A New Parallel Adaptive DSMC Algorithm for Unsteady Flows in Complex Geometries

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***Abstract*—We present an efficient parallel multi-scale Direct Simulation Monte Carlo (DSMC) algorithm for the simulation of three-dimensional unsteady rarefied gas flows over complex geometries. The flow domain is represented by a hierarchical octree-based Cartesian grid where three-dimensional solid objects with triangulated surfaces are incorporated using a cut-cell algorithm. The hierarchical octree domain representation allows the method to provide straightforward and efficient data management suitable for a particle-tracing and dynamic grid refinement and coarsening. The algorithm implements a spatial adaptivity scheme that is based on the gradients of statistically averaged macro-properties of the flow. The proposed DSMC algorithm employs a novel parallelization scheme suitable for simulating strongly unsteady, non-equilibrium flows. The parallelization scheme, implemented using Open Multi-Processing (OpenMP) for multicore Central Processing Units (CPUs), significantly reduces the computational cost of modeling these flows. The proposed DSMC algorithm is assessed for two fundamental flows in the slip and transition-continuum regimes.**

Keywords–DSMC; Octree hierarchical grid; Spatially adaptive; Parallel; Rarefied gas flow; Ray tracing; Unsteady; Complex geometry.

I. INTRODUCTION

Rapid developments in micro and nano-technologies call for computational tools that efficiently and accurately predict the flow dynamics at these scales. The Direct Simulation Monte Carlo (DSMC) method has become the most widely used computational tool for simulating rarefied gas flows in the slip and transition regimes, characterized by the Knudsen number range $0.001 < \mathrm{Kn} < 10$ [1]. Applications include investigation of the dynamics of the squeeze-film surrounding a microstructure undergoing oscillations of large amplitudes [2], investigation of the Knudsen thermal force on the performance of a low-pressure micro gas sensor [3], and prediction of rarefied flow fields in various micro/nano-systems [4], among others.

The geometry model in DSMC simulations refers to both the computational mesh and surface representation. Two primary approaches for the geometry model in existing state-of-the-art DSMC solvers include the unstructured body-fitted grids and the Cartesian-based grids. DSMC solvers can run with a single processor or in parallel using the Message Passaging Interface (MPI) library on multiple processors. Parallelization is carried out by decomposition of the spatial domain among the processors. This flavor of parallelization suffers from two drawbacks. The first is the challenge of load balancing and distributed storage of the computational domain within a spatial-temporal adaptive algorithm that dynamically adjusts the computational grid and time step in response to the evolving flow field structures in unsteady flows. The second challenge is that the criteria for spatial-temporal adaptivity are based on macroscopic properties computed as averages over a statistically meaningful number of realizations (a realization is a DSMC simulation initiated from a unique random number generator seed). This latter observation suggests parallelization over independent realizations. In the proposed framework, each thread or core processes a realization of the simulation of the unsteady flow over the entire computational domain.

In this paper, we present a three-dimensional DSMC algorithm parallelized over realizations, rendering it suitable for simulating unsteady flows. The flow domain is represented by a hybrid mesh consisting of a hierarchical octree-based Cartesian grid, whereas the surfaces of solid objects are represented by a triangular mesh. To allow for accurate DSMC simulations of flows over objects of complex boundaries, a cut-cell method is implemented [5]. The method, which calculates the volume of each flow cell cut by a solid boundary, enables accurate modeling of molecular collisions in these cells. The cut-cell method also allows for decoupling of the flow field mesh from the solid boundaries surface mesh, making it suitable for simulating near-continuum flows with large density variations. In addition, the method employs a dynamic spatial adaptation algorithm. The spatial adaptation criterion is based on the local macroscopic flow properties, which are computed as statistical averages over a number of realizations. The hierarchical octree-based Cartesian grid representation of the domain allows for an efficient data storage and management that is compatible with the spatial adaptation algorithm. Such representation significantly improves memory requirement when compared to unstructured meshes and, as such, is more suitable for simulating large-scale DSMC problems. It also enables a potentially more general scheme for varying cell volumes over a large range of the molecular length scales. The hybrid mesh scheme enables simple integration of a variety of effective geometric tools used in computer graphics, including fast particle-tracing algorithms. The scheme also enables spatial grid adaptation, molecular movement, and re-sorting to be performed with fewer operations. A key feature of the DSMC algorithm proposed in this work is that it is optimized for simulating unsteady flows in parallel over multiple cores. In contrast with distributing the domain over the cores, the independent realizations are distributed over the cores. Due to the lack of communication between the cores when each is handling an independent realization, the parallelization efficiency is almost 100 %. In addition, this type of parallelization is optimal when simulating highly unsteady rarefied flows over complex geometries. These flows typically experience considerable variability in the spatial gradients of the macroscopic thermodynamics properties, and as such,

