Coupled Navier-Stokes/DSMC Method for Transient and Steady-State Gas Flows

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Abstract. An adaptatively coupled continuum-DSMC approach for compressible, viscous gas flows has been developed. The continuum domain is described by the unsteady Navier-Stokes equations, solved using a finite volume formulation in compressible form to capture the shock. The molecular domain is solved by the Direct Simulation Monte Carlo method (DSMC). The coupling procedure is an overlapped Schwarz method with Dirichlet-Dirichlet boundary conditions. The domains are determined automatically by computing the Kn number with respect to the local gradients length scale. The method has been applied to simulate a 1-D shock tube problem and a 2-D expanding jet in a low pressure chamber.

Keywords: Direct Simulation Monte Carlo; Coupled Method; Hybrid Method; Rarefied Gas Flow; Navier-Stokes solver.

1 Introduction

In several applications we are faced with the challenge to model a gas flow transition from continuum to rarefied regime. Examples include: flow around vehicles at high altitudes [1], flow through microfluidic gas devices [2], small cold thruster nozzle and plume flows [3], and low pressure thin film deposition processes or gas jets [4].

It is always very complicated to describe this kind of flows; in the continuum regime ($Kn \ll 1$), Navier-Stokes equations can be used to model the flow, whereas free molecular flow ($Kn \gg 1$) can be modelled using Molecular Dynamics models. For the intermediate Knudsen number ranges ($Kn = 0.01 - 10$), neither of the approaches is suitable. In this regime the best method to use is DSMC (Direct Simulation Monte Carlo). The computational demands of DSMC, however, scale with Kn^{-4} and when the Knudsen number is less than ~ 0.05 , its time and memory expenses become inadmissible.

Different solutions have been proposed to compute such flows. The most standard uses a continuum solver with analytical slip boundary conditions [5]. This method is suitable only in conditions where $Kn < 0.1$ and the precise formulation of the slip boundary conditions is strongly geometry dependent. For this reason, several hybrid continuum/molecular models have been proposed, for instance: Molecular Dynamics (MD) and Navier-Stokes (N-S) equations [6], Boltzmann and N-S equations [7], Direct Simulation Monte Carlo (DSMC) and Stokes equations [2], DSMC and incompressible N-S equations [8], and DSMC and N-S equations [9,10,11,12,13].

In particular, Garcia et al.[9] constructed a hybrid particle/continuum method with an adaptive mesh and algorithm refinement. It was a flux-based coupling method with no overlapping between the continuum and the DSMC regions. On the contrary, Wu and al. [10] and Schwartzenruber and al. [11,12] proposed an 'iterative' coupled CFD-DSMC method where the coupling is achieved through an overlapped Schwarz method with Dirichlet-Dirichlet type boundary conditions. However, both Wu and al. [10] and Schwartzenruber and al. [11,12] methods are only suitable for gas flow simulations under steady-state conditions, while the method that we propose has been applied both to transient and steady-state gas flow simulations.

We consider, in the continuum regime, the compressible N-S equations and, in the transitional regime, DSMC because it is several order of magnitude more efficient than MD and the Boltzmann equations solvers. The coupling of the two models is reached through an overlapped Schwarz method [10] with Dirichlet-Dirichlet boundary conditions. It is an adaptive method in which, during the computations, the Kn number with respect to the local gradients is computed to determine and divide the CFD (Computational Fluid Dynamics) domain from the DSMC one.

2 The Coupling Method

2.1 The CFD Solver

The CFD code used is a 2-D, unsteady code based on a finite volume formulation in compressible form to capture the shock. It uses an explicit, second-order, flux-splitting, MUSCL scheme for the Navier-Stokes equations.

Because a high temperature flow has to be modelled, a power-law temperature dependence was used for the viscosity μ and a model coming from kinetic gas theory for the thermal conductivity κ . The density was computed from the ideal gas law.

2.2 The Molecular Algorithm: DSMC

The 2-D DSMC code developed is based on the algorithm described in [14].

A "particle reservoirs" approach was used to implement the inlet (outlet) boundary conditions. A Maxwell-Boltzmann or a Chapman-Enskog velocity distributions can be used to generate molecules in those reservoirs.

2.3 Schwarz Coupling

We describe in this section two different strategies developed and implemented to couple the Navier-Stokes based CFD code to the DSMC code: One for steady state flow simulation, the other for unsteady flow simulations.

