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Improved parallelized hybrid DSMC–NS method

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ABSTRACT

In this paper, an improved parallelized hybrid DSMC–NS (Navier–Stokes method) algorithm, as compared to the previous work [1], is presented. A detailed kinetic velocity sampling study is conducted with a two-dimensional supersonic flow ($M_\infty = 4$) past a 25° finite wedge. It shows most of the boundary layer region is in nearly thermal equilibrium, even with very high continuum breakdown parameter based on velocity, velocity gradient and local mean free path. A new continuum breakdown parameter based on pressure is designed to effectively "exclude" the "false" breakdown region such as the boundary layer. An improved hybrid DSMC–NS algorithm is verified using the same wedge flow case. Results show that the improved algorithm can greatly reduce the computational cost while maintaining essentially the same accuracy. A hypersonic flow ($M_\infty = 12$) past a square cylinder is also employed to exhibit the capability of the improved hybrid DSMC–NS method.

1. Introduction

Several technically important flow problems often involve continuum and rarefied regions in the flow field at the same time. Examples include expanding reaction control system plumes from a space vehicle [2,3], hypersonic flows past a blunt body [4], expanding plumes from a rocket at high altitude [5], high compression ratio turbomolecular pump [6] and jet-type chemical vapor deposition [7], to name a few. Unfortunately, neither continuum nor rarefied flow solver can be used alone accurately and efficiently to solve the entire flow field. Thus, how to efficiently and accurately simulate this kind of flows represents a great challenge to the computational fluid dynamics community at large.

Prior studies in solving flow fields involving continuum and rarified regions employed the hybrid DSMC–NS schemes with various approaches of coupling the particle and continuum methods. Detailed reviews of these approaches can be found in Schwartzentruber and Boyd [8,9], Wu et al. [1] and references cited therein. In general, a hybrid DSMC–NS method applies the concept of spatial domain decomposition to distinguish the computational domain of rarefaction or thermal non-equilibrium to be modeled by the DSMC method, and the computational domain of continuum to be solved by the CFD (NS, Euler or Stokes) solver. Success of such hybrid numerical method relies upon three important issues: (1) accurate and efficient method in determining the continuum breakdown region; (2) proper and efficient flow properties exchange at breakdown interface; (3) the effect of steadiness of the flow solution on designing data exchange at the interface. In the present paper, we focus on the first issue that can further improve the efficiency of the hybrid DSMC–NS algorithm.

Wu's group [1] developed a parallelized hybrid DSMC–NS scheme with unstructured grids, and used two modified breakdown parameters to decompose the spatial domain of the flow fields. One of these two breakdown parameters was the *continuum breakdown parameter*:

$$Kn_{\max} = \max[Kn_D, Kn_V, Kn_T] \quad (1)$$

where Kn_Q is the local maximum Knudsen number defined as the ratio of the local mean free path and local characteristic length based on gradient of property Q:

$$Kn_Q = \frac{\lambda}{Q}|\nabla Q| \quad (2)$$

And the other was the thermal non-equilibrium indicator:

$$P_{\mathrm{Tne}} = |(T_{\mathrm{tr}} - T_{\mathrm{rot}})|/T_{\mathrm{tr}} \quad (3)$$

where T_{tr} and T_{rot} are translational and rotational temperature, respectively. A domain overlapping strategy, taking advantage of unstructured data format, with Dirichlet–Dirichlet type boundary conditions based on these two breakdown parameters was used iteratively to determine the choice of solvers in the spatial domain. These breakdown regions were simulated using the more expensive DSMC method, while other regions were simulated using the relatively cheaper NS equation solver. Normally, the size of the overlapping region was about four layers extending from the particle side towards continuum side to make sure the Maxwellian distribution could be applied accurately at solver-solver boundaries. Results

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showed that, not only the leading edge and shock, but also the boundary layer regions were identified as breakdown regions, in which large velocity gradient due to high-speed flows was often the dominating factor in determining Kn_{max} .

There are still several issues that require further investigation. *First*, the inclusion of the boundary layer as the continuum breakdown region often causes slow convergence or even wrong solution of the coupling, which was also found by Schwartzentruber et al. [11]. Now question arises: is it truly continuum breakdown in the whole domain of boundary layer? *Second*, the computational cost could be higher than the pure DSMC solution mainly due to the expensive DSMC simulations for several couplings. Any strategy of reducing the computational cost due to DMSC should be highly welcomed. This issue has been partially addressed by Schwartzentruber and Boyd [8,9] by using so-called "sub-relaxation" scheme in DSMC sampling and will not be discussed here. In this paper, we intend to address the first issue as mentioned earlier and hopefully we can improve the hybrid DSMC–NS algorithm to become a more practical tool in simulating flow field involving continuum and continuum/thermal-equilibrium breakdown regions, such as hypersonic flows.