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spatial adaptation is frequently carried out. With each core being assigned a DSMC realization, local flow properties at different time steps are collected simultaneously in parallel and averaged over the multicores for local mesh refinement.

This paper is organized as follows: Section 2 summarizes the DSMC methodology. Section 3 presents the three-dimensional unsteady parallel DSMC algorithm. Validation of our algorithm through benchmark DSMC simulations of the micro-channel Poiseuille flow and the slider bearing flow problem is presented in Section 4. The conclusion is presented in Section 5.

II. DSMC METHODOLOGY

DSMC, pioneered by G. A. Bird in the 1960s [6], is the most widely used particle-based simulation method for the study of rarefied gas flows. The DSMC method is described in detail in the monograph by Bird [6]. A brief summary of the method, highlighting key aspects relevant to the algorithm we are proposing in this work, is presented next.

Based on the well-developed kinetic theory of gases, DSMC is a stochastic particle method that computationally solves the non-linear Boltzmann equation by emulating the physics of a real gas. The microscopic behaviour of the gas is modeled by tracking thousands or millions of randomly selected simulated particles, each representing a large number of physical molecules or atoms. The DSMC algorithm involves four major processes: 1) moving the particles over a time step and model their interactions with boundaries, 2) indexing and tracking the particles within the grid of collision cells, 3) selecting particles for collision on a probabilistic basis and applying the appropriate collision model, and 4) sampling the macroscopic flow properties.

For the DSMC method to produce physically realistic and accurate solutions, the time step, and grid cell size must be chosen as follows. The collision grid cell size, Δx, must be small compared to the local mean free path, $\lambda \sim |\pi/\nabla\pi|$; the length scale characterizing the spatial variations of the macroscopic properties, λ. So, we choose $\Delta x \ll \lambda$, where λ generally varies with space and time. The simulation time step Δt over which molecular motions and collisions are uncoupled must be smaller than the local mean collision time, $\Delta t < \tau_c = \lambda/\mathrm{V_{MP}}$, where $\mathrm{V_{MP}}$ is the most probable velocity. In order to preserve collision statistics and to yield a reasonable approximation of the local velocity distribution function, the number of simulated gas molecules per cubic mean free path, N, must be larger than a minimum (typically 20).

In DSMC, simulated molecules move, collide with each other and with the physical boundaries. Different types of boundary conditions are employed in DSMC simulations. These include solid wall boundary conditions (thermal walls and periodic boundaries), and inflow/outflow boundary conditions. The interaction between a gas molecule and a solid boundary can be treated as being fully specular, fully diffuse, or a combination of the two. The inflow/outflow boundary conditions can accommodate supersonic and subsonic flows. They are implemented by injecting particles into the computational domain at the external flow conditions. The inflow/outflow boundary conditions can be implemented in DSMC using the standard method or the reservoir method. The standard method involves a particle emission surface set at the flow boundary [6]. The well-known Maxwellian Reservoir Method employs ghost cells at the boundaries of the DSMC computational domain that act as sinks and sources of the simulation particles [7]. The velocity of the molecules entering the flow field is generated according to the velocity distribution of the external flow.

