Parallel Hybrid Particle-Continuum (DSMC-NS) Flow Simulations Using 3-D Unstructured Mesh

J.-S Wu[1]*, Y.-Y. Lian[1], G. Cheng[2] and Y.-S. Chen[3]

[1]Department of Mechanical Engineering
National Chiao Tung University
Hsinchu City 300, TAIWAN

[2]Department of Mechanical Engineering
University of Alabama at Birmingham
AL 35294-4461, USA

[3]National Space Organization
Hsinchu City 300, TAIWAN
E-mail: Dr. J.-S. Wu, chongsin@faculty.nctu.edu.tw

Key Words: Parallel computing, Hybrid particle-continuum flow simulation

ABSTRACT

In this paper, a recently proposed parallel hybrid particle-continuum (DSMC-NS) scheme employing 3D unstructured grid for solving steady-state gas flows involving continuum and rarefied regions is described [1]. Substitution of a density-based NS solver to a pressure-based one that greatly enhances the capability of the proposed hybrid scheme and several practical experiences of implementation learned from the development and verifications are highlighted. At the end, we present some simulation results of a realistic RCS nozzle plume, which is considered very challenging using either a continuum or particle solver alone, to demonstrate the capability of the proposed hybrid DSMC-NS method.

Introduction

Several important gas flows involve flow fields having continuum and rarefied regions, e.g., hypersonic flows [2], vacuum-pump flows with high compression ratio [3], expanding RCS (reaction control system) nozzle plumes in aerospace and space applications [4], physical vapor deposition processes with heated sources [5], pulsed-pressure chemical vapor deposition processes [6], among other things. Understanding of the underlying physics through simulation and modeling in the above flows are important for the success of these disciplines, in addition to the usual experiemental studies.

In general, these flow problems are governed by the Boltzmann equation, which is very difficult to solve numerically or analytically due to the existence of collision integral and high number of phase-space dimensions (up to seven). It is well known the direct simulation Monte Carlo (DSMC) method [7] can provide more physically accurate results in flows having rarefied and non-equilibrium regions than the continuum flow models such as the NS equations. However, the DSMC method is extremely computational expensive especially in the near-continuum and continuum regions, which prohibits its applications to practical problems with large domains. In contrast, the computational fluid dynamics (CFD) method, employed to solve the Navier-Stokes (NS) or Euler equation for continuum flows, is computationally efficient in simulating a wide variety of flow problems. But the use of continuum theories for the flow problems involving the rarefied gas or very small length scales (equivalently large Knudsen numbers) can produce

inaccurate results due to the breakdown of continuum assumption or thermal equilibrium. A practical approach for solving the flow fields having near-continuum to rarefied gas is to develop a numerical model combining the CFD method for the continuum regime with the DSMC method for the rarefied and thermal non-equilibrium regime. A well-designed hybrid scheme is expected to take advantage of both the computational efficiency and accuracy of the NS solver in the continuum regime and the physical accuracy of the DSMC method in the rarefied or thermal non-equilibrium regime.

In the past, there were several efforts in developing the hybrid particle-continuum scheme. Most studies employed structured grid for both the particle and continuum solvers [8-12], in which the location of breakdown interfaces between continuum and rarefied regions was specified in advance [8,9,11,12] or identified after 뱋ne-shot? CFD simulation [10]. One immediate disadvantage by employing structured grid is that the pre-specified breakdown interface does not follow faithfully the interface determinde by some breakdown parameters [7, 13], which may in turn either increases the runtime or induce inaccuracies of the solution. In addition, some techniques, such as particle cloning [12], overlapped region [8,12] and iteration [8] between particle and continuum regions, are used to reduced the statistical uncertainties in coupling the two solvers. Among these, the hybrid schemes developed by Wang *et al.* [11] and Roveda *et al.* [12] are potentially suitable for simulating unsteady flows, while the others were only designed for simulating steady flows. In the above, only one-dimensional and two-dimensional flows were demonstrated and extension to parallel or three-dimensional simulation has not been reported to the best knowledge of the authors.

