Application Of Local Mesh Refinement
In The DSMC Method

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ABSTRACT. The implementation of an adaptive mesh embedding (h-refinement) schemes using unstructured grid in two-dimensional Direct Simulation Monte Carlo (DSMC) method is reported. In this technique, local isotropic refinement is used to introduce new meshes where local cell Knudsen number is less than some preset value. This simple scheme, however, has several severe consequences affecting the performance of the DSMC method. Thus, we have applied a technique to remove the hanging mode, by introducing anisotropic refinement in the interfacial cells. This is completed by simply connect the hanging node(s) with the other non-hanging node(s) in the non-refined, interfacial cells. In contrast, this remedy increases negligible amount of work; however, it removes all the difficulties presented in the first scheme with hanging nodes. We have tested the proposed scheme for Argon gas using different types of mesh, such as triangular and quadrilateral or mixed, to high-speed driven cavity flow. The results show an improved flow resolution as compared with that of unadaptive mesh. Finally, we have triangular adaptive mesh to compute two near-continuum gas flows, including a supersonic flow over a cylinder and a supersonic flow over a 35° compression ramp. The results show fairly good agreement with previous studies. In summary, the computational penalties by the proposed adaptive schemes are found to be small as compared with the DSMC computation itself. Nevertheless, we have concluded that the proposed scheme is superior to the original unadaptive scheme considering the accuracy of the solution.

INTRODUCTION

For the past decade, the development of CFD using adaptive unstructured meshes has greatly extended the capability of predicting complex flow fields. Several adaptive mesh techniques have been developed to increase the resolution of “important” region and decrease the resolution of “unimportant” region within the flow field, as reviewed by Powell et al. [2].

In general, mesh adaptation can be categorized into three methods [3]: (1) remeshing (mesh generation), (2) mesh movement, and (3) mesh enrichment (or h-refinement). For the first method, a solution based on the initial mesh is obtained, and then the mesh is regenerated which the mesh points are more concentrated on where resolution of the solution is needed. This new mesh may contain more or fewer mesh points than the original mesh. For the second method, the total mesh points remain the same in the computational domain. It is common to use a spring analogy, in which the nodes of the mesh are connected by springs whose stiffness is proportional to certain measure of solution activity over the spring. The mesh points are moved closer into the region where solution gradients are relatively large. This is often applied to the spatial adaptation of a structured mesh. For the final method, mesh enrichment, mesh points are added or embedded into the regions where relatively large solution gradients are detected, while the global mesh topology remains intact. It is generally regarded that mesh enrichment method has certain advantages over the first two methods [3,4]. One of the most important advantages is that the mesh enrichment technique is in general many times faster and robust than the remeshing technique [4]. In Ref. 3, it is mentioned that the disadvantage, however, is that the implementation of mesh enrichment involves a significant modification to existing numerical schemes due to the appearance of hanging nodes. This can be easily overcome, however, by some simple methods through the elimination of hanging nodes, proposed by Kallinderis and Vijayan [5].

The corresponding development and the application of the adaptive mesh technique in particle method, such as the DSMC method, has been largely ignored. Applying adaptive mesh technique in the DSMC method, as in CFD, not only improves the flow field resolution without increasing the computational cost much, but also more or less equalizes the statistical uncertainties in the averaging process of obtaining the macroscopic quantities.

Among the very few studies about this subject, Wong and Harvey [6] has first applied solution-based,
re-meshing adaptive grid technique (mesh regeneration using the advancing front method) in unstructured meshes to study the hypersonic flow field with highly non-uniform density involving shocks. Later on in the same group, Robinson [7] has applied a similar technique to compute a hypersonic flow over a flat plate with a ramp at different angles. However, some unexpected results such as lower accuracy for a refined mesh, as compared with a coarse mesh, arose due to some reasons yet to be clarified.

Cybyb et al. [8] have developed a technique using the Monotonic Lagrangian Grid (MLG) in the DSMC method, which provides a time-varying grid system that automatically adapts to local number densities within the flow field. However, the application of this MLG technique to external gas flows is not promising due to the particle sorting problems inhered in the scheme. Additionally, this technique highly restricts the time-step size as compared with the traditional DSMC method, which makes the cost of obtaining the steady-state solution comparably high.

Garcia and Bell [9] have developed an adaptive mesh and algorithm refinement (AMAR) embedding the DSMC method within a continuum method (N-S equation solver) at the finest level of an adaptive mesh refinement (AMR) hierarchy. This method can cope with problems possessing several orders of magnitude of length scale.