Steady Formulation: We propose a hybrid coupling method based on the Schwarz method [10] and consisting of two stages.

In the first stage the unsteady N-S equations are integrated in time on the entire domain Ω until a steady state is reached. From this solution, local Kn numbers with respect to the local gradients length scales [15] are computed according to

$$Kn_Q = \frac{\lambda}{Q} |\nabla Q| \quad (1)$$

where λ is the mean free path length and Q is a flow property (density, temperature etc.); The values of Kn_Q are used to split Ω in the subdomains Ω_{DSMC} ($Kn > Kn_{split} - \Delta Kn$), where the flow field will be evaluated using the DSMC technique, and Ω_{CFD} ($Kn < Kn_{split}$), where N-S equation will be solved. For Kn_{split} a value of 0.05 was used. Between the DSMC and CFD regions an overlap region is considered, where the flow is computed with both the DSMC and the CFD solver; the value of ΔKn can be chosen in "ad hoc" manner in order to vary the overlap region size.

In the second stage, DSMC and CFD are run in their respective subdomains with their own time steps (Δt_{DSMC} and Δt_{CFD} , respectively), until a steady state is reached. First DSMC is applied; molecules are allocated in the DSMC subdomain according to the density, velocity and temperature obtained from the initial CFD solution. A Maxwell-Boltzmann or a Chapmann-Enskog distributions can be chosen to create molecules. It is important to say that the grid is automatically refined in the DSMC region in order to respect the DSMC requirements. The boundary conditions to the DSMC region come from the solution in the CFD region. As described in the previous section for the inlet (outlet) boundary, outside the overlapping region some "particle reservoirs" are considered. In these cells molecules are created according to density, velocity, temperature and their gradients of the solution in the CFD region, with a Maxwell-Boltzmann or a Chapmann-Enskog distributions. After running the DSMC, the N-S equations are solved in the CFD region. The boundary conditions comes from the solution in the DSMC region averaged over the CFD cells.

Once a steady state solution has been obtained in both the DSMC and N-S region, the local Kn_Q numbers are re-evaluated and a new boundary between the two regions is computed. This second stage is iterated until in the overlapping region DSMC and CFD solutions differ less than a prescribed value.

We made an extensive study of the influence of various coupling parameters, such as the size of the overlap region (4 – 59 mean free path lengths) and the amount of averaging applied to the reduce DSMC statistical scatter (averaging over 5, 30 and 50 repeated runs). The influence of these parameters on the final solution was found to be small.

Unsteady Formulation: In the unsteady formulation, the described coupling method is re-iterated every coupling time step $\Delta t_{coupling} \gg \Delta t_{DSMC}, \Delta t_{CFD}$, starting on the solution at the previous time step. As expected, in order to avoid instabilities, it was necessary to keep the Courant number (based on the coupling time step, the molecules most probable velocity, and the CFD grid cell size) below one.

In the second stage, after every coupling step, the program compares the predicted DSMC region with the one of the previous step. In the cells that still belong to the DSMC region, we consider the same molecules of the previous time step whose properties were recorded. Molecules that are in the cells that no longer belong to the DSMC region are deleted. In cells that have changed from CFD into a DSMC cell, new molecules are created with a Maxwell-Boltzmann or a Chapmann-Enskog distribution, according to the density, velocity and temperature of the CFD solution at the previous time step.

At the end of the every coupling step molecule properties are recorded to set the initial conditions in the DSMC region for the next coupling step.

3 Results

3.1 1-D Shock-Tube Problem

The unsteady coupling method was applied to the unsteady shock tube test case (fig.1).

Fig. 1. Shock tube test case

The code models a flow of Argon inside an 0.5 m long tube between two tanks in different thermo-fluid-dynamic conditions. In the left tank there are a pressure of 2000 Pa and a temperature of 12000 K , while in the tube and in the right tank there are a pressure of 100 Pa and a temperature of 2000 K . When the membrane that separates the two regions breaks a shock travels in the tube from left to right. Upstream from the shock, the gas has high temperature and pressure, but gradient length scales are very small. Downstream of it both temperature and pressure are lower, but gradient length scales are large. As a result, the local Kn number Kn_Q is high upstream of the shock and low downstream. In the hybrid DSMC-CFD approach, DSMC is therefore applied upstream, and CFD downstream. The continuum grid is composed of 100 cells in x direction and 1 cell in y direction, while the code automatically refines the mesh in the DSMC region to fulfill its requirements. In the DSMC region molecules were created with the Chapman-Enskog distribution. It was demonstrated, in fact, that in a

