The hybrid Grid Implemented DSMC Method used in 2D Triangular Micro Cavity Flows

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Abstract In this study a new hybrid grid is implemented in a 2D DSMC solver to be used in 2D triangular micro cavity flows. Currently DSMC is the prominent method to analyze micro scale gas flows which are rarefied. Because of the computational cost, DSMC solvers are generally used in rarefied gas conditions in which continuum based solvers are useless. If the efficiency of DSMC solvers is improved, the application range of these solvers can be increased further where the continuum based solvers dominate. Indexing the particles according to their cells is one of the main steps in the DSMC method. Either the particles are traced cell-by-cell along their trajectories or coordinate transformation techniques are used in this step. The first option requires complex trigonometric operations and search algorithms which are computationally expensive. But it can be used in both structured and unstructured grids. Although the second option is computationally more efficient, it demands specially tailored structured grids which are more geometry dependent compared to the unstructured grids. Here it is shown that a novel hybrid grid structure can be used successfully in 2D DSMC solver to analyze triangular shaped lid-driven micro cavity flows. Hybrid grids used in this study are much less dependent of the geometry like unstructured grids. Additionally, hybrid grids like structured grids facilitate coordinate transformation techniques in order to increase the efficiency of the particle indexing step in the DSMC method.

Keywords: Triangular Lid-Driven Micro Cavity Flow, DSMC, Hybrid Grids, MEMS

1. Introduction

Rapid growths of micro-electro-mechanical systems (MEMS) greatly benefit from the mature production methods used in the field of semiconductor industry. Typical dimensions of these MEMS devices are between 1 millimeter and 1 micrometer **(Gad-el-Hak, 2001)**. Some MEMS devices include not only mechanical and electrical systems but also the fluids. Micro-nozzles, micro-sensors, micro-channels, micro-valves and micro-turbo-machines are the examples of some MEMS devices using fluids. Fluid flows inside or around the MEMS devices are classified as micro flows because of the small characteristic dimensions of these devices. Characteristic length (L) of the MEMS devices approaches the mean-free-path (λ) of the gas. Rarefaction of the gas flows is measured by the dimensional Knudsen number which is the ratio of the characteristic length to the mean-free-path. Consequently, micro gas flows can be considered as rarefied because of their relatively high Knudsen numbers.

In rarefied gas conditions, flows locally depart from thermal equilibrium because of the inadequate molecular collisions. As the gas flow becomes rarefied, velocity slips and temperature jumps arise at the boundaries. Subsequently, linear relations not only between velocity gradient and shear stress, but also temperature gradient and heat conduction are lost. As a result continuum based Navier-Stokes and Euler equations cannot be used, because these equations operate with linear constitutive equations. Experimental studies show that micro scale gas flows behave differently from the large scaled ones, which are generally studied with hydrodynamic models. For safer results in micro gas flow studies, it is better to use rarefied gas analyzing methods.

In micro scale flows, generally molecular

methods are preferred. Molecular dynamic (MD) is the best known physical molecular method **(Allen and Tildesley, 1987)**. MD is generally used to analyze liquids and dense gas flows in nanometer scales because of the excessive number of molecules. For the rarefied gases, direct simulation Monte Carlo (DSMC) which is another physical molecular method is utilized **(Bird, 1994)**. The DSMC method is computationally more expensive, as the Knudsen number gets lower. New approaches are needed to shorten the calculation time of the DSMC method. In this study a hybrid grid structure is proposed. This new grid is less dependent on the geometry like unstructured grids and additionally it can be used with the coordinate transformation technique to increase efficiency of the DSMC method.

2. Lid-Driven Micro Cavity Flows

In lid-driven cavity flows, a viscous fluid surrounded by the solid walls are driven by a moving edge through the shear stress. In the fluid mechanics, lid-driven cavity flow is an important test problem for the numerical algorithms **(Ribbens et al., 1994)**. Lid-driven cavity flow studies are first started with the square cavities **(Ghia et al., 1982; Erturk et al., 2005; Albensoeder and Kuhlmann, 2005)** and later continued with the triangular shape cavities **(Erturk and Gokcol, 2007; Li and Tang, 1996)**. Computational fluid dynamics (CFD) methods are employed in these studies. Recently, new solvers based on the Lattice Boltzmann Method (LBM) are appeared in the literature **(He et al., 2005; Fudhail et al., 2010)**. These new solvers are important alternatives to the continuum based CFD solvers.

