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Extension of the low diffusion particle method for near-continuum two-phase flow simulations

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Abstract The low diffusion (LD) particle method, proposed by Burt and Boyd, is modified for the near-continuum two-phase flow simulations. The LD method has the advantages of easily coupling with the direct simulation Monte Carlo (DSMC) method for multi-scale flow simulations and dramatically reducing the numerical diffusion error and statistical scatter of the equilibrium particle methods. Liquid- or solid-phase particles are introduced in the LD method. Their velocity and temperature updating are respectively, calculated from the motion equation and the temperature equation according to the local gas properties. Coupling effects from condensed phase to gas phase are modeled as momentum and energy sources, which are respectively, equal to the negative values of the total momentum and energy increase in liquid or solid phase. The modified method is compared with theoretical results for unsteady flows, and good agreements are obtained to indicate the reliability of the one-way gas-to-particle coupling models. Hybrid LD–DSMC algorithm is implemented and performed for nozzle discharging gas–liquid flow to show the prospect of the LD–DSMC scheme for multi-scale two-phase flow simulations.

1. Introduction

In a number of aerospace engineering applications, gas flows involving a wide range of flow regimes are required to be simulated with accurate and efficient computational aerothermodynamics models. They can be characterized by the overall Knudsen number (*Kn*) and assorted with three different regimes.[1] The overall Knudsen number is calculated as

$$Kn = \frac{\lambda}{L} \tag{1}$$

where λ is the mean free path and L a characteristic length scale. The flow is treated to be continuum if the Knudsen number is smaller than 0.01. In this regime, intermolecular collisions dominate over other processes and equilibrate the inner structure of the gas. When the Knudsen number is much higher than 10, the flow regime is free-molecular and particle collisions with the surface play a critical role. Between the continuum regime and the free-molecular regime, there is the transitional regime, in which both the intermolecular collisions and the molecular–surface interactions are important.

Physical and computational aerothermodynamics models have been proposed for different flow regimes. In continuum regions, the gas velocity distributions are within small departure from equilibrium and the Navier–Stokes (N–S) or Euler equations are appropriate. Traditional computational fluid dynamics (CFD) schemes, which involve direct numerical

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solutions for the governing equations, have been applied for the simulations of these flows. As the Knudsen number increases, the gas velocity distributions deviate a lot from equilibrium. The continuum assumption breaks down and models tied to kinetic theory are required to describe the gas flows. The Boltzmann equation, which is derived following the assumptions of molecular chaos and binary intermolecular collisions, is the governing equation for gas flows at arbitrary Knudsen numbers. However, the Boltzmann equation is a nonlinear integro-differential equation amenable to analytical solutions only for a small number of special problems, and numerical algorithms are required to solve this equation. The most widely used approach to solve the Boltzmann equation is the direct simulation Monte Carlo (DSMC) method, which has been developed since the early 1960s and has been successfully applied to a wide range of rarefied gas dynamics problems. The DSMC method abandons the form of the Boltzmann equation and computes gas flows through simulating the random evolution of a representative particle system.[2] Within a simulation time step, a collection of representative particles are tracked through a computation grid, which move and collide following the phenomenological models. The gas velocity distributions are represented by the velocities of those particles and the macroscopic properties of the flow are obtained by sampling the properties of the representative particles. Although the DSMC method is a mature approach for dilute gas simulations, the physical nature of the DSMC method, which requires high resolution of the mean free path and the collision rate by appropriate cell size and simulation time step, leads to higher computational expense at low Knudsen numbers when compared to traditional CFD schemes for the N–S equations, which often prohibits its application in near-continuum regimes.[3]

Efficient multi-scale computational models are needed to simulate multi-scale flows. Both traditional CFD and DSMC methods are usually applied. The CFD techniques are utilized in continuum regimes and the DSMC method is used where the continuum breaks down. Many researchers have focused on this type of computational model and proposed several simulation strategies. The simplest hybrid approach decouples the CFD and DSMC methods, which firstly performs the CFD simulation on a domain including a wide range of flow regimes and then defines inflow boundary for the independent DSMC simulation from the CFD results.[4,5] This uncoupled scheme is only used to simulate the steady state with the DSMC downstream of the CFD regions and the interface between the two regions is uniformly supersonic.[5] For more complex flow simulations, a coupled CFD–DSMC method is necessary. However, the large statistical scatter associated with the Monte Carlo method brings difficulties to information transfer across the interface, and scatter reductions also bring complexity and challenges to the numerical frameworks.

