A DSMC-based variance reduction formulation for low-signal flows

H.A. Al-Mohssen husain@mit.edu
N. G. Hadji Constantinou ngh@mit.edu

Mechanical Engineering Dept., MIT
September 2009
Motivation

❖ Boltzmann Equation (BE): describes the evolution of PDF $f=f(x,c,t)$

$$\frac{\partial f}{\partial t} + c \cdot \frac{\partial f}{\partial x} = \left[ \frac{\partial f}{\partial t} \right]_{\text{Collision}} = \frac{1}{2} \int \int \int (\delta' + \delta' - \delta_1 - \delta_2) f_1 f_2 c_{12} \sigma d\Omega d\epsilon_1 d\epsilon_2$$

❖ Direct Simulation Monte Carlo simulates the BE, the uncertainty in "measurement" is:

$$\sigma_{\text{Uncertainty}} = \frac{\sigma_{\text{Thermal}}}{\sqrt{N_{\text{Samples}}}}$$

⇒ problems in low signal (≡ deviation from equilibrium) flows (eg. low Ma flows).

❖ We want:

$$\sigma_{\text{Uncertainty}} = \frac{\sigma(\text{Signal})}{\sqrt{N_{\text{Samples}}}}$$

s.t. $\sigma(\text{Signal}) \to 0$ as Signal $\to 0$

❖ Related Work:

 Serif Öttinger, 1997: polymer simulation
 Serif Chun and Koch, 2005: linearized BE
Let \( \langle R \rangle \) be a property of interest (e.g., \( u_x = \langle c_x \rangle, \langle c_x^4 \rangle \) etc.). In general, it can be written as:

\[
\langle R \rangle = \int R(c) f(c) \, dc \quad \text{and likewise for } f_{eq} \neq f, \quad \langle R \rangle_{eq} = \int R(c) f_{eq}(c) \, dc
\]

Where \( f_{eq} \) is an arbitrary reference (equilibrium) distribution.

An estimate of this quantity (that we will call \( \bar{R} \)) can be calculated by generating samples \( c_i \) from \( f(c_i) \):

\[
\Rightarrow \bar{R} \approx \frac{1}{N} \sum_{i=1}^{N} R(c_i)
\]
Variance Reduction Approach

\[ I = \int f(c) \, dc \Rightarrow I = \frac{1}{N} \sum_{i=1}^{N} f(c_i) \]  \hspace{1cm} (1)

\[ I = \int \{f(c) - g(c)\} \, dc + \int g(c) \, dc \]  \hspace{1cm} (2)

if \( \int g(c) \, dc \) is known deterministically & \( f(c) \approx g(c) \)
Variance Reduction Approach

\[ \int f(c) \, dc \]

\[ \int g(c) \, dc \]

\[ \int \{f(c) - g(c)\} \, dc \]
Variance Reduction Approach

\[ I = \int f(c) \, dc \Rightarrow I = \frac{1}{N} \sum_{i=1}^{N} f(c_i) \]  
\[ \downarrow \]

\[ I = \int \{f(c) - g(c)\} \, dc + \int g(c) \, dc \]  
\[ \downarrow \]

if \( \int g(c) \, dc \) is known deterministically & \( f(c) \approx g(c) \)

(2) can be estimated more efficiently than (1)
**Variance Reduction Approach**

\[ I = \int f(c) \, dc \Rightarrow I = \frac{1}{N} \sum_{i=1}^{N} f(c_i) \quad (1) \]

\[ I = \int \{f(c) - g(c)\} \, dc + \int g(c) \, dc \quad (2) \]

if \( \int g(c) \, dc \) is known deterministically & \( f(c) \approx g(c) \)

(2) can be estimated more efficiently than (1)

\[ I \approx \left\{ \int f(c) - g(c) \, dc \right\} + \int g(c) \, dc \]

Simulate using deviational particles

Hadjiconstantinou, Baker, Homolle, Radtke
Variance Reduction Approach

\[ I = \int f(e) \, de \Rightarrow I = \frac{1}{N} \sum_{i=1}^{N} f(e_i) \]  