The present paper is organized as follows. Direct kinetic velocity sampling from a pure DSMC simulation for a supersonic nitrogen flow past a 2-D wedge flow is described in detail in Section 2. Improved hybrid DSMC–NS algorithm is then proposed in Section 3, emphasizing the modifications as compared to the original version [1], which include the definition of a new breakdown parameter in applying this new breakdown parameter. This improved algorithm is then verified in detail in Section 4 by simulating a supersonic flow past a 25° wedge. Simulation of hypersonic flow past a square cylinder is demonstrated in Section 5. Finally, the major findings of the present study are summarized in Section 6.

2. Kinetic velocity sampling

To probe whether the boundary layer is a thermal non-equilibrium region, a direct kinetic sampling study for a supersonic wedge flow case is conducted, as schematically shown in Fig. 1. Sampling locations and distribution of continuum breakdown parameter Kn_{max} based on flow density, temperatures and velocities, resulting from a pure DSMC simulation, are indicated in Fig. 1. Important flow conditions are briefly summarized as: nitrogen gas, Mach number of 4 (1111 m/s), free-stream temperature of 185.6 K and wedge wall-temperature of 293.3 K. DSMC related simulation conditions are shown in Table 1. Note the Knudsen number based on the length of the wedge and the free-stream conditions is 0.0017. In addition, the thermal non-equilibrium indicator is further generalized in the present study as follows:

$$P^{*}_{\text{Tne}} = \sqrt{\frac{\left(\frac{T_x}{T_{\text{tot}}}-1\right)^2+\left(\frac{T_y}{T_{\text{tot}}}-1\right)^2+\left(\frac{T_z}{T_{\text{tot}}}-1\right)^2+\zeta_{\text{rot}}\left(\frac{T_{\text{rot}}}{T_{\text{tot}}}-1\right)^2+\zeta_v\left(\frac{T_v}{T_{\text{tot}}}-1\right)^2}{(3+\zeta_{\text{rot}}+\zeta_v)}} \quad (4)$$

where T_x, T_y and T_z are translational temperature in the *x*-, *y*-, *z*-direction, respectively. T_{rot}, T_v and T_{tot} are rotational, vibrational and average temperature, respectively. ζ_{rot} and ζ_v are the number of degree of freedom of rotation and vibration, respectively.

Totally 52 points, including near leading edge, oblique shock, boundary layer and expanding fan, are selected in the computational domain. Velocity distributions of three Cartesian directions at each selected point are sampled for particles up to at least 0.3 million and then are compared with the corresponding local Maxwell–Boltzmann velocity distributions to calculate the degree of continuum breakdown in these representative points. In addition, the thermal non-equilibrium indicator P^{*}_{Tne} is also calculated at each selected point based on the DSMC results. In general, the Kn_D and Kn_T dominate most part of the computational domain and across the oblique shock, respectively; while Kn_V dominates near the solid wall due to the high velocity gradient in the boundary layer and wake regions.

As shown in Fig. 1 at Points 26–30 and Points 31–35 in the boundary layer, very large breakdown parameter Kn_{max} occurs due to the large velocity gradient, especially near the solid wall ($Kn_{max} > 0.4$). Normally these two regions in the boundary layer would be considered as continuum breakdown domains based on previously proposed criterion of Kn_{max}. Fig. 2b–d shows the particle random velocity distributions at Points 26–30 near the boundary layer along with the local Maxwell–Boltzmann distribution. Note that Points 26–30 are at locations closer to the leading edge,