After completing molecular movements, intermolecular collisions are simulated probabilistically using molecular collision models. Several collision models, designed to reproduce the real flow macroscopic behaviour, were applied successfully within the framework of DSMC. These models include the inverse power law model, the hard sphere (HS) model, the variable hard sphere model (VHS), and the variable soft sphere (VSS) model [6]. In the VSS model, the mean free path is given as:

$$\lambda_{\mathrm{VSS}} = \frac{4\alpha(7-2\omega)(5-2\omega)}{5(\alpha+1)(\alpha+2)} \left(\frac{\mu}{n}\right) (2\pi m k_B T)^{-1/2}$$
$$\mu = \mu_{\mathrm{ref}} \left(\frac{T}{T_{\mathrm{ref}}}\right)^{\omega} \quad (1)$$

where m is the molecular mass, $n = \rho/m$ is the number density, μ_{ref} is the viscosity at reference temperature, and α is the scattering parameter ($\alpha = 1$ for VHS model). The viscosity index ω is related to the power exponent η in the inverse power law model as $\omega = \frac{1}{2}\frac{\eta+3}{\eta+1}$. In the HS model, the mean free path is expressed as:

$$\lambda_{\mathrm{HS}} = \frac{1}{\sqrt{2}\pi d^2 n} \quad (2)$$

where d is the molecular diameter.

The DSMC method is an explicit time marching simulation algorithm. As such, it always produces unsteady flow simulations. The statistical scatter of DSMC computation varies according to the inverse square root of the sample size. Figure 1 illustrates two sampling methods used in DSMC: the steady and the unsteady sampling techniques. For predicting a steady flow field, a time average over a number of time steps is required to obtain smooth results. In this case, averaging must be carried out after the transient phase elapses and a steady behaviour is established. For simulating unsteady flows, ensemble-averaging is performed where the entire flow evolution is calculated repeatedly. The flow field is sampled at the appropriate flow sampling time steps. To compute the flow fields of the macroscopic thermodynamic properties, the samples are averaged over a sufficiently large number of flow realizations, each originating from a different random number generator seed.

III. THREE-DIMENSIONAL UNSTEADY DSMC ALGORITHM

In the current study, an octree-based Cartesian grid divides the computational domain into cubic cells, whereas the surface of the 3D solid object is triangulated using the preprocessing open-source software SALOME 7.5.1 [9]. Tree-based methods with the simple Cartesian structure and embedded hierarchy make use of recursive encoding schemes. These schemes render processes such as mesh adaptation, rebuilding, data access, and handling of fluid-solid interaction both simple and efficient.

Each solid object is bounded by a rectangular box. An axis-aligned box-box intersection test [10] is then carried out to identify collision cells neighbors and all cubic cells that

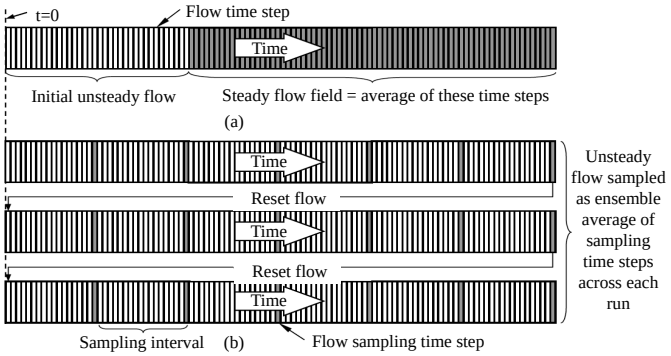

Figure 1. (a) The schematic of the time-averaging of the flow properties over a long interval of simulation time. (b) The schematic of the ensemble-averaging of the flow properties over many runs [8].

overlap with the bounding box surface. In addition, the fast 3D triangle-box overlap test by Moller [11] is implemented to test overlapping between triangular elements of the solid object surface mesh and cubic cells inside the bounding box. This test enables linking each surface mesh triangular element to the overlapping Cartesian cells. Figure 2(a) shows a schematic diagram illustrating the hybrid mesh scheme. Figure 2(b) shows a zoomed-in view of the box bounding the solid object (sphere). It also shows the cut-cell representation, where triangular solid surface elements cut the cubic cells in the adaptively refined Cartesian mesh. The resulting cut-cell volume is estimated using the Monte Carlo technique described in [5]. This volume is needed to accurately model collisions and predicts the macroscopic properties in the cut-cell. The proposed three-dimensional hybrid mesh scheme employs a flexible data structure which enables simulation of particles movement and sorting processes with fewer operations, thereby reducing the CPU time.