This paper begins with the Introduction, followed by the DSMC Method with Mesh Adaptation, then the Benchmark Test, Applications to Realistic Flows, and finally the Conclusions.

THE DSMC METHOD WITH MESH ADAPTATION

Based on the reviews in previous chapter and considering the application to DSMC, the general features of an adaptive mesh generation scheme are proposed as follows: (1) unstructured mesh (triangular or quadrilateral or hybrid); (2) h-refinement with mesh embedding; (3) local cell Knudsen number (inversely proportional to density) as the mesh adaptation parameters; (4) upper limit on maximum number of levels of mesh adaptation.

Adaptation Parameters and Criteria

All mesh adaptation methods need some means to detect the requirement of local mesh refinement to better resolve the features in the flow fields and hence to achieve more accurate numerical solutions. This also applies to DSMC. It is important for the adaptation parameters to detect a variety of flow features but does not cost too much computationally. Often gradient of properties such as pressure, density or velocity is used as the adaptation parameter to detect rapid changes of the flow-field solution in traditional CFD. However, by considering the statistical nature of the DSMC method, density is adopted instead as the adaptation parameter. Using density as the adaptation parameter in DSMC is justified since it is generally required that the mesh size be much smaller than the local mean free path to better resolve the flow features.

To use the density as an adaptation parameter, a local cell Knudsen number is instead defined as

\[ Kn = \frac{\lambda}{\sqrt{A_i}} \]  

(1)

where \( \lambda \) is the local cell mean free path and \( A_i \) is the local cell area. When the mesh adaptation module is initiated, local Knudsen number at each cell is computed and compared with a preset value, say, 2. If this value is less than the preset value, then mesh refinement is required. If not, check the next cell until all cells are checked. This adaptation parameter is expected to be most stringent on mesh refinement (more cells are added); hence, the impact to DSMC computational cost might be high.

Consider the practical applications of mesh adaptation in some cases, we have added another constraint, \( |\phi| > \phi_0 \), where \( \phi \) (free-stream parameter) is defined as

\[ \phi = \frac{P - P_-}{\rho_-} \]  

(2)

and \( \phi_0 \) is a preset value case by case. Not only the above constraint helps to reduce the total refined cell numbers to an acceptable level, but also alleviates the problem of too few particles per cell in the interfacial cells between refined and unrefined cells. This will be demonstrated clearly in later chapters.

Mesh Adaptation Procedures

Before outlining the procedures of mesh adaptation, two general rules is described as follows.

(1) Isotropic mesh refinement is employed for those cells, which flag for mesh refinement. A new node is
added on each edge (face) of a parent cell and connecting them to form four child cells. This rule applies to quadrilateral, triangular mesh, as illustrated in Fig. 1. In general, this will create one to three hanging nodes in the cell, which is not refined, next to the cell(s), which is refined isotropically. Existence of hanging node(s) not only complicates the particle movement, but also increases the cost of the cell-by-cell particle tracking due to the increase of face numbers. The remedy is proposed as follows in item (2).

(2) Anisotropic mesh refinement is utilized in the (interfacial) cells next to those cells have just been isotropically refined. Triangular child cells are formed no matter what type of the interfacial cell is, considering the generality of the programming. Typical methods of interfacial mesh refinement in the quadrilateral cells are also shown in Fig. 1. Similar methods are employed to triangular cells. For an interfacial cell with \( (n-1) \) hanging nodes, where \( n \) is the face number of the interfacial cell, an isotropic cell refinement is conducted and then followed by an anisotropic mesh refinement in the new created interfacial cell. The removal of hanging node(s) in the interfacial cells does increase the computational cost; it is, however, trivial as compared with the disadvantages caused by the hanging node(s).

In summary, the following steps describe the procedures for mesh refinement:

1. Set up initial grids and input data.
2. Proceed DSMC computation until enough sampled data are gathered at each cell.
3. Compute the adaptation parameter using Eqs. (1) and (2).
4. Refine all the cells in which the \( Kn_c \) is less than the preset \( Kn_{cc} \) by conducting isotropic mesh refinement.
5. Create and update the neighbor identifying arrays, coordinates, face numbers and sampled data for the new and old cells, respectively. Reduce the simulation time step to half.
6. Check if there are any hanging nodes at each cell. If it does, then conduct anisotropic mesh refinement. Also create and update associated cell data as described in step (5).
7. Return to (2) if the accumulated adaptation levels are less than the preset maximum value.
8. If the accumulated adaptation levels are greater than the preset value or no mesh refinement is required, then reset all sampled data and proceed the DSMC computation as normal.

Note that the proposed mesh adaptation is capable of refining the meshes close to the body surface following the real surface geometry if the surface contour can be cast into a parametric function.

**BENCHMARK TESTS**

A high-speed driven cavity flow, as schematically sketched in Fig. 2, is tested with flow conditions set as follows: \( Kn=\lambda_i/H=0.04 \), aspect ratio \( L/H=1 \), initial number density \( n=6.47E17 \), bottom plate speed \( V_{plate}=8*C_{mp} \) and wall temperature \( T_w=300 \), where \( C_{mp} \) represents the most probable speed based on wall temperature. Initial gas temperatures are 300 K. VHS model is used to model Argon gas with molecular data adopted from Bird [1]. This problem is chosen as the test problem due to its simple geometry and expected high particle density at corners.

Initial 2500 uniform unstructured quadrilateral cells are used. Corresponding simulation time step is 1.17E-4 seconds. Same particle numbers (62500) as the unadaptive mesh are used. The \( Kn_c \) criterion (\( Kn_{cc} \)) is set as 0.95. Evolution of adaptive mesh at each level of adaptation is illustrated in Fig. 3. As illustrated, the maximum adaptation level of adaptive mesh is 3, although the actual number of adaptation levels is 7. The adaptive mesh for adaptation level greater than 3 is not shown due to the limited graphic resolution. Number of mesh adaptation levels at the top corners (right- and left-hand) and bottom corner (right-hand) are one and seven, respectively. The number of cells increases from 2500 of the original mesh to 2929 of the final refined mesh (level 7).

**APPLICATIONS TO REALISTIC FLOWS**

Proposed mesh adaptation scheme has been verified successfully by the benchmark problems stated previously using the local cell Knudsen number as the adaptation parameter. Thus, to demonstrate the powerful capability of the current mesh adaptation, we have applied it to compute two realistic flows, including a hypersonic flow over a cylinder (Fig. 4) and a hypersonic flow over a 35° compression ramp (Fig. 5). The results are then compared with previous simulated or experimental studies available in the literature. Note that the discussion of flow physics is brief since we are only interested in demonstrating the capability of the current DSMC implementation.
A Hypersonic Flow Over a Cylinder

Flow and Simulation Conditions

The flow conditions are listed as follows: VHS Nitrogen gas, free-stream Mach number \( M_\infty = 20 \), free-stream number density \( n_\infty = 5.1775 \times 10^{19} \) particles/m\(^3\), free-stream temperature \( T_\infty = 20K \), fully thermal accommodated and diffusive cylinder wall with \( T_w/T_\infty = 0.18 \), where \( T_w \) and \( T_\infty \) are the wall and the stagnation temperatures, respectively. The corresponding free-stream Knudsen number \( K_n = (\lambda/D) \) is 0.025. These flow conditions represent the experiments conducted by Butefisch [10]. Temperature dependent rotational energy exchange model of Parker [1] is used to model the diatomic Nitrogen gas.

Mesh Adaptation Concerns

This flow problem is chosen to demonstrate the capability of resolving the expected high density in the stagnation region and the high-density gradient across the detached bow shock around the cylinder. In addition, it also serves to verify the conformation of adaptive mesh to the parametric surface ("circular" in this case). Corresponding adaptation criteria for mesh adaptation are \( K_{nc} = 1.0 \) but with maximum number of adaptation levels equal to 5. Additional constraint, \( \phi_w = 1.05 \), which reduces greatly the final refined total cell numbers, is used not to refine those cells with normalized density ratio close to unity (within 5% in this case). The side effect of this constraint might increase the skew of the interfacial cells between unadaptive and adaptive cells. The impact on DSMC, however, is minimal as compared with that on CFD since the cells in DSMC are only used for collision and sampling. Initial 5281 triangular cells and approximately 370,000 particles are used for the simulation.

Adaptive Mesh

Evolution of adaptive mesh at each level is presented in both Fig. 6. The cell numbers increase from 5,281 to 88,959 after five levels of mesh adaptation. The number of cells is less than that used by Kuora and Takahira [11], which had 200,000 cells, but the positioning of the cells in the present study might be superior to theirs due to the mesh adaptation. As illustrated in Figs. 6a-6c, the mesh is refined across the strong bow shock around the cylinder (levels 1-2) as well as the stagnation region (levels 1-5) in front of the cylinder. It is clearly that the proposed mesh adaptation method captures the important flow features such as shocks in this case.

Properties Along the Stagnation Line

Results of normalized number density \( (n/n_\infty) \) along the stagnation line are presented in Figs. 7 and 8, respectively. Previous experimental data of Butefisch [10] and DSMC data of Koura and Takahira [11] are also included in these figures. The present data agree well with both the available experimental data and simulated data in front of and behind the cylinder. The maximum density ratio (23) of the present study is, however, larger than that (~16) of Koura and Takahira [11] due to the highly refined mesh in the stagnation region. Similar agreement is also found for translational and rotational temperatures.

A Hypersonic Flow Over a 35° Compression Ramp

The second demonstration case is the supersonic flow over a 35° compression ramp. This corresponds to the experiments conducted by Chun [12] and the associated computation by Moss et al. [13,14] and Robinson [7]. The hypersonic flat plate problem has been historically important for DSMC computation as it provides the most convincing validations of the method [15]. The author's interest is to resolve the complicated flow fields, which include shock/shock and shock/boundary layer interactions, using the newly developed mesh adaptation method. Although several studies about these phenomena using DSMC have been completed [16,17], application of the adaptive mesh should enable higher resolution of the flow features.

General Flow Features of the Compression Ramp

These have been thoroughly discussed in Robinson [7] and are only briefly described here. There are two major points of interest in the flow field, i.e., the tip flow and shock/shock interactions, as illustrated in the exploded sketch of Fig. 5. The flat plate generates a weak leading-edge shock and a viscous boundary layer, which both propagate downstream the flat plate. The pressure rise caused by the compression ramp influences the plate flow through the subsonic boundary layer, which thickens the boundary layer. For some
range of Mach numbers, Reynolds numbers and ramp angle, the momentum in the laminar boundary layer may not be able to overcome the viscous friction of the plate and adverse pressure generated by the compression ramp, and the layer will separate, leading to a recirculation region in the ramp corner. The free shear layer reattaches further downstream on the ramp due to the pressure rise in the inviscid outer flow because of flow turning. In order to turn the flow along the ramp, a compression fan forms on the outside of the viscous boundary layer, which gradually coalesces into an oblique shock. The pressure rise caused by the resultant shock will thin the viscous boundary layer further downstream on the ramp, until it reaches a point of minimum thickness, or, "neck". Downstream of this point, the boundary layer returns to a normal state with weak interaction with the free stream.

As described in the above, the flow field of a hypersonic flow over a compression ramp is rather complicated. Thus, it is a good test to see if the proposed mesh adaptation can capture the important features of the flow.

**Flow and Simulation Conditions**

The corresponding flow conditions are listed as follows: VHS Nitrogen gas, free-stream Mach number $M_\infty=24.3$, free-stream number density $n_\infty=5.213\times10^18$ particles/m$^3$, free-stream temperature $T_\infty=8.6$K, fully thermal accommodated and diffusive wall with $T_w=394$K. The corresponding free-stream Knudsen number $Kn_\infty=0.003478$. Temperature dependent rotational energy exchange model of Parker [1] is used to model the diatomic Nitrogen gas. Total initial 4013 triangular cells and approximately $4\times10^5$ particles at steady state are used for the simulation.

Since the simulation results of the current study will compare with those of Moss et al. [13,14] and Robinson [7].

**Adaptive Mesh**

Corresponding adaptation criteria for mesh adaptation are $Kn_{cc}=1.0$ and $\phi_\theta=1.05$ but with maximum number of adaptation levels equal to 2, considering the tremendous reduction of particle numbers per cell due to increase of cell numbers. The results of adaptive mesh at each level are illustrated in both Fig. 8. The cell numbers increase from 7,938 to 58,054 after two levels of mesh adaptation, while the corresponding minimum $Kn_\infty$ increases from 0.045 to 0.177. The number of cells is higher than that used by Robinson [7] (~21,000) and Moss et al. [13,14] (~23,800), but the positioning of the cells might be superior to theirs due to the mesh adaptation. As illustrated in Figs. 8, the meshes are refined around the tip of the flat plate (levels 1-2), across the leading-edge shock (levels 1-2) and the interaction regime of the boundary layer and the oblique shock on the ramp (levels 1-2). It is clearly that the proposed mesh adaptation method captures the important flow features such as the leading-edge shock, interactions of both shock/boundary layer and shock/shock in this case. We would expect the results in these regions are improved greatly as compared with unadapted mesh.