Recently, Wu *et al.* [1] has developed a parallel hybrid DSMC-NS scheme using 3D unstructured mesh. Parallel implementation is realized on memory-distributed parallel machines, e.g., PC-cluster system. In this method, a domain overlapping strategy, taking advantage of unstructured data format, with Dirichlet-Dirichlet type boundary conditions based on two breakdown parameters, was used iteratively to determine the choice of solvers in the spatial domain. The selected breakdown parameters for this study include: 1) a local maximum Knudsen number, proposed by Wang and Boyd [13], defined as the ratio of the local mean free path and local characteristic length based on property gradient and 2) a thermal non-equilibrium indicator defined as the ratio of the difference between translational and rotational temperatures to the translational temperature. A supersonic nitrogen flow (M_∞=4) over a quasi-2-D 25° wedge and a nitrogen flow, which two near-continuum parallel orifice jets underexpand into a near-vacuum environment, were simulated to, respectively, verify its validity and demonstrate its capability in solving realistic 3-D gas flows. Effects of the size of overlapping regions and the choice of breakdown parameters on the convergence history are also discussed in detail.

In the present paper, this recently developed hybrid DSMC-NS scheme is described briefly for completeness. Improvement of the NS solver by using a pressure-based solver is described next. Then, several practical experiences learned from the development and verifications of the implementation are shown in detail. Finally, simulation results for several challenging flows are presented to demonstrate its capability.

Hybrid DSMC-NS Scheme Using 3D Unstructured Mesh

In the proposed coupled DSMC-NS method [1], steady-state flow calculation is assumed. There were two numerical flow solvers included: one is the 3-D DSMC code for rarefied and thermally non-equilibrium regions, named PDSC (Parallel Direct Simulation Monte Carlo Code), developed by Wu뒽 group [e.g, 14] and the other is HYB3D, a density-based 3-D Euler and Navier-Stokes solver for continuum regions, developed by Koomullil [e.g, 15]. In the present study for nozzle plume, a pressure-based NS solver, named UNIC-UNS, using 3D unstructured mesh, developed by Chen and his coworkers [e.g., 16-17] that is applicable at all speeds, is used for continuum regions. It is rather straightforward to exchange the information between the PDSC and this UNIC solver in the proposed DSMC-NS scheme because both methods use the unstructured grid topology with parallel computing. However, proposed coupling procedures between DSMC and NS solvers are not limited to any specific codes, and selection of these two

solvers is for the purpose of demonstration. Both codes are introduced briefly in the following, respectively, for completeness.

DSMC Solver (PDSC)

Details of the features of the PDSC code can be found in the reference [14] and are only briefly described here for brevity. PDSC features 3-D unstructured grid, parallel computing with dynamic domain decomposition using MPI, variable time-step scheme with adaptive mesh refinement and treatment of high-temperature chemical reacting flows. It can be implemented efficicntly on general memory-distributed parallel machines, such as PC-cluster system.

Navier-Stokes Solver

The present Navier-Stokes solver employs an unstructured-grid topology and has the following important features: 1) Cell-centered finite-volume for the numerical integration of governing equations, 2) An upwind method with linear reconstruction scheme for convective flux evaluation, 3) Modified pressure-velocity-density coupling algorithm of the SIMPLE type with added pressure damping term, 4) Parallel computing based on domain decomposition with message passing interface (MPI), 5) Turbulent flow simulation capability with the standard and extended k-ε turbulence models, and 6) General chemical reacting flow treatment. One of the most important features of this NS solver is the use of pressure-based method which allows accurate simulaiton of the flows at all speeds. Either implicit first-order Euler time-marching or second-order time-centered scheme can be used for time integration. A second order spatial accuracy is achieved using Taylor뭘series expansion and the gradients of the flow properties are computed using a least-square method. The creation of local extreme during the higher order linear reconstruction is eliminated by the application of limter proposed by Barth and Jespersen [18]. Parallel computing of the NS solver also incorporates the graph-partition tool, METIS, which is the same as that in the PDSC.