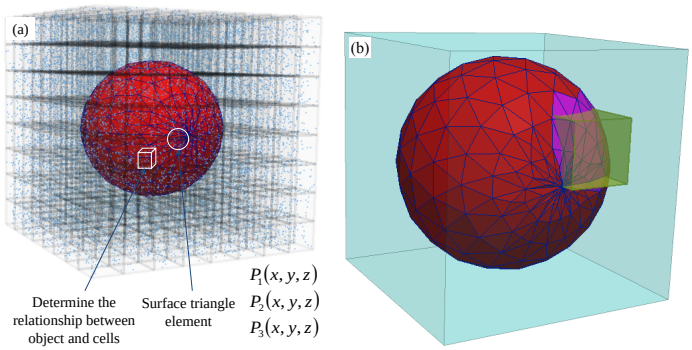

Figure 2. (a) Schematic representation of a triangulated surface mesh of a sphere embedded in a 3D octree Cartesian grid. (b) Bounding box and a cut-cell representation.

In the presence of complex solid boundaries (and/or when the surface to volume ratio of the flow domain is large), the computational cost of molecular movement amounts to a significant fraction of the computational cost of a DSMC simulation. To efficiently track the particle movement within the hierarchical octree-based Cartesian grid, a special particle ray-tracing technique is employed. This technique is used in the vicinity of the solid object surface where the region of the bounding box is treated as follows. During a single time step, a molecule cannot move more than one collision cell size along each dimension (a DSMC time constraint). Ray tracing is performed only for particles that leave their assigned cell and intersect the box bounding the solid object. If an intersection with the bounding box occurs, a cell-by-cell particle tracking procedure is performed to determine whether the particle reaches a boundary surface triangle, stays in or leaves the current cell. If no ray-triangle intersection occurs, the particle's position is updated if the particle stays in the current cell; otherwise, ray-box intersection tests with all possible neighbour collision cells are performed to track the particle from the current cell to its nearest neighbour collision cell. The particle-tracking algorithm is then invoked again to move the particle over the remainder of the time step. At the completion of the molecular movement phase, each particle is automatically stored within its final cell by the sort subroutine. In summary, the hierarchical octree-based data structure allows for efficient intersection testing within the ray tracing algorithm. We point out here that the grid cells are axis-aligned boxes whose edges are all parallel to the basis vector, which enhances the efficiency.

Another special feature of the proposed algorithm is that it runs transient parallel Monte Carlo simulations simultaneously and independently on multicore CPUs. Figure 3 shows a schematic representation of the parallel algorithm using multiple cores. Each simulation consists of m transient solutions with n realizations each. Most DSMC solvers are parallelized through decomposition of the physical domain into groups of cells that are distributed among the processors. The efficiency of such parallelization scheme may suffer due to the intensive communications between the processors and load imbalance among the processors. In addition, this parallelization scheme is more convenient in simulating low speed flows where a uniform Cartesian grid is used and/or in simulating high-gradient flows where grid resolution in both space and time is evoked once before steady state is reached.

The proposed algorithm is also adaptive where refinement of the spatial grid is employed to simulate flows with length scales that vary considerably over the domain. Accurate prediction of these flows require variable resolution of different flow regions. Figure 4 shows the flow chart for the implemented DSMC method using the adaptive method. Prior to the adaptation process, the DSMC simulation starts with a uniform mesh. As depicted in the inset figure at the top right corner of Figure 3, periodic spatial adaptivity tests are carried out in the course of an unsteady simulation. The inset also shows the sampling times for predicting the transient macroscopic behaviour. Refinement or coarsening of collision grids is based on the averaged local flow variables over the multicores, which allows accurate prediction of these properties within a computationally efficient framework.