One of the efficient ways to overcome the difficulties of the hybrid CFD–DSMC scheme is to extend the DSMC method to near-continuum flow regimes. Among ''all-particle'' hybrid schemes, there are two main types of approaches. One is to modify the DSMC method to reduce its high computational expense in near-continuum regions, by either restricting the collisions of particles[6] or replacing them with resampling particle velocities from Maxwell distribution (equilibrium distribution).[7] The other is intermediated between the particle method and a conventional finite-volume solver for continuum flows, which represents the macroscopic flux by representative particles sampled from a certain shape of velocity distribution.[8] All these schemes are on the basis of local thermal equilibrium assumption (hence named equilibrium particle simulation method, EPSM) and provide results equivalent to a numerical solution of the compressible Euler equations. The utilization of same particles allows two-way strong information transfer in the hybrid scheme.[9] However, one of the main problems of these equilibrium particle methods is the large numerical diffusion errors. The probable reason is that the random molecular motions, which should be suppressed on the macroscopic level in near-continuum flows, are reproduced on the scales of computational cell sizes.[10]

An alternative approach to the equilibrium particle method for simulating near-continuum flows in the hybrid scheme has been proposed recently and named the low diffusion (LD) particle method.[9–15] In this DSMC similar method, a collection of representative particles are tracked through the grid in such a way that every particle maintains a constant relative position within a Lagrangian cell. The Lagrangian cell is a virtual cell that is coincident with the fixed computation grid at the beginning of each time step. During the time interval, the Lagrangian cells move and deform according to local flow properties. Particles follow the macroscopic motions of Lagrangian cells and random motions are suppressed. As a result, numerical diffusion error and statistical scatter associated with the existing continuum particle methods are greatly reduced. The LD method is firstly presented for the simulation of compressible inviscid gas flows and one-dimensional and two-dimensional test cases show it gives an equivalent solution to the Euler equations.[9] Then the LD method couples with the DSMC method to simulate multi-scale flows. The hybrid scheme is easily integrated in one numerical framework and easily implements two-way strong information transfer.[10] Many other modifications have been introduced to improve the LD method, including additions of viscosity effect,[11] rotational and vibrational nonequilibrium energy models,[12] determination of transport coefficients of gas mixtures,[13] and diffusive transport of nonequilibrium internal energy modes.[14] Subcell procedures, numerical weight and time step adaptations have also been applied to reduce cell size sensitivity and computational expense in the hybrid scheme. The LD–DSMC hybrid method has shown a promising prospect for simulations of high altitude rocket exhaust flows, flows around hypersonic reentry vehicles, and many other gas flows involving a wide range of characteristic length scales.[15]

In particular, two-phase flows consisting of liquid or solid particles in a carrier gas are commonly found in rocket exhaust plumes. These flows involve a wide range of flow regimes. Due to the combustion processes in the propulsion systems, the condensed phase particles are formed with very different sizes and properties. Unburnt drops of liquid propellants are one of the important classes of particles. Because of their small mass fractions, they might not affect the gas flow. However, they may cause significant contamination problems. There are several recorded accidents which were caused by plume contaminant. Additionally, in all types of aluminized propellants, aluminum oxide particles compose a large mass fraction of the exhaust and may significantly impact the gas flow properties. Soot must also be considered for liquid propellant thrusters, which are very important to the plume radiation characteristics.[16] Hence, numerical analysis should be carefully conducted for these flow simulations.