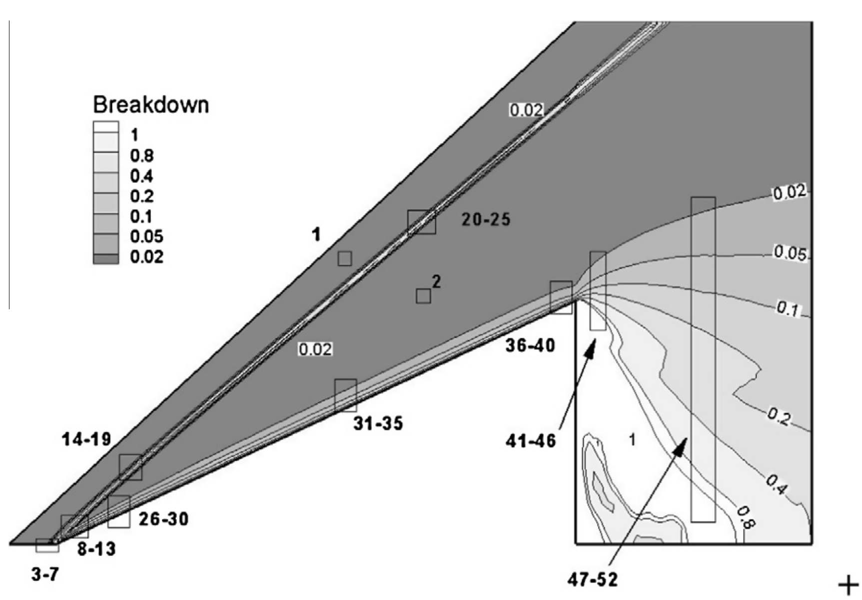

Fig. 1. Sketch of the kinetic velocity sampling locations and distribution of continuum breakdown parameter (based on velocities, density and temperatures) of 2-D 25° wedge flow resulting from a pure DSMC simulation.

Table 1
Simulational conditions of supersonic flow past quasi-2-D 25° wedge with pure DSMC simulation for the kinetic study.

Method	DSMC for the kinetic study
Cell no.	103,520
Sim. particle no.	~7,700,000
Reference, Δt (s)	2.2E−08
Sampling time steps	92,000

*Velocity distributions at each selected point are sampled for particles up to at least 0.3 million.

which are expected to have larger property gradients. However, the particle random velocity distributions at Points 26 and 28 are quite consistent with the local Maxwell–Boltzmann distribution. Even at Point 30, which is very near the solid wall, the maximum temperature deviation to the average temperature is less than 5–6% (P^{*}_{Tne} = 0.034). Astonishingly, at Points 31–35 the velocity distributions are in very good agreement with the local Maxwell–Boltzmann distribution and the temperature variation among different degrees of freedom is very small (not shown here), even with very large value of $Kn_{\max}$ (all higher than 0.05 as shown in Fig. 1). We attribute the non-breakdown of continuum and thermal equilibrium among various degrees of freedom of thermal energy (translation, rotation and vibration) in the boundary layer to that the particles frequently collide with the isothermal solid wall and are thermalized to the wall-temperature before emitting into the region near the wall.

Based on the $Kn^{\mathrm{Thr}}_{\max}$ = 0.05 (the threshold value of $Kn_{\max}$ for continuum region) as recommended by Wang and Boyd [10], the boundary layer would be assigned as the breakdown region. Thus, we can conclude that the degree of the continuum breakdown in these locations, such as Points 31–35, is overestimated based on the previously proposed criterion of $Kn_{\max}$. The above kinetic studies indicate that it is not necessary to utilize the DSMC method in the whole boundary layer, even the continuum breakdown parameter $Kn_{\max}$ is very large. The detailed kinetic velocity sampling