IV. Benchmark Test Cases

To validate the proposed three-dimensional parallel DSMC algorithm, numerical simulations of two fundamental flows in the slip and transition-continuum regimes are presented. The Poiseuille flow is taken as an example to assess the spatial adaptation scheme in the slip flow regime. A three-dimensional flat slider gas bearing problem is considered to evaluate the hybrid mesh scheme in transition flow regime. The simulations

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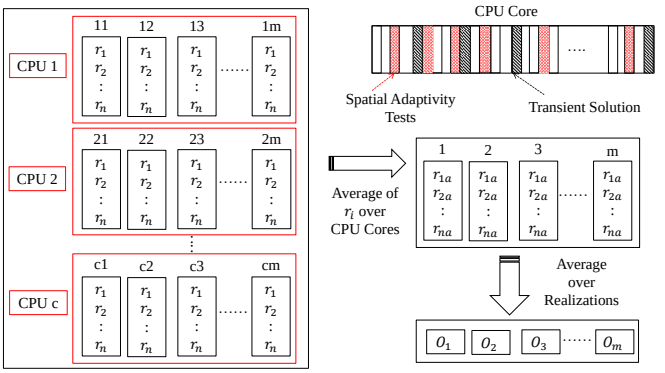

Figure 3. The schematic of running transient DSMC simulations on different CPU cores. The upper right figure displays the local adaptive and the flow sampling time steps.

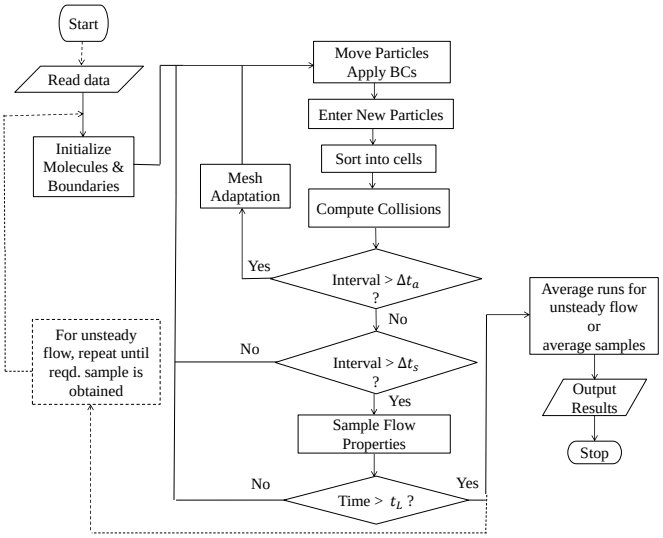

Figure 4. Simplified flow chart of the implemented DSMC algorithm. Δt_a: adaptive time; Δt_s: sampling time; t_L: Long time.

were carried out using Fortran in CentOS Linux 7 on 16 core Intel Xeon(R) CPU E5-2650 v2 running at 2.6 GHz.

A. Poiseuille Flow

The pressure-driven Poiseuille gas flow in a rectangular microchannel between two parallel plates is considered. The channel axis is along the x direction. The plates, of length L along the flow direction (x), are separated by a distance H, where $L/H \gg 1$. The flow is two dimensional in the $x-z$ plane; the channel dimension, W, along the y direction is much larger than H; $W \gg H$. Since the flow is two dimensional in the $x-z$ plane, the computational domain consists of one grid cell in the y direction. The following boundary conditions were imposed: (i) solid-walls are assumed to be perfectly accommodating, (ii) periodic boundary conditions are enforced at the $x-z$ planes on either size of the domain, and (iii) the Maxwellian reservoir method is used for the inflow/outflow boundary conditions at the inlet and outlet of the channel. The simulated fluid is argon gas (VHS gas) initially at ambient conditions. The channel length is $L = 5\,\mu m$, the channel aspect ratio is $L/H = 5$, the inlet flow stream temperature is $T_{in} = 300\,K$, the inlet to exit pressure ratio, $P_{in}/P_e = 3$, and the inlet pressure is $P_{in} = 160.839\,kPa$. To assess the spatial adaptivity scheme in our DSMC algorithm, this flow is simulated with and without dynamic grid adaptation. For the non-adaptive simulation, the grid spacing was chosen to be $\Delta x \sim 1/5\lambda_0$, where λ_0 is the mean free path at the initial conditions. For the adaptive simulation, the grid spacing is computed as $\Delta x \sim \lambda/3$, where at each adaptation time interval, λ for each cell is computed using Eq. (1), where T and n for the cell are averaged over all the cores. Figure 5 shows the steady state centreline pressure distribution using the proposed DSMC algorithm with and without grid adaptation. Our results are in good agreement with the simulated pressure profile by Wu et al. [12], with the pressure profile predicted using the adaptive scheme closer to that predicted by Wu et al. [12]. The figure also shows the flow field refined mesh