Breakdown Parameters

A continuum breakdown parameter, proposed by Wang and Boyd [13] for hypersonic flows, is employed in the present hybrid DSMC-NS method as one of the criteria for selecting proper solvers. The continuum breakdown parameter Kn_{max} is defined as

$$Kn_{max} = \max[Kn_D, Kn_V, Kn_T] \tag{1}$$

where Kn_D, Kn_V and Kn_T are the local Knudsen numbers based on density, velocity and temperature, respectively. They can be calculated from the following general formula

$$Kn_Q = \frac{\lambda}{Q}|\nabla Q| \tag{2}$$

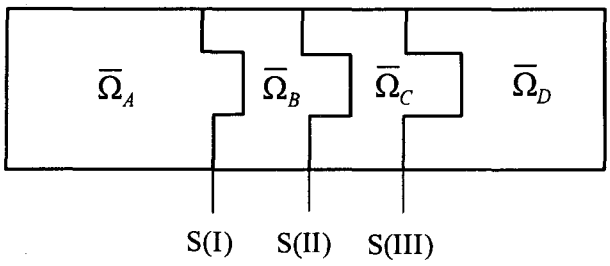
where Q is the specific flow property (density, velocity and temperature) and λ is the local mean free path. If the calculated value of the continuum breakdown parameter in a region is larger than a preset threshold value $Kn_{max}^{Thr.}$, then it cannot be modeled using the NS equation. Instead, a particle solver like DSMC has to be used for that region.

In addition, another breakdown parameter is used to identify regions that exhibit thermal non-equilibrium among various degrees of freedom. In the current study, this thermal non-equilibrium indicator is defined as

$$P_{Tne} = \left|\frac{T_{Tr} - T_R}{T_{Tr}}\right| \tag{3}$$

where T_{Tr} and T_R are translational and rotational temperature, respectively. If the value of the computed thermal non-equilibrium indicator in a region is larger than some preset threshold value $P_{Tne}^{Thr.}$ in the current study, then this flow region cannot be modeled correctly by the

present thermal-equilibrium NS solver, which assumes thermal equilibrium among various degrees of freedom. Hence, the DSMC method has to be used for that region instead.



S(I) = $\overline{\Omega}_A \cap \overline{\Omega}_B$: Boundary-I (Dirichlet B.C.) for NS simulations

S(II) = $\overline{\Omega}_B \cap \overline{\Omega}_C$: Boundary-II for updated solution using different solvers

S(III) = $\overline{\Omega}_C \cap \overline{\Omega}_D$: Boundary-III (Dirchlet B.C.) for DSMC simulations

Figure 1 Sketch of numerical domain distribution of the present coupled DSMC-NS method with overlapping regions and boundaries.

Overlapping regions between DSMC and NS domain

Figure 1 shows the sketch of overlapping regions and boundaries near the interface of the DSMC and NS solvers at an intermediate step (other than the first CFD simulation step for the whole domain). The general iterative procedure of the present coupling framework is that running the DSMC solver first after the breakdown regions are identified, and then running the NS solver next with the boundary values calculated from DSMC simulations. Note that all domains mentioned in the following include the boundaries surrounding them. Domain $\overline{\Omega}_A \cup \overline{\Omega}_B \cup \overline{\Omega}_C$ represents the DSMC simulation region, while domain $\overline{\Omega}_B \cup \overline{\Omega}_C \cup \overline{\Omega}_D$ represents the NS simulation region; thus, domain $\overline{\Omega}_B \cup \overline{\Omega}_C$ is the designated overlapping region. Boundary conditions (Dirichlet-type) on Boundary-I ($=\overline{\Omega}_A \cap \overline{\Omega}_B$) for NS simulation come from part of the previous iterative DSMC simulation, while boundary conditions (Dirichlet-type) on Boundary-III ($=\overline{\Omega}_C \cap \overline{\Omega}_D$) for DSMC simulation come from part of the previous iterative NS solution. Location of Boundary-I is determined from strict comparison of breakdown parameters ($Kn_{\max}$ and P_{Tne}), computed based on previous iterative solution of domain $\overline{\Omega}_A \cup \overline{\Omega}_B \cup \overline{\Omega}_C \cup \overline{\Omega}_D$, with the preset criteria. Location of Boundaries-II and -III are then determined by extending from Boundary-I towards the neighboring continuum region. In addition, the 빫hickness? (number of cell layers) of domains $\overline{\Omega}_B$ and $\overline{\Omega}_C$ can be adjusted to achieve better convergence for the coupling procedure. Furthermore, in the current coupled DSMC-NS method the choice of solution update for each cell is based on its domain type. Domain $\overline{\Omega}_A \cup \overline{\Omega}_B$ is the region where the updated solution comes from the DSMC simulation, while domain $\overline{\Omega}_C \cup \overline{\Omega}_D$ is the region where the updated solution comes from the NS simulation.

