 can be replaced with their second order finite difference approximations as

$$\frac{\partial P}{\partial X} = \frac{1}{2\Delta X} [P_{i+1,j} - P_{i-1,j}] \quad (5.19)$$

$$\frac{\partial^2 P}{\partial X^2} = \frac{1}{\Delta X^2} [P_{i+1,j} - 2P_{i,j} + P_{i-1,j}] \quad (5.20)$$

The spatial derivatives of H can be easily evaluated since the height of the slider air bearing at the different node points (i, j) is known. At the inflow and outflow boundary the pressure is known and is specified as ambient pressure ($P = 1 \text{ atm}$). So at

the nodes along the inflow and outflow boundary, Dirichlet boundary conditions can be specified (i.e. $P = 1$). The resulting set of non-linear equations formed can be solved by an iterative technique like the Newton's method to obtain the three-dimensional pressure field in the slider bearing. The various slip corrected and the Fukui-Kaneko Reynolds equation models have been solved using codes which have been written for the purpose in MATLAB.

5.3 Reynolds Equation Solutions

5.3.1 Two-Dimensional Solutions

The continuum and various slip corrected Reynolds equation models have been tested and implemented for validation purposes. A slider bearing of configuration $L = 5\mu m$, $H_1 = 100nm$, $H_0 = 50nm$ and $U = 25m/s$ has been considered for the purpose. Ambient conditions have been assumed i.e. $P_0 = 1atm$, $T_0 = 273K$ and the viscosity of the gas considered is $\mu = 2.08 \times 10^{-5}Ns/m^2$.

The solutions of the various Reynolds equation models have been compared with the DSMC result, which is considered as the exact solution for the same slider bearing in Fig 5.2. From the figure it can be seen that the continuum model fails to predict the flow condition in the air bearing accurately, the maximum deviation being about 40% for this particular case. The first order slip model overestimates the pressure, while the second order slip model underestimates the pressure. The 1.5 order slip model and the stress-density ratio model predict a much better estimate for the solutions of pressure close to that of the DSMC solution. The Fukui Kaneko model of the Reynolds equation closely matches with the DSMC solution confirming the validity of this model. The Fukui and Kaneko model has been selected for all further computations using the Reynolds equation in this work.

Figure 5.2: Comparison of solutions of various Reynolds equation models with DSMC

5.3.2 Three-Dimensional Solutions

The pressure profile in a three-dimensional slider air bearing has also been computed using the Fukui-Kaneko Reynolds equation model. Two cases of slider air bearing geometry of configuration $L = 4\mu m$, $W = 3.3\mu m$, $U = 25 m/s$ with different cases of flying height, viz. $H_0 = 25 nm$ and $H_0 = 15 nm$ has been considered. The different views of the computed three-dimensional pressure profiles for the two cases are shown in Fig 5.3 and Fig 5.4.

Figure 5.3: Computed pressure profiles for $L = 4\mu m$, $W = 3.3\mu m$, $H_0 = 25 nm$ and $U = 25 m/s$

Figure 5.4: Computed pressure profiles for $L = 4\mu m$, $W = 3.3\mu m$, $H_0 = 10 nm$ and $U = 25 m/s$

5.4 A Coupled Reynolds-DSMC Approach for HDI Gap Flow Modeling

A coupled Reynolds-DSMC model to couple the Reynolds equation model solutions to the DSMC model, in instances where a detailed atomistic simulation is required in any localized region in the HDI region is discussed in this section. The DSMC method although computationally expensive, has many advantages over the Reynolds equation model in that many of the assumptions required by the lubrication theory can be relaxed and thus can capture the exact physics. For example at the inflow and outflow regions of the slider air bearing, the Reynolds equation assumes fully developed flow conditions and assumes a boundary condition of one atm. However in a real slider this need not be the case because of the slowing down of the flow in these regions. Also the basic Reynolds equation assumes the flow to be plane flow and doesn't directly take care of any surface roughness effects. The flow is also considered to be isothermal throughout. However this need not be the case always, especially near the read/write head region either due to partial contact, "thermally assisted" recording or when a small region near the read/write head is heated by external means to reduce the head-media spacing during read/write which in turn helps in the design of increased the recording capacity. Besides the Fukui Kaneko Reynolds equation model based on the solution of a linearized Boltzmann equation in a two-dimensional channel results in a logarithmic increase in the Poiseuille flow rate in the free molecular region. This is contrary to the three-dimensional behavior as noted by Bahukudumbi and Beskok [75], which might affect the accuracy of the flow solutions in the free molecular region.

In instances where a detailed atomistic simulation is required near the HDI region to capture the exact physics, DSMC method needs to be employed. In this work, a method for coupling the solutions from the Reynolds equation model to the DSMC model in such regions is described, the motivation being to achieve economic computation of accurate solutions in the HDI regions of the slider air bearing. A simple one-way coupled Reynolds-DSMC method has been employed to match the pressure solutions obtained from the Reynolds equation method with the DSMC method in localized small regions

such as the HDI region. It is shown how the pressure solutions in the rest of the slider bearing region merges with that near the read/write head region.

The slider bearing region is divided into two sub-domains as shown in Fig. 5.5. Flow field in the sub-domain Ω_R of length l_r is modeled by the Fukui-Kaneko Reynolds equation model, while the flow in sub-domain Ω_D of length l_d is modeled by the DSMC method. The span of the Reynolds sub-domain Ω_R considered is such that it is farther away from the read/write head region where the assumptions of the Reynolds equation hold. The DSMC sub-domain Ω_D considered is an extremely small region compared to the rest of the slider bearing such that it is computationally feasible to be modeled by the DSMC method. In a real slider the length of the slider bearing region is about 1 mm and Ω_D represents the read/write head region of length about 1-2 microns. The inflow boundary condition for this region is not known *a priori* and needs to be determined from the Reynolds equation model.

