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Efficient Deterministic Modelling of Three-Dimensional Rarefied Gas Flows

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Abstract. The paper is devoted to the development of an efficient deterministic framework for modelling of three-dimensional rarefied gas flows on the basis of the numerical solution of the Boltzmann kinetic equation with the model collision integrals. The framework consists of a high-order accurate implicit advection scheme on arbitrary unstructured meshes, the conservative procedure for the calculation of the model collision integral and efficient implementation on parallel machines. The main application area of the suggested methods is micro-scale flows. Performance of the proposed approach is demonstrated on a rarefied gas flow through the finite-length circular pipe. The results show good accuracy of the proposed algorithm across all flow regimes and its high efficiency and excellent parallel scalability for up to 512 cores.

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1 Introduction

Past few years have seen rapid development of numerical methods and associated computer codes for solving the Boltzmann kinetic equation with the exact or model collision integrals for three-dimensional problems. The accurate numerical solution of this equation is important in mathematical modelling of gaseous flows inside micro-scale systems, for which popular statistical methods [8] are inefficient. In existing approaches for solving three-dimensional kinetic problems in complex geometries time marching methods are typically used for both steady-state and unsteady calculations, with the only exception reported in [5] for plasma thruster modelling. In [27, 28] a second-order accurate

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structured finite-difference solver for the model kinetic equations was reported. In a series of publications [6, 22, 23] a semi-unstructured Cartesian solver for the Boltzmann equation with both exact and several model collision integrals was developed. Another first-order accurate unstructured-mesh solver was presented [2, 18, 19]. The performance of these methods has been illustrated by computing a number of rarefied gas flows.

Although the above-mentioned methods and associated computer codes represent a significant advance in computational rarefied gas dynamics, there is still much room for improvement. Firstly, the cited three-dimensional methods [2,6,18,19,22,23,27,28] use explicit time evolution with splitting with respect to processes and are thus not efficient for computing steady-state solutions. Existing one- and two-dimensional implicit methods for single-block structured meshes [31, 54, 56] are not easily extendable to complex three-dimensional geometries. Secondly, with the exception [27, 28] their spatial discretization methods do not allow for an accurate and economical resolution for the near-wall layers, which is important in the transitional and near-transitional regime. Thirdly, the scalability of the methods on modern massively parallel clusters has not been properly demonstrated. Since the computational problems associated with the direct numerical solution of the Boltzmann equation are typically large, good parallel performance is very important. Therefore, the development of more effective and universal methods for solving three-dimensional kinetic applications is still an open problem.

The present paper is devoted to the development of a new numerical framework for obtaining three-dimensional solutions of the Boltzmann kinetic equation with the model collision integrals, which circumvents the deficiencies of the existing methods, outlined above. The framework consists of the three main blocks: high-order accurate implicit advection scheme on hybrid unstructured meshes, conservative procedure for the calculation of the model collision integral and a simple and efficient implementation on modern high-performance clusters. The use of unstructured meshes in physical space simplifies the computations in three-dimensional domains of complex geometry and allows for efficient and accurate resolution of near-wall layers. The high-order accurate total variation diminishing (TVD) advection scheme works well for both large Knudsen numbers, when discontinuities of distribution function play an important role, and for moderate and small Knudsen numbers, for which the high order of accuracy is important. The one-step implicit time discretization method accelerates convergence to a steady state by at least an order of magnitude as compared with explicit time evolution methods. Finally, good scalability of the method makes it possible to use relatively fine meshes with moderate computational time required.

The performance of the proposed method is demonstrated on the problem of a rarefied gas flow through a circular micro-scale pipe of finite length driven by pressure difference between the reservoirs attached to the ends of the pipe. The gas flow through a circular orifice (channel of zero length) was studied as early as in 1974 in [38] using a finite-difference method. More recently, flow through a finite-length tube was studied on the basis of the statistical modelling techniques [52]. In the present work the gas flow in the finite-length tube with length to diameter ratio of 10 is used as a relevant computa-