QuiPS: How a Discrete Velocity Technique Morphed into Monte Carlo Simulation

Philip Varghese

Department of Aerospace Engineering & Engineering Mechanics Oden Institute for Computational Engineering and Sciences The University of Texas at Austin Austin, TX 78712 varghese@mail.utexas.edu

I will describe the evolution of the quasi-particle scheme (QuiPS) for solving the Boltzmann equation from a discrete velocity method [1-3] to something that looks a lot like DSMC [4]. QuiPS can be viewed as Monte Carlo simulation using fixed velocity particles with variable statistical weight and is complementary to conventional DSMC that uses variable velocity particles with fixed statistical weight [5]. In general, QuiPS permits resolution of the tails of the velocity and internal state distributions at lower computational cost than conventional DSMC, which is critical to accurate calculation of chemical reaction and ionization rates in some applications [6]. QuiPS can also model transient flows more than DSMC efficiently and provides the opportunity to implement some novel adaptive schemes [7-9]. I will provide illustrative results of QuiPS calculations and discuss possible extension and developments.

- Z.-Q. Tan, Y.-K. Chen, P. L. Varghese, and J. R. Howell, "New Numerical Strategy to Evaluate the Collision Integral of the Boltzmann Equation." *Rarefied Gas Dynamics: Theoretical and Computational Techniques*, E. P. Muntz, D. P. Weaver, and D. H. Campbell, (eds.), Progress in Aeronautics and Astronautics **118**, AIAA, pp. 359-373, 1989.
- [2] Z. Tan and P. L. Varghese, "The $\Delta \varepsilon$ Method for the Boltzmann Equation," J. Computational Physics 110, 327-340 (1994).
- [3] A. B. Morris, P. L. Varghese, and D. B. Goldstein, "Monte Carlo Solution of the Boltzmann Equation via a Discrete Velocity Model," J. Computational Physics 230, 1265-1280 (2011).
- [4] G. A. Bird, Molecular Gas Dynamics and the Direct Simulation of Gas Flows, Oxford University Press, Oxford, UK (1994).
- [5] P. Clarke, P. Varghese, and D. Goldstein, "A low noise discrete velocity method for the Boltzmann equation with quantized rotational and vibrational energy," J. Computational Physics 352, 326-340, (2018).
- [6] Y. Poondla, D. Goldstein, P. Varghese, P. Clarke, and C. Moore, "Modeling Rarefied Gas Chemistry with QuiPS, a novel quasi-particle method," *Theoretical and Computational Fluid Dynamics* **36**, 81-116, (2022).
- [7] P. Varghese, A. Sekaran, S. Estes, and D. Goldstein, "Lid-Driven Cavity Flow Using a Discrete Velocity Method for Solving the Boltzmann Equation," *Rarefied Gas Dynamics: 30th International Symposium, AIP Conference Proceedings* **1786**, 040011 (2016).
- [8] A. Sekaran, P. Varghese, and D. Goldstein, "An analysis of numerical convergence in discrete velocity gas dynamics for internal flows," *J. Computational Physics* **365**, 226-242 (2018).
- [9] G. Oblapenko, D. Goldstein, P. Varghese, and C. Moore "A velocity space hybridization-based Boltzmann equation solver," J. Computational Physics 408, 109302, (2020).