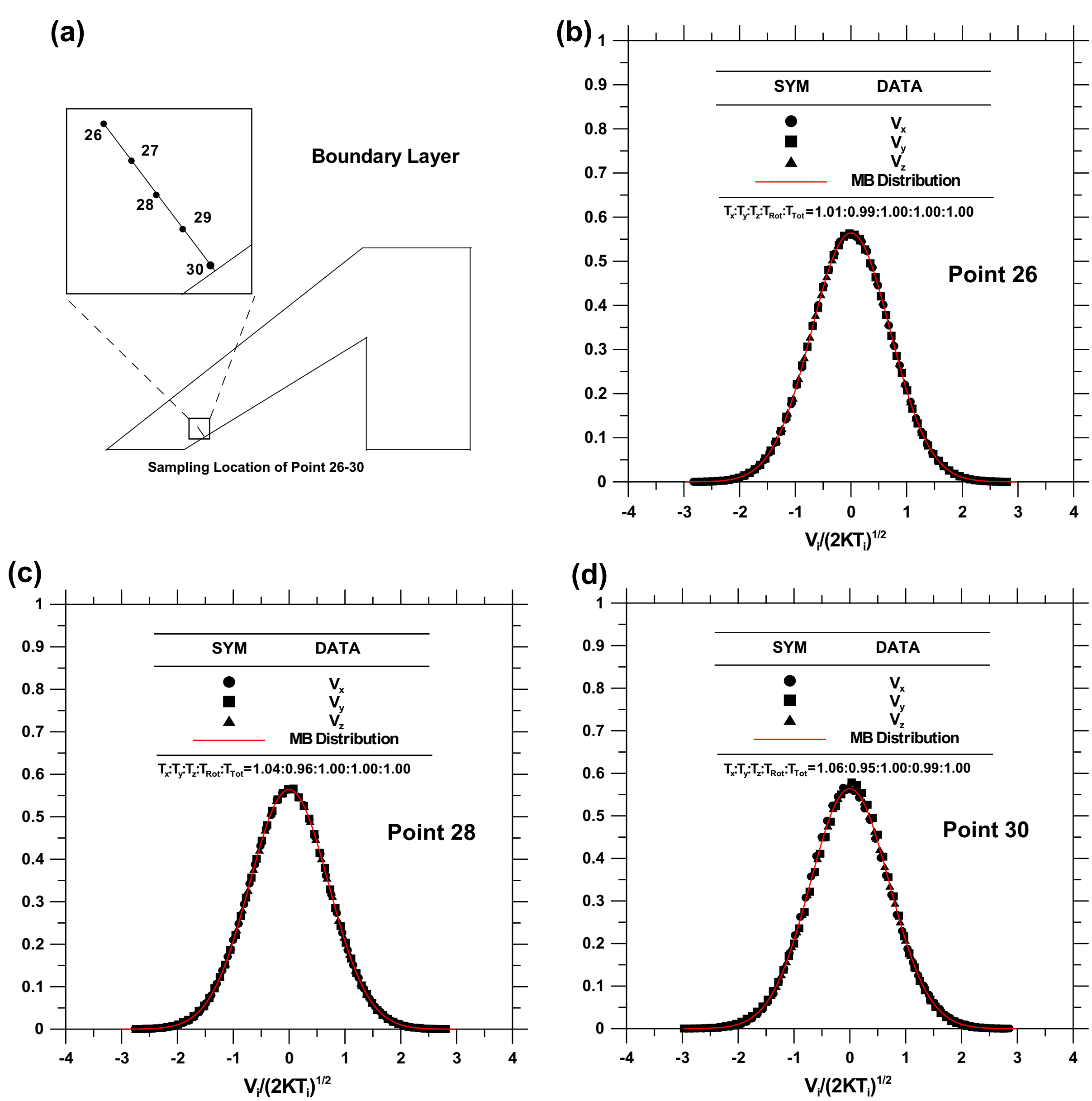

Fig. 2. (a) Location of sampling points across the boundary layer; random velocity distributions in each direction at Point (b) 26; (c) 28; (d) 30, along with translational and rotational temperatures.

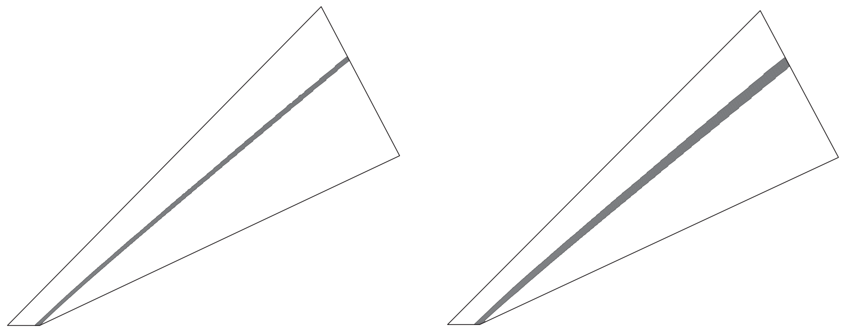

Fig. 3. Breakdown domain based on one-shot NS solution with new continuum breakdown criteria. (a) Breakdown region (b) DSMC domain including the overlapping regions ($Kn_p > 0.05$).

Table 2
Simulation sets with different breakdown criteria in supersonic flow past a quasi-2-D 25° wedge.

Set	Old breakdown criteria	New breakdown criteria
Overlapping layers for non-BL	4	4
Overlapping layers for BL	4	25
Kn^{Thr}	$Kn_{\max} > 0.05$	$Kn_p > 0.05$
$P_{\mathrm{Tne}}^{\mathrm{Thr}}$	0.03	0.03
Final DSMC cells	~18,000	~14,000
Sim. particle number	~2060,000	~1230,000
Reference, Δt (s)	3.0E−09	
Sampling time steps	10,000	

*Total cell number of computational domain for coupled DSMC–NS method is ~68,000. Ten processors are used throughout the simulation.

proves that previously defined continuum breakdown parameter $Kn_{\max}$ can generally predict the continuum breakdown well, except in the regions of the boundary layer, where the thermal equilibrium generally holds well. Thus, an alternative continuum and thermal-equilibrium breakdown determining strategy is required to effectively "exclude" this boundary layer region to generalize the proposed hybrid DSMC–NS algorithm.