As the interest in the MEMS devices are increased, studies for the lid driven micro cavities are also becoming apparent. Although these flows are rather simple in geometry, they display all the details of micro flows **(Perumal et al., 2010)**. Different methods such as Linearized Boltzmann Equation (LBE), Molecular Dynamics (MD), Navier-Stokes-Fourier Equations (NSF), Finite Volume Element (FVE) and Direct Simulation Monte Carlo (DSMC) are used by different researchers **(Naris and Valougeorgis, 2005; Qian and Wang, 2005; Mizzi et al., 2007; Darbandi et al., 2008; Mukinovich and Brenner, 2009; Benzi et al., 2010)**.

Best of the author's knowledge a study for the triangular shaped lid-driven micro cavity flow using the DSMC method is not introduced until now. In this study, triangular shaped lid-driven cavity flows is analyzed with the 2D DSMC solver using a novel hybrid grid. It is expected that the vortex structure in these flows will be different from the square shaped cavities.

3. Conventional 2D DSMC Grids

Although gridless DSMC methods exist in the literature **(Olson and Christlieb, 2008)**, most of the current DSMC solvers depend on the grids. Grids are used to simplify the four basic steps of the DSMC method. The first purpose of the grids is to determine the close proximity molecules in the “indexing” step after the “movement” step. This information is required to choose the collision pairs in the “collision” step. Secondly, grids are used to calculate the macroscopic values from molecular properties in the “sampling” step. Most time consuming part of the DSMC method is to determine in which cells DSMC molecules are positioned. If this information is figured out fast, the efficiency of the DSMC method is increased inherently.

The simplest DSMC solvers are limited with structured grids and rectangular geometries. In these types of solvers, molecule indexing according to the positions can be handled very fast using simple arithmetic operations. But geometry may not be always rectangular or grids may not be structured. When this is the case, either DSMC molecules are traced cell-by-cell or non-rectangular geometry should be mapped to a rectangular geometry using coordinate transformation techniques **(Shimada and Abe, 1989)**. The small regions between the grids are defined as cells in the DSMC method. In cell-by-cell technique, both structured and unstructured cells can be used.

Although different cell-by-cell tracing techniques are presented, these techniques require complicated trigonometric operations which are computationally expensive. In the case of the coordinate transformations, non-rectangular physical flow region can be mapped to a square computational domain. Computational domain consists of structured grids to increase the efficiency of the "indexing" step. If direct spatial relations between two domains are exist, DSMC "movement" step is carried out in the physical domain. Following, "indexing" step is realized in the computational domain. In case, direct spatial relations do not exist between two domains, "movement" step is also performed in the computational domain in addition to the "indexing" step. Because of the curved trajectories, solving equations of motions in the computational domain is rather time consuming in comparison to the physical domain and neutralizes efficiency increase of "indexing" step of the computational domain **(Abe, 1989)**. Consequently, in order to increase the efficiency of the DSMC method, primarily physical domains are needed to map to the rectangular computational domains. Secondly, tailored grids should be generated in the physical domain in order to calculate molecule cell data fast in the computational domain.

In a former study, the cell-by-cell and the coordinate transformation techniques are compared to the same problem. It was demonstrated that the efficiency of the DSMC method is increased to almost two folds, if coordinate transformation technique is used instead of cell-by-cell technique **(Sengil and Edis, 2011)**. But the mentioned study is limited to the 2D quadrilateral geometries and structured grids.

Grids can be classified fundamentally in two types; as structured and unstructured grids. If grid connections are defined by a general rule, meshes are considered as structured. When grid connections different at each grid point, these types of grids are called unstructured grids. These grids typically composed of triangles in 2D, and tetrahedral in 3D. Unstructured grids are more capable to discretize complex geometries comparing to the structured grids.

