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Construction and comparison of parallel implicit kinetic solvers in three spatial dimensions

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ABSTRACT

The paper is devoted to the further development and systematic performance evaluation of a recent deterministic framework Nesvetay-3D for modelling three-dimensional rarefied gas flows. Firstly, a review of the existing discretization and parallelization strategies for solving numerically the Boltzmann kinetic equation with various model collision integrals is carried out. Secondly, a new parallelization strategy for the implicit time evolution method is implemented which improves scaling on large CPU clusters. Accuracy and scalability of the methods are demonstrated on a pressure-driven rarefied gas flow through a finite-length circular pipe as well as an external supersonic flow over a three-dimensional re-entry geometry of complicated aerodynamic shape.

1. Introduction

In the last ten years or so there has been rapid development of explicit numerical methods and associated computer codes for solving the kinetic equations of the rarefied gas dynamics in three space dimensions [20,17,2,13]. A more recent approach is the high-order unstructured implicit Nesvetay-3D framework [38,39]. The main advantages of Nesvetay-3D over other existing three-dimensional numerical methods for kinetic equations are two-fold. Firstly, its ability to use arbitrary unstructured meshes, comprising not only tetrahedrons, but also elements of other shapes, makes Nesvetay-3D suitable for industrial problems with complex geometries and various flow regimes. Secondly, the use of the efficient one-step implicit time evolution method significantly accelerates convergence for steady-state problems. A recent application of the method is the calculation of the flow in long finite-length pipes across a wide range of Knudsen numbers [42,41]. Results were provided for length to radius ratios up to fifty, which so far has not been achieved by using other methods and codes.

The current implementation of the framework on parallel computers uses the Message Passing Interface (MPI) and is based on the decomposition of the molecular velocity mesh while keeping the spatial mesh as a single block. Such approach is simple and strictly equivalent to the sequential implementation. However, it has restrictions on the size of the spatial mesh on the most of the existing high-performance computing systems. This is because the data structure of the complete spatial mesh is stored at each processor and the amount of the required memory for its storage does not decrease with

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the increasing number of processors used. Another problem is that the use of the data reduction operators can affect the scalability of the parallel code, see e.g. [40] for the studies of the analogous methods in two space dimensions.

The present work is a follow-on to [39] and has two objectives. Firstly, the developments of the existing implicit parallel method over the last four years are reviewed and further improvements are introduced. Secondly, the multi-block version of the numerical framework is presented, which does not use the data exchange between blocks during the solution of the linear system of equations for the time increments in the implicit scheme. Although the resulting parallel method is not strictly equivalent to the single-block method, the resulting method is free of the problems of the single-block parallel implementation and is simple enough for practical implementation.

The convergence properties and parallel scalability of various versions of the method are compared on two test problems. The first problem concerns rarefied gas flow through a short circular pipe, connecting two reservoirs with gas under different pressures. The difficulty here is to compute the solution with satisfactory accuracy across all degrees of gas rarefaction from the free-molecular to nearly-continuum flow. In the present work for the first time a spatial mesh convergence study is presented, using three consequently refined meshes. The results of three advection schemes are compared with one another and with the well-resolved DSMC calculations [48]. It is known that the use of mesh partitioning may seriously degrade the convergence properties of the implicit time-marching schemes [34]. The results are presented that demonstrate the behaviour of the present implicit method for multi-block meshes.

The second problem concerns an external supersonic flow over a model winged re-entry space vehicle (RSV), proposed by Central Aerohydrodynamic Institute (TsAGI). The model has a rather complex shape, which includes a blunt fuselage, swept wings, keel and flap. Recently, the aerodynamics of this vehicle has been extensively studied on the basis of the compressible Euler equations for a wide range free-stream Mach numbers [43,44]. In the present work the rarefied regime of the flow is examined for a moderate free-stream velocity for the conditions, approximately corresponding to 100 km of altitude. To the best of our knowledge, it is the first time when the flow over such a complex vehicle has been computed using the kinetic equations.

The selected test problems require the ability to handle three-dimensional geometries and flow features with steep gradients at very different degrees of rarefaction. They are thus very suitable for testing the accuracy and robustness of the numerical methods for kinetic equations.

The rest of the paper is organized as follows. The governing equations are presented in Section 1. The sequential numerical algorithm is described in Section 2. The parallel strategies are discussed in Section 4. Numerical results are presented in Section 5 and conclusions are drawn in Section 6.

2. Governing equations

The present work concerns the monatomic rarefied gas flows. A three-dimensional state of the rarefied gas is determined by the velocity distribution function $f(\boldsymbol{x},\boldsymbol{\xi})$, where $\boldsymbol{\xi}=(\xi_1,\xi_2,\xi_3)$ are the components of the molecular velocity vector in the spatial directions $\boldsymbol{x}=(x_1,x_2,x_3)=(x,y,z)$. Let l_*, p_*, T_*, μ_* be characteristic scales of length, pressure, temperature and viscosity, respectively; $\beta_*=\sqrt{2kT_*/m}$ is used as the characteristic scale of velocity, $t_*=l_*/\beta_*$ is the scale of temporal variable. Here m is mass of a molecule, k is the Boltzmann constant. The non-dimensional macroscopic quantities, such as number density n, temperature T, mean velocity $\boldsymbol{u}=(u_1,u_2,u_3)$ and heat flux $\boldsymbol{q}=(q_1,q_2,q_3)$ vectors are defined as the integrals of the velocity distribution function with respect to the molecular velocity:

$$\begin{pmatrix} n \\ n\boldsymbol{u} \\ n(\frac{3}{2}T+u^2) \\ \boldsymbol{q} \end{pmatrix} = \int \begin{pmatrix} 1 \\ \boldsymbol{\xi} \\ \xi^2 \\ \frac{1}{2}\boldsymbol{v}v^2 \end{pmatrix} f\,d\boldsymbol{\xi}, \tag{1}$$

where $u^2=u_\alpha u_\alpha$, $\xi^2=\xi_\alpha\xi_\alpha$, $v^2=v_\alpha v_\alpha$, $d\boldsymbol{\xi}=d\xi_1\,d\xi_2\,d\xi_3$.

In the non-dimensional variables the Boltzmann equation with the S-model collision integral [29,30] for the distribution function f has the following form:

$$\begin{aligned} &\xi_1\frac{\partial f}{\partial x}+\xi_2\frac{\partial f}{\partial y}+\xi_3\frac{\partial f}{\partial z}=\nu\left(f^{(S)}-f\right),\quad \nu=\frac{nT}{\mu}\delta,\quad \delta=\frac{l_*p_*}{\mu_*\beta_*},\\ &f^{(S)}=f_M\left[1+\frac{4}{5}(1-\mathrm{Pr})S_\alpha c_\alpha\left(c^2-\frac{5}{2}\right)\right],\quad f_M=\frac{n}{(\pi T)^{3/2}}\exp\left(-c^2\right),\\ &v_i=\xi_i-u_i,\quad c_i=\frac{v_i}{\sqrt{T}},\quad c^2=c_\alpha c_\alpha,\quad S_i=\frac{2q_i}{nT^{3/2}}. \end{aligned} \tag{2}$$

Here rarefaction parameter δ defines the degree of gas rarefaction and is inversely proportional to the Knudsen number Kn; summation of over the repeated Greek indexes is assumed. For a monatomic gas the Prandtl number $\mathrm{Pr}=2/3$. The hard-sphere intermolecular interaction $\mu=\sqrt{T}$ is used in all calculations.

The kinetic equation (2) has to be augmented with the boundary conditions. Let $\boldsymbol{n}=(n_1,n_2,n_3)$ be the unit normal vector to a boundary surface, pointing in the outward direction to the surface. Assuming the diffuse molecular scattering