Coupling Procedures

In brief summary, major procedures of the present hybrid DSMC-NS method are listed as follows, referring to the overlapped region as shown in **Figure 1**:

1. Apply the NS code to simulate the whole flow field as continuum;
2. Determine the locations of Boundary-I and -III and, thus, the DSMC simulation domain ($\overline{\Omega}_A \cup \overline{\Omega}_B \cup \overline{\Omega}_C$).
3. Impose Dirichlet-type boundary conditions (velocities, temperature and number density) on Boundary-III, obtained from latest NS simulation, for the next DSMC simulation domain ($\overline{\Omega}_A \cup \overline{\Omega}_B \cup \overline{\Omega}_C$).

4. Simulate and sample the flow field in the DSMC domain ($\Omega_A \cup \Omega_B \cup \Omega_C$), using the PDSC code, until acceptable statistical uncertainties are reached.
5. Impose Dirichlet-type boundary conditions (velocities, temperature and density) on Boundary-I, obtained from latest DSMC simulation, for the next NS simulation domain ($\overline{\Omega}_B \cup \overline{\Omega}_C \cup \overline{\Omega}_D$).
6. Conduct flow simulation in the NS domain ($\overline{\Omega}_B \cup \overline{\Omega}_C \cup \overline{\Omega}_D$), using the NS code, to obtain a converged steady-state solution.
7. Update solution of the whole computational domain.
8. Repeat from Steps 2 to 7 until the maximum number of coupling iterations is exceeded or the preset convergence criterion is reached.

Practical Implementation

Numerical simulations with the hybrid DSMC-NS code are conducted on a memory-distributed PC cluster system (64 Nodes, dual processors, 2GB RAM per node, Gbit switching hub) running under a Linux operating system. 32 processors are used throughout this study, unless otherwise specified. The PDSC and the NS codes are coupled through a simple shell script on Linux system. Thus, the hybrid DSMC-NS code is expected to be highly portable among parallel machines with distributed memory. Most importantly, our experience shows that the I/O time related to the switching of solver and read/write files is negligible comparing to the simulation time used by each solver.

Table 1 Free-stream conditions in supersonic flow over quasi-2-D 25o wedge.

Gas	ρ_∞	U_∞	T_∞	M_∞
N_2	6.545E-4kg/m^3	1111m/s	185.6K	4

Table 2 Sonic conditions at the orifice exiting plane in two parallel near-continuum orifice free jets flow.

Gas	ρ_{throat}	U_{throat}	T_{throat}	Re_{throat}
N_2	6.52E-3 kg/m^3	314 m/s	237.5 K	401

Results and Discussions

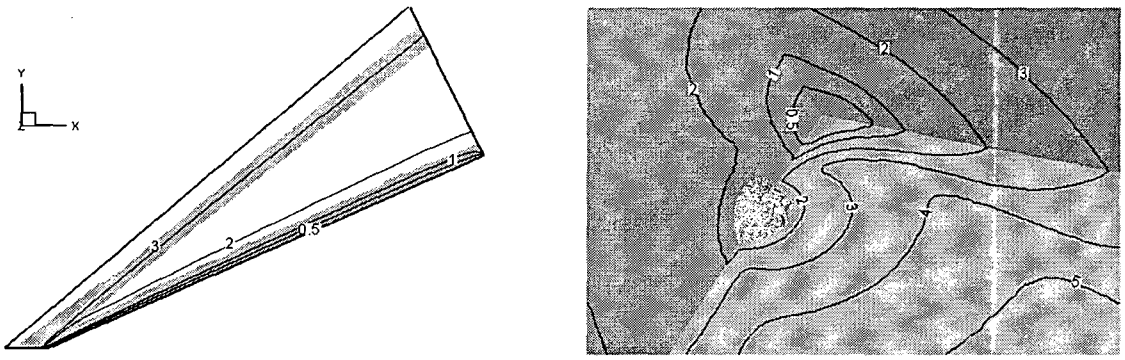
Validations

Completed parallel hybrid DSMC-NS code was tested using a supersonic nitrogen flow (M_∞=4) over a quasi-2-D 25° wedge and a nitrogen flow, which two near-continuum parallel orifice jets underexpand into a near-vacuum environment, were simulated to verify its validity and demonstrate its capability in solving realistic 3-D gas flows [1]. Corresponding flow conditions are shown in **Table 1** (wedge flow) and **Table 2** (orifice jet) for completeness. Simulation data compared excellently with the benchmark simulation results using DSMC for the quasi-2-D wedge flow, and reasonably well with the experimental data for the 3-D orifice jet flow. Details of the description can be found in [1] and are skipped here for brevity.