If the grid lines and surfaces are coinciding with coordinate lines and surfaces, these grids are called coordinate grids. These kinds of grids require interpolation schemes usage for calculations. These schemes should be avoided in DSMC simulations because of the accuracy problems. If boundaries are defined analytically and configured as the grid lines or surfaces, these types of grids are called boundary-fitted grids **(Liseikin, 2007)**. Boundary-fitting grids are calculated using algebraic, differential and variational methods. In algebraic methods, different interpolation schemes are used to generate grid points inside the physical domain. This method is simple and fast if used with smooth boundaries. In this study only the algebraic method is discussed because this method provides direct analytical relations between physical and computational domains. Differential and variational methods are discussed in other sources in detail **(Blazek, 2005)**.

The quality of the grid strongly influences the accuracy and the efficiency of the DSMC simulations. Ideal DSMC grids have some important requirements **(Bird, 1994)**. Firstly, an ideal DSMC grid should be computationally efficient. Secondly, these grids should be fitted to complex geometries. Next, grid sizes should be correlated with the mean free path and local gradients. Following, grids can be adapted to the changing local flow conditions. And finally, sub-cell construction should be straightforward.

Structured grids are preferred if efficiency is critical. But the application of the structured grids is generally geometry dependent.

3.1 Hybrid Grids for 2D triangles

In the case of the flow geometry diverging from quadrilateral to the triangular, cell area quality decreases if structured grids are used. This deficiency can be resolved by employing unstructured grids **(Naris and Valougeorgis, 2008)**. Comparison of cell area qualities can be seen in Figure 1. But in this case DSMC molecules should be traced cell-by-cell to calculate the cell data. The cell-by-cell tracing

technique is less efficient in comparison to the coordinate transformation technique. A new type of hybrid grid can be a better option. Firstly, it should not as geometry dependent as structured grids. Secondly, this grid should be used with the coordinate transformation technique in order to increase the efficiency.

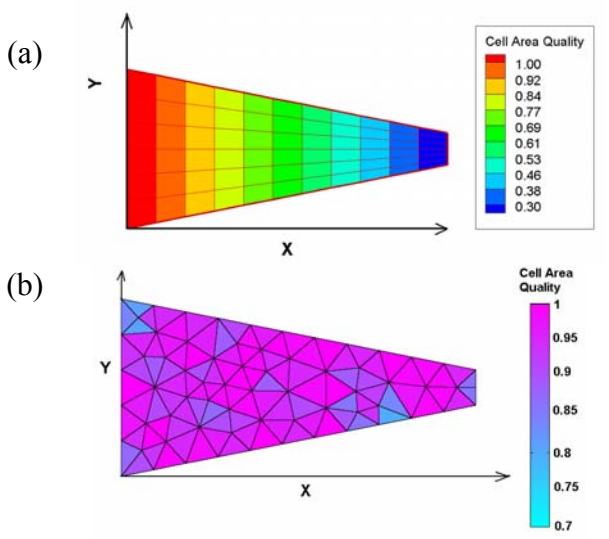

Fig. 1. Comparison of cell area qualities of a quadrilateral geometry. (a) Structured grids. (b) Unstructured grids.

Starting with a scalene triangle, a new method is proposed to construct the hybrid grids in triangular shaped geometries. As a first step, in order to generate algebraic meshes, a 2D scalene triangle rotate around one of its corners, until its vertical edge coincidence with the y-axis as shown in Figure 2.

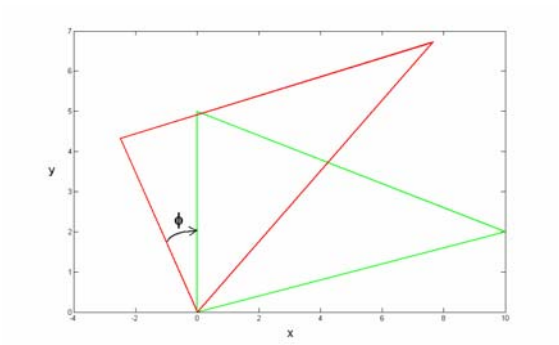

Fig. 2. Scalene triangle (red) is rotated until its vertical edge coincidences with the y-axis (green).