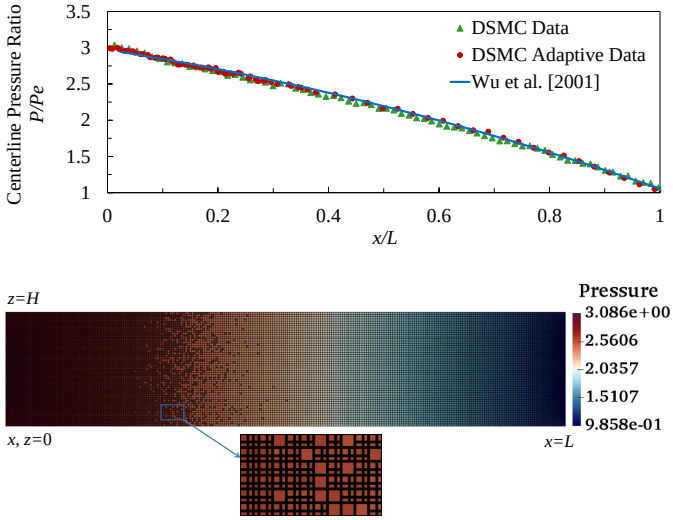

Figure 5. Centreline pressure distribution (top figure) and flow field refined mesh for a microchannel in the slip flow regime.

upon spatial adaptation where the size of an inlet collision cell is adapted to half the size of a collision cell at the exit; $\lambda_{in}/\lambda_e \sim P_{in}/P_e$. With $P_{in}/P_e = 3$ and since the octree divides a cell by integer powers of 2, λ_{in}/λ_e was set to 1/2.

The transient solution and spatial adaptivity sampling intervals are presented in Table I, among other parameters. The table also shows that at the end of the simulation, the number of cells in the adaptive simulation increased from 13056 to 48084, which is comparable to that used in the non-adaptive case. The computational cost of the adaptive simulation is, however, less by a factor of 7.7.

B. Slider Bearing Problem

Figure 6 shows a typical three-dimensional flat slider gas bearing configuration. A channel is formed by a moving horizontal bottom surface and a stationary slightly inclined surface whose length is $L = 5\,\mu m$ and height at the trailing edge is $H_o = 50\,nm$. The simulation used argon hard sphere particles initially at ambient conditions. Thus, the Knudsen number at the exit is $\mathrm{Kn}_o = \lambda/H_o = 1.25$. The lower surface moving at a speed of $U = 25\,m/s$ and the bearing number is $\Lambda = 61.6$ (defined as $\Lambda = 6\mu UL/p_a H_o^2$; p_a

TABLE I. COMPARISON OF ELAPSED TIME PER DSMC REALIZATION FOR NON-ADAPTIVE AND ADAPTIVE POISEUILLE FLOW.

	Non-Adaptive	*Adaptive*
Time step	14.48 ps	28.96 ps
Sampling time	55.3 ns	55.3 ns
Transient solution sampling interval	27.45 ns	27.45 ns
Spatial adaptivity sampling interval		18.299 ns
Total no. of time steps	3800	1900
Total Time per Realization per core	45910.5 s	5931.76 s
Initial no. of Cells	52224	13056
Final no. of Cells	52224	48084

is the ambient pressure and μ is the viscosity of the gas). As for the boundary condition, the solid-walls are assumed to be perfectly accommodating, periodic boundary conditions are enforced at the $x-z$ planes on either side of the 3D domain, and the Maxwellian reservoir method is used for the inflow/outflow boundary conditions at the inlet and outlet. Our

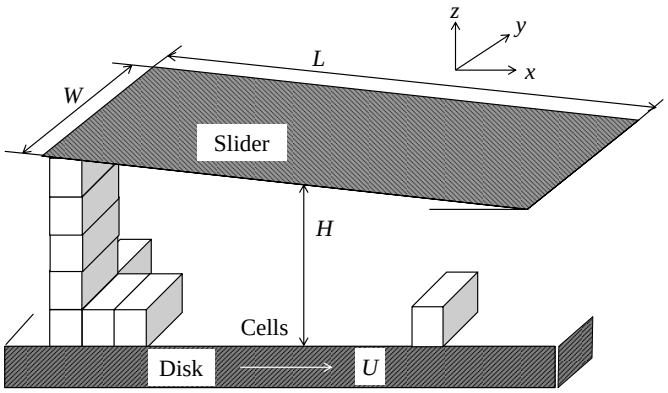

Figure 6. Schematic of the slider bearing geometry, $L = 5\mu m$, $H_o = 5\mu m$, $U = 25m/s$.

DSMC results are in excellent agreement with the previously published DSMC solution by Garcia et al. [13].

Table II shows the simulation time per time step per core distributed among the particles movement, sorting and collision time steps. It can be observed that the molecular motion in the slider bearing flow takes the longest time. This is due to the cost of the ray-tracing operations using the hybrid mesh constructed near the inclined surface.

TABLE II. ELAPSED TIME(S) OF DSMC PROCESSES AT FLOW SAMPLING TIME STEP FOR BENCHMARK SIMULATIONS.

	Non-Adaptive Poiseuille	*Adaptive Poiseuille*	*Slider Bearing*
Move Molecules	3.269	0.917	4.240
Sort Molecules	2.165	0.729	0.084
Perform Collisions	0.354	0.215	0.019

V. CONCLUSION

We presented a parallel three-dimensional DSMC algorithm to model rarefied gas flows in domains with complex solid boundaries. The algorithm employs a hierarchical octree-based Cartesian grid, accompanied by a cut-cell algorithm to incorporate complex 3D geometries with triangulated surfaces

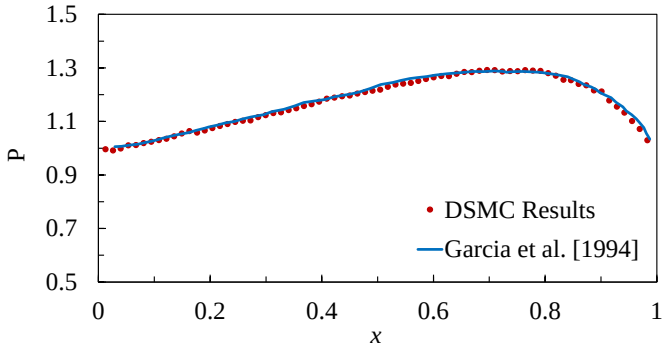

Figure 7. Slider bearing normalized pressure profile for $\mathrm{Kn}_o = 1.25$, $\Lambda = 61.6$, $\mathrm{Ma} = 0.08$.

within the grid cells. It also incorporates a multi-level spatial adaptivity scheme based on the macroscopic average of local flow properties. An original method of running parallel unsteady DSMC simulations simultaneously and independently on multicores is proposed. The selected geometry model is characterized by its low memory storage requirements compared to the use of non-Cartesian meshes, its ability to employ an efficient ray-tracing particle movement scheme, and its flexibility to enable a fully dynamic three-dimensional spatial adaptive scheme that maintains DSMC constraints consistent with the local variations of flow field properties. Correlation of computational results and experimental data clearly show the capability of the unsteady DSMC algorithm to provide accurate flow field predictions. In future work, we expect to complement the spatial adaptivity with a novel temporal adaptivity scheme and then showcase the efficiency and accuracy of the method in predicting unsteady flows in complex geometries encountered in micro- and nano-electromechanical systems (MEMS/NEMS).

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