Yet another variance reduction method for direct monte carlo simulations of low-signal flows

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1 Motivation(1/2)

The Boltzmann Equation(BE): describes the evolution of PDF $f = f(\boldsymbol{x}, \boldsymbol{c}, t)$. It can be written as:

$$\frac{\partial f}{\partial t} + \boldsymbol{c} \cdot \frac{\partial f}{\partial \boldsymbol{x}} = \left[\frac{\partial f}{\partial t}\right]_{\text{Collision}} = \frac{1}{2} \int\int\int (\delta_1' + \delta_2' - \delta_1 - \delta_2)\, f_1\, f_2\, c_{12}\, \sigma\, d\Omega\, d\boldsymbol{c}_1\, d\boldsymbol{c}_2$$

The BE is relevant when the Knudsen number $\text{Kn} = \lambda / L > 0.1$where λ is the gas mean free path and L is problem characteristic length scale

- **The Direct Simulation Monte Carlo method allows us to simulate the BE**

1 Motivation(2/2)

- **In DSMC properties are explicitly sampled**
- **The uncertainty in "measurement" is:**

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

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

- **We want:**

$$\sigma_{\text{Uncertainty}} = \frac{\sigma(\text{Signal})}{\sqrt{N_{\text{Samples}}}} \qquad s.t.\ \sigma(\text{Signal}) \to 0 \text{ as Signal} \to 0,\ \text{eg. } \sigma(\text{Signal}) \propto \text{Signal}$$

1.1 Previous Work

- **Baker & Hadjiconstantinou: Variance Reduction by simulating deviation from equilibrium**

  —DSMC-like particle method simulating deviation from **global** equilibrium (particle number diverges for Kn < 1)
  —Discontinuous Galerkin solution using variance-reduced collision integral evaluation (Talk tomorrow, Session 22-3-B)

- **Chun & Koch: Particle method simulating deviation from global equilibrium using the linearized Boltzmann equation**

  (Essentially equivalent to above particle method, ie. particle number diverges for Kn < 1)

- **Homolle & Hadjiconstantinou: DSMC-like Particle method can be stabilized by simulating deviation from local equilibrium (LVDSMC)**

  ~Stable
  ~Currently only for hardsphere collision integral
  ~Extension to other collision models in progress
  ~Very powerful

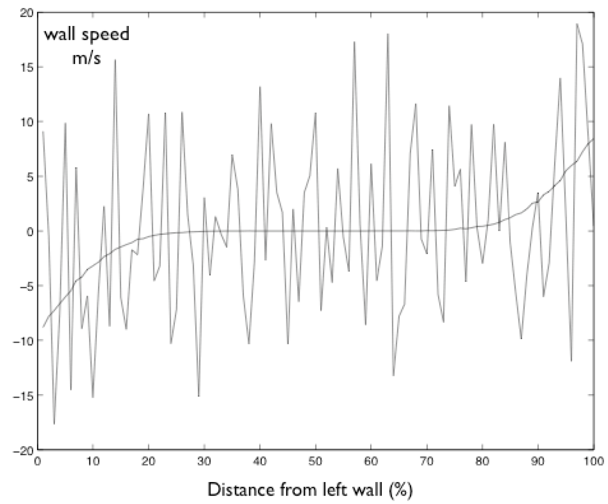


Illustration of variance reduction : 1 ensemble, 3000 particles/cell, wall velocity 0.05 (normalized)

1.2 Objective

- **Can we develop a variance-reduction technique that:**
  - **Uses DSMC as its main ingredient**
  - **Does not substantially increase computational requirements**

(Still Under Construction)

2.0 Solution Approach: Variance Reduction Using Likelihood Ratios

- **Consider the following moments:**

$$\langle R \rangle = \int R(\boldsymbol{c})\, f(\boldsymbol{c})\, d\boldsymbol{c}$$

$$\langle R \rangle_{\text{eq}} = \int R(\boldsymbol{c})\, f_{\text{eq}}(\boldsymbol{c})\, dc = \int R(\boldsymbol{c}) \left(\frac{f_{\text{eq}}(\boldsymbol{c})}{f(\boldsymbol{c})} \right) f(\boldsymbol{c})\, d\boldsymbol{c} = \int R(\boldsymbol{c})\, W(\boldsymbol{c})\, f(\boldsymbol{c})\, d\boldsymbol{c}$$