Rotation of the scalene triangle is implemented with the use of following relationships,

$$x' = x.\cos\phi - y.\sin\phi$$
$$y' = y.\cos\phi + x.\sin\phi. \qquad (1)$$

Mapping of the 2D triangle to a square computational domain is carried out using the direct analytical relations,

$$\eta = \frac{x - x_1}{x_2 - x_1}$$
$$\xi = \frac{y - y_d(x)}{y_u(x) - y_d(x)} \qquad (2)$$

Here, x and y are the positions in the physical domain, while x_1 , x_2 $y_d(x)$ and $y_u(x)$ are the minimum, maximum x values and lower and upper edge functions of the 2D triangle respectively. The computational domain is shown in Figure 3. Not all the cells are necessarily quadrilateral. The last cell in the right corner is triangular in shape.

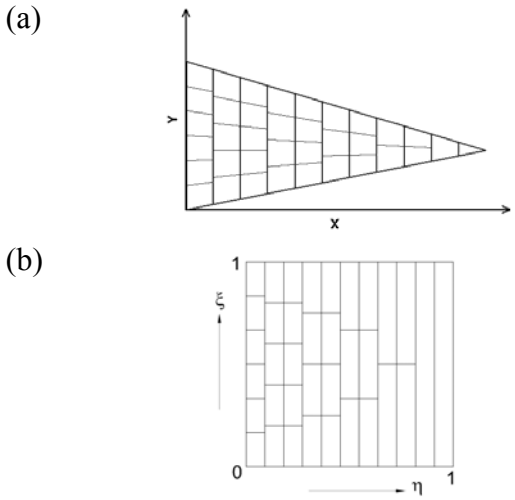

Fig. 3. Hybrid meshes (a) Physical domain. (b) Computational domain.

After the grid size is determined, the triangle is first sliced along x-direction. The edges of the slices are parallel to y-axis. These slices divided again, along the y - direction according to the predetermined grid size. These grids are generated using algebraic grid production techniques.
Primarily, DSMC "movement" step is implemented in the physical domain. Later, molecule positions are transformed to

computational domain using analytical relations between two domains. Following, in which slice DSMC molecule positioned is calculated. This operation is quite simple because the distance between slices is chosen equal. Knowing the cell numbers in each slice, calculation of the cell data is also simplified. As a result DSMC "indexing" step is carried out in the computational domain. In Figure 3, both hybrid grids in the physical domain and the computation domain are displayed. In this method, DSMC molecules are not traced cell-by-cell as in conventional DSMC solvers and calculation time is saved. Also, this method increases the cell area quality considerably, except a few cells, which are located at the right corner as can be seen in Figure 4-a. Consequently, the study is extended to triangular geometries with curved edges, as shown in Figure 4-b.

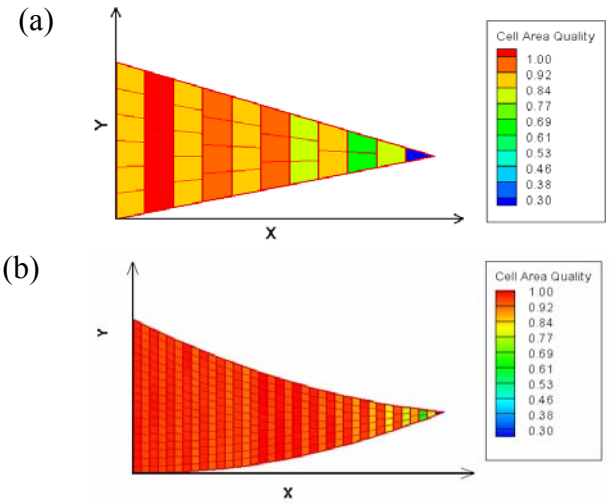

Fig. 4. (a) Scalene triangle with hybrid meshes. (b) Curved edged triangle with hybrid meshes.

This type of geometries is considered more important, because the general polygons are made up of curved edge triangular. This method can have a considerable application area, if polygons are divided to curved edged triangular as shown in Figure 5.