Figure 5.5: Schematic of the two-dimensional computation domain showing the two sub-domains

The inflow boundary of the DSMC sub-domain is located such that it falls along the centre of a Reynolds equation cell. In the present approach of coupling, first the Reynolds equation model has been used to compute the pressure field in the entire slider bearing region. The computed pressure solution at the coupling boundary obtained from

the Reynolds equation model is extracted and this forms the Dirichlet boundary condition at the inflow for solving the DSMC sub-domain, while at the outflow, ambient pressure conditions are imposed. The DSMC sub-domain can be then solved by employing the pressure boundary conditions at the inflow and outflow by the implicit boundary treatment method as described in section 3.3. The velocity field in Ω_R can be obtained indirectly from the computed pressure solutions using the analytical expressions from the Beskok model [75].

A similar one-way coupling procedure has been done for a three-dimensional coupled Reynolds-DSMC modeling. The three-dimensional slider configuration is shown in Fig. 5.6, which also shows the coupling plane (yz plane), oriented along the z direction and perpendicular to the xy plane along which the coupling could be done.

Figure 5.6: Schematic of the three-dimensional computation domain

The inflow boundary condition for the small DSMC region is not known *a priori* and must be determined from the Reynolds sub-domain to provide the inflow boundary conditions required to simulate the flow conditions in the DSMC region. The Reynolds equation model is first employed to obtain the pressure field in the entire slider bearing region. In the three-dimensional case however, pressure also varies along the z direction, in the coupling plane. The computed pressure profile from the Reynolds equation along the coupling plane is extracted and this pressure solution can be imposed as the inflow boundary condition for the DSMC region. This has been implemented by imposing the

corresponding pressure solution in the cells at different sections along the coupling plane and applying the implicit boundary treatment to derive other flow variables. All the other three sides of the slider have been treated as outflow where ambient pressure is fixed as the boundary condition. The simulation then proceeds in a similar manner to that for the two-dimensional case. It is to be noted that although here the read/write region of the slider has been considered as the DSMC region, in principle this approach can be extended to any selected region in which a detailed atomistic simulation is required. A similar procedure can be implemented for such a case for coupling the solutions between the two sub-domains.

5.4.1 Coupled Reynolds-DSMC Solutions

A simple case has been considered first to check the feasibility of the coupled Reynolds-DSMC method. A slider bearing geometry of length $L = 4\mu m$, flying height $H_0 = 25nm$, and disk velocity $U = 25m/s$ is considered. The gas and wall surfaces have been assumed to be kept at a constant temperature $T_0 = 273K$. The Reynolds and DSMC sub-domains are taken such that $l_r = 2\mu m$ and $l_d = 2\mu m$ as shown in the Fig. 5.5. The computed pressure profile obtained using the coupled approach is compared with the DSMC solutions in the entire domain and is shown in Fig. 5.7. In the figures *full Reynolds* and *full DSMC* denote the solutions in the entire domain obtained using Reynolds equation and DSMC method respectively. *Coupled DSMC* denotes the solutions in the DSMC sub-domain Ω_D obtained from the coupled Reynolds-DSMC method. With the DSMC solution in the full domain considered as the exact solution, the maximum deviation for the pressure solution between the coupled model and the exact DSMC solution is less than 5%. As an additional check the flow velocity at the disk surface in the DSMC sub-domain is also compared with the full domain DSMC solutions in Fig. 5.8. The coupled DSMC solutions compare well when compared to that for the full domain.

Figure 5.7: Comparison of *coupled DSMC* pressure solution with *full DSMC* solutions

Figure 5.8: Comparison of *coupled DSMC* flow velocity solution with the *full DSMC* solution

In order to further verify the coupled Reynolds-DSMC approach, another case has been considered for which the pressure solution from the Reynolds equation model differs from the DSMC solutions significantly. This has been done by applying different wall temperatures to different segments of the slider configuration. The same slider configuration of dimensions $L = 4\mu m$, $H_0 = 25nm$ and $U = 25m/s$ is considered. A higher wall temperature of $323K$ is considered at both the bottom and top plates in a small region of length $0.5\mu m$ towards the trailing edge of the slider. In rest of the region of length $3.5\mu m$, a wall temperature of $273K$ is considered. The region with a higher wall temperature is extremely small considered to the rest of the slider bearing region and so it can be safely assumed for this case that farther away from the read/write head region, the flow field conditions are not affected and are isothermal. Physically the higher temperature can be interpreted as due to heat generation due to partial contact. This could lead to a higher peak pressure and correspondingly a higher load carrying capacity due to the higher temperature and thermal creep effects. The coupled Reynolds-DSMC approach can be employed to explore how the solutions in the Reynolds equation sub-domain merges with the exact DSMC solutions near the read/write head region. The Reynolds and DSMC sub-domains are taken such that $l_r = 2\mu m$ and $l_d = 2\mu m$ as in the previous case. The coupled pressure solution in the DSMC sub-domain is compared with the Reynolds and DSMC solutions for the entire domain and shown in Fig. 5.9. The *full DSMC* solution can be considered as the exact solution. It can be seen from the figure that the Reynolds equation solution deviates considerably from the exact solution in the vicinity of the region where a higher wall temperature is imposed. The coupled Reynolds-DSMC solutions are in good agreement with the exact solution. This shows that in instances where a detailed atomistic simulation is required near the read/write head region, DSMC can be employed while being coupled to the Reynolds equation solutions in the rest of the region.