- **Using importance sampling :**

$$\overline{R} \simeq \frac{1}{N} \sum_{i=1}^{N} R(\boldsymbol{c}_i)$$

$$\overline{R}_{\text{eq}} \simeq \frac{1}{N} \sum_{i=1}^{N} \frac{f_{\text{eq}}(\boldsymbol{c}_i)}{f(\boldsymbol{c}_i)}\, R(\boldsymbol{c}_i) = \frac{1}{N} \sum_{i=1}^{N} W_i\, R(\boldsymbol{c}_i)$$

where $W_i = W(\boldsymbol{c}_i) = \dfrac{f_{\text{eq}}(\boldsymbol{c}_i)}{f(\boldsymbol{c}_i)}$

In words: we can evaluate both $\overline{R}$ and $\overline{R}_{\text{eq}}$ using samples from $f(c)$ only (provided the relative likelihood ratios W_is are known)

2.1 Variance Reduction Using Likelihood Ratios

This formulation can be used to yield variance reduction if $\langle R \rangle_{\text{eq}}$ is known by writing,

$$\overline{R}^{\text{VR}} = \overline{R} - \overline{R}_{\text{eq}} + \langle R \rangle_{\text{eq}} = \frac{1}{N} \sum_{i=1}^{N} (1 - W_i)\, R(\boldsymbol{c}_i) + \langle R \rangle_{\text{eq}}$$

When f is close to f_{eq}, i.e. $|W_i - 1| \ll 1$, we can show that

$$\sigma^2 \{\overline{R}^{\text{VR}}\} = \frac{1}{N^2} \sum_{j=1}^{N} \sum_{i=1}^{N} (1 - W_i)\left(1 - W_j\right) R(\boldsymbol{c}_i)\, R\left(\boldsymbol{c}_j\right) \left(\delta_{i,j} N - 1\right) \quad \& \quad \sigma^2 \{\overline{R}\} = \frac{1}{N^2} \sum_{j=1}^{N} \sum_{i=1}^{N} R(\boldsymbol{c}_i)\, R\left(\boldsymbol{c}_j\right) \left(\delta_{i,j} N - 1\right)$$

$\Rightarrow$

$$\sigma^2 \{\overline{R}^{\text{VR}}\} \ll \sigma^2 \{\overline{R}\}$$

2.2 Likelihood ratios: Illustrative Numerical Example

For $N = 10\,000$ let us take N samples c_i from $f(c) = \text{Normal}(\mathbf{0.1}, 1)$

$\bar{c} = \frac{1}{N} \sum_{i=1}^{N} c_i = 0.111786$ (±0.01 error)

Let $f_{\text{eq}}(c) = \text{Normal}(\mathbf{0}, 1)$. Instead of directly sampling $f_{\text{eq}}(c)$ we use the previous samples by defining $W_i = f_{\text{eq}}(c_i) \big/ f(c_i)$

- **Using the samples c_i and weights w_i we can measure the mean of f_{eq}:**

$\bar{c}_{\text{eq}} = \frac{1}{N} \sum_{i=1}^{N} W_i \, c_i = 0.0119512$ (again ±0.01 error)

- **Using the fact that $\langle c \rangle_{\text{eq}}$ is known we get variance reduction by**

$\bar{c}^{\text{VR}} = \bar{c} - \bar{c}_{\text{eq}} + \langle c \rangle_{\text{eq}} = \frac{1}{N} \sum_{i=1}^{N} (1 - W_i) \, c_i = 0.0998347$ (±0.001 error)

3 VR DSMC Using Likelihood Ratios

- **Can the above methodology be applied to DSMC?**
- **How?**

By introducing an auxiliary simulation which uses the DSMC data but simulates f_{eq}

- **What are the auxiliary simulation's Initial Condition and Boundary Condition?**

Yes, from the definition $W_i = \frac{f_{\text{eq}}(\boldsymbol{c}_i)}{f(\boldsymbol{c}_i)}$

- **What about Particle Dynamics?**

Convenient to look at advection and collision process separately (like DSMC)

3.1 Auxiliary Simulation: Advection

DSMC simulates the non-equilibrium BE. For the auxiliary simulation the governing equation is:

$$\frac{\partial f_{\text{eq}}}{\partial t} + \boldsymbol{c} \cdot \frac{\partial f_{\text{eq}}}{\partial \boldsymbol{x}} = 0$$

