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

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Motivation

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

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

- **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. $\sigma(\text{Signal}) \rightarrow 0$ as $\text{Signal} \rightarrow 0$

- **Related Work:**
  - Öttinger, 1997: polymer simulation
  - Chun and Koch, 2005: linearized BE
  - Hadjiconstantionu, et el. 2004-2009: deviational particles

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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:**

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

  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 $\boldsymbol{c}_i$ from $f(\boldsymbol{c}_i)$**

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

Variance Reduction Approach

$$I = \int f(\boldsymbol{c})\, d\boldsymbol{c} \;\Rightarrow\; \bar{I} = \frac{1}{N}\sum_{i=1}^{N} f(\boldsymbol{c}_i) \tag{1}$$

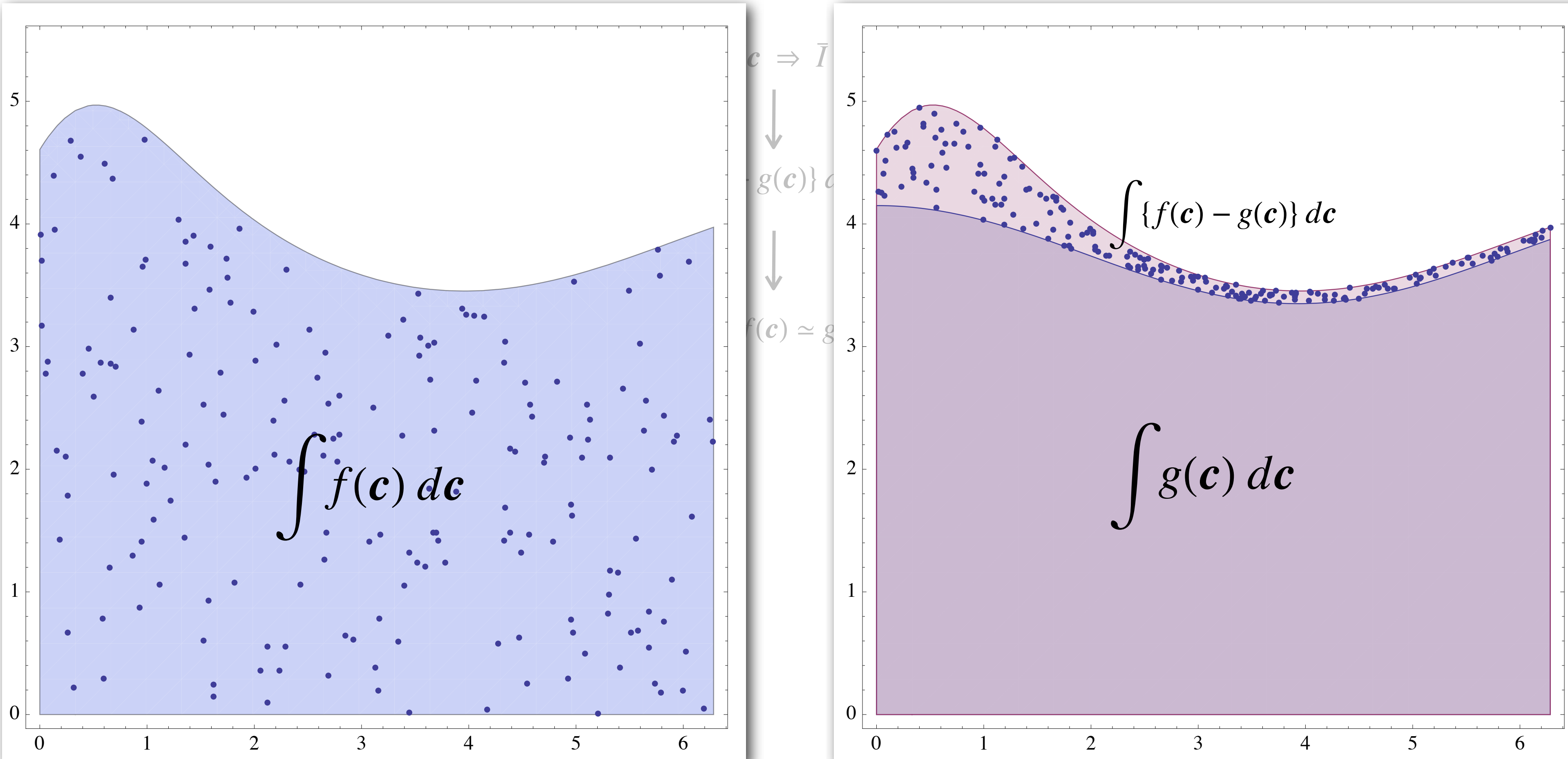
$$\downarrow$$

$$I = \int \{f(\boldsymbol{c}) - g(\boldsymbol{c})\}\, d\boldsymbol{c} \;+ \int g(\boldsymbol{c})\, d\boldsymbol{c} \tag{2}$$

$$\downarrow$$

if $\int g(\boldsymbol{c})\, d\boldsymbol{c}$ is known deterministically & $f(\boldsymbol{c}) \simeq g(\boldsymbol{c})$

Variance Reduction Approach



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$$I \simeq \underbrace{\left\{\int f(\boldsymbol{c}) - g(\boldsymbol{c})\, d\boldsymbol{c}\right\}} \; + \int g(\boldsymbol{c})\, d\boldsymbol{c}$$

Simulate using deviational particles

Hadjiconstantinou, Baker, Homolle, Radtke

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Simulate using deviational particles

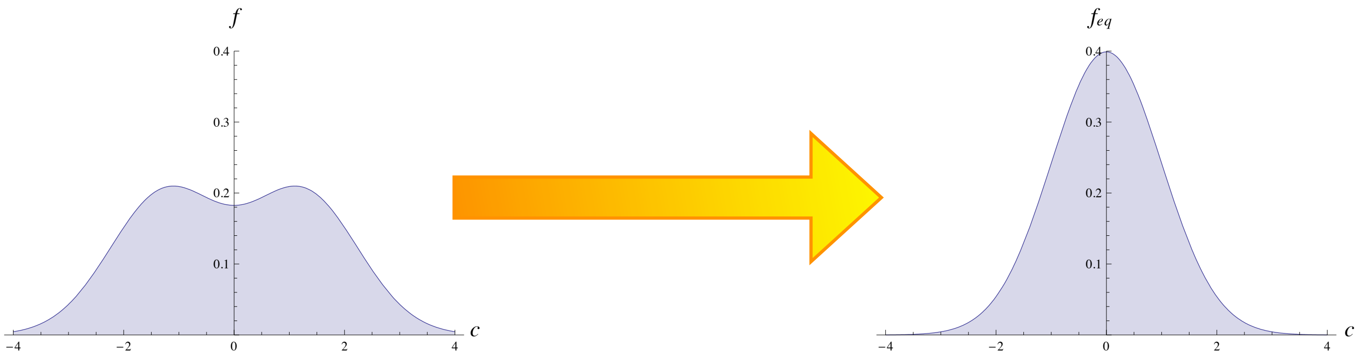
Hadjiconstantinou, Baker, Homolle, Radtke

$$I \simeq \underbrace{\left\{\int f(\boldsymbol{c})\, d\boldsymbol{c}\right\}} - \underbrace{\left\{\int g(\boldsymbol{c})\, d\boldsymbol{c}\right\}} + \int g(c)\, \mathrm{dc}$$