Figure 5.9: Comparison of *coupled DSMC* pressure solution with *full DSMC* solutions

Next a slider bearing of realistic length $L = 1 \text{ mm}$ has been considered which is representative of an actual slider in a modern HDD. The flying height considered is $H_0 = 50 \text{ nm}$ and $H_1/H_0 = 2$. To apply the coupled Reynolds-DSMC approach for this slider configuration, the Reynolds and DSMC sub-domains are taken such that $l_r = 997 \text{ }\mu\text{m}$ and $l_d = 4 \text{ }\mu\text{m}$. The Reynolds equation solution for pressure in entire slider bearing is shown in Fig. 5.10. The coupled Reynolds-DSMC pressure solution obtained is compared with the full Reynolds solution in Fig. 5.11. It can be seen from the figure that the coupled DSMC solution coincides closely with the full Reynolds solution.

Figure 5.10: Pressure profile from the Reynolds Equation model for the full domain

Figure 5.11: Comparison of coupled Reynolds-DSMC pressure solution with the *full Reynolds* solution

The feasibility of predicting the flow in the three-dimensional slider-air bearing using the coupled Reynolds-DSMC method has also been considered. For the purpose, a simple case of the slider air bearing of $L = 4\mu m$, $H_0 = 25\text{ nm}$ and $U = 25\text{ m/s}$ has been considered. The Reynolds equation is used to compute the solutions in the full slider configuration and different views of the computed three-dimensional pressure profile is shown in Fig. 5.12. The DSMC sub-domain considered is of length $l_r = 2\mu m$ similar to that taken for the two-dimensional slider. The coupling plane for the three-dimensional Reynolds-DSMC coupling is as shown in Fig. 5.6. Along the coupling plane the pressure varies and is maximum along the centre line of the slider. The pressure profile obtained from the Reynolds equation along the coupling plane is shown in Fig. 5.13. At the inflow of the DSMC region, this pressure profile is imposed as the boundary condition. This is implemented by imposing the corresponding pressure information at the cells at different sections along the coupling plane. On all the other three sides of the slider considered as outflow, ambient pressure is fixed as the boundary condition. The implicit boundary treatment is then applied to the cells at the inflow and outflow regions to derive other properties such as velocity as the simulation progresses.

Figure 5.12: Different views of three-dimensional pressure profile obtained using Reynolds equation

Figure 5.13: Variation of pressure profile along the coupling plane Γ_D

For the DSMC computations a total of about 8000 cells, 40 cells along the x direction, 52 cells along the z direction and 4 cells along the y direction have been taken. About 240,000 particles have been taken initially for the simulations. Particles accumulate in the computational domain with each iteration and upon reaching steady state, fluctuate about a constant number after a certain number of iterations as shown in Fig. 5.14. Sampling is done for over a period of about 100000 time steps, once steady state has been reached. Different views of the three-dimensional pressure profile obtained for the DSMC region is shown in Fig. 5.15. A comparison of the coupled DSMC pressure solutions along the coupling plane is made with the imposed pressure boundary conditions from the Reynolds equation model in Fig. 5.16. Good agreement is observed indicating the accuracy of the imposed pressure boundary conditions. A comparison of the variation of the coupled Reynolds-DSMC pressure solutions with the full Reynolds solution along the visualization plane is made in Fig. 5.17. Good agreement is observed between the pressure solution in the coupled DSMC domain and the pressure solutions in the full domain.

Figure 5.14: Particle Accumulation in the computation domain as a function of iteration number

Figure 5.15: Coupled three-dimensional DSMC pressure profiles obtained in the DSMC sub-domain

Figure 5.16: Comparison of the *coupled DSMC* pressure solution along Γ_D with the *full Reynolds* solution

Figure 5.17: Comparison of the *coupled DSMC* pressure solution with the *full Reynolds* equation solution along the visualization plane

CHAPTER 6

HYBRID CONTINUUM-ATOMISTIC (NAVIER-STOKES - DSMC) MODELING IN THE HEAD- DISK INTERFACE GAP

6.1 Introduction

Rarefied gas flow applications often involve regions of both continuum and rarefaction and spans a wide range of Knudsen numbers. The DSMC method can model the entire Knudsen number regime accurately, but is a computationally prohibitive method to model the entire domain. This means that an atomistic model like DSMC must be limited to regions where it is really warranted. Multi-scale methods must be employed which can couple DSMC which is modeled only in rarefied regions to continuum models in the rest of the region. The continuum and atomistic sub-domains describe two different physical descriptions and the coupling method should involve methods to accurately exchange information between the two sub-domains. In an HDD enclosure the flow outside the slider falls in the continuum regime, while the flow in the HDI region falls in the transition regime as shown schematically in the Knudsen number demarcation plot in Fig 1.2. The global flow fields outside the HDI gap in the HDD enclosure can be accurately modeled using the incompressible Navier-Stokes equations. A hybrid continuum-atomistic method must be employed to couple the DSMC model in the HDI region to the flow outside the slider modeled by Navier-Stokes equation. In this work various modeling aspects have been discussed for the case of a hybrid continuum-atomistic simulation and a multi-scale model based on the Schwarz Alternating method is applied to couple the Navier-Stokes solution to the DSMC model to compute flow near the vicinity of the HDI gap.