From these two simulations, we have found that the number of couplings between DSMC and NS solvers strongly depends upon the flow conditions near the breakdown interfaces, which is described in the following.

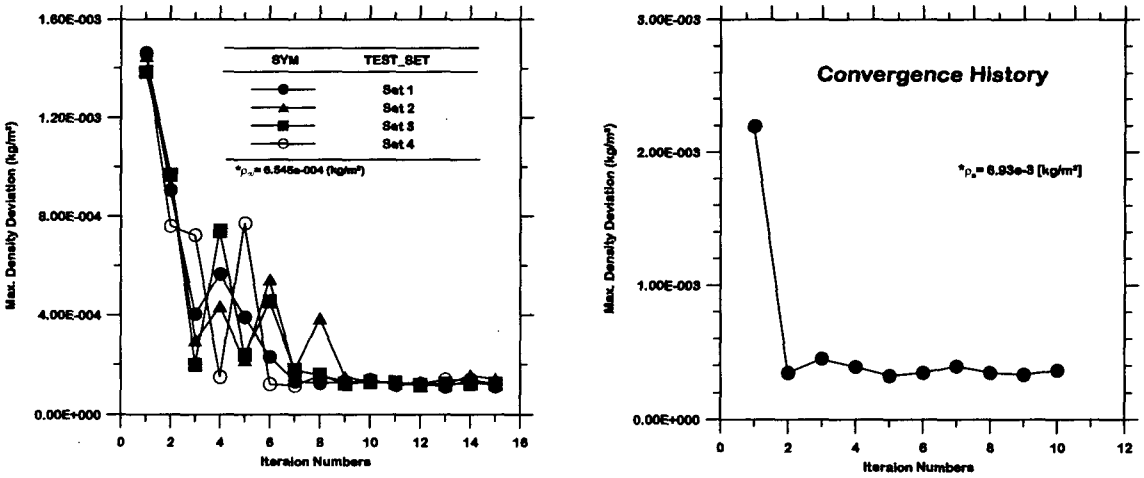
In the case of supersonic flow past a quasi-2-D wedge (**Figure 2a**), subsonic flow dominates in the regions near the breakdown interface above the boundary layer along the wedge wall that necessitates more number of couplings to exchange the information between two solvers

(**Figure 3a**), although supersonic flow dominates in the regions near the breakdown interface around the oblique shock. Note the four sets of data represent different simulation conditions in the number of cell layers of the overlapped region (1~4) and the threshold values of breakdown parameters ($Kn_{max}^{Thr.}$=0.02~0.04, $P_{Tne}^{Thr.}$=0.03~0.06), which all have the similar trend. However, in **Figure 2b**, supersonic flow dominates near the breakdown interface around entrance regime of orifice jets, which greatly reduces the number of couplings (**Figure 3b**) required for convergence as seen from the simulation. The above observation is very important from the viewpoints of practical implementation. For example, in the early stage of simulation we can determine the number of couplings required for convergence by simply monitoring to which the flow regime (supersonic or subsonic) near the breakdown interface belongs. If most flows near the breakdown interface are supersonic, then two coupling iterations should be enough for convergence. If not, more coupling iterations (e.g., less than ten) are required to have a converged solution. Further investigation in determining the optimum number of coupling iterations is required in practical applications of the current hybrid method



(a) (b)

Figure 2 Mach number distribution of: **a)** quasi-2-D supersonic wedge flow; **b)** two parallel near-continuum free jets near orifice (gray areas: DSMC domain; others: NS domain).