hybrid DSMC/CFD method a Chapman-Enskog distribution is required when the viscous fluxes are taken into account, while a simple Maxwellian distribution is adequate when the continuum region is well approximated by the Euler equations [9]. The particle cross section was evaluated using the Variable Soft Sphere (VSS) model because it is more accurate than the Variable Hard Sphere (VHS) one to model viscous effect. The coupling time step is $\Delta t_{coupling} = 2.0 \times 10^{-6} sec.$ and the ensemble averages of the DSMC solution to reduce the scattering were made on 30 repeated runs. In addition to the hybrid approach, the problem was also solved using CFD only and DSMC only (which was feasible because of the 1-D nature of the problem). The latter is considered to be the most accurate. In fig.2 the pressure inside the tube after $3.0 \times 10^{-5} sec.$, evaluated with the hybrid (Schwarz coupling) method is compared with the results of the full DSMC simulation and the full CFD simulation.

Fig. 2. Pressure and Kn number in the tube after $3.0 \times 10^{-5} sec$

In the same picture also local Knudsen number Kn_Q , computed using the hybrid method, is compared with the full CFD simulation.

From the results shown in fig.2, it is clear that the full CFD approach fails due to the high values of the local Kn number caused by the shock presence. The full CFD approach predicts a shock thickness less than 1 cm, which is unrealistic considering the fact that the mean free path near the shock is of the order of several centimeters. In the full DSMC approach, therefore, the shock is smeared over almost 20 cm. The results obtained with the hybrid approach are virtually identical to those obtained with the full DSMC solver, but they were obtained in less than one fifth of the CPU time.

3.2 2-D Expanding Jet in a Low Pressure Chamber

The steady-state coupling method was applied to a steady state expanding neutral gas jet in a low pressure chamber (fig.3).

The code models an Argon jet, at a temperature of $6000K$ and Mach number 1, injected from the top in a 2-D chamber of dimensions $0.32m \times 0.8m$, through a slot of $0.032m$. The pressure inside the chamber is kept at a value of $10Pa$ through two slots of $0.04m$ wide disposed on its lateral sides at a distance $0.6m$ from the top. Walls are cooled at a temperature of $400K$. The continuum grid

Fig. 3. Expanding jet in a low pressure deposition chamber test case

Fig. 4. Kn number and CFD/DSMC domains splitting

is composed of 50 cells in x direction and 160 in y direction while the code automatically refines the mesh in the DSMC region to fulfill its requirements. In the DSMC region, molecules were created with the Chapman-Enskog distribution and the particle cross section was evaluated using the VSS model. Fig.4 shows the Knudsen number in the chamber, respectively evaluated with reference to the inlet dimension (Kn_L) and to the local temperature gradient length scale (Kn_T). The pressure does not change a lot in the domain. Around the inlet the temperature is high and, because of the presence of a shock, gradient length scales are small. In the rest of the chamber the temperature is lower and

Fig. 5. Velocity and temperature fields in the deposition chamber

gradient length scales are large. As a result the Kn number is high around the inlet and low in the rest of the domain. In the right-hand side of Fig.4, the resulting division between the DSMC, CFD and overlapping regions is shown.

In fig.5 the velocity and temperature fields, evaluated with the hybrid (Schwarz coupling) method, are compared with the results of a full CFD simulation. It is evident that the DSMC region influences the flow field and its effects are present in a region wider than the DSMC and overlapping regions alone. Far away from the DSMC region, however, the full CFD and the hybrid method give the very similar results.

4 Conclusions

A hybrid continuum-rarefied flow simulation method was developed to couple a Navier-Stokes description of a continuum flow field with a DSMC description of a rarefied one. The coupling is achieved by an overlapped Schwarz method implemented both for steady state and transient flows. Continuum subdomain boundary conditions are imposed on the molecular subdomain via particle reservoirs. The molecular subdomain boundary conditions are imposed on the continuum subdomain using simple averaging. The subdomains are determined automatically by computing the Kn number with respect to the local gradients length scale on a preliminary Navier-Stokes solution.

The method has been applied to a shock tube and to a 2-D expanding jet in a low pressure chamber problems showing its capability of predicting the flow field even where a CFD solver fails.

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