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Development and verification of a coupled DSMC–NS scheme using unstructured mesh

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Abstract

An efficient and accurate parallel coupled DSMC–NS method using three-dimensional unstructured grid topology is proposed and verified for the simulation of high-speed gas flows involving continuum and rarefied regimes. A domain overlapping strategy, taking advantage of unstructured data format, with Dirichlet–Dirichlet type boundary conditions based on two breakdown parameters is 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 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 flow ($M_\infty = 4$) over a quasi-2-D 25° wedge is employed as the first step in verifying the present coupled method. The results of simulation using the coupled method are in excellent agreement with those of the pure DSMC method, which is taken as the benchmark solution. Effects of the size of overlapping regions and the choice of breakdown parameters on the convergence history are discussed. Results show that the proposed iteratively coupled method predicts the results more accurately as compared to the "one-shot" coupled method, which has been often used in practice. Further, a realistic 3-D nitrogen flow, which two near-continuum parallel orifice jets underexpand into a near-vacuum environment, is simulated using the present coupled method to demonstrate its capability. Finally, developments in extending the present method are also outlined in this paper.

Keywords: Direct simulation Monte Carlo; Coupled method; Rarefied gas flow; Navier–Stokes solver; Supersonic flows

1. Introduction

Hypersonic flows of practical importance often involve flow fields having continuum and rarefied regions, e.g. blunt body wakes, sharp leading edges, and expanding reaction control system plumes [1,2]. It is well known the direct simulation Monte Carlo (DSMC) method [3] can provide more physically accurate results

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in flows having rarefied and non-equilibrium regions than continuum flow models. However, the DSMC method is extremely computational expensive especially in the near-continuum region, which prohibits its applications to practical problems with complex geometries and 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. Past efforts in developing such a hybrid method are reviewed and summarized below.

Aktas and Aluru [4] proposed a multi-scale method that combines the Stokes equation solver with the DSMC method, which was used for the analysis of micro-fluidic filters. The continuum regions were governed by Stokes equations solved by a scattered point finite cloud method. The continuum and DSMC regions were coupled through an overlapped Schwarz alternating method with Dirichlet–Dirichlet type boundary conditions. However, the interface location between two solvers was specified in advance. Garcia et al. [5] constructed a hybrid particle/continuum algorithm with an adaptive mesh and algorithm refinement, which was designed to treat multi-scale flow problems. The DSMC method was used as a particle method embedded within a Godunov-type compressible Navier–Stokes solver. This methodology is especially useful when local mesh refinement for the continuum solver becomes inappropriate as the grid size approaches the molecular scales. Glass and Gnoffo [6] proposed "one-shot" coupled 3-D CFD–DSMC method for the simulation of highly blunt bodies using the structured grid under steady-state conditions. Interfacial location between the CFD and DSMC zones was identified manually after one-shot CFD simulation. Results of CFD simulation at this interface were then used as the inflow boundary conditions (Dirichlet type) for the DSMC method in the rarefied regions. Wang et al. [7] proposed a hybrid information preservation/Navier–Stokes (IP-NS) method to reduce statistical uncertainties during the process of coupling. This method is potentially suitable for simulating unsteady flows. Roveda et al. [8] also proposed a hybrid Euler–DSMC approach for unsteady flow simulations. Two special approaches were designed to reduce statistical uncertainties at the interface during the coupling procedures: (1) use of an overlapped region between the DSMC and Euler zones and (2) use of a "ghost level structure" to reduce statistical uncertainties. However, cloning of particles is required in this approach and may be problematic in a particle method such as DSMC. At present, only one-dimensional and two-dimensional flows were demonstrated in the literature and extension to parallel or three-dimensional simulation has not been reported to the best knowledge of the authors.

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 factors: (1) Correctness in identifying the location of spatial interface between the DSMC and continuum method during computation. Proper location of the interface not only guarantees a physically correct simulation, but also helps to possibly optimize (or reduce) the computational time. It is expected to design some criteria that can be used to efficiently and accurately identify the interface and be easily evaluated during runtime. (2) Properly and efficiently exchanging interfacial information (or flow properties) during runtime. In practice, one side of the interface is the DSMC method with accuracy strongly depending upon the sampling statistics. The computational efficiency and accuracy of the continuum solver can be potentially jeopardized by the possibly noisy boundary conditions if the uncertainty of statistical sampling is large. (3) The effect of steadiness of the flow solution on designing data exchange at the interface. In the case of unsteady simulations, the algorithm for data exchange can be very complicated in order to keep the statistical uncertainties of the particle method as low as possible.

In the current study, a parallel coupled DSMC–NS method using three-dimensional unstructured mesh, capable of efficiently and correctly simulating steady flows, consisting of both continuum and rarefied regions is proposed and verified. Steady-state simulations were performed to reduce the complexity in the coupling