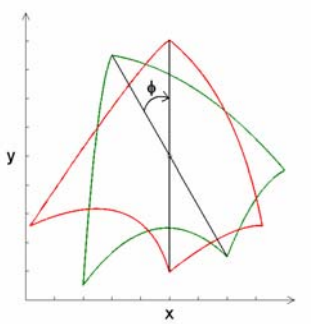

Fig. 5. Quadrilateral (green) rotated and divided into curved edge triangles (red).

4. DSMC Simulations

The physical dimensions of the cells are in the same order with the mean-free-path (λ) of the gas flow **(Bird, 1994)**. But depends on the different flow requirements, sizes of the collision and sampling cells can be different. In this study cell size are chosen as half of the mean-free-path (λ) and the same cells are used both for the "indexing" and "sampling" purposes.

Both in Case1 and Case 2 studies, DSMC molecules are reflected from fully diffusive walls. Walls' temperatures are fixed to $T_w = 300\ K$. The pressure and the temperature inside the cavities are taken $P_i = 1\ atm.$, and $T_i = 300\ K$ as initially. Flowing gas is nitrogen (N_2). DSMC molecule collisions are realized using Variable Hard Sphere (VHS) model.

4.1 Triangular shaped 2D micro cavity

The dimensions of this micro cavity can be seen in Figure 6. Both upper and lower edges of the cavity are straight lines. The analytical equations of the lines are,

$$\begin{aligned} y_u &= -0.3\,x + 5\times10^{-7}, \\ y_d &= 0.2\,x. \end{aligned} \qquad (3)$$

Moving lid is chosen as the bottom wall. The speed of moving wall is 100 m/s. After 3000 time steps, flow become steady and a circulation is formed as expected in a lid-driven micro cavities. A total of 368 hybrid cells is used. A velocity slip is developed by

the walls as expected. The Knudsen number is calculated as 0.1.

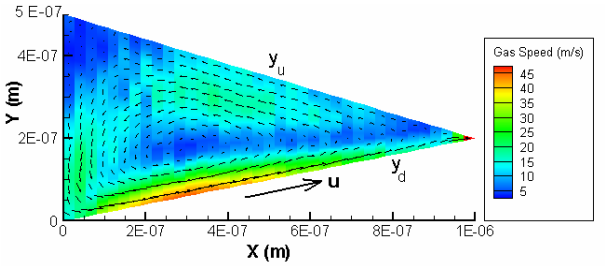

Fig. 6. The gas speed contours of the triangular shaped micro cavity.

4.2 Triangular shaped 2D micro cavity with curved edges

The dimensions of this micro cavity can be seen in Figure 7. Both upper and lower edges of the cavity are curved. The analytical equations of the curves are,

$$y_u = 2\times10^5\ x^2,$$
$$y_d = 2\times10^5\ x^2 - 0.5\,x + 5\times10^{-7}. \qquad (4)$$

Moving lid is chosen as the curved bottom wall. The speed of moving wall is 100 m/s. After 3000 time steps, flow become steady and a circulation is formed as expected in a lid-driven micro cavities. A total of 368 hybrid cells is used. A velocity slip is developed by the walls as expected. The Knudsen number is calculated as 0.1.

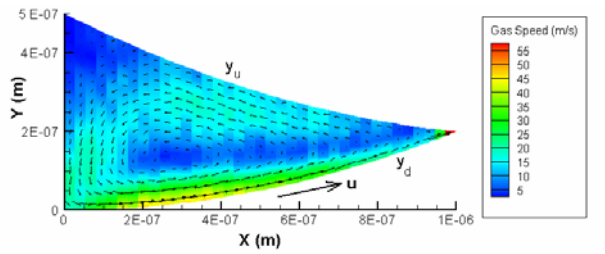

Fig. 7. The gas speed contours of the triangularly shaped micro cavity with curved edges

5. Conclusions

In lid-driven micro cavities, DSMC is one of the prominent methods to acquire gas flow properties. Computation time of the DSMC method is directly related to the Knudsen number. In low Knudsen numbers, solution time of the DSMC method can be intolerable. Using more efficient techniques, the application range of the DSMC method can be increased further. It is shown that, using hybrid grids, cell area quality can be improved as high as the unstructured grids in triangular shaped geometries. Additionally, these types of grids make it possible to implement the coordinate transformation technique which is known more efficient compared to the cell-by-cell tracing technique

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