Unmodified DSMC **Auxiliary** Weighted DSMC

This Work

Illustration



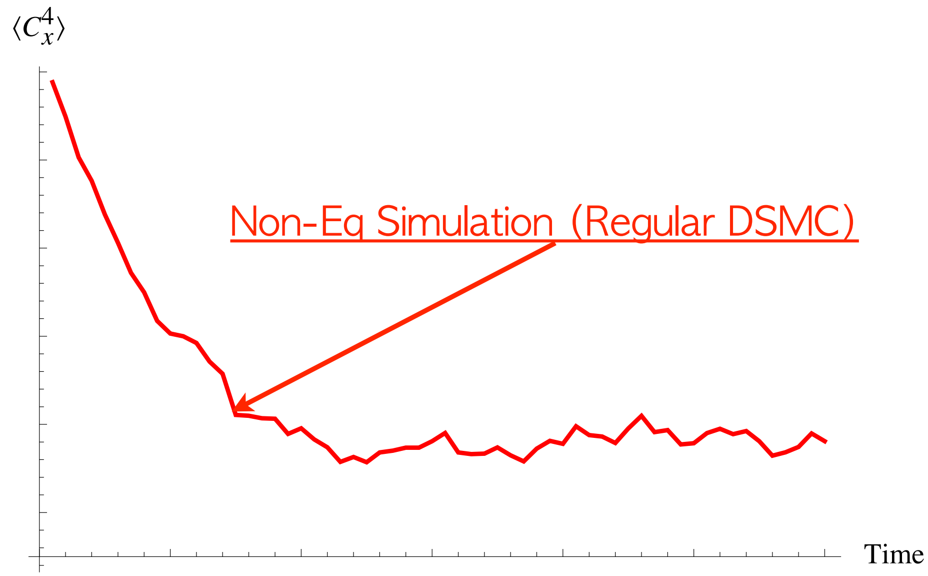