**Surface Properties Along the Solid Wall**

Normalized surface properties, including pressure coefficient is defined as follows:

$$C_p = \frac{P_s - P_w}{\frac{1}{2}P_wu_m^2}$$  

Fig. 9 illustrate the corresponding surface property coefficient for the initial mesh and adaptive meshes along with the simulation data by Moss et al [13,14] and Robinson [7] against streamwise location $x$. The agreement for this coefficient from the level-1 mesh with previous studies [7,13,14] along the streamwise location is fairly well. Hence, we will concentrate on discussing the level-1 results unless otherwise specified. However, discrepancies exist in the recirculation and compression ramp regions. Current computational results agree well with both the results from Moss et al [13,14] and Robinson [7] except at the end of the compression ramp, where the current pressure coefficient is higher than the other two results. The discrepancies between the current results and the other two results are unexpected since $C_p$ is generally regarded as least sensitive to the computational details. In addition, it is believed that the rapid decrease of $C_p$ is caused by the weak expansion wave generated by the type VI interaction.

As illustrated in Fig. 9, we have found that the results of level-1 mesh agree best with previous DSMC data. For approximately constant particle number, the discrepancy resulting from level-2 mesh is caused by too few particles per cell since too many cells created after two levels of mesh adaptation. In addition, the
disagreement resulting from initial mesh is caused by the resolution problem since too few cells in the regions of interest. As illustrated in Fig. 10, very few particles per cell (< 1) occurs at level-2 mesh in some refined region, e.g., the compression ramp shock. This will cause the strong correlation between simulated particles due to the collision processes.

Note that the comparison with previous DSMC data is not served as code validation due to the lack of experimental data in the literature. It can only be seen as qualitative comparison to see if most of the flow features are duplicated. We believe that this is well done in the current study.

CONCLUSIONS

In the current study, a DSMC method using the adaptive unstructured mesh is proposed. In this method, an isotropic mesh refinement is used to enrich the cell where the adaptation parameter, \( K_n \), is smaller than the preset value. Additional constraint, free-stream parameter, \( \phi \phi_0 \), is used in some cases to help reduce the total refined cell numbers by relaxing the adaptation criteria in the free-stream cells. An anisotropic mesh refinement is then used to remove the hanging nodes in the interfacial cells created during the isotropic refinement process. Benchmark problem is used to verify the proposed method. Result shows that the current method of mesh adaptation using unstructured mesh is efficient and robust. Finally, the developed method of mesh adaptation is applied to two cases, including a hypersonic flow over a cylinder and a hypersonic flow over a flat plate with 35° ramp. Results are in good agreement with previous experimental or simulation data.

In summary, major findings of the current research are listed as follows.

1. A mesh adaptation method using unstructured mesh, combining the DSMC method, is proposed and tested successfully on several benchmark problems.
2. The proposed method alleviates the burden often required on creating a suitable mesh considering the solution variations, which is not known \textit{a priori}. It automatically generates a solution-based mesh in the current proposed method.
3. Applications of the propose method to two realistic hypersonic flows show that the solution-based adaptive mesh can resolve several important flow features such as shock, interactions of shock/shock and shock/boundary layer.

REFERENCES


Fig. 1 Mesh refinement rules for quadrilateral and triangular cell

Fig. 2 Sketch of High-speed driven cavity flow (V_p=8*V_{mp}, T_w=300K, Ar gas L/H=1, Kn=0.04)

Fig. 3 Evolution of unstructured quadrilateral mesh of a high-speed driven cavity flow (a) initial (b) level 1 (c) level 2 (Kn=0.04, Kn_r=0.95)

Fig. 4 Sketch of a hypersonic flow over a cylinder (Ma=20, T_\infty=20k, T_w=291.6k, N_2 gas, Kn=0.025)

Fig. 5 Sketch of a hypersonic flow over a flat plate with a 35° ramp (Ma=11.42, T_\infty=20k, T_w=394k, N_2 gas, L=71.4mm, Kn=0.003478)

Fig. 6 Evolution of unstructured triangular mesh for a hypersonic flow over a cylinder (a) initial (b) level 1 (c) level 5 (Kn=0.025, Kn_r=1.0, \phi=1.05)
Fig. 7 Normalized number density along the stagnation line for a hypersonic flow over a cylinder (Kn∞=0.025)

Fig. 8 Evolution of adaptive mesh for a hypersonic flow over a 35° compression ramp (a) initial (b) level 1 (c) level 2 (Kn∞=0.003478)

Fig. 9 Pressure coefficient against streamwise location for a hypersonic flow over a 35° compression ramp (Kn∞=0.003478)

Fig. 10 Distribution of particle numbers in per cell (Kn∞=0.003478)