(a) (b)

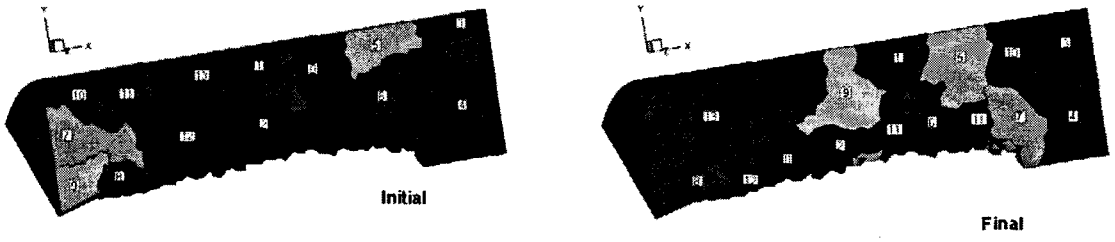
Figure 3 Convergence history of maximum density deviation for: **(a)** the quasi-2-D 25° wedge flow; **(b)** two parallel near-continuum orifice free jets flow.

RCS Nozzle Plume Simulation

We applied the present hybrid DSMC-NS method to simulate the plume flow field issuing from a realistic flown RCS nozzle. Important flow conditions include: nitrogen gas, stagnation pressure of 1~8.75bar, stagnation temperatur of 500~875K, throat diameter of 4.36 mm, length

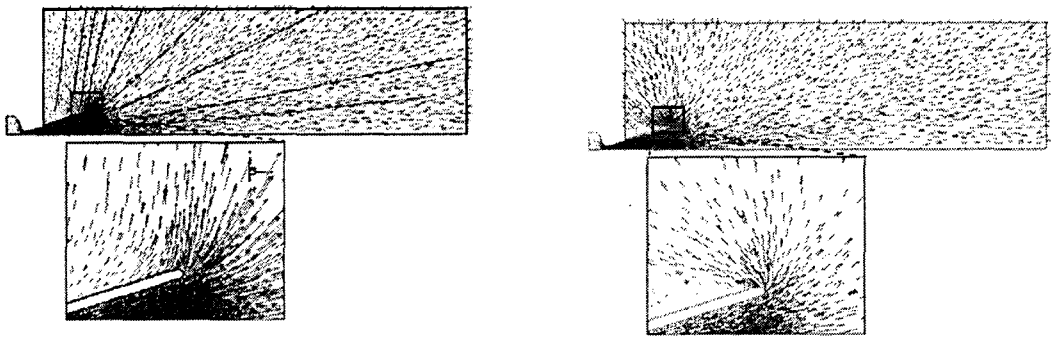
of the convergent part of 8 mm, length of the divergent part of 50 mm, and area expansion ratio of 60. Only some prelimanry results for the case of P_0=8.75bar and T_0=875K are presented in the following, while details of other cases will be presented in the meeting. In the simulation, breakdown parameters are set as $Kn_{max}^{Thr.}$=0.07 and $P_{Tne}^{Thr.}$=0.04. Only 1/6 of the physical domain are used due to symmetry with 14 processors for this simulation. Influence of these parameters will be discussed in the meeting.

Figure 4 illustrates the initial and final distribution of domain decomposition in the DSMC solver during the first the coupled iteration. It is clear that the spatially uniform decomposition at the initial stage has evolved to the spatially non-uniform decomposition, which reflects the correct density distribution at the end. **Figure 5** shows the velocity vector plot using 뱅ne-shot? NS simulation and hybrid DSMC-NS simulation after the 1st iteration. With the present hybrid method, it can clearly capture the backflows near the nozzle lip even with only one coupling, which cannot be predicted using the NS simulation alone.



(a) (b)

Figure 4 Domain distribution in DSMC simulation region (**a**) Initial (**b**) Final



(a) (b)

Figure 5 Velocity vector plot of the RCS plume simulation: **a**) initial NS solution; **b**) coupled DSMC-NS solution with 1st coupling iteration.

Conclusions

A hybrid DSMC-NS approach for steady-state flows using 3-D unstructured mesh is presented to combine the high computational efficiency of the NS solver in continuum and thermal-equilibrium regions with high fidelity of the DSMC method in 뱐reakdown? regions. Flexible overlapping regions between DSMC and NS simulation domains are designed by taking advantage of the unstructured grid topology in both solvers. Two breakdown parameters, including a continuum breakdown parameter proposed by Wang and Boyd [13] and a thermal non-equilibrium indicator, are employed to determine the DSMC simulation and NS simulation domains, in addition to the concept of overlapping regions. Proposed hybrid DSMC-NS scheme was verified using a quasi-2D supersonic wedge flow and a realistic 3D flows with two parallel near-continuum orifice jets expands into a near-vacuum environment. Results show that the number of couplings for convergence between two solvers is approximately 2-3 if supersonic flows dominate near the breakdown interface, while it increases up to 8-10 if subsonic flows dominate near the breakdown interface. At the end, proposed hybrid scheme is employed to simulate a realistic RCS plume to demonstrate it capability in handling realistic challenging problems.