(1)

\[ I = \int \{ f(e) - g(e) \} \, de + \int g(e) \, de \]  

(2)

if \( \int g(e) \, de \) is known deterministically & \( f(e) \approx g(e) \)

(2) can be estimated more efficiently than (1)

\[ I \approx \left\{ \int f(e) \, de \right\} + \int g(e) \, de \]  

Simulate using deviational particles

Hadjiconstantinou, Baker, Homolle, Radtke

\[ I \approx \left\{ \int f(e) \, de \right\} - \left\{ \int g(e) \, de \right\} + \int g(e) \, de \]  

Unmodified DSMC  Auxiliary Weighted DSMC

This Work
Illustration

Non-Eq Simulation (Regular DSMC)
\[ \bar{R}_{VR} = \bar{R} - \bar{R}_{eq} + \langle R \rangle_{eq} \]

Illustration

Non-Eq Simulation (DSMC VR)

Non-Eq Simulation (Regular DSMC)

Eq Simulation (Weighted DSMC Auxiliary Simulation)

Analytical Eq Value

\[ \langle c_x^4 \rangle \]

Time
Formulation

Our Formulation:

- Use an unmodified DSMC to directly calculate $\bar{R}$

$$\bar{R} \approx \frac{1}{N} \sum_{i=1}^{N} R(c_i)$$

- Use an auxiliary simulation to calculate $\bar{R}_{eq}$. The auxiliary simulation does not perturb the main DSMC simulation and uses the same samples $c_i$

- How can we calculate both $\bar{R}$ and $\bar{R}_{eq}$ from the same set of data?
  - Use weights!
Auxiliary Simulation Using Weights

✿ Likelihood ratios \((W_i \equiv W(c_i) \equiv f_{eq}(c_i)/f(c_i))\):

\[
\langle R \rangle_{eq} = \int R(c) f_{eq}(c) \, dc = \int R(c) \left( \frac{f_{eq}(c)}{f(c)} \right) f(c) \, dc = \int R(c) W(c) f(c) \, dc
\]

⇒ \(\bar{R}_{eq} = \frac{1}{N} \sum_{i=1}^{N} W_i R(c_i)\)

✿ As a result:

\[
\bar{R}_{VR} = \bar{R} - \bar{R}_{eq} + \langle R \rangle_{eq} = \frac{1}{N} \sum_{i=1}^{N} (1 - W_i) R(c_i) + \langle R \rangle_{eq}
\]
Algorithm Overview

Regular DSMC

1. Initialize $N$ particles
2. Advection Step
3. Collision Step
4. Select $i$ & $j$
   - Accept with probability $c_r / MX$
   - If rejected, $c_i \rightarrow c_i', c_j \rightarrow c_j'$
5. Sample equilibrium and non-equilibrium properties
Algorithm Overview

Regular DSMC + VR DSMC

Initialize $N$ particles at $c_i$ & $W_i = ?? ??$

Advection Step

Collision Step

Select $i$ & $j$
Accept with probability $\hat{c}_r = c_r / MX$

$c_i \rightarrow c'_i, c_j \rightarrow c'_j$
$W'_i = ?? ?? & W'_j = ?? ??$

Accepted

$c_i \rightarrow c_i, c_j \rightarrow c_j$
$W'_i = ?? ?? & W'_j = ?? ??$

Rejected

Sample equilibrium and non-equilibrium properties
Conditional Weight Update Rules

- For every particle at $c_i$ there will be on average $P_{c_i \rightarrow c'_i}$ particles at $c'$. If we have $x$ particles at $c_i$ there will be (at $c'_i$)
  - $xP_{eq:c_i \rightarrow c'_i}$ particles in an Equilibrium simulation
  - $xP_{c_i \rightarrow c'_i}$ particles in a Non-equilibrium simulation

- Since we advance particles per the Non-equilibrium rules each particle at $c_i$ needs to simulate:
  
  \[
  \frac{P_{eq:c_i \rightarrow c'_i}}{P_{c_i \rightarrow c'_i}}
  \]

