Introduction:

- Non-equilibrium flows, e.g., in MEMS, hypersonic flight, vacuum technology require a molecular solution approach.
- The Boltzmann equation for single particle velocity distribution function (f)
  \[ \frac{\partial f}{\partial t} + \mathbf{F} \cdot \nabla f + \frac{\partial f}{\partial \mathbf{c}} + \mathbf{c} \cdot \nabla f + \sigma d\Omega d\mathbf{c} = 0 \]

assumes 1) dilute gas 2) molecular chaos 3) instantaneous collisions 4) f is constant in the phase space volume
- The direct simulation Monte Carlo (DSMC) method[1] is a stochastic approach that can be used to solve the Boltzmann equation.

Deterministic methods such as the ellipsoidal-statistical Bhatnagar-Gross-Krook (ES-BGK) method become invalid when statistical fluctuations are significant as in rough contacting surfaces.

Objectives:

- Illustrate the application of the DSMC method for a hypersonic flow and a microscale low-speed flow.
- Apply the Bayesian method for calibration of critical gas-surface interaction parameters based on past experiments and DSMC simulations.
- Study the feasibility of using the DSMC method for microscale flows and hence as validation for approximate solutions to the Boltzmann equation such as model kinetic equations.
- Being a stochastic method, the DSMC technique requires the sampling of flow properties making it more suitable for steady flows.

Molecular Models for Gas-Gas Collisions:

- The collisions in DSMC are binary which is a good approximation for dilute gases (p < 2 atm).
- A widely used approximation for the distribution function of molecules reflected after interaction with a solid surface is the Maxwell model.
- A fraction of molecules 1-α of the molecules are reflected specularly while the remaining are reflected diffusely.

VHS Velocity:

\[ \mu_{\text{vhs}} = \frac{T}{W} \]

LJ Viscosity:

\[ \mu = \frac{5}{8} \frac{m k T}{\sigma^3 \sqrt{2 \pi}} \]

\( W(2) \) is the velocity collision integral

Maxwell Model for Gas-Surface Interaction:

- A widely used approximation for the distribution function of molecules reflected after interaction with a solid surface is the Maxwell Model.
- A fraction of molecules 1-α of the molecules are reflected specularly while the remaining are reflected diffusely.

DSMC Applications

Uncertainty Quantification and Bayesian Calibration of Model Parameters for DSMC

- DSMC simulations rely on microscopic parameters (such as accommodation coefficient, viscosity exponent, molecular diameters) that cannot be measured directly.
- Uncertainties in these parameters can produce significant uncertainty in calculated macroscopic properties.
- The critical DSMC parameters can be calibrated by comparing macroscopic properties obtained from DSMC simulations to experiments.

Conclusions:

- Microscopic gas-surface interaction parameter required by DSMC simulations were extracted from experiments using the Bayesian method.
- DSMC simulations of microscale gas flows without explicit variance reduction techniques suffer from significant statistical scatter making deterministic approaches (such as model kinetic equations) more suitable for this weak disturbance flows.

References