3. Improved hybrid DSMC–NS algorithm

In the previously proposed hybrid DSMC–NS algorithm using unstructured grids [1], steady-state flow calculation was assumed. Two breakdown parameters were used to identify the breakdown region and were defined earlier in Section 1. General procedures of iterative coupling between DSMC and NS solvers are summarized as: (**1**) simulate the whole domain using the NS solver; (**2**) determine the breakdown regions based on distribution of breakdown parameters $Kn_{\max}$ and P_{Tne}; (**3**) extend the breakdown domain with few overlapping layers towards continuum domain; (**4**) simulate the breakdown domain using the DSMC solver; (**5**) repeat step (**1**) (but only for the continuum domain) through step (**4**) until convergence is reached.

In the present paper, we use the UNIC-UNS NS solver [12,13], instead of the HYB3D [14] as used in our previous study [1]. The present Navier–Stokes equation solver, developed by Chen and his coworkers [12,13], employs the cell-centered finite-volume method with a hybrid 2D/3D unstructured-grid topology. Details of various numerical and physical modules embedded in this solver can be found in [12,13] and are skipped here for brevity. Only three important features are mentioned here. The first is the use of pressure-based method, which allows accurate simulation of the flows at all speeds. The second is the automatic slip velocity and temperature jump boundary conditions near solid wall. The third is parallel computing of the NS equation solver also incorporates the graph-partition tool, PMETIS [15], which is the same as that in the present parallelized DSMC solver [16–18] (PDSC).

As mentioned earlier, by applying the $Kn_{\max}$ as the breakdown parameter in addition to the thermal non-equilibrium indicator P_{Tne}, the boundary layer region is generally included as the breakdown DSMC domain for high-speed flows, which generally slows down the convergence of the coupling between two numerical

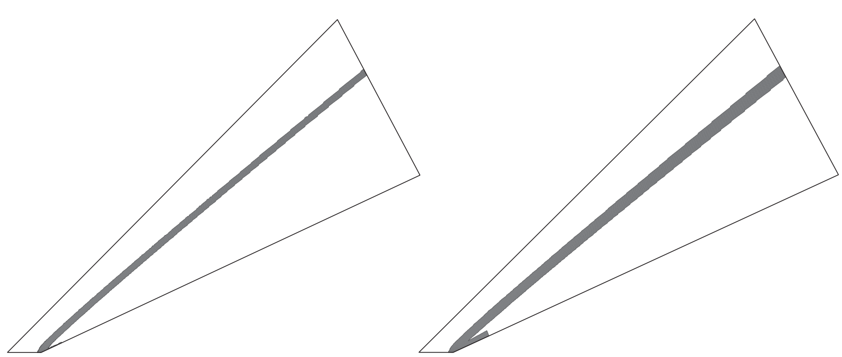

Fig. 4. Breakdown domain distribution at 20th hybrid iteration with new continuum breakdown criteria. (a) Breakdown region (b) DSMC domain including the overlapping regions.

Table 3
Total computational time (h) in supersonic flow past quasi-2-D 25° wedge.

	Pure NS	Pure DSMC	New coupled method (four iterations)			coupled method (six iterations)		
			One-shot			One-shot		
			NS	DSMC	NS	NS	DSMC	NS
			1.25	3.03	0.63	1.25	9.10	0.57
Total time	1.25	9.33		4.91			10.92	

*The computational time in each iteration for *new* coupled method is about 0.85 h, while that for *old* coupled method is 1.5 h.

solvers. In the present study, we define a new continuum breakdown parameter Kn_p to replace the role of $Kn_{\max}$ as follows,

$$Kn_p = \frac{\lambda}{p}|\nabla p| \tag{5}$$

For example, Fig. 3 shows the initial breakdown domains using the new breakdown parameter ($Kn_p > 0.05$) based on the solution of initial NS simulation. With this new breakdown parameter, most of the boundary layer can be excluded as one of the breakdown regions, in which the more efficient NS equation solver can solve the flow field with proper slip boundary conditions at wall.

In brief summary, general procedures of newly proposed hybrid algorithm are summarized as follows: (**1**) simulate the whole domain using the NS solver; (**2**) calculate breakdown parameters, Kn_p and P_{Tne} based one-shot NS simulation or the hybrid solution from NS equation and DSMC solvers; (**3**) determine the breakdown regions based on these two breakdown parameters in the whole flow field; (**4**) estimate the location of thermal breakdown interface in regions near boundary layer by extending more layers; (**5**) extend the breakdown domain with few overlapping layers towards continuum domain; (**6**) simulate the breakdown domain using the DSMC solver; (**7**) repeat step (**1**) (but only for the continuum domain) through step (**6**) until convergence is reached.