REFERENCES

[1] J.-S. Wu, Y.-Y. Lian, G. Cheng, R. P. Koomullil and K.-C. Tseng, (2006). 밆evelopment and Verification of a Coupled DSMC-NS Scheme Using Unstructured Mesh? *Journal of Computational Physics* (accepted).

[2] J. N. Moss, J. M. Price, (1997). 밪urvey of Blunt Body Flows Including Wakes at Hypersonic Low-Density Conditions? *Journal of Thermophysics & Heat Transfer*, Vol. **11**, pp. 321-329.

[3] H.-P. Cheng, R.-Y. Jou, F.-Z. Chen, and Y.-W. Chang, (2000). 밪hree-dimensional flow analysis of spiral-grooved turbo booster pump in slip and continuum flow? *Journal of Vacuum Science & Technology A: Vacuum, Surfaces, and Films*, Vol. **18**, pp. 543-551.

[4] M. Taniguchi, H. Mori, R. Nishihira, T. Niimi, Experimental analyses of flow field structures around clustered linear aerospike nozzles, *24th International Symposium on Rarefied Gas Dynamics* (2004).

[5] S. T. Junker, R. W. Birkmire, F. J. Doyle III, (2005). 밠 ass and heat transfer modeling of a physical vapor deposition effusion source? *AIChE Journal*, Vol. **51**, pp. 878-894.

[6] V. Versteeg, C. T. Avedisian, R. Raj, Method and apparatus for CVD using liquid delivery system with an ultrasonic nozzle, *U.S Patent Number: 5,451,260* (1994).

[7] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Oxford Univ. Press, New York, 1994).

[8] O. Aktas, N. R. Aluru, (2002). 밟 combined continuum/DSMC technique for multiscale analysis of microfluidic filters? *J. Comput. Phys.*, Vol. **178**, pp. 342-372.

[9] A. L. Garcia, J. B. Bell , W. Y. Crutchfield , B. J. Alder, (1999). 밟daptive mesh and algorithm refinement using direct simulation Monte Carlo? *J. Comput. Phys.*, Vol. **154**, pp. 134-155.

[10] C. E. Glass, P. A. Gnoffo, A 3-D Coupled CFD-DSMC Solution Method With Application to the Mars Sample Return Orbiter, *NASA report TM-2000-210322* (2000).

[11] W.-L. Wang, Q.-H. Sun, I.D. Boyd, Towards development of a hybrid DSMC-CFD method for simulating hypersonic interacting flows, *8th AIAA/ASME Joint Thermophysics and Heat Transfer Conference* (AIAA Paper 2002-3099, 2002).

[12] R. Roveda, D. B. Goldstein, P. L.Varghese, (1998). 밐 ybrid Euler/particle approach for continuum/rarefied flows? *J. Spacecraft & Rockets*, Vol. **35**, pp. 258-265.

[13] W.-L Wang, I. D. Boyd, (2003). 봒redicting Continuum Breakdown in Hypersonic Viscous Flows? *Physics of Fluids*, Vol. **15**, pp. 91-100.

[14] J.-S. Wu, K.-C. Tseng, U.-M. Lee, Y.-Y. Lian, Development of a general parallel three-dimensional direct simulation Monte Carlo code, *24th International Symposium on Rarefied Gas Dynamics* (2004).

[15] R. P. Koomullil, B. K. Soni, (1999). 밠low simulation using generalized static and dynamics grids? *AIAA Journal*, Vol. **37**, pp. 1551-1557.

[16] H. M. Shang, M. H. Shih, Y.-S. Chen, P. Liaw, Flow Calculation on Unstructured Grids with a Pressure-Based Method, *Proceedings of 6th International Symposium on Computational Fluid Dynamics* (1995).

[17] H. M. Shang, Y.-S. Chen, Unstructured Adaptive Grid Method for Reacting Flow Computation (AIAA Paper 97-3183 1977).

[18] T. J. Barth, D. C. Jespersen, The Design and Application of Upwind Schemes on Unstructured meshes (AIAA Paper 89-0366, 1989).