- The final collision rules
  - Accepted
    \[W_i \& W_j \rightarrow W_i W_j\]
  - Rejected
    \[W_i \rightarrow W_i \frac{1 - W_j \hat{c}_r}{1 - \hat{c}_r} \quad \text{and} \quad W_j \rightarrow W_j \frac{1 - W_i \hat{c}_r}{1 - \hat{c}_r}\]
Stability

Problem:
- These weight update rules are not stable $\Rightarrow$ loss of Variance Reduction

Solution:
- From definition $W_i = f_{eq}(c_i)/f(c_i) \Rightarrow$ we need knowledge of PDF
- Re-construct the PDF from samples, this is a standard numerical method known as Kernel Density Estimation. Specifically, for every particle at $c$ replace
  \[
  f(c_i) \rightarrow \hat{f}(c_i) = \int K(c' - c) f(c') \, dc'
  \]
  since $\hat{f}(c_i) \rightarrow f(c_i)$ as $K(\Delta c) \rightarrow \delta(\Delta c)$

Implementation:
- For accepted particles
  \[
  W_i \rightarrow \hat{W}_i = \frac{1}{\|S_i\|} \sum_{j \in S_i} W_j
  \]
  (average weights within a sphere of radius $\varepsilon$ in velocity space)
**Final Algorithm**

\[ \hat{W}_i = \frac{1}{\|S_i\|} \sum_{j \in S_i} W_j \]  

(1)
**Results: Bias (error) vs. \( \varepsilon \) in 0D**

- Error

\[
N_{\text{Cell}} \frac{\varepsilon^3}{C_{mp}^3} >> 1
\]

- Error = A / B

\[
\frac{\varepsilon}{C_{mp}}
\]

\[
\frac{c_1}{c_0}
\]
Results: 1D Transient Couette Flow

\[ \frac{T}{T_0} \]

\[ \frac{\rho}{\rho_0} \]

\[ \frac{q_y}{q_{y0}} \]

\[ \frac{u_y}{c_0} \]

\[ N_{Cell} = 500 \]

\[ Kn = 1.0 \]

\~1\% Relative Error
Relative Sampling Uncertainty

\[ \sigma_u \]

\[ 1,000,000 \text{ less samples for the same uncertainty at 5cm/s!} \]
For stability at a fixed $\varepsilon$

$\text{Kn} \downarrow \Rightarrow \| S_i \| \uparrow$

$\Rightarrow N_{\text{Cell}} \uparrow$
Conclusions

- **Variance reduction using likelihood ratios is viable and exciting**
  - Main advantage: the DSMC simulation is never perturbed

- **Small increase in computational cost**
  - Need to find NN of some particle ⇒ total cost scales as $O(N_{cell} \log(N_{cell}))$

- **Stability Issues:**
  - KDE introduces bias that is a function of $\varepsilon$
  - for low $Kn$, $N_{cell} \uparrow$ for a Stable and Accurate solution

- **Looking forward:**
  - Other collision Models
    - BGK
    - Maxwell
  - Improve bias for a given $N_{cell}$
Q&A

More info including sample code:
http://web.mit.edu/husain/www
Appendix
DSMC with weights: Scattering probability

- DSMC is a set of probabilistic steps
- Start by selecting the same number of candidate particles:
  \[ \text{Candidates} = N_{\text{Eff}} N_{\text{Cell}} (N_{\text{Cell}} - 1) M X \sigma \Delta t / V_{\text{Cell}} \]
- If we choose particles of velocity classes \( c_i \) and \( c_j \) with weights \( W_i \) and \( W_j \) respectively there will be:
  \[ (N_{\text{Eff}})^2 W_i W_j C_{ij} \sigma \Delta t / V_{\text{Cell}} \text{ Collisions} \]
- To correctly account for this we use the following collision probabilities:
  \[
  P_i = \frac{W_j c_{ij}}{M X} \\
  P_j = \frac{W_i c_{ij}}{M X}
  \]