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Fast Kinetic Scheme: Efficient MPI Parallelization Strategy for 3D Boltzmann Equation

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Abstract. In this paper we present a parallelization strategy on distributed memory systems for the Fast Kinetic Scheme — a semi-Lagrangian scheme developed in [J. Comput. Phys., Vol. 255, 2013, pp 680-698] for solving kinetic equations. The original algorithm was proposed for the BGK approximation of the collision kernel. In this work we deal with its extension to the full Boltzmann equation in six dimensions, where the collision operator is resolved by means of fast spectral method. We present close to ideal scalability of the proposed algorithm on tera- and peta-scale systems.

AMS subject classifications: 65Y05, 65M70, 76P05

Key words: Boltzmann equation, kinetic equations, semi-Lagrangian schemes, spectral schemes, 3D/3D, MPI.

1 Introduction

Kinetic equations provide a statistical description of non equilibrium particle gases. The evolution of the system is described by a ballistic motion of particles interacting only by two-body collisions [11, 22]. The Boltzmann model derived originally in 1870s for rarefied gases that are far from thermodynamic equilibrium is nowadays used in a variety of applications: ranging from plasma physics to astrophysics, quantum physics, biology and social science. In the Boltzmann description, the state of the system is described by a distribution function defined in seven independent dimensions, the physical space, the velocity space and time. Moreover, the interaction term requires multiple integrals over velocity space to be evaluated at every space point and for every time step of the numerical method [24,45]. This makes the kinetic theory very challenging from numerical view point.

There are two major strategies to approach the Boltzmann equation numerically. The first is to apply probabilistic methods such as Direct Simulation Monte Carlo (DSMC)

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[5, 8, 9, 36, 37, 42]. The second is to choose a deterministic scheme such as finite volume or spectral methods [2, 22, 25, 27, 38, 40, 43]. The probabilistic approach is characterized in general by low order and slow convergence rate but is more efficient for hypersonic flows.

In this work we choose a semi-Lagrangian approach [13, 14, 25, 26, 34, 47] applied to the transport part of the Boltzmann equation coupled with spectral methods to solve the collision operator [7, 10, 23, 24, 26, 31–33, 44, 46, 52–55]. In particular, we consider a Fast Kinetic Scheme (FKS) developed originally for the Bhatnagar-Gross-Krook (BGK) operator [4] in [15, 16, 19]. The FKS applies the Discrete Velocity Model (DVM) technique, where the velocity space is truncated and discretized with a set of fixed discrete velocities. As a result, the original continuous kinetic equation is replaced by a discrete set of transport equations that can be solved exactly in the semi-Lagrangian framework at practically no cost. In the original method for the BGK operator, where the collisions are modelled as a relaxation towards the local thermodynamic equilibrium, the coupling between equations was included in the computation of the local macroscopic variables (density, momentum, temperature) used to approximate the local equilibrium state. We extend herein the FKS solver to take into account more complex collision models, such as the Boltzmann operator [5, 11]. We make use of the fast spectral method allowing to compute the collision operator in $\mathcal{O}(N_v \log N_v)$, where N_v is a number of discrete velocity points in three dimensions [23, 24, 41].

The curse of dimensionality makes numerical simulations of the Boltzmann equation prohibitive on sequential machines even if fast numerical schemes are employed. That is why the need for efficient parallelization strategies arises. The parallel computing in the context of kinetic equations was already explored in [28–30], where the authors made use of Graphics Processing Unit (GPU) to solve the BGK equation with probabilistic methods. In [39] the authors have implemented the Boltzmann collision kernel on GPU, OpenMP and MPI algorithms were explored in [1, 3, 35, 48–50]. The FKS parallelization on shared memory systems under OpenMP on GPU was proposed in [17] for the BGK collision kernel. In [18] a simple parallelization strategy on distributed memory systems was proposed for the FKS coupled with Boltzmann collision kernel. The goal of this article is to study in more detail the performance of the FKS on tera- and peta-scale systems. In particular, we propose an efficient hybrid MPI/OpenMP implementation of the scheme with strong scaling close to ideal on available systems.

The article is organized as follows. Section 2 introduces the kinetic equation, the Fast Kinetic Scheme and some collision operators. Section 3 discusses the particle of the FKS interpretation as particularly well suited for parallelization, Section 4 proposes a parallel algorithm and finally Section 5 gives scalability results and some profiling information.

2 Kinetic equations and Fast Kinetic Scheme

In the kinetic theory of rarefied gases, the state of the system is described by a non negative distribution function $f(x,v,t)$. This distribution function describes a density of parti-