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

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Motivation

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

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

- **Used to describe flows with** $Kn = \lambda / L > 0.1$

  λ is the gas mean free path and L is problem characteristic length scale

- **Direct Simulation Monte Carlo: simulates the BE**

  The uncertainty in "measurement" is:

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

$\Rightarrow$ problems in low signal($\equiv$ deviation from equilibrium) flows (eg. low Ma flows).

- **Ideally, we want:**

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

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

Previous Work & Objective

Previous Work:

- Baker & Hadjiconstantinou: Variance reduction by simulating only deviation from equilibrium (unstable for $Kn<1.0$ without particle cancellation)
- Chun & Koch: Particle method simulating deviation from global equilibrium using the linearized Boltzmann equation (unstable for $Kn<1.0$ without particle cancellation)
- Homolle & Hadjiconstantinou: Low-variance deviational simulation Monte Carlo (LVDSMC)

Objective: develop a VR method that is

- directly based on DSMC
- easily incorporates more complex interaction models
- more general (see later)

Notation:

- **Let $\langle R \rangle$ be a property of interest (eg. $u_x = \langle c_x \rangle$, $\langle c_x^4 \rangle$ etc.). In general, it can be written as:**

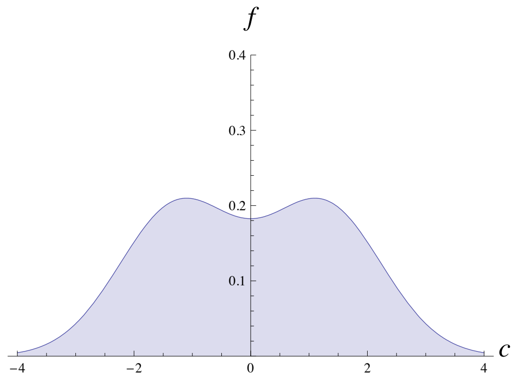
$$\langle R \rangle = \int R(\boldsymbol{c})\, f(\boldsymbol{c})\, d\boldsymbol{c} \qquad \text{and likewise for } f_{eq} \neq f, \quad \langle R \rangle_{\text{eq}} = \int R(\boldsymbol{c})\, f_{\text{eq}}(\boldsymbol{c})\, d\boldsymbol{c}$$

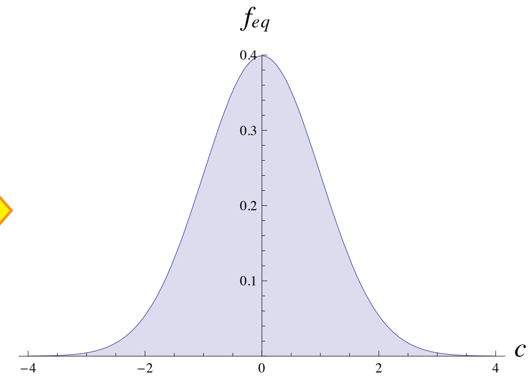
Where f_{eq} is an arbitrary reference equilibrium distribution

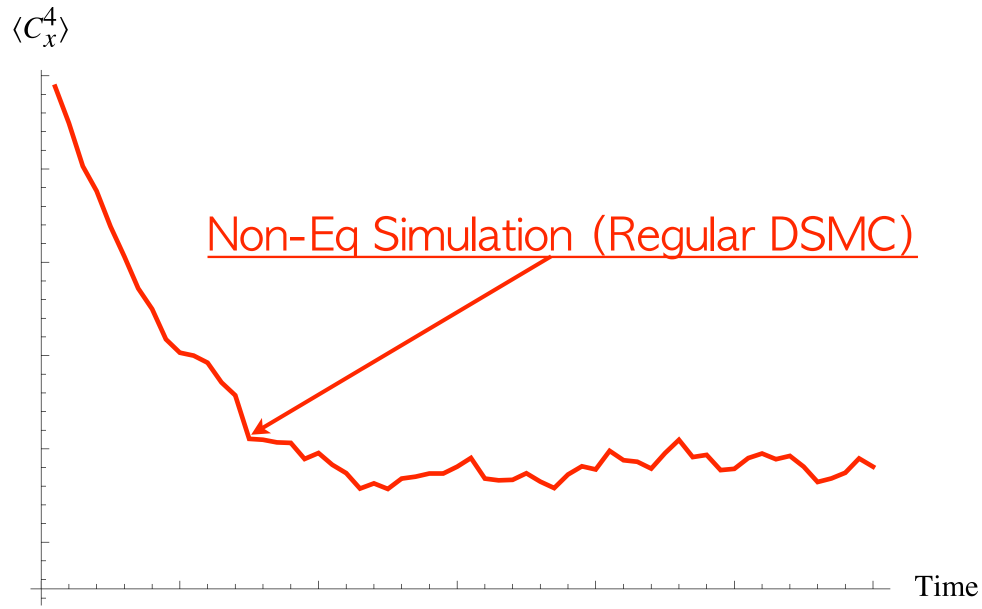
- **An estimate of this quantity (that we will call $\overline{R}$) can be calculated by generating samples c_i from $f(c_i)$**

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

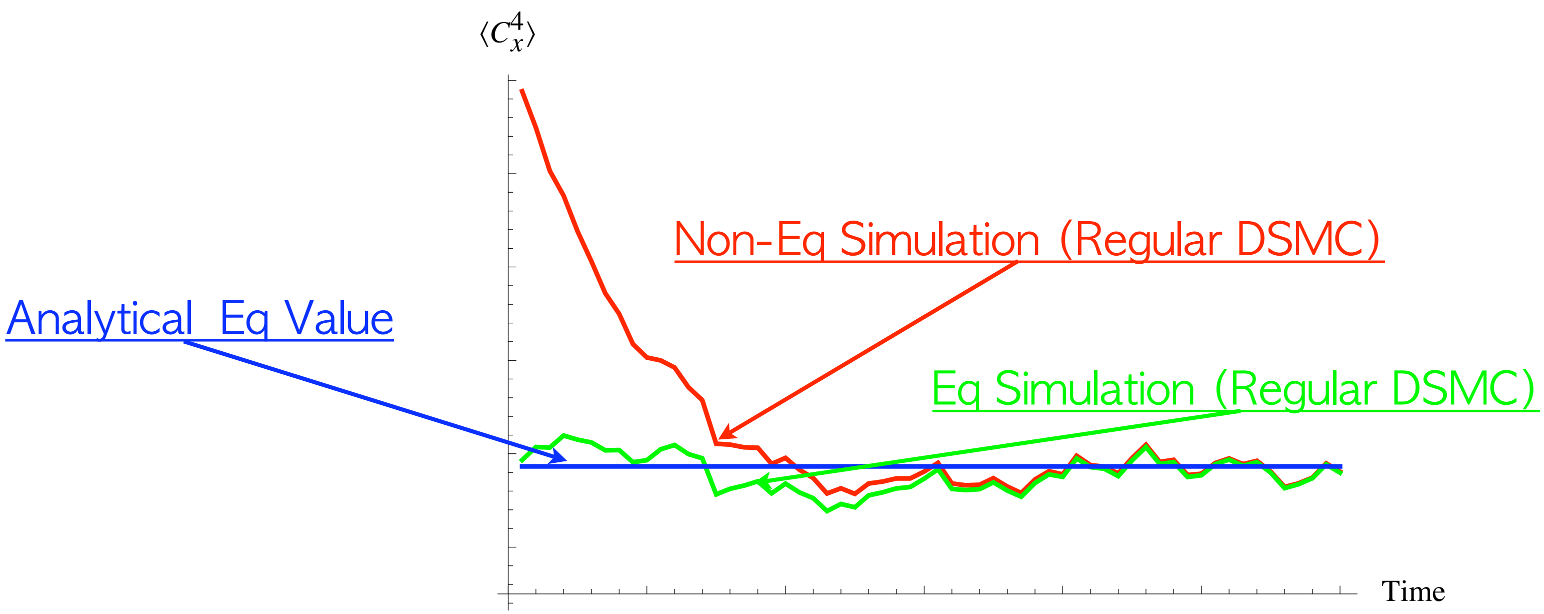
Variance Reduction Approach





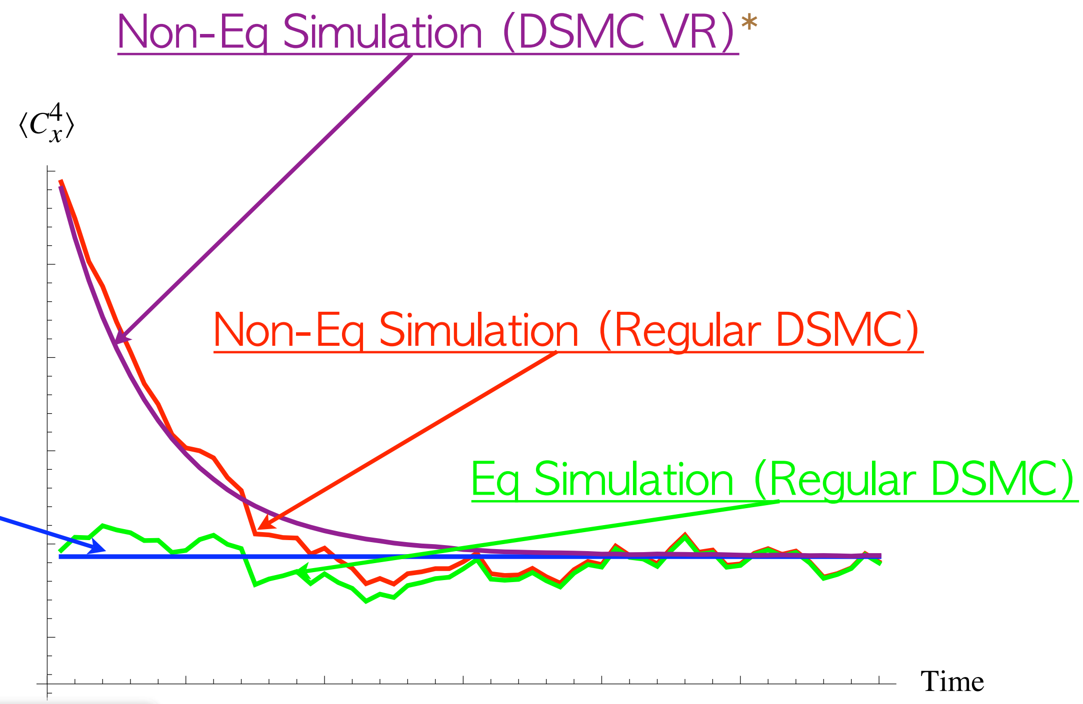


Variance Reduction Approach



Variance Reduction Approach

$$\overline{R}^{\mathrm{VR}} = \overline{R} - \overline{R}_{\mathrm{eq}} + \langle R \rangle_{\mathrm{eq}}$$



* Actual Simulation Results!

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Formulation

- **How can we use above concept (previously used in polymer simulation [Öttinger,1997]) to produce low-variance solutions using DSMC?**

- **Our Formulation:**
  - Use an **unmodified** DSMC to directly calculate $\overline{R}$

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

  - Use an **auxiliary** simulation to calculate $\overline{R}_{eq}$. The auxiliary simulation does not perturb the main DSMC simulation and uses the same samples $\boldsymbol{c}_i$

Auxiliary Simulation Using Likelihood Ratios

- **How can we calculate both $\overline{R}$ and $\overline{R}_{eq}$ from the same set of data?**
- **Likelihood ratios** $(W_i \equiv W(\boldsymbol{c}_i) \equiv f_{eq}(\boldsymbol{c}_i)/f(\boldsymbol{c}_i))$**:**

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

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

- **As a result:**

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

Evolution of W_i

0. Initialize N particles at $\boldsymbol{c}_i$ & $W_i = ??$

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

2. Collisions:

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

   Accepted: Scatter both particles & $W_i^* = ??$

   Rejected: Keep same velocity & $W_i^* = ??$

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

4. Repeat steps 1, 2, 3 & 4

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Evolution of W_i

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

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

2. Collisions:

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

    Accepted: Scatter both particles & $W_i^* = W_i W_j$

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

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

4. Take $W_i^* \rightarrow W_i$, repeat steps 1, 2, 3 & 4

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Stability

- **Problem:**
  - These weight update rules are not stable ⇒ loss of Variance Reduction

- **Solution:**
  - From definition $W_i = f_{eq}(\boldsymbol{c}_i)/f(\boldsymbol{c}_i)$ ⇒ 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 $\boldsymbol{c}$

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

- **Implementation:**
  - For each particle i with W_i @ $\boldsymbol{c}_i$ we replace post-collision weight with average weights within a sphere (in velocity space) of radius ε.

Final Algorithm Summary

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

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

2. Collisions:

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

    Accepted: Scatter both particles & $W_i^* = W_i\, W_j$

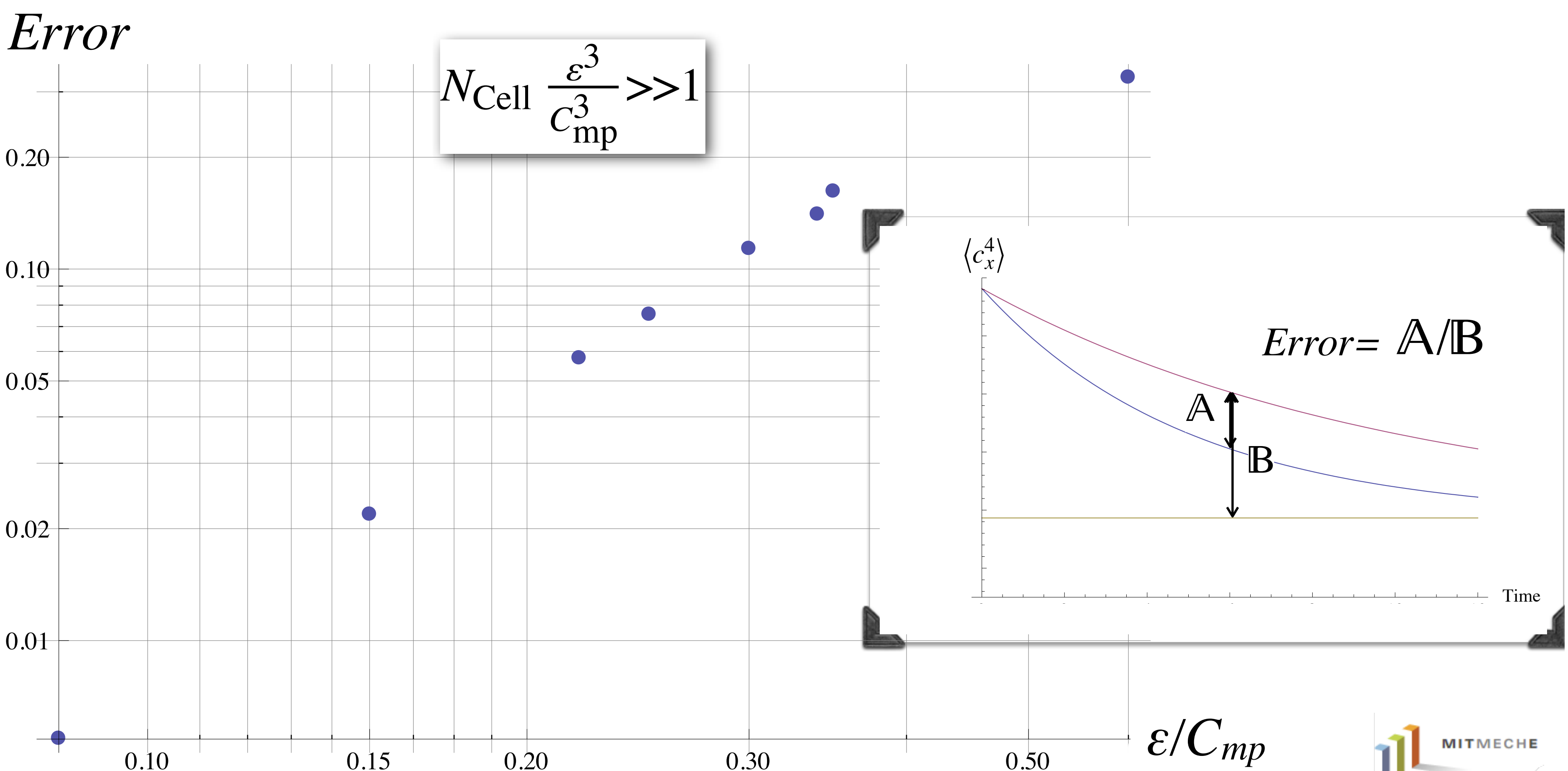
    Rejected: Keep same velocity & $W_i^* = W_i \frac{1 - W_j P_{\text{NE}}}{1 - P_{\text{NE}}}$

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 $W'_i \rightarrow W_i$, repeat steps 1, 2, 3, 4 & 5

Results: Error vs. ε



Conclusions

- **Variance reduction using likelihood ratios is viable and promising**
- **Main advantage: the DSMC simulation is never perturbed**
- **Small increase in computational cost**
  - need to find NN of particle at end of every step making the total cost *O(N Log(N))*

- **We are working on:**
  - improving the efficiency and robustness of stabilizing scheme
  - moving into multi-dimensional problems
  - More details to appear in:
    - Al-Mohssen, H. A., Hadjiconstantinou, N.G.; Yet another variance reduction method for direct Monte Carlo simulations of low-signal flows, 26th International Symposium on Rarefied Gas Dynamics, July 21-25, 2008.

Appendixes

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,

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

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

$$\sigma^2 \{\overline{R}^{\text{VR}}\} = \frac{1}{N^2} \sum_{j=1}^{N} \sum_{i=1}^{N} (1 - W_i)(1 - W_j)\, R(c_i)\, R(c_j)\, (\delta_{i,j} N - 1) \qquad \& \qquad \sigma^2 \{\overline{R}\} = \frac{1}{N^2} \sum_{j=1}^{N} \sum_{i=1}^{N} R(c_i)\, R(c_j)\, (\delta_{i,j} N - 1)$$

$\Rightarrow$

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

3.1 Auxiliary Simulation: Advection

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

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

Making the substitution $f_{eq} \rightarrow W f$ we obtain

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

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

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

$\Rightarrow$ Advecting weights satisfies the BE for equilibrium

3.2 Auxiliary Simulation: Collision (1/2)

Collision integral for equilibrium:

$$\left[\frac{\partial f_{\mathrm{eq}}}{\partial t}\right]_{\mathrm{Collision}} = \frac{1}{2}\int\int\int(\delta_1' + \delta_2' - \delta_1 - \delta_2)\, f_{\mathrm{eq},1}\, f_{\mathrm{eq},2}\, c_{12}\, \sigma\, d\Omega\, dc_1\, dc_2$$

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

$$\left[\frac{\partial f_{\mathrm{eq}}}{\partial t}\right]_{\mathrm{Collision}} = \frac{\mathrm{MX}}{2}\int\int\int(\delta_1' + \delta_2' - (\delta_1 + \delta_2))\, W_1\, W_2\, f_1\, f_2\, \frac{c_{12}}{\mathrm{MX}}\, \sigma\, d\Omega\, dc_1\, dc_2$$

Which can be re-written as:

$$\frac{1}{2}\mathrm{MX}\int\int\int\left(-\frac{\delta_1}{W_2} - \frac{\delta_2}{W_1} + \delta_1' + \delta_2'\right) W_1\, W_2\, f_1\, f_2 \left(\frac{c_{12}}{\mathrm{MX}}\right) \sigma\, d\Omega\, dc_1\, dc_2 \;+\; \frac{1}{2}\mathrm{MX}\int\int\int\left(\frac{\delta_1}{W_2} + \frac{\delta_2}{W_1} - \delta_1 - \delta_2\right) \frac{c_{12}/\mathrm{MX}}{\left(1 - \frac{c_{12}}{\mathrm{MX}}\right)}\, W_1\, W_2\, f_1\, f_2\, \sigma \left(1 - \frac{c_{12}}{\mathrm{MX}}\right) d\Omega\, dc_1\, dc_2$$

$$= \text{"acceptance"} \quad + \quad \text{"rejection"}$$

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

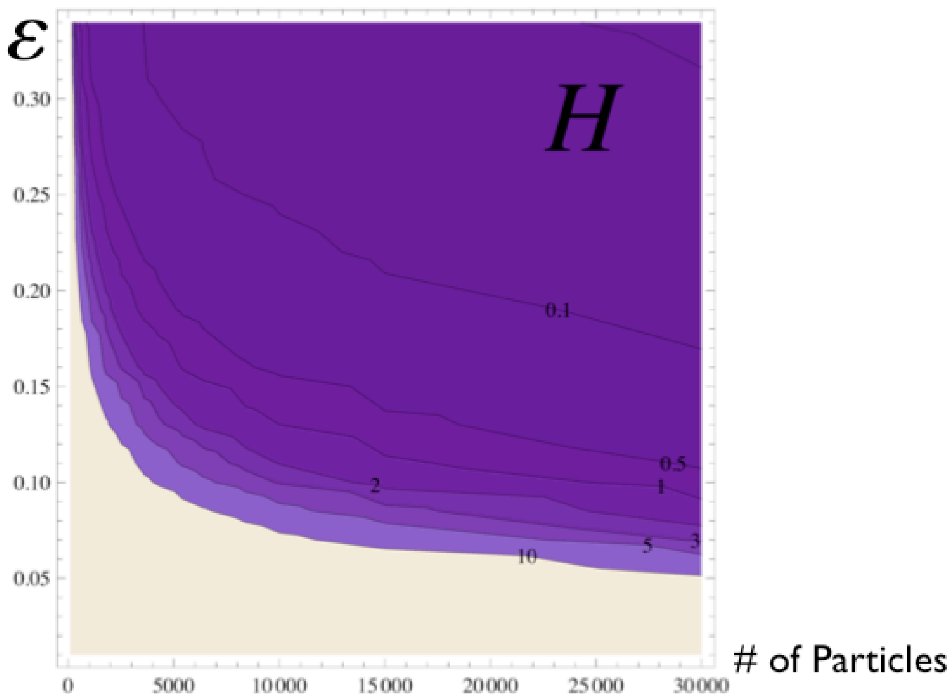
3.2 Auxiliary Simulation: Collision (2/2)

- **Weight "bookkeeping"**

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

5 Stability Results

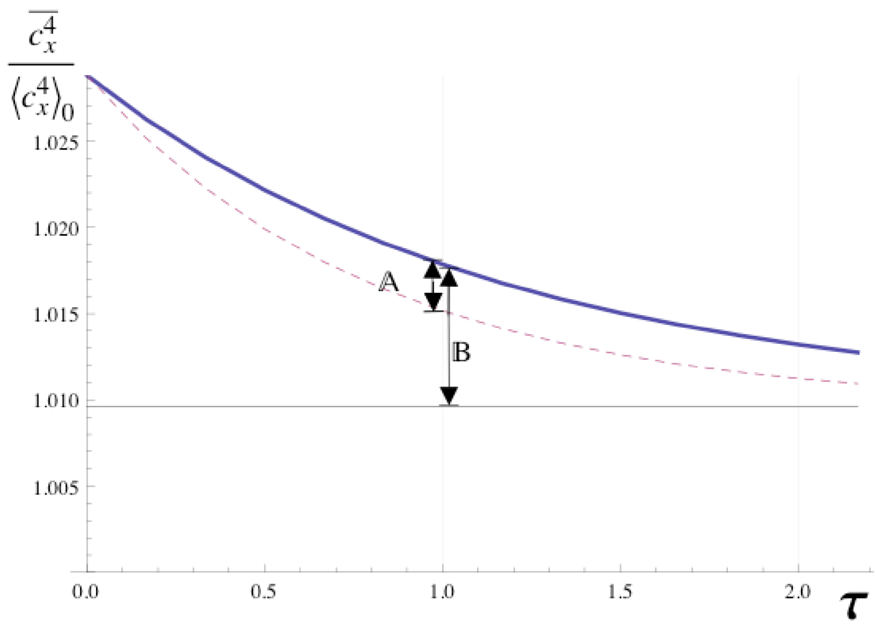
Defining our stability parameter $H = \frac{\text{Variance at time } 4\,\tau}{\text{Initial Variance}} = \frac{\text{Var}\left\{\left(1-W_i\right) c_{x,i}^4\right\}_{\text{at time}=4\,\tau}}{\text{Var}\left\{\left(1-W_i\right) c_{x,i}^4\right\}_{\text{at time}=0\,\tau}}$



5 Results: Problem Setup

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

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



Variance Reduction: — α=0.1 ⇒ VR = 400

— α=0.01 ⇒ VR = 6.25×10^6