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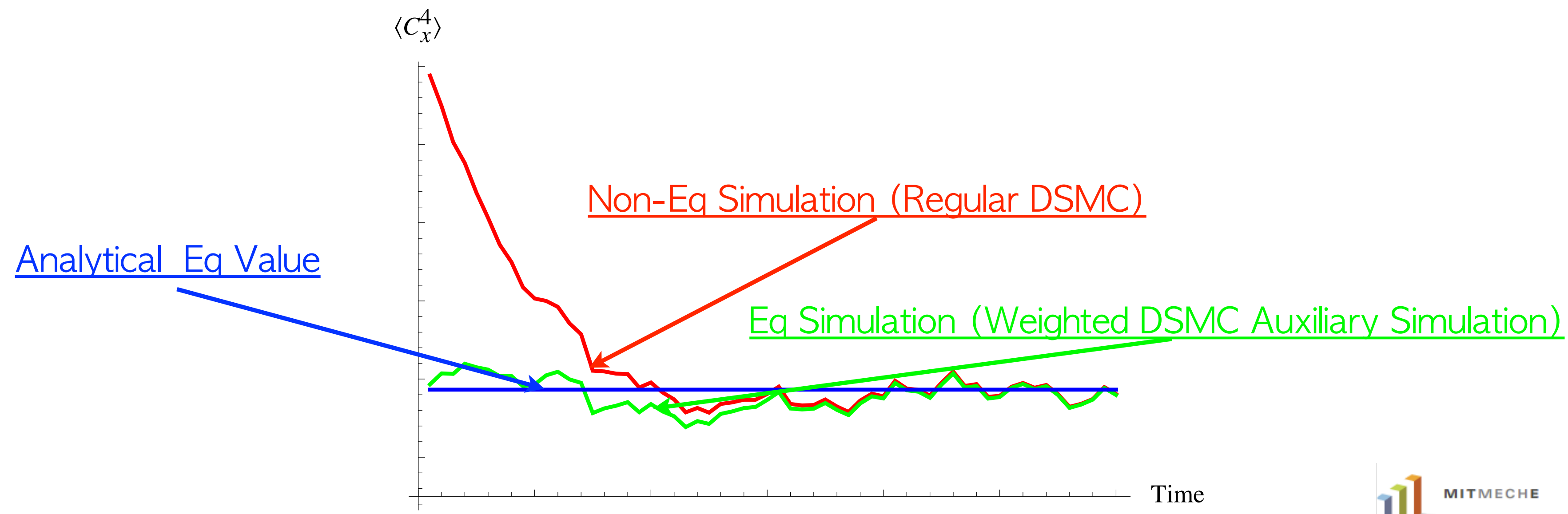
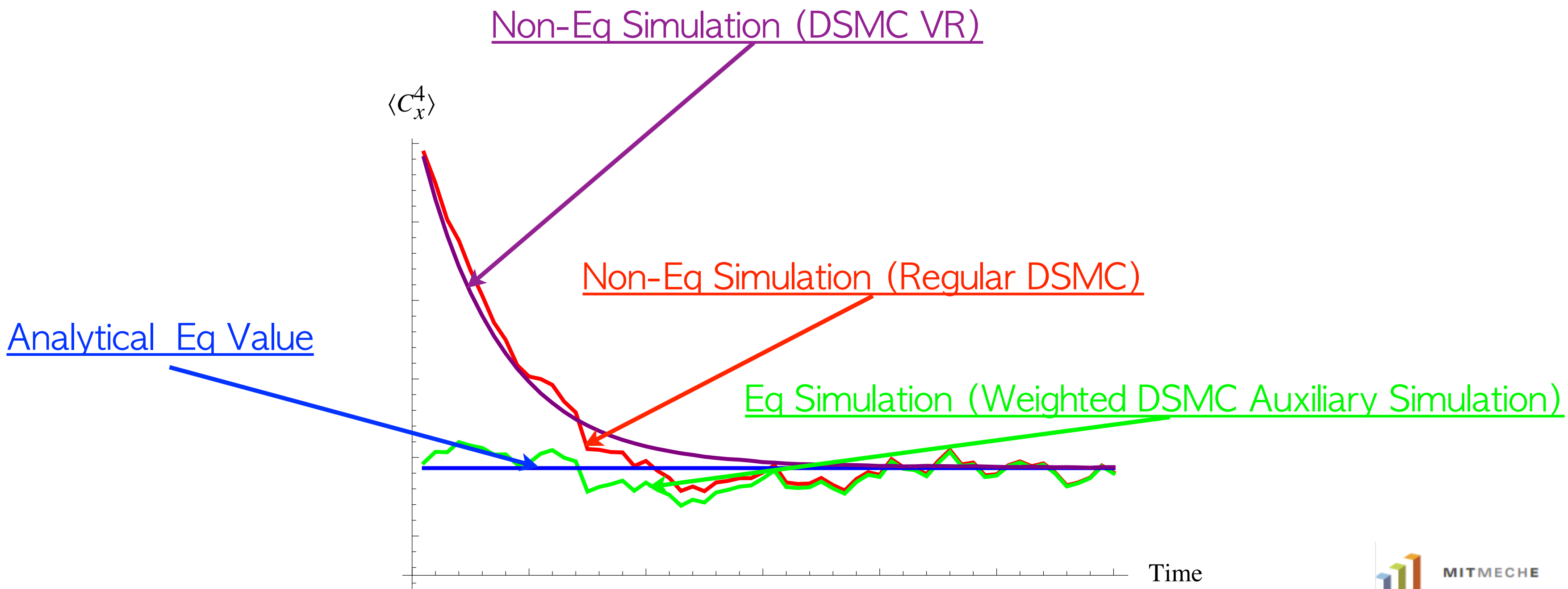
Illustration