4. Test problem

4.1. Flow and simulation conditions

A supersonic nitrogen flow ($M_\infty = 4$) past a 2-D wedge of 25° half-angle with a length of 60.69 mm is chosen as the test problem for the new hybrid algorithm. All simulation conditions are the same as those in previous study [1] and are summarized in Table 2. In this study, number of extension layers is fixed as four, except near the boundary layer close to the leading edge. Some of the simulation conditions are mentioned in the following, as it is necessary. In addition, 10 processors are used throughout the study. Results of flow properties obtained by the new hybrid algorithm are essentially the same as those by the old hybrid algorithm [1] and are not shown here due to the page limit.

4.2. Distribution of breakdown domains

The final distribution of breakdown domains using Kn_p and P_{Tne} after 20 coupling iterations is illustrated in Fig. 4. Note the criterion for Kn_p and P_{Tne} is set as 0.05 and 0.03, respectively, in this study, unless otherwise specified. Note the breakdown domain only includes the regions across the shock and regions near the leading edge, in which most boundary layer regions are excluded, which the NS equation solver can be used to obtain the flow field more efficiently, while accurately enough.

4.3. Comparison of convergence between the old and new coupled algorithms

Table 2 summarizes the simulation conditions along with the breakdown criteria for the old and new coupled algorithm for this specific test case. Results show that fewer DSMC cells are included in the new algorithm as compared to that in the old one. This reduction of number of DSMC cells and fewer coupled iterations required attributes to the shorter simulation time as summarized

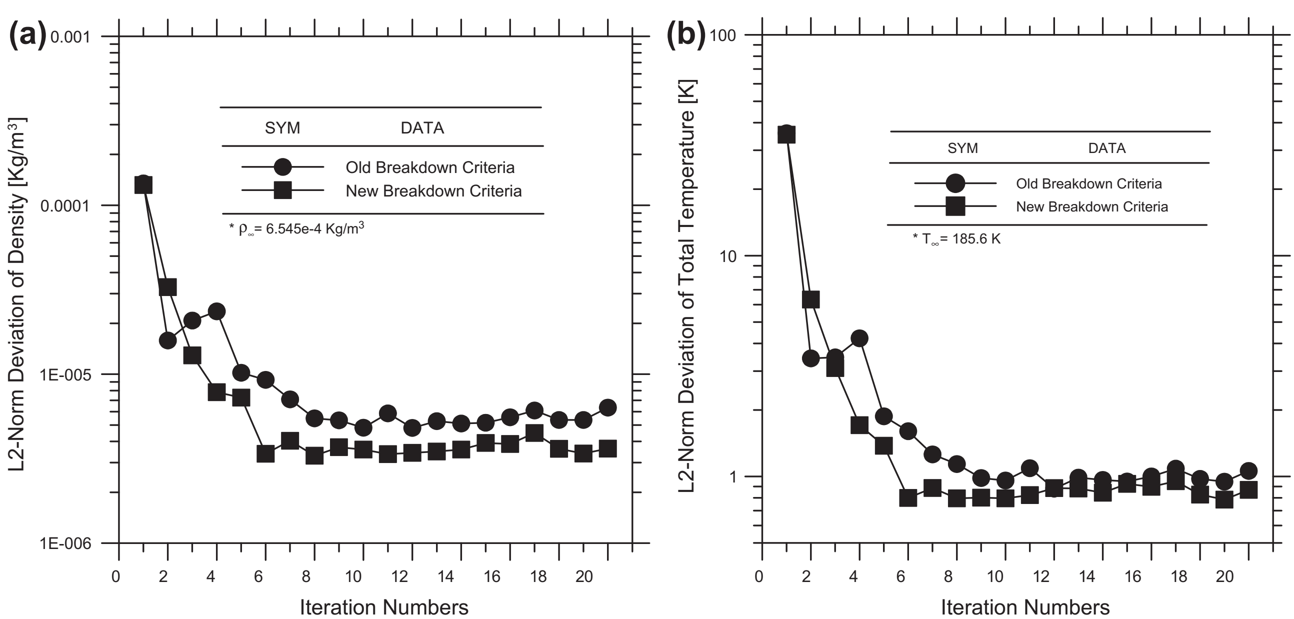

Fig. 5. Convergence history of L2-norm deviation of (a) density and (b) overall temperature between different continuum breakdown criteria in quasi-2-D 25° wedge flow.

in Table 3. New algorithm can save up to 50% of the computational cost with the same convergence criteria for the present test case. Note this problem is chosen such that the pure DSMC solution can be obtained in a short period of time.