Making the substitution $f_{\text{eq}} \to W\, f$ we obtain

$$f\left(\frac{\partial W}{\partial t} + \boldsymbol{c} \cdot \frac{\partial W}{\partial \boldsymbol{x}}\right) + W\left(\frac{\partial f}{\partial t} + \boldsymbol{c} \cdot \frac{\partial f}{\partial \boldsymbol{x}}\right) = 0$$

The main DSMC simulation causes the 2nd term to drop giving us:

$$\frac{\partial W}{\partial t} + \boldsymbol{c} \cdot \frac{\partial W}{\partial \boldsymbol{x}} = 0$$

$\Rightarrow$ Advecting weights satisfies the BE for equilibrium

3.2 Auxiliary Simulation: Collision (1/2)

Collision integral for equilibrium:

$$\left[\frac{\partial f_{eq}}{\partial t}\right]_{\text{Collision}} = \frac{1}{2}\int\int\int (\delta_1' + \delta_2' - \delta_1 - \delta_2)\, f_{eq,1}\, f_{eq,2}\, c_{12}\, \sigma\, d\Omega\, d\boldsymbol{c}_1\, d\boldsymbol{c}_2$$

Making the substitution $f_{eq} \to W f \Rightarrow$

$$\left[\frac{\partial f_{eq}}{\partial t}\right]_{\text{Collision}} = \frac{\text{MX}}{2}\int\int\int (\delta_1' + \delta_2' - (\delta_1 + \delta_2))\, W_1\, W_2\, f_1\, f_2\, \frac{c_{12}}{\text{MX}}\, \sigma\, d\Omega\, d\boldsymbol{c}_1\, d\boldsymbol{c}_2$$

Which can be re-written as:

$$\frac{1}{2}\text{MX}\int\int\int\left(-\frac{\delta_1}{W_2} - \frac{\delta_2}{W_1} + \delta_1' + \delta_2'\right) W_1\, W_2\, f_1\, f_2 \left(\frac{c_{12}}{\text{MX}}\right) \sigma\, d\Omega\, d\boldsymbol{c}_1\, d\boldsymbol{c}_2 \;+\; \frac{1}{2}\text{MX}\int\int\int\left(\frac{\delta_1}{W_2} + \frac{\delta_2}{W_1} - \delta_1 - \delta_2\right) \frac{c_{12}/\text{MX}}{\left(1 - \frac{c_{12}}{\text{MX}}\right)}\, W_1\, W_2\, f_1\, f_2\, \sigma \left(1 - \frac{c_{12}}{\text{MX}}\right) d\Omega\, d\boldsymbol{c}_1\, d\boldsymbol{c}_2$$

= "acceptance" **+ "rejection"**

$\text{MX} = \text{Max}\{\, W\, c_{12}\}$

3.2 Auxiliary Simulation: Collision (2/2)

- **Weight "bookkeeping"**

Event	In	Intermediate Steps	Final Result
Accepted (**Prob.** = C_{12}/MX)	W_1 @ $\boldsymbol{C_1}$ W_2 @ $\boldsymbol{C_2}$	Create : $W_1\,W_2$ @ $\boldsymbol{C'_1}$ & $W_1\,W_2$ @ $\boldsymbol{C'_2}$ Annihilate : W_1 @ $\boldsymbol{C_1}$, W_2 @ $\boldsymbol{C_2}$	$W_1\,W_2$ @ $\boldsymbol{C'_1}$ and $W_1\,W_2$ @ $\boldsymbol{C'_2}$
Rejected (**Prob.** = $1 - C_{12}$/MX)	W_1 @ $\boldsymbol{C_1}$ W_2 @ $\boldsymbol{C_2}$	Create : $W_1 \frac{C_{12}}{\mathrm{MX}} \Big/ \left(1 - \frac{C_{12}}{\mathrm{MX}}\right)$ @ $\boldsymbol{C_1}$ $W_2 \frac{C_{12}}{\mathrm{MX}} \Big/ \left(1 - \frac{C_{12}}{\mathrm{MX}}\right)$ @ $\boldsymbol{C_2}$ Annihilate : $W_1\,W_2 \frac{C_{12}}{\mathrm{MX}} \Big/ \left(1 - \frac{C_{12}}{\mathrm{MX}}\right)$ @ C_1 & C_2	$\frac{1-W_2 \frac{C_{12}}{\mathrm{MX}}}{1-\frac{C_{12}}{\mathrm{MX}}} W_1$ @ $\boldsymbol{C_1}$ $\frac{1-W_1 \frac{C_{12}}{\mathrm{MX}}}{1-\frac{C_{12}}{\mathrm{MX}}} W_2$ @ $\boldsymbol{C_2}$