Illustration

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



Formulation

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 $\boldsymbol{c}_i$

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

Auxiliary Simulation Using Weights

- **Likelihood ratios** *($W_i \equiv W(\boldsymbol{c}_i) \equiv f_{eq}(\boldsymbol{c}_i)/f(\boldsymbol{c}_i)$)***:**

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

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

- **As a result:**

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

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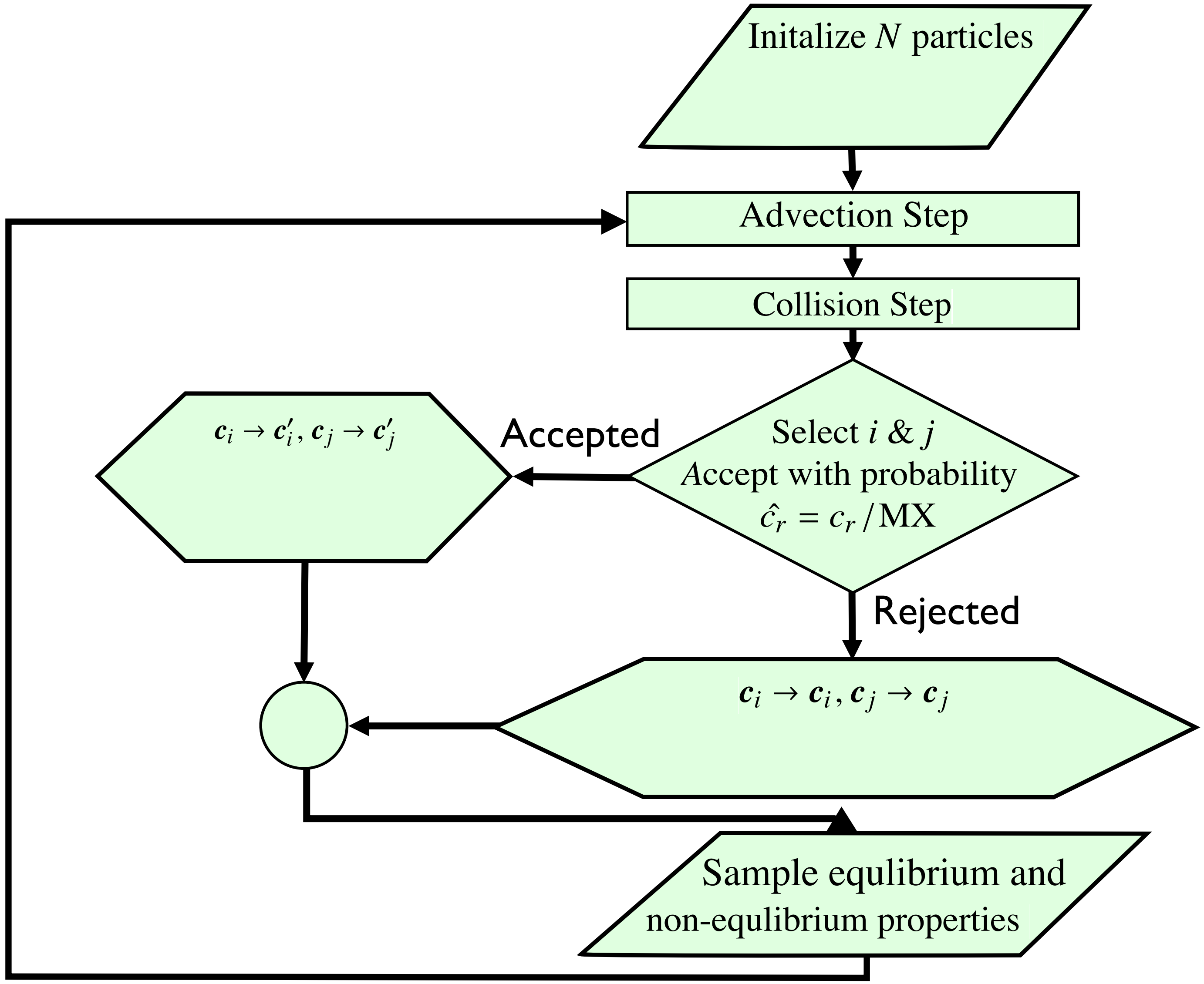
Algorithm Overview

