## A unified gas-kinetic scheme for continuum and rarefied flows, direct modeling, and full Boltzmann collision term

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All fluid dynamic equations are valid in their modeling scales, such as the kinetic scale for the Boltzmann equation and the hydrodynamic scale for the Navier–Stokes (NS) equations. There is no such an equation which is valid in all scales. With the variation of the modeling scales, there should have a continuum spectrum of fluid dynamic equations, instead of the a few well-defined ones. The unified gas-kinetic scheme (UGKS) is a direct modeling method, and its modeling scale is the mesh size and time step. Different from the single scale modeling methods, such as the direct simulation Monte Carlo (DSMC) and direct Boltzmann solver, the mesh size and time step used in UGKS are not limited by the particle mean free path and collision time. With the variation of the ratio between the numerical cell size and local particle mean free path, the UGKS covers flow physics from the kinetic scale particle transport and collision to the hydrodynamic scale wave propagation. Even with past success, the modeling in UGKS is mainly based on the time evolution of kinetic model equations. In the kinetic regime with the mesh size and time step being less than the particle mean free path and collision time, there is still dynamic difference between the kinetic collision model and the full Boltzmann collision term, even though the difference diminishes as the time step becomes larger than the particle collision time. This work is about the further development of the UGKS by implementing the full Boltzmann collision term in the regime needed, and to construct an accurate and efficient UGKS in all flow regimes. The central ingredient of the finite volume UGKS is the coupled particle transport and collision in the flux evaluation across a cell interface. The molecular free transport and the hydrodynamic NS gas evolution become two limiting solutions in the flux modeling. The UGKS has the asymptotic preserving property of recovering the NS solutions in the continuum flow regime, and the Boltzmann solution in the rarefied regime. In the transition regime, the UGKS itself provides a valid solution. With a continuous variation of modeling scales, the UGKS presents a continuous spectrum of numerical governing equations. The solutions in all flow regime can be captured accurately by the UGKS.

The UGKS scheme is verified by numerical test cases from kinetic scale to hydrody-

namic scale, for example, we simulate the shock structure of argon gas at mach number 5 under a nonuniform mesh and local time. The result from UGKS shows good agreement with MD simulation [2] as shown in Fig.1. On the other hand we simulate the lid driven cavity flow at different *Kn* numbers. In the continuum regime with  $Kn = 1.42 \times 10^{-4}$  or Re = 1000, Fig.2 shows the UGKS results and reference Navier–Stokes solutions [1], which clearly demonstrates that the UGKS converges to the NS solutions accurately in the hydrodynamic limit. In the transition regime with  $Kn = 2.85 \times 10^{-2}$  or Re = 5, the velocity profiles between UGKS and GKS are similar. However, the heat flux shows quite different properties. As shown in Fig.3, the heat flux from UGKS is not necessarily perpendicular to the temperature contour level, which is the basic assumption of the Fourier's law. We believe that the UGKS provides more accurate physical solutions than the NS does. So, the UGKS is an indispensable tool in the study of non-equilibrium flow at near continuum flow regime.

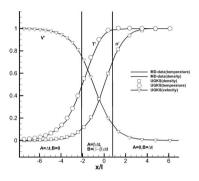


Fig. 1 Normalized number density, temperature and velocity distributions from UGKS (symbols) and MD solutions (lines) [2]

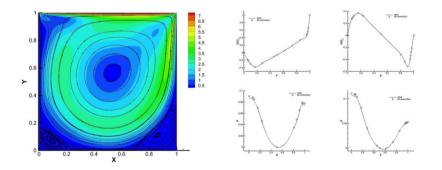
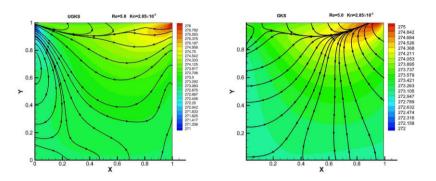


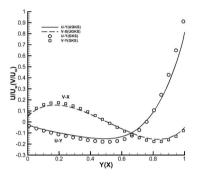
Fig. 2 Left: cavity flow at  $Kn = 1.42 \times 10^{-4}$  and  $Re = 1\,000$ . Right: velocity stream lines with temperature background; *U*-velocity along the central vertical line, *V*-velocity along the central horizontal line, pressure along the central vertical line, and pressure along the central horizontal line (circles: NS solution, line: UGKS)

## Boltzmann and Related Equations



(a) Temperature contour and heat flux: UGKS

(b) Temperature contour and heat flux: GKS



(c) U-velocity along the central vertical line and V-velocity along the central horizontal line (circles: GKS, line: UGKS)

**Fig. 3** Cavity simulation using UGKS and GKS at  $Kn = 2.85 \times 10^{-2}$  and Re = 5

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## References

- 1. Ghia U, Ghia K N, Shin C. High-resolutions for incompressible flow using the Navier–Stokes equations and a multigrid method. *J. Comput. Phys.*, **48**: 387–411 (1982)
- 2. Valentini P, Schwartzentruber T E. Large-scale molecular dynamics simulations of normal shock waves in dilute argon. *Phys. Fluids*, **21**: 066101 (2009)
- 3. Xu K. A gas-kinetic BGK scheme for the Navier-Stokes equations and its connection with artificial dissipation and Godunov method. *J. Comput. Phys.*, **171**: 289–335 (2001)
- Xu K, Huang J C. A unifed gas-kinetic scheme for continuum and rarefied fows. J. Compute. Phys., 220: 7747–7765 (2010)
- Xu K, Kim C, Martinelli L, et al. BGK-based schemes for the simulation of compressible flow. *Int. J. Comput. Fluid Dyn.*, 7: 213–234 (1996)