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Multiscale Modeling and Simulation of Gaseous Microflows

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We study gaseous flows in micro-scales by using molecular dynamics (MD), kinetic equation, and hydrodynamic equations, acrossing micro-, meso-, and macro-scopic scales. First, we solve the linearized Boltzmann equation in a wide range of Knudsen number by using an efficient high-order collocation method [1]. We obtain accurate solutions of the singular integral equation derived from the linearized BGK equation. Based the solution of the integral equation, we construct various approximated solutions which can be modeled by macroscopic equations [1]. We extend the approximated model for molecular flows including van der Waals interaction between gas molecules and walls, which can only be modeled by MD [2]. We use Couette flow in two-dimensions as the specific example to illustrate our ideas.

References:

7. W. Li, L.-S. Luo, and J. Shen, *Computers & Fluids,* **111**, 18-32 (2015).
2. W. Li, Z. Guo, and L.-S. Luo, *Preprint* (2015).