4 Stability (1/2)

- **These weight update rules are not stable**
- **Weights grow exponentially ⇒ loss of Variance Reduction**

- **Why does the instability happen?**

A number of ways to think of this :

- **1. No conservation of mass, momentum and energy**

Weights are not conserved in steps. Since the weight update formula is a function of weight values themselves the random walk quickly diverges.

- **2. We are calculating probabilities of samples and not of a local PDF**

These weight update rules calculate $P_{\text{eq}}\left(\boldsymbol{c}_i^{t+1} \,\middle|\, I^t \,\middle|\, I^{t-1} \ldots.\right)$ not $f_{\text{eq}}(\boldsymbol{c}_i)$ only the latter PDF is expected to converge to f at long time.

4 Stability (2/2)

- **From definition $W_i = f_{eq}(c_i) / f(c_i)$ ⇒ we need knowledge of PDF**
- **Solution: Need to *reconstruct* the PDF from samples**

  This is a standard numerical method known as Kernel Density Estimation

- **Specifically, for every particle at c**

$$f(\boldsymbol{c}) \simeq \int K(c' - c)\, f(c')\, d\boldsymbol{c}'$$

$$f_{eq}(\boldsymbol{c}) \simeq \int K(c' - c)\, f_{eq}(\boldsymbol{c}')\, d\boldsymbol{c}' = \int K(\boldsymbol{c}' - \boldsymbol{c})\, W(\boldsymbol{c}')\, f(\boldsymbol{c}')\, d\boldsymbol{c}'$$

Using sampling we can get:

$$W'_j = \left(\sum_{i=1}^{S_j} (W_i)^*\right) \Big/ \left(\sum_{i=1}^{S_j} 1\right)$$

$$S_j = \{\text{particles within } \varepsilon \text{ of } \boldsymbol{c}_j\}$$

4 Final Algorithm Summary

0. Initialize N particles at $\boldsymbol{c}_i$ & $W_i = \frac{f_{\text{eq}}(c, t=0)}{f(c, t=0)}$

1. Advection: $\boldsymbol{x}_i' = \boldsymbol{x}_i + \Delta\text{t}\, \boldsymbol{c}_i$

2. Collisions:

   2.1 Select candidates (i and j) & process with $P_{\text{NE}} = c_{\text{ij}} / \text{MX}$ & $P_{\text{eq}} = W_j\, c_{\text{ij}} / \text{MX}$

   Accepted: Scatter both particles & $W_i^* = W_i \frac{P_{\text{eq}}}{P_{\text{NE}}}$

   Rejected: Keep same velocity & $W_i^* = W_i \frac{1-P_{\text{eq}}}{1-P_{\text{NE}}}$

3. Sample: $\overline{R}^{\text{VR}} = \frac{1}{N} \sum_{i=1}^{N} (1 - W_i)\, R(c_i) + \langle R \rangle_{\text{eq}}$

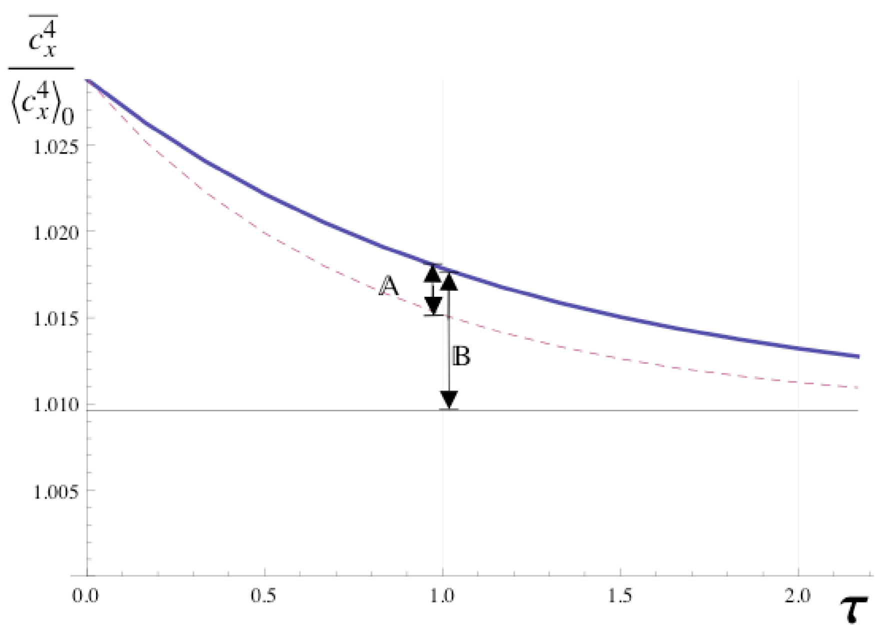
4. Use Kernel Density Estimation to produce W_i' from W_i^* of all particles around c_i

