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A hybrid continuum-particle solver for unsteady rarefied gas flows

S. Pantazis [a, *], H. Rusche [b]

[a] Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin, Germany
[b] WIKKI GmbH, Görgestraße 24, 38118 Braunschweig, Germany

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ABSTRACT

The implementation of a hybrid simulation algorithm based on the compressible Navier–Stokes equations and the Direct Simulation Monte Carlo (DSMC) method is discussed, with emphasis on problems of transient nature. The coupling of the two methods at their common interface is achieved by the generation of particles according to the local Maxwellian distribution and the imposition of macroscopic quantities for the continuum solver. Dynamic characteristics of the continuum-particle decomposition scheme lead to a flexible and fully configurable determination of the two regions. The parallelization scheme and the ability to consider arbitrary geometries allow the consideration of the method for non-trivial, practical applications. The validation of the code is performed for two benchmark problems, namely those of shock tube flow and unsteady flow through an orifice.

1. Introduction

The simulation of unsteady rarefied gas flows remains a challenging task. Such problems have received more attention only recently [1–3]. Even though some progress has been made in this field, insurmountable difficulties may occur when the density levels are mixed throughout the domain, which is often the case in practice in the field of vacuum technology [4]. Structures like strong shocks as well as regions of stagnant gas may be found in the same flow domain. The conditions may be such that the Knudsen number spans in its whole range throughout the flow domain, from the hydrodynamic (viscous) up to the free molecular regime, and with large variations in time. Significant modeling errors as well as numerical difficulties may occur when the Navier–Stokes equations are used due to the inherent hypothesis of the gas as continuum. Even though the applicability of continuum-based methods may be consistently extended up to $Kn = 0.1$ to include non-equilibrium phenomena [5], this may be insufficient for some problems. On the other hand, the computational cost of methods based on the Kinetic Theory of Gases, such as the Direct Simulation Monte Carlo (DSMC) method [6], increases significantly as the Knudsen number decreases and/or the flow velocity drops. As a result, it may be unrealistic to apply them in the complete flow field for some applications. These limitations are significantly stricter for phenomena of unsteady nature in comparison with steady state flows.

A possible solution methodology is to concentrate the usage of kinetic approaches only in areas of high departure from local equilibrium, coupling the kinetic solver with a hydrodynamic method. This approach belongs to the family of hybrid methods and the most commonly used combination involves the usage of the Navier–Stokes equations with the DSMC method (see for examples [7–20]). All of the above referred works employ the concept of overlapping buffer cells due to the enhanced accuracy this scheme offers in the communication between the two methods. Various criteria for the most appropriate decomposition of the flow domain have also been investigated in some of these works [7,12], with the gradient local length Knudsen number being the most commonly accepted one. By using hybrid methods, the accuracy may be enhanced while keeping the computational requirements within acceptable limits. Some authors have reported a significant reduction in the computational load, by factors higher than 20 [14,15] in comparison to DSMC in its standard form.

Hybrid methods are frequently used for steady state problems due to their easy application using two independent solvers, a hydrodynamic and a kinetic based one, in their appropriate domain of applicability and in an iterative manner. Data is exchanged between the solvers only after completing each run. Thus, the two solvers can be independent from one another and the programming expertise required is relatively low. Moreover, closed source commercial code may even be used for this purpose.

* Corresponding author.
E-mail addresses: sarantis.pantazis@ptb.de (S. Pantazis), h.rusche@wikki-gmbh.de (H. Rusche).

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In contrast to previous works, the two methods cannot be decoupled for problems of unsteady nature, since the iterative process would result to a very large computational effort. Very few solvers of the hybrid type are still available for time-dependent problems [10,13,16,17], especially for 3-dimensional arbitrary geometries. Several difficulties need to be considered in this case, such as stronger numerical instabilities than in the steady state, dynamic domain decomposition and parallelization difficulties. If we also consider the fact that memory demands may be unpredictable and the parallel effort distribution may be unbalanced among the processors, it is easily seen why such problems have received less attention.

In this work, we investigate the possibility of a hybrid particle-continuum method within the framework of the OpenFOAM® computational suite. The two regions are connected through a Schwarz-type technique involving buffer cells [7]. Unsteady problems have been considered in the validation stage, performed through a comparison with analytical and DSMC results for the problems of shock tube and starting orifice flow. The novelty of the current work lies in the three-dimensional nature of the solver and its ability to deal with arbitrary geometries. The use of unstructured meshes with arbitrary cell shape leads to high flexibility and may be used to consider non-trivial geometries. The application in the framework of OpenFOAM® creates the potential of combining the solver with other existing libraries of the same suite to model advanced characteristics, such as moving meshes, fluid–structure interaction and conjugate heat transfer. The parallelization scheme used here allows for an efficient application in highly demanding problems with a good scaling.

An outline of the paper is as follows: In the next Section, the details of the numerical method implementation are given. A brief description of the two parallelization methods applied here, as well as the resulting computational efficiency of the method, are given in the third Section. The validation of the solver through two indicative problems is discussed in the following Section. Finally, some concluding remarks are given to summarize the progress of the current work and indicate future applications.

2. Numerical method

In an effort to develop a hybrid solver, it is important to carefully choose the decomposition criterion, determining which solver will be used for each cell. The quantity and the threshold value used for this purpose are very important for the accuracy, validity and efficiency of the solver. The decomposition criterion used here is based on the gradient local length Knudsen number for the density, defined as [6]

$$Kn_{\mathrm{GLL}} = \frac{\lambda}{\rho}|\nabla\rho| \tag{1}$$

where ρ is the density and λ is the molecular mean free path. The selection of density as the critical quantity has been made after running several test sessions. Besides Kn_{GLL}, other quantities which may play a role in our decomposition are the density and temperature values themselves. If any of these two quantities is below a certain level, the DSMC solver is applied again to avoid divisions by zero in the hydrodynamic solver and to compensate for the lack of thermodynamic data. The latter is caused by the limited range of the polynomials used by the hydrodynamic solver for the thermal capacity, enthalpy and entropy (e.g. $T > 80$–100 K for $p = 1$ bar when nitrogen is considered). The current hybrid algorithm is completely dynamic, i.e. the particle region is re-established every few time steps according to this criterion and particles are removed, created or regenerated based on the characteristics of each cell.

The most challenging aspect of hybrid methods is the proper interaction between the two methods at their common interface. The two domains overlap in a layer of a few “buffer” cells, in order to ensure the smooth transition between the two methods. During the DSMC step, particles are regenerated in the overlapping regions every few time steps according to the local Maxwellian distribution and are allowed to enter or exit the DSMC field. A more detailed description of this procedure may be found in previous works, such as [7]. The Chapman-Enskog distribution has not been used to avoid difficulties due to negative values of the distribution function, as well as an increase in the computational effort [11,15]. Particles entering the continuum field are deleted. During the continuum solver step, state variables such as pressure, velocity and temperature, are updated at the buffer cells according to the sampling properties of the particles in the corresponding areas. Besides the sampling, an averaging also takes place for several DSMC time steps. Moreover, the mass fluxes of the finite volume hydrodynamic solver at the interface boundaries are corrected according to the number of particles crossing each face.

The algorithm consists of the following steps:

1. Initialize the macroscopic fields (p, U, T).
2. Determine the DSMC region according to the local Knudsen and extend to the neighboring cells to get the buffer layer.
3. Initialize particles in new DSMC cells and in buffer cells according to the local Maxwellian distribution using the macroscopic fields.
4. Delete particles elsewhere if present, i.e. if a DSMC cell has been converted to a continuum cell.
5. Apply DSMC in the corresponding region and the buffer cells for several time steps of size Δt_{DSMC}.
6. Sample and average the particle properties in the DSMC and buffer regions for this time period to calculate p, U, T and the mass flux across the interface.
7. Fix p, U, T at the DSMC cells and the mass flux across the interface for the continuum solver.
8. Simulate the continuum and buffer cell parts using the hydrodynamic solver for one time step of size $\Delta t_{\mathrm{hydro}}$ ($>\Delta t_{\mathrm{DSMC}}$).
9. Delete particles in buffer cells.
10. Repeat steps 2–9 until the final time is reached.

The OpenFOAM® open source platform [21] has been employed for the simulations after appropriately modifying the computational code. A strong advantage is the availability of reliable and efficient continuum and particle solvers. Structured or unstructured three-dimensional meshes may be considered and execution times are reduced via a parallelization scheme. The rhoPimpleFoam density-based solver has been used for the hydrodynamic part of the simulations. The solver employs the PIMPLE algorithm, i.e. the PISO algorithm [22] with an addition of two characteristics: (a) the same time step is repeated using the last iteration value as initial guess for the next iteration and (b) underrelaxation is included in the algorithm. It is capable of simulating viscous, compressible flow, based on a finite volume discretization of the Navier–Stokes equations. The dsmcFoam solver is based on the classical DSMC method as described elsewhere [6] and its validity has been confirmed through several benchmark problems [23]. For the simulations shown below, collision pairs are selected according to the non-time counter (NTC) scheme [6]. Collisions are then realized using the Variable Hard Sphere potential. A redistribution of internal energy is possible according to the Larsen-Borgnakke model [24], if the gas has any internal degrees of freedom. There is no requirement for a direct connection of the various DSMC parts, i.e. they can be located in completely different parts of the domain. However, for reasons of efficiency, if two different DSMC parts are