6.2 Hybrid Continuum-Atomistic Modeling

The choice of the hybrid coupling method depends on the physics of the problem involved. Hadjiconstantinou [78] provides a review of the recent developments in the field of hybrid continuum-atomistic methods. The applicability of various coupling schemes to different flow problems have been studied in Wijesinghe and Hadjiconstantinou [28, 79]. Explicit flux based coupling method is appropriate for hypersonic flows for which the characteristic timescale is comparable to the DSMC time step. Multi-scale methods applied to hypersonic compressible flow problems reported in literature include that by Garcia et al. [25], Hash and Hassan [26], and Wadsworth and Erwin [27]. More recently hybrid methods have been applied for incompressible flow problems especially for modeling of microfluidics in MEMS applications. A hybrid continuum-atomistic method which relies on an explicit state based coupling scheme at each time step for hypersonic non-equilibrium flow applications have been reported recently by Schwartzentruber and Boyd [80]. However for low speed flows, as typically encountered in MEMS applications, there is a wide disparity between the timescales of atomistic and continuum models and implicit methods provide a framework for coupled solutions. As a result explicit flux based coupling for incompressible flow problems might be computationally prohibitive especially if the continuum sub-domain is very large. Also flux based coupling is not suitable for low speed flows because of the high statistical noise of the flux variables when compared with the state variables such as velocity. The Schwarz alternating method provides an implicit framework for obtaining coupled solutions for such cases.

The Schwarz method which has been originally developed as a domain decomposition method outlined in Quarteroni and Valli [81] for solving partial differential equations has been extended for hybrid continuum-atomistic coupling and was first applied to liquid flows by Hadjiconstantinou [82] and later for dense fluids by Werder et al. [83]. Wijesinghe and Hadjiconstantinou [28] demonstrated the Schwarz hybrid coupling for a driven cavity test problem by employing overlap regions in both x and y directions (two-dimensional coupling) and employed the Chapman-Enskog

distribution. Real applications of the Schwarz Alternating method to hybrid continuum-atomistic methods for gaseous flows in MEMS devices are in paucity in literature. The Schwarz method has been applied recently by Aktas et al. [29, 84] to predict the flow field in microfluidic filters. They had considered an overlap region in just one direction (one dimensional coupling) for the hybrid coupling of the continuum and atomistic sub-domains and employed the Maxwellian distribution function. A flux based coupling scheme have been employed previously for the coupling of continuum and DSMC solutions for the slider bearing problem by Memnonov [85]. Initial results of the hybrid coupling by the Schwarz Alternating method for the slider bearing problem have been reported in Benzi and Damodaran [86]. In the present work the Schwarz Alternating method has been employed for the hybrid coupling of continuum and atomistic sub-domains to compute flow in the vicinity of the HDI gap and the impact of overlap size on the convergence behavior of the Schwarz method is investigated in detail. By the Schwarz Alternating method, the coupling between the continuum and atomistic sub-domains is attained implicitly by iterating between the steady state solutions of the two sub-domains. An overlap region between the Navier-Stokes (NS) and atomistic regions facilitates the information exchange between the two domains in the form of Dirichlet boundary conditions. Exchange of flow variables such as velocity components etc., when compared to the exchange of flux variables ensures that the statistical errors associated with DSMC can be minimized [87]. Schwarz iterations are done with updated boundary conditions in each sub-domain until solutions of both sub-domains are identical in the overlap region. From the point of view of computational efficiency the atomistic region modeled by the DSMC method must be confined to rarefied regions while the remaining larger domain must be modeled as part of the continuum regime. One-dimensional Schwarz coupling employed by considering overlap region along one direction implies that the region modeled by DSMC for each Schwarz iteration could be very large resulting in poor computational efficiency. Thus for an optimum computational efficiency a two-dimensional coupling must be employed by considering overlap regions along both x and y directions. In this work the application of Schwarz coupling has been demonstrated in two-dimensions using the Chapman-Enskog distribution for boundary condition imposition from the continuum region to the DSMC region. The schematic of

the two-dimensional geometry with the decomposition of the simulation domain into Navier-Stokes and DSMC sub-domains is shown in Fig 6.1. In the continuum domain, the incompressible Navier-Stokes equation is solved using the commercial flow solver *Fluent* [10] which uses the finite volume method with the pressure equation derived using the SIMPLE method. The region under the slider and additional regions near the inflow and outflow is considered as the atomistic region which is modeled by DSMC, while rest of the region is considered as the continuum domain modeled by the Navier-Stokes equations. The slider bearing region considered is of length $L = 4\mu m$, flying height $H_0 = 25nm$, pitch angle $\alpha = 0.01 rad$ and the bottom wall velocity $U_w = 50 m/s$. Additional regions of length $l_{ext} = 1.5\mu m$ and height $h_{ext} = 156nm$ at either side of the slider are also considered part of the DSMC sub-domain as shown.

Figure 6.1: Schematic of two-dimensional computational domain showing DSMC and NS sub-domains with overlap region

In Fig 6.1, the solid lines AA_1A_2 and $A_3A_4A_5$ represent the atomistic boundary which receives the flow variables from the continuum domain while the dotted lines CC_1C_2 and $C_3C_4C_5$ represent the continuum sub-domain boundary which receives flow variables from the atomistic sub-domain. Schwarz coupling has been done in two dimensions, for which overlap regions are considered both along the x and y directions as

shown. The overlap along the x direction will be referred to as x -overlap which is of width $l_{x,ov}$ while the overlap along the y direction will be referred to as y -overlap which is of width $l_{y,ov}$. A similar overlap width is considered at both the inflow and outflow section with $l_{x,ov} = 0.5\mu m$ and $l_{y,ov} = 39nm$. A small selected region upstream of the slider denoted by the dotted rectangular region $DEFG$ as shown in Fig 6.1 is chosen to make contour plots of the hybrid solution obtained. In the Navier-Stokes sub-domain the flow conditions are considered as incompressible and isothermal. The no slip boundary condition is applied at all the walls denoted by W_{1-6} in the NS sub-domain as shown. The inlet boundary of the computational domain denoted by I in the figure is treated as a *Pressure Inlet*, while the outlet boundary denoted by O is specified as *Pressure Outlet* by which ambient pressure conditions of $P_0 = 1atm$ is specified.