5. Take $W_i' \to W_i$, repeat steps 1, 2,3,4&5

5 Results: Problem Setup

We study the relaxation of $\int c_x^4 \, f(\boldsymbol{c}) \, d\boldsymbol{c}$ in a homogeneous calculation from the initial condition:

$$f(c) = \beta \left(\text{Exp}\left[- \frac{(c_x - \alpha)^2 + c_y^2 + c_z^2}{c_0^2} \right] + \text{Exp}\left[- \frac{(c_x + \alpha)^2 + c_y^2 + c_z^2}{c_0^2} \right] \right)$$

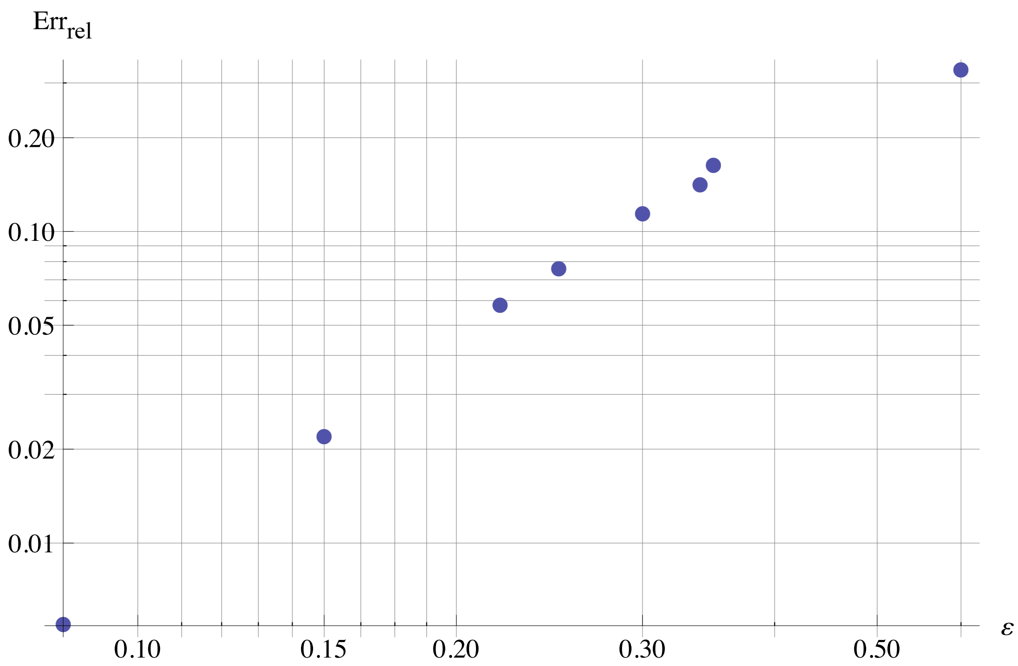


Variance Reduction: — α=0.1 ⇒ VR = 400

— α=0.01 ⇒ VR = 6.25×10^6

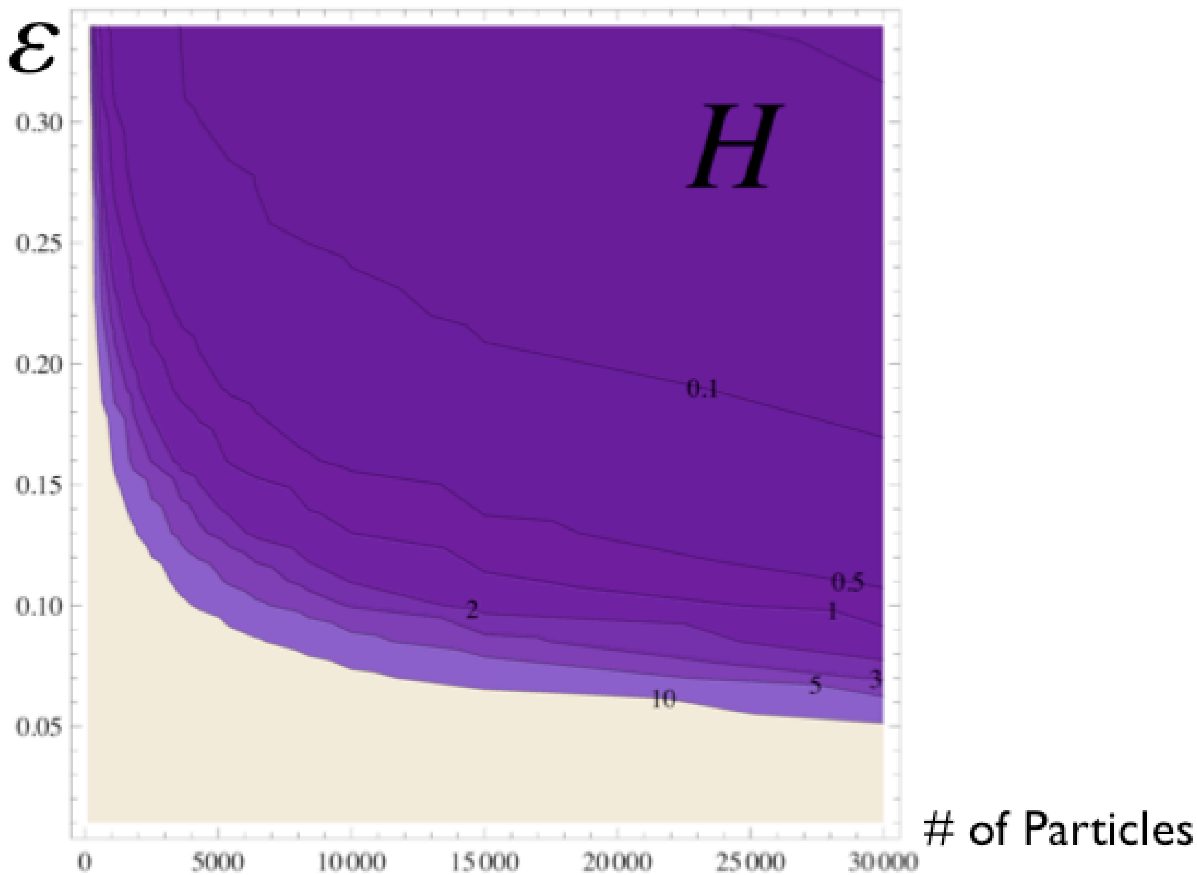
5 Results: Error vs. ε

$$\mathrm{Err}_{\mathrm{Rel}}(\varepsilon, t) = \frac{\mathbb{A}(\varepsilon, t)}{\mathbb{B}(t)} = \left(\frac{\langle c_x^4 \rangle_{\text{NE,Exact Solution}} - \overline{\langle c_x{}^4 \rangle}_{@\,\varepsilon}}{\langle c_x^4 \rangle_{\text{NE,Exact Solution}} - \langle c_x^4 \rangle_{\text{SS}}} \right)_{\text{Evaluated at time}=t}$$



5 Stability Results

Defining our stability parameter $H = \frac{\text{Variance at time } 4\,\tau}{\text{Initial Variance}} = \frac{\text{Var}\left\{(1-W_i)\,c_{x,i}^4\right\}_{\text{at time}=4\,\tau}}{\text{Var}\left\{(1-W_i)\,c_{x,i}^4\right\}_{\text{at time}=0\,\tau}}$



6 Conclusions

- **Variance reduction using likelihood ratios is viable and promising**
- **The main DSMC simulation is never perturbed. This is one of the advantages compared to other variance reduction techniques developed by our group**
- **Need to find NN of particle at end of every step making the total cost $O(N \operatorname{Log}(N))$**
- **Current kernel density estimator very crude.
Only looks at c_i's within ε of sample point**
- **There is a trade-off between stability and numerical error**