Advances in Applied Mathematics and Mechanics
Adv. Appl. Math. Mech., Vol. **12**, No. 5, pp. 1247-1260

DOI: 10.4208/aamm.OA-2019-0147
October 2020

Performance Comparison on Parallel CPU and GPU Algorithms for Two Dimensional Unified Gas-Kinetic Scheme

Jizhou Liu[1], Xiaodong Li[1,*] and Fang Q. Hu[2]

[1] *School of Energy and Power Engineering, Beihang University, Beijing 100191, China*
[2] *Department of Mathematics and Statistics, Old Dominion University, Norfolk, VA 23529, USA*

Received 21 May 2019; Accepted (in revised version) 24 November 2019

Abstract. This paper intends to explore the acceleration performances of parallel algorithms on CPU and GPU devices for two-dimensional Unified Gas-Kinetic Scheme (UGKS) in a comparative way. Such a comparison could provide guidance when the UGKS needs to be accelerated. To accomplish this goal, parallel algorithms on CPU and GPU devices are implemented and the speedup performances are investigated by a case of two-dimensional channel flow. Based on the multiscale feature of UGKS, a two-level fine-grain parallel strategy for both spatial and velocity spaces is adopted for GPU algorithm. The parallel CPU algorithm applies a two dimensional block layout that also parallelizes the spatial and velocity coordinates. A series of meshes with different sizes are tested to reveal the performance evolution of the two algorithms. Special attention is paid to cases where the discrete velocity space is large. The comparisons show that the proposed fine-grain GPU algorithm could take advantage of the feature of UGKS and provides significant speedups especially with the latest GPU version. On the other hand, parallel CPU strategy might provide more predictable and preferable performances when velocity space grid point number is large.

AMS subject classifications: 65Y05

Key words: UGKS, GPU acceleration, parallel algorithm, performance comparison.

1 Introduction

The Unified Gas-Kinetic Scheme (UGKS) is a direct gas flow modeling that is valid in a broad range of Knudsen numbers [1, 2]. Due to its multiscale property, it has become a promising tool in simulating microscale flow of transitional regime [3] and supersonic

*Corresponding author.
Email: lixd@buaa.edu.cn (X. D. Li)

high speed flows where characteristic length scale and particle mean free path vary significantly [4].

The overwhelming advantage of the UGKS is its ability to capture continuum as well as rarefied gas properties in one scheme. However, the computation speed is slowed down owing to this multiscale ability or dual mechanisms. To capture particle free transport in the rarefied regime, the UGKS adopts a kinetic formulation where fully-resolved distribution function in velocity space is included. At every spatial position, additional velocity coordinates need to be discretized. This usually makes the UGKS several orders of magnitude slower than other conventional N-S flow solvers for continuum regime. On the other side, the UGKS would also be expected to be slower than other kinetic methods. This is because the particle collision mechanism needs also to be considered for being able to deal with the continuum flow regime.

Although the UGKS is intrinsically less efficient from a computational point of view, it finds many suitable applications for multiscale flow problems in transitional regime. However, even for relatively small size problems, single core algorithm usually could not afford desirable computing speed if discrete velocity number is large. Such as simulations of hypersonic flow [6] and modeling particle phase with UGKS [7]. For these two applications, the Mach number practically exceeds 5. To guarantee a well-resolved distribution function, a wide velocity interval with a large number of discrete velocity grid points is needed. Therefore, acceleration in computing speed is necessary starting from two dimensional simulations.

To improve the computational speed, MPI parallelization on CPU chips has been developed for the UGKS [8–10]. In Li et al. [8], both the physical and velocity spaces are parallelized. Two-dimensional Cartesian topology is used to arrange the physical and velocity blocks. Tests on small-scale and large-scale grids show quasi-linear and even super-linear speedups. Based on the same parallel structure, Tan et al. [9] extends the UGKS for multi-group neutron transport. In Ragta et al. [10], parallelized UGKS on Cartesian grid is constructed and tested on very large problems. Canonical turbulence at low Knudsen numbers are correctly simulated with parallelized UGKS code.

Beside algorithm on connected CPU devices, parallel computing with Graphics Processing Unit (GPU) has become an emerging solution for accelerating calculations in image processing [11] and biomolecule analysis [12]. It has also been applied to the field of Computational Fluid Dynamics(CFD). Depending on the method and problem size, speedups ranging from $10\times$ to $100\times$ could be reached by implementing fine-grain GPU programming [13, 14]. Karantasis et al. [15] implement a highly accelerated finite difference WENO scheme on GPU card. A maximum $50\times$ speedup is obtained which shows the promising potential of GPU in solving turbulent flow at high Reynolds number. Lou et al. [16] establish a GPU accelerated *p*-multigrid discontinuous Galerkin (DG) method based on OpenACC for 3D unstructured grid. The application of their method on realistic engineering problems shows a speedup value between $5\times$ and $10\times$. Besides, GPU acceleration has also been implemented to kinetic methods. Boroni et al. [17] build a fully parallel GPU implementation of LBM in combination with Immersed Boundary Condi-