Fig. 5a and b illustrates the convergence history of L2-norm deviation of density and overall temperature, respectively, using two different breakdown criteria. Result shows the L2-norm deviations of the new hybrid algorithm level off starting at the 6th iteration, while they take up to 10 iterations with obviously higher values for the old hybrid algorithm. The adoption of the new breakdown criteria indeed improves the efficiency of coupling convergence. As compared to the results after 20 iterations, it only takes four coupling iterations with new breakdown criterion Kn_p for reaching a well converged solution, while it needs at least 6 or 7 using the old Kn_{max}.

5. Application case

5.1. Flow and simulation conditions

Hypersonic nitrogen flow past a 2-D square cylinder shown in Fig. 6 is chosen as the application case for the new hybrid algorithm. Free-stream conditions for this test case include: a Mach number (M_∞) of 12, a velocity (U_∞) of 1547 m/s, a density (ρ_∞) of 9.54E−5 kg/m^3 and a temperature (T_∞) of 40 K and the solid wall boundary is adiabatic. Note the threshold values for Kn_p and P_{Tne} are set as 0.05 and 0.1, respectively. Related simulation conditions are also summarized in Table 4 for reference. Results of flow properties obtained by the new hybrid algorithm are also very favorable

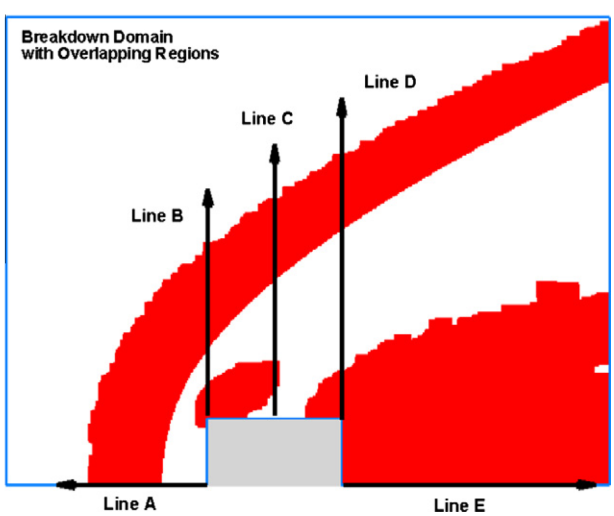

Fig. 6. Final breakdown regions and locations of Lines A–E (for 20th iterations). Breakdown regions are shown in red color. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 4
Simulation condition in hypersonic flow over a square cylinder.

Set	New breakdown criteria
Overlapping layers	4
Kn_p^{Thr}	0.05
P_{Tne}^{Thr}	0.1
Final DSMC cells	~53,541 (for 20th iteration)
Sim. particle number	~712,000
Reference, Δt (s)	7.36E−08
Sampling time steps	11,000 (same as in pure DSMC)

*Total cell number of computational domain for coupled DSMC–NS method is 152,500. Ten processors are used.