Regular DSMC

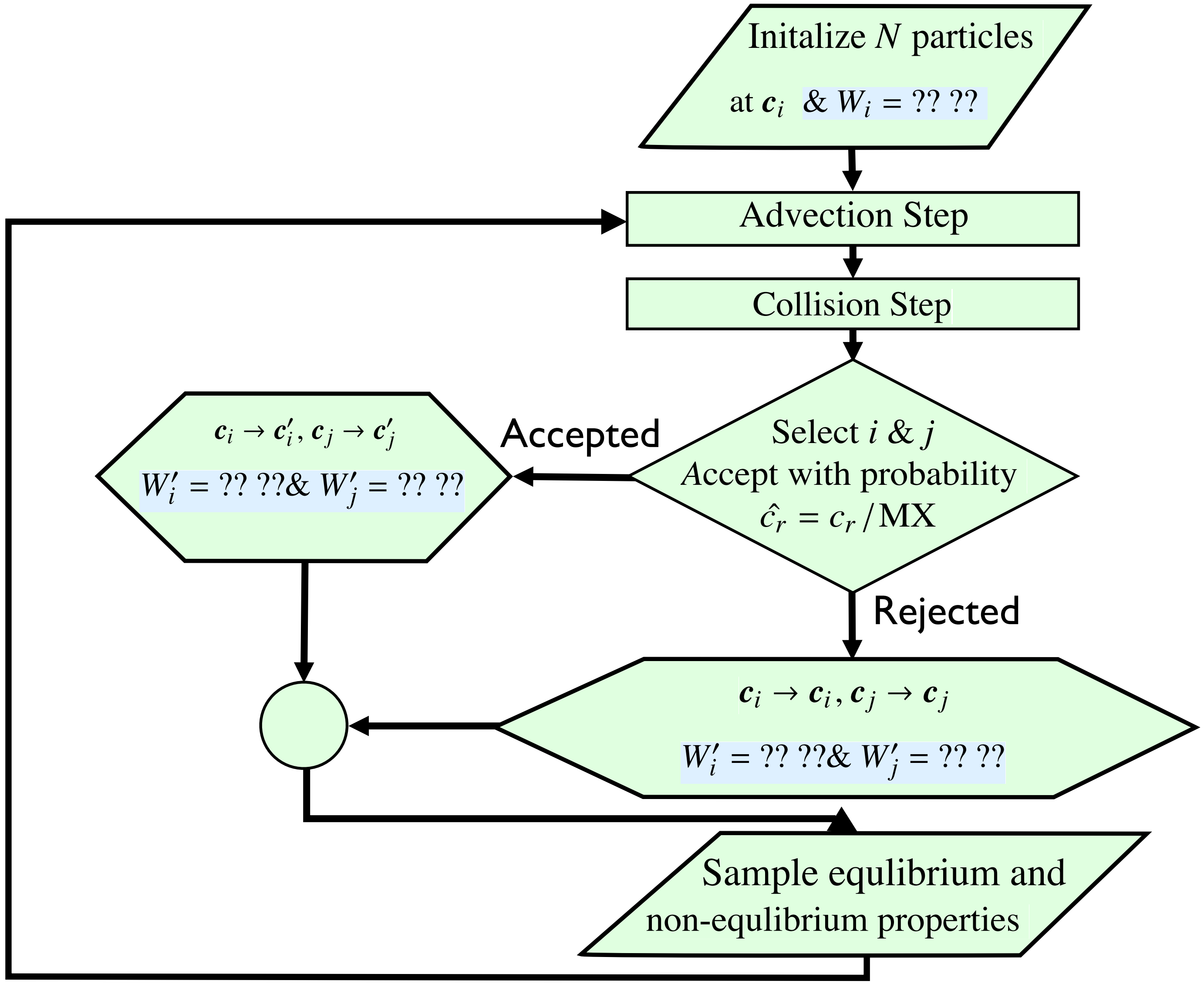


Algorithm Overview

Regular DSMC

\+

VR DSMC



Conditional Weight Update Rules

- **For every particle at c_i there will be <u>on average</u> $P_{c_i \to c_i'}$ particles at c_i'. If we have x particles at c_i there will be (at c_i')**
  - $x P_{\text{eq}:c_i \to c_i'}$ particles in an Equilibrium simulation
  - $x P_{c_i \to c_i'}$ particles in a Non-equilibrium simulations
- **Since we advance particles per the Non-equilibrium rules each particle at needs to simulate:**

$$\frac{P_{\text{eq}:c_i \to c_i'}}{P_{c_i \to c_i'}}$$

- **The final collision rules**
  - Accepted

$$W_i \;\&\; W_j \;\to\; W_i \; W_j$$

  - Rejected

$$W_i \to \; W_i \, \frac{1 - W_j \, \hat{c}_r}{1 - \hat{c}_r} \;\; \& \; W_j \to \; W_j \, \frac{1 - W_i \, \hat{c}_r}{1 - \hat{c}_r}$$

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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 $\boldsymbol{c}$ replace

$$f(\boldsymbol{c}_i) \to \hat{f}(\boldsymbol{c}_i) = \int K(\boldsymbol{c}' - \boldsymbol{c})\, f(\boldsymbol{c}')\, d\,\boldsymbol{c}' \qquad \text{since} \qquad \hat{f}(\boldsymbol{c}_i) \to f(\boldsymbol{c}_i) \text{ as } K(\Delta\boldsymbol{c}) \to \delta(\Delta\boