2D hybrid meshes for direct simulation Monte Carlo solvers

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2D hybrid meshes for direct simulation Monte Carlo solvers

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Abstract. The efficiency of the direct simulation Monte Carlo (DSMC) method decreases considerably if gas is not rarefied. In order to extend the application range of the DSMC method towards non-rarefied gas regimes, the computational efficiency of the DSMC method should be increased further. One of the most time consuming parts of the DSMC method is to determine which DSMC molecules are in close proximity. If this information is calculated quickly, the efficiency of the DSMC method will be increased. Although some meshless methods are proposed, mostly structured or non-structured meshes are used to obtain this information. The simplest DSMC solvers are limited with the structured meshes. In these types of solvers, molecule indexing according to the positions can be handled very fast using simple arithmetic operations. But structured meshes are geometry dependent. Complicated geometries require the use of unstructured meshes. In this case, DSMC molecules are traced cell-by-cell. Different cell-by-cell tracing techniques exist. But, these techniques require complicated trigonometric operations or search algorithms. Both techniques are computationally expensive.

In this study, a hybrid mesh structure is proposed. Hybrid meshes are both less dependent on the geometry like unstructured meshes and computationally efficient like structured meshes.

1. Introduction

Direct simulation Monte Carlo (DSMC) is a molecular based stochastic method to analyze gas flows in the rarefied flow regimes where continuum based solvers are found unsatisfactory. In DSMC method, one particle can represent many physical molecules. Additionally, molecular collisions and movements are decoupled to increase the efficiency in terms of the solution time [1].

Although gridless DSMC methods exist in the literature [2], most of the current DSMC solvers depend on the grids. First DSMC solvers are embedded with the structured grids [3] because of the simplicity of the code maintenance and efficiency. To deal with more complicated geometries, unstructured grids are also implemented in the DSMC method [4]. Currently both structured and unstructured meshes are used in current DSMC solvers.

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. Grid based DSMC solvers display a certain compromise between solution time efficiency and geometry dependence. In this study we propose a hybrid grid system. This new grid system is computationally as efficient as the structured grids. But at the same these grids are adaptable to complex geometries like unstructured grids [1].
2. DSMC 2D grid cell area qualities

The quality of the grid system is defined such that, DSMC cell area values should be as equal as possible and aspect ratios should be close to unity. The number of cells is chosen around 60.

2.1. Structured grids

If grid connections are defined by a general rule, grids are considered as structured [5]. The simplest DSMC solvers are constructed on the structured grids. These kinds of grids are computationally efficient. Additionally, DSMC solvers developed with structured codes are quick to develop and easily maintainable. But these grids are geometry dependent.

![Figure 1](image1.png)

**Figure 1.** (a) Normalized cell area values of a triangle with structured grids (b) Normalized cell area distribution of 66 structured cells.

2.2. Unstructured grids

When grid connections different at each grid point, these types of grids are called unstructured grids. Unstructured grids are more capable to mesh complex geometries comparing to the structured grids. The cell area values and their aspect ratios are more uniform compare to the structured grids as shown in figure 2.

![Figure 2](image2.png)

**Figure 2.** (a) Normalized cell area values of a triangle with unstructured grids (b) Normalized cell area distribution of 60 unstructured cells.

2.3. Hybrid grids

In this study, a hybrid type grid is proposed to mesh a triangular geometry. 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 as shown in figure 3. The cell area values and their aspect ratios are more uniform compare to the structured grids.

![Figure 3](image3.png)

**Figure 3.** (a) Normalized cell area values of a triangle with hybrid grids (b) Normalized cell area distribution of 64 hybrid cells.
3. DSMC 2D grid computational efficiencies

In this part of the study we measure the computational efficiency figures of the structured, unstructured and hybrid grids. Cell dimensions are scaled with the local mean-free-path. After these grids are constructed, one DSMC cell is filled with 10,000 DSMC molecules. Each DSMC molecule is positioned randomly in this cell and assigned velocity components sampled from the Maxwellian distribution. The time step is configured such that DSMC molecules travel no more than one cell length which is physically consistent. In “movement” step, these DSMC molecules change their positions. They either position in the original cell or move to the neighbor cells. After completion of the “movement” step, computer clock is resettled. In “indexing” step all the DSMC molecules are assigned to their new cells in which they positioned. When “indexing” step is completed, computer clock is recorded. Comparisons of the time differences during “indexing” step enables us to assess how efficient the grid systems are.

3.1. Structured grids

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. When geometry is not a rectangular, non-rectangular physical domain should be mapped to a square computational domain geometry using coordinate transformation techniques [6] as shown in figure 4. 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. Tailored grids should be generated in the physical domain in order to calculate molecule cell data fast in the square computational domain with structured grids. Cell data calculation of all 10,000 DSMC molecules takes 0.002 Sec.

3.2. Unstructured grids

DSMC molecules should be traced cell-by-cell to calculate the cell data if unstructured grids are employed as shown in figure 5. The cell-by-cell tracing technique is less efficient in comparison to the coordinate transformation technique. To calculate the efficiency of the DSMC method based on unstructured meshes, first 10000 DSMC molecules are randomly placed inside the cell marked with cell number 59. After “movement” step, all the cells in which DSMC molecules positioned are calculated. Although many methods are existed to calculate the cell data, we only use three different techniques. In the first technique, we searched all the cells sequentially to find out in which cells DSMC molecules positioned. The calculation time for this technique is 0.125 Sec. Secondly; we searched the cells starting from the neighbor cells. This technique takes only 0.011 Sec. Our calculations show that %92.1 of the DSMC molecules either positioned in the originated (59) or neighbor cells on the edges (55,57,58). Finally, we trace the DSMC molecules in these cells only. If DSMC molecules are not located these cells, they are searched in other cells. Calculation time of this third technique is 0.006 Sec.
3.3. Hybrid grids

Hybrid grids can be used with the coordinate transformation technique unlike the unstructured grids in order to increase the efficiency. 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. 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 6, both hybrid grids in the physical domain and the computation domain are displayed. It takes only 0.002 Sec to calculate in which cells DSMC molecules travel.

4. Conclusion

In this study different grid techniques used in 2-dimensional DSMC method are compared in terms of the cell area quality and the computational efficiency. Structured grids are computationally efficient. Moreover they are simple to develop and easily maintainable in the DSMC solvers. But their cell area quality can be significantly degraded when it comes to the complex geometries. Consequently new DSMC solvers embedded with unstructured grids are developed. In these DSMC solvers, molecules are traced cell-by-cell. However this technique is quite inefficient in terms of the computational time. To take advantage of the best parts of these grid systems, we proposed a hybrid type of grid. It is shown that hybrid grids display high cell area qualities like unstructured grids. Besides hybrid grids exhibit efficiency figures as high as the structured grids. In the future, the implementation of the hybrid grids will be further extended to the 3-dimensional DSMC solvers.

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