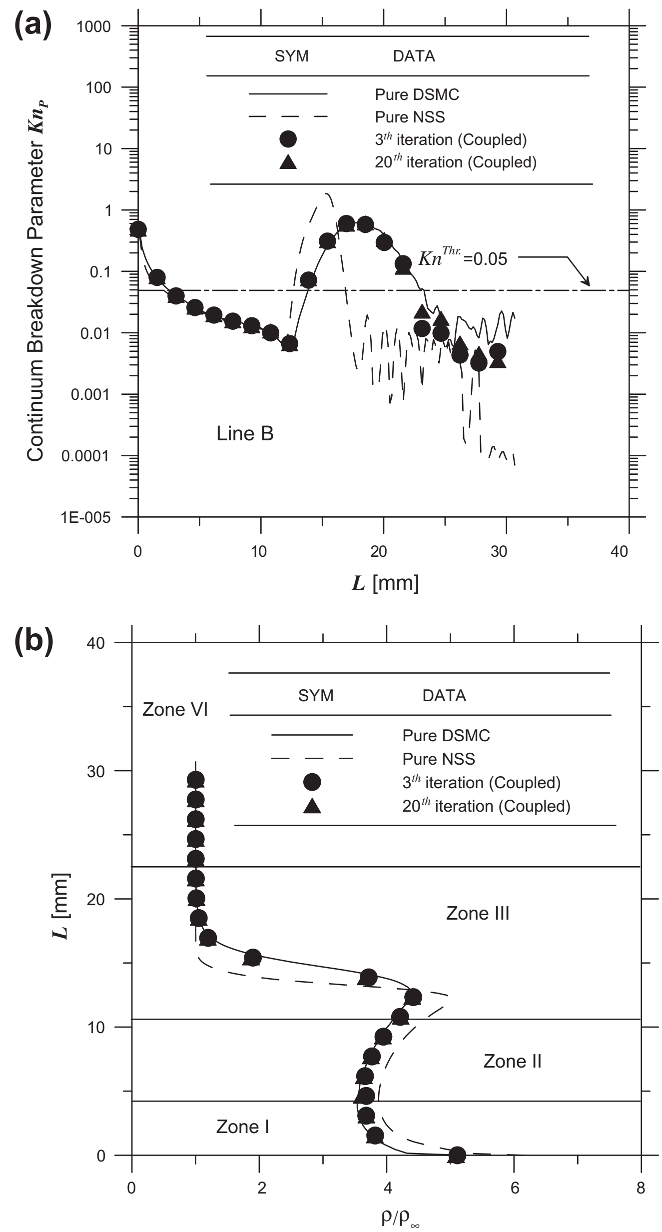

Fig. 7. Profiles of (a) continuum breakdown parameter and (b) density along Line B for 20 iterations.

to those obtained by full DSMC simulations, although they are not shown here due to the page limit.

5.2. Distribution of breakdown domains and typical results

Fig. 6 shows the final breakdown regions after 20 coupling iterations based on the simulation condition. Lines A–E are selected to compare the results among pure DSMC, pure NS equation solver (NSS), 3 and 20 hybrid DSMC–NS iterations. Note the breakdown

Table 5
Total computational time (h) in hypersonic flow past a square cylinder.

	Pure NS	Pure DSMC	New coupled method (four iterations)		
			One-shot NS	DSMC	NS
Total time	1.48	4.17	1.48	2.97 5.00	0.55

domain only includes the regions across the shock, and zones near the leading edge and wake region. We can see most boundary layer regions are excluded, which the NS equation solver can be used to obtain the flow field more efficiently.

One typical example is shown in Fig. 7 which illustrates the profiles of continuum breakdown parameter Kn_p and density along Line B. The horizontal dashed line showing the threshold value $Kn^{Thr.}$ of the new continuum breakdown parameter is the borderlines above which the continuum breaks down and the NS equation solver cannot be used. General trend of the Kn_p distribution shows that the value is rather large (up to 0.4 or larger) near the shoulder of square cylinder due to large property gradients in leading edge region, and decreases to rather small value in the region between the boundary layer and the bow shock, and finally becomes large again across the bow shock (up to 0.5 or less). Obviously, the Kn_p distribution from either 3 or 20 coupled DSMC–NS iteration is in good agreement with those by pure DSMC simulation while pure NS equation solver predicts a much thinner shock thickness and different location of bow shock. Based on the calculated breakdown parameters (Kn_p and P_{Tne}), the flow region is divided into four sub-domains, as shown in Fig. 7b: Zones I and III are the DSMC solution domains, while the other two regions (II and VI) are the NS solution domains. At this location (along Line B), the result of the NS equation solver deviate appreciably from those of both pure DSMC simulation and the coupled method (after either 3 or 20 iterations). Results of the present hybrid methods are still in excellent agreement with those of pure DSMC simulation for the entire domain. It also shows three hybrid iterations are good enough to reach convergence of the hybrid algorithm. Related computational timings are listed in Table 5 for reference.

6. Conclusion

An improved parallel hybrid DSMC–NS algorithm is proposed and verified in the present paper. Direct kinetic velocity sampling is conducted to point out that previously defined continuum breakdown parameter Kn_{max} could overestimate the degree of the continuum breakdown in most region of the boundary layer, where the thermal equilibrium generally holds well. A new breakdown Kn_P based on pressure is designed to effectively "exclude" such that boundary layer region. A 2-D 25° wedge flow ($M_\infty = 4$) was used as the test case for verification of the improved hybrid method. Most of the boundary layer region can be excluded as the breakdown region, if the breakdown parameter Kn_p is employed. With this new hybrid algorithm, simulation converges faster as compared to the old one. Then, this improved algorithm is applied to a hypersonic flow ($M_\infty = 12$) past a square cylinder case. Results show that, with the proposed coupled algorithm, simulation can obtain a good solution within three coupling iterations.

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