Fig 6.2 illustrates the boundary condition transfer for the hybrid coupling using the Schwarz Alternating method. The DSMC and continuum sub-domains are tessellated using uniformly spaced rectangular cells. Dotted rectangular lines represent the cells in the continuum sub-domain, and solid rectangular cells represent the DSMC cells. The macroscopic flow velocities (U_{DSMC}, V_{DSMC}) computed in the DSMC cells can be imposed directly as Dirichlet boundary conditions at the face centers of the continuum domain boundary Γ_{NS} . The macroscopic velocities are obtained by time averaging the molecular velocities as normally done during the sampling phase in any standard DSMC procedure as follows

$$U_{DSMC} = \frac{1}{N_c} \sum_{i=1}^{N_c} u_i \quad (6.1)$$

$$V_{DSMC} = \frac{1}{N_c} \sum_{i=1}^{N_c} v_i \quad (6.2)$$

where N_c is the number of particles in the cell, (u_i, v_i) are the molecular velocity components. The computed flow velocity field from the DSMC cells are extracted and used in the continuum domain (in which Navier-Stokes equations are solved using

Fluent) as a boundary profile or via a user defined function (UDF) in *Fluent*. In order to mitigate interpolation errors at the continuum boundary, the face centers of the continuum cells along Γ_{NS} are aligned with the centers of the DSMC cells as shown in Fig 6.2.

Figure 6.2: Schematic illustration of the Schwarz coupling method

The boundary conditions from the continuum sub-domain to the DSMC sub-domain are imposed using buffer cells (located adjacent to the boundary of the DSMC sub-domain Γ_{DSMC}) which act as volume reservoirs filled with particles according to the density and velocity distribution corresponding to the Navier-Stokes solution in the continuum cells such that the number of particles generated correspond to the density information ρ_{NS} in the continuum cells. The Chapman-Enskog molecular velocity distribution is used to generate particles corresponding to the flow velocity (U_{NS}, V_{NS}) and velocity gradients in the Navier-Stokes sub-domain. The reservoir region is of length l_R as shown in Fig 6.2 and l_R is assumed such that it is sufficient to represent the entire range of velocity distribution function including the portion of the distribution function corresponding to the high velocity fraction. The length of the reservoir region for the

Chapman-Enskog distribution is the same as that for the Maxwellian distribution function. In the presence of a mean flow velocity U , the length of the reservoir region is taken as $l_R = v_{cutoff} \times \Delta t$ where $v_{cutoff} = 6 \times (V_{mp} + U)$ is the cutoff velocity, V_{mp} is the most probable velocity and Δt is the time step. This ensures that the length of the reservoir is adequate enough to represent the entire range of Chapman-Enskog velocity distribution. The Chapman-Enskog distribution can be generated numerically by the acceptance-rejection method as outlined in Garcia and Alder [88]. The Chapman Enskog velocity distribution $f(C)$ is given as follows

$$f(C) = f_0(C) \Gamma(C) \quad (6.3)$$

where, $f_0(C)$ is the Maxwellian distribution and C is the normalized thermal velocity whose components (C_x, C_y, C_z) are given by

$$C_x = (u - U_{NS}) / c_0, \quad C_y = (v - V_{NS}) / c_0, \quad C_z = (w) / c_0 \quad (6.4)$$

where (u, v, w) represents the molecular velocity components and c_0 is the most probable velocity given by $c_0 = (2kT / m)^{1/2}$.

$$f_0(C) = \frac{1}{\pi^{3/2}} e^{-C^2} \quad (6.5)$$

$\Gamma(C)$ is given by

$$\begin{aligned} \Gamma(C) = & 1 + (q_x C_x + q_y C_y + q_z C_z) \left(\frac{2}{5} C^2 - 1 \right) - 2(\tau_{xy} C_x C_y + \tau_{xz} C_x C_z + \tau_{yz} C_y C_z) \\ & - \tau_{xx} (C_x^2 - C_z^2) - \tau_{yy} (C_y^2 - C_z^2) \end{aligned} \quad (6.6)$$

$$q_i = -\frac{k}{P} \left(\frac{2m}{kT} \right)^{1/2} \left(\frac{\partial T}{\partial x_i} \right) \quad (6.7)$$

$$\tau_{ij} = \frac{\mu}{P} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3} \frac{\partial v_k}{\partial x_k} \delta_{i,j} \right) \quad (6.8)$$

where q_i and τ_{ij} are the dimensionless heat flux and stress tensor, μ is the dynamic viscosity of air, k is the thermal conductivity, P is the pressure and $v=(U_{NS}, V_{NS})$ is the mean velocity. To implement the Chapman-Enskog distribution function numerically by acceptance-rejection theorem, the velocity components (U_{NS}, V_{NS}) and the velocity gradients $\partial U_{NS}/\partial x$, $\partial U_{NS}/\partial y$, $\partial V_{NS}/\partial x$ and $\partial V_{NS}/\partial y$ from the continuum domain are used to compute the values for $\Gamma(C)$. The cell centered values of the velocity and their gradients across any required section are obtained using *Fluent*. At each time step the reservoir is filled with particles and convected. Those particles which enter the simulation domain are retained while the rest are discarded. To reduce the computational time associated with the DSMC method, the DSMC code solving the atomistic regime has been parallelized. Eight processors have been deployed for the computation and to ensure a reasonable load balance among the processors, the partitioning of the computational domain is done such that each processor has approximately the same number of cells. The partitioning of the DSMC computational domain between processors to enable parallel computation is shown in Fig 6.3.

Figure 6.3: Schematic representation of partitioning of the DSMC sub-domain among eight processors for parallel processing

6.3 Results and Discussion

6.3.1 Hybrid Continuum-Atomistic Flow Solutions Using the Schwarz Method

The Schwarz alternating method is applied to the slider bearing problem to obtain hybrid continuum-atomistic solutions. For the first Schwarz iteration, the DSMC sub-domain is solved using an initial guessed boundary condition of $P = 1 \text{ atm}$, $U_{NS} = 0 \text{ m/s}$, $V_{NS} = 0 \text{ m/s}$ at all the DSMC inflow and outflow boundaries. Additional Schwarz iterations are done using updated boundary conditions for each iteration until the solutions converge in the overlap region. All the DSMC simulations, at each Schwarz iteration have been carried out by employing about 50 particles per cell and the sampling process has been done for over a period of about 300,000 iterations to minimize the scatter associated with the DSMC method. The convergence of the Schwarz method can be assessed from the variation in the velocity and pressure boundary conditions transferred from the continuum sub-domain to the DSMC sub-domain, with every Schwarz iteration. The variation in the transferred velocity and pressure boundary conditions as a function of the Schwarz iteration along the x -overlap and y -overlap are plotted in Figures 6.4 and 6.5. The boundary condition value along the x -overlap is plotted by taking the corresponding value from the buffer cell at $h_{ext}/2$, while the boundary condition value along the y -overlap is plotted by taking the corresponding value from the buffer cell at $l_{ext}/2$. It can be observed from the figures that convergence is attained in about five iterations after which the variations in the transferred boundary conditions are negligible.

Fig 6.6 shows the variation of the computed velocity components and pressure fields in the DSMC sub-domain with Schwarz iterations along a straight line located at a height $0.15H_1$ above the bottom wall, where H_1 is the slider height at the leading edge and the region between the two vertical lines denote the slider bearing region. It can be seen that the converged solutions for both pressure and velocity are obtained in about five iterations after which the solutions remain unchanged. The computed velocity contours from the hybrid solutions obtained by combining the solutions in the continuum and

atomistic regions across the selected plane *DEFG* (shown in Fig. 6.1) located upstream of the slider is shown in Fig. 6.7. The region between the dotted lines in the figure represents the overlap region.

Figure 6.4: Convergence of a) velocity and b) pressure boundary conditions transferred from Continuum to DSMC along *x-overlap*

Figure 6.5: Convergence of a) velocity and b) pressure boundary conditions transferred from Continuum to DSMC along *y-overlap*

Figure 6.6: Variation of flow solutions of a) pressure b) x -velocity and c) y -velocity in the DSMC sub-domain with Schwarz iterations. (The vertical lines in the figure represent the inflow and outflow sections of the slider.)

Figure 6.7: Velocity Contours from the hybrid solution across a selected region upstream of the slider. (The region between the dotted lines represents the overlap region)

Fig 6.8 compares the converged hybrid solutions of pressure and x -velocity with the exact solution in the entire domain. The DSMC solution in the entire domain is considered as the exact solution and comparisons are made across two selected sections by plotting the velocities along two straight lines located at a height of $0.15H_1$ and $0.35H_1$ above the bottom wall. Comparison of pressure is made across just one section which is at a height of $0.15H_1$ above the bottom wall, since the variation of pressure is negligible along the thickness of the bearing. In the figure, the vertical lines denote the overlap region. The solutions of both pressure and velocity show good correlation with the exact solutions with a maximum deviation of about 5 % observed. From the plots it can be observed that the pressure in the region outside the slider remains about the ambient pressure, while that at the inflow and outflow of the slider deviates from the ambient pressure of one atm. At the inflow there is a significant increase in pressure

while at the outflow the pressure drops below the ambient pressure, which affects the pressure profile in the slider bearing region. From the solutions of velocity, it can be observed that the velocity values under the slider is characterized by slip and rises to a peak value at the trailing edge of the slider where there is a sudden pressure drop.

The transition of the hybrid flow solutions at the interface region could be dependent on a variety of factors such as the accuracy in the transfer of boundary conditions across the two sub-domains. For example there could be inherent statistical errors in the DSMC solutions which might affect the accuracy of the transfer of boundary conditions from the DSMC sub-domain to the continuum sub-domain. The other factors that could affect the accuracy of the hybrid solutions could be associated with the convergence of the Schwarz Alternating method. The effect of various factors such as compressibility, Mach number and Reynolds number on the convergence of the Schwarz Alternating method for the case of a hybrid continuum-atomistic simulation is not very well known and is something that deserves future study.

6.3.2 Effect of Size of Overlap Region on Convergence of Solution

The effect of overlap size on the convergence of the hybrid Schwarz method has been investigated by considering different overlap widths along the *y-overlap* region. The plots of variation of velocity and pressure boundary conditions transferred from the continuum domain to the DSMC sub-domain with different overlap width size is shown in Fig 6.9. The boundary condition value along the *y-overlap* is plotted by taking the corresponding values of pressure and velocity from the buffer cell at $l_{ext}/2$. The error in the transferred boundary conditions of pressure and velocity from the continuum domain to the DSMC sub-domain along the *y-overlap* region is shown in Fig 6.10 by plotting the relative error norm with respect to the exact solution. For example the relative error norm for pressure is calculated as $\sum \sqrt{(P_{exact} - P)^2 / P_{exact}^2}$, where P_{exact} is the exact solution.

It is observed from Fig 6.9 and Fig 6.10 that the Schwarz method for NS/DSMC coupling does not converge when the overlap is zero. Both the pressure and velocity

values appear to diverge with Schwarz iterations in the absence of an overlap region. For all the other cases of overlap width considered viz; $w = 26nm, 39nm, 52nm$, the convergence is not significantly affected with variation in overlap. With increasing overlap size the convergence is only slightly improved, with no significant variations observed. The results indicate that the hybrid coupling by the Schwarz coupling is weakly dependent on the size of the overlap region. However a finite overlap must be employed to facilitate the exchange of boundary conditions as the hybrid solution has been found to diverge with zero overlap.

6.3.3 Comparison of Continuum solutions with Hybrid Solutions

An investigation has been done to study the impact of rarefied flow effects on flow prediction in the vicinity of the HDI region by computing the flow field in the entire domain using the Navier-Stokes equations. The continuum solutions are then compared with the hybrid continuum-atomistic solution in the entire domain. The comparisons of the continuum solutions of pressure and velocity with the hybrid solutions along the disk surface are plotted in Fig 6.11. The region between the two vertical lines denotes the slider bearing region. The continuum solutions over predict the solutions of both pressure and velocity. The peak pressure predicted by the continuum method varies by about 50% from the hybrid solutions. The flow in the slider falls in the transition regime and hence the continuum solutions cannot predict the rarefied flow effects such as velocity slip, as could be observed from the velocity plot comparison.

(a)

(b)

Figure 6.8: Comparison of hybrid solutions of a) pressure and b) x -velocity with the exact solution in the entire domain. (The region between the vertical lines denotes the overlap region. The lines L_1 and L_2 represent the lines AA_1 and CC_1 in Fig 6.1, where as the lines L_3 and L_4 denote represents the lines C_4C_5 and A_4A_5 in Fig 6.1.)

(a)

(b)

Figure 6.9: Convergence of a) pressure and b) *x-velocity* with Schwarz iterations as a function of overlap size

(a)

(b)

Figure 6.10: Convergence of relative error norm of (a) pressure and (b) x -velocity component along the y -overlap boundary with Schwarz iterations as a function of overlap size

(a)

(b)

Figure 6.11: Comparison of Navier-Stokes (continuum) solutions of a) pressure and b) x -velocity with the hybrid solutions in the entire domain. (The lines L_1 and L_2 represent the lines AA_1 and CC_1 in Fig 6.1, where as the lines L_3 and L_4 denote represent the lines C_4C_5 and A_4A_5 in Fig 6.1. The region between the dotted lines in the figure represents the slider bearing region.)

CHAPTER 7

CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE WORK

As flow at micro- and nano-scales deviate significantly from the continuum hypothesis it cannot be modeled by conventional continuum methods. With the advent of miniaturization and wide application of MEMS devices, there is an increasing need for developing computational models which can predict accurately the rarefied flow phenomenon associated with micro flows. The main aim of this thesis has been towards the development of appropriate computational models which can predict rarefied and non-equilibrium flow accurately in micro flow applications such as that in the HDI gap.

This dissertation focuses on the modeling of air flow characteristics in the vicinity of the HDI gap using the DSMC method. Although the DSMC is a computationally intensive method, the combination of rapid technological developments in high performance computing platforms with parallelization of numerical algorithms implies that the DSMC method can be efficiently used for the computation of rarefied flows. During the course of the thesis, several aspects have been studied such as multi-scale modeling and incorporation of two-phase computations in the DSMC model. Flow modeling aspects for a stand-alone DSMC computation and for a hybrid continuum-atomistic simulation coupling the Navier-Stokes (NS) equations to a DSMC solver are addressed in this work. In order to achieve the objectives of this thesis work, a significant part of the work involved the developing and writing the computer codes in C/C++ for parallel DSMC and hybrid continuum-atomistic models.

The DSMC method has been initially applied to micro flows such as Couette and Poiseuille flows to identify and validate various flow features associated with flows at micro- and nano- scales. As DSMC is a computationally intensive method, parallel three-

dimensional DSMC codes have been developed to compute the flow in the HDI gap region. Parallel DSMC method has been implemented on several local advanced computing platforms and a PC cluster and the corresponding parallel performance metrics analyzed. The parallel DSMC method demonstrated good scalability on the different computing platforms considered. Super linear speedup has been obtained on all the computing platforms considered resulting in significant computational savings. The issue of load balancing has also been addressed and a dynamic load balancing scheme has been implemented to achieve further computational economy.

The work considered here also focused on the implementation of appropriate boundary conditions for DSMC simulation of micro flows. An appropriate implicit boundary treatment method is used for fixing the pressure boundary conditions at the inflow and outflow boundaries and has been extended to the case of a three-dimensional DSMC micro flow simulation. Accuracy considerations in terms of the number of cells, number of particles and time step size required for an accurate DSMC simulation of the HDI gap have also been addressed. An investigation into the number of cells required for an accurate DSMC simulation of the HDI gap reveals that the linear cell dimensions along the length and width of the slider can be much greater than the mean free path because of very small velocity gradients along these directions. This effectively reduces the total number of cells and particles required to ensure an accurate DSMC simulation of the HDI gap. Various slip corrected Reynolds equation gas lubrication models and the popular Fukui-Kaneko model have also been solved using the finite difference method to compute the pressure distribution in the slider bearing region. A coupled Reynolds-DSMC model has also been proposed to couple the Reynolds equation model solutions to the DSMC model, in instances where a detailed atomistic simulation is required in any localized region in the HDI region both for the two-dimensional and three-dimensional case. By this coupled approach the DSMC method can be employed for a detailed investigation in any small selected region of interest to capture the true physics, while being coupled to the rest of the slider bearing region modeled by the Reynolds equation. The coupling approach provides a frame work for coupling the Reynolds equation model to the region modeled by DSMC.

Two-phase (gas-solid particle) flow modeling using the DSMC method to enable the modeling of particle laden flow in the HDI gap has also been attempted in the present work. The two-phase model to compute particle trajectories has been implemented based on a one-way coupled method, by computing the forces on a particle under the assumption of locally free molecular flow conditions. The two-phase model has been incorporated both in the two-dimensional and three-dimensional parallel DSMC models. Representative particle trajectories have been computed for particles that may enter the HDI region for which the flow falls entirely in the transition regime. The study has been done for particles which are of a few nanometer diameter sizes and for various cases of material density.

Multi-scale methods are required to couple continuum solutions governed by the Navier-Stokes solution to atomistic solutions governed by the DSMC model. A hybrid continuum-atomistic method for micro flows based on the Schwarz alternating method has also been developed and applied to compute flow in the HDI gap. This hybrid coupling has been demonstrated in two-dimensions by considering overlap regions along both x and y directions to demonstrate proof-of concept application. Boundary condition imposition from the continuum region to the DSMC region has been achieved using buffer cells and Chapman-Enskog velocity distribution. To reduce the computational cost the DSMC sub-domain has been parallelized. Converged hybrid flow solutions are obtained in about five iterations and the hybrid NS-DSMC solutions show good agreement with the exact solutions in the entire domain considered. A study on the impact of the size of the overlap region on the convergence behavior of the Schwarz method shows that a finite overlap region is essential for the convergence of the Schwarz method, as the hybrid solutions have been found to diverge when an overlap of zero width is considered. For all other cases of finite overlap sizes no significant variations in the convergence behavior have been noted. It has been found from the hybrid results that near the inflow of the slider there is a significant increase in pressure while at the outflow the pressure drops below the ambient pressure, which affects the pressure profile in the slider bearing region. The impact of rarefied flow effects on the flow prediction in the vicinity of the HDI region has also been investigated by comparing the flow field

obtained using the Navier-Stokes equations in the entire domain with the accurate hybrid solutions.

The current work provides ample scope for conducting further numerical simulations for flow prediction in the HDI gap. During the read/write operation in a HDD, the slider could operate under various conditions of flying height and disk speeds. Optimum slider configurations correspond to shapes which maintain a steady flying height and which ensure minimum particle contamination in regions near the read/write head under different operating conditions. The computation of the three-dimensional flow field in the HDI gap using the DSMC method for various cases of slider orientation with respect to the spinning disk will be pursued in the future. The possibility of integrating the flow field in the slider air bearing dynamically with the six degree of freedom (6-DOF) slider motion using the DSMC method can also be explored. The equations of motion of the slider along various translational directions and rotational directions such as the pitch, roll and skew directions can be solved simultaneously with the pressure distribution obtained from the unsteady DSMC model at various times to obtain the dynamic response of the slider. The study of dynamic motion of the slider at different instants of time and under various operating conditions could identify the parameters that affect the sensitivity of the slider flying height the most. To enable the work, the current DSMC codes need to be enhanced to model unsteady DSMC simulation which requires further study on various issues such as optimum time step and cell shapes. The two-phase DSMC models developed in the current work can provide the basis for investigating the motion of nanometer sized particles in more complex slider bearing geometries with grooved surfaces. The current DSMC models could be modified to simulate the flow in step sliders with cavities in the slider geometry. Detailed investigation of particle motion could also be studied for particles which may enter from the continuum flow outside the slider into the HDI gap. The particle contamination patterns in the HDI gap for various cases of slider geometry shapes can provide useful information for the design of optimum slider shapes and also shapes of small grooves which can be etched on the surface of the slider to alter the pressure distribution locally so as to achieve minimum particle contamination in the HDI region.

Although the flow in the HDI gap can be considered to be isothermal throughout (as is the case in this study in view) this need not be the case always, especially near the read/write head region if there is a slider-disk interaction corresponding to the case of “thermally assisted” recording or when a small region near the read/write head is heated by external means to reduce the head-media spacing during read/write which in turn helps in the design of increased the recording capacity. In such cases the DSMC method can be used to study the effect of heat transfer on the flow in the HDI gap. Also of interest here will be the study of particle motion in the presence of a temperature gradient. The thermophoretic forces acting on particles which may enter the HDI gap and their resulting motion due to the heat transfer could be computed using the two-phase DSMC method. The two-phase parallel DSMC code can be modified to include the computations for finding the net heat transfer acting on a particle from the gas phase under locally free molecular flow conditions. The effect of thermophoresis on the motion of nanometer sized particles can be assessed for a range of Knudsen number. Another logical work that could be pursued is the development of a three-dimensional hybrid continuum-atomistic model based on the Schwarz Alternating method. The continuum model for the hybrid coupling will be solved using the Navier-Stokes equation in *Fluent* software. The effect of various factors such as compressibility and Reynolds number on the convergence of the Schwarz Alternating method for micro flow simulations also requires further study. The codes developed in the current work can easily be extended and enhanced to address all these proposed activities and could provide the framework for enabling hybrid NS-DSMC simulations in other micro flow applications and also for hypersonic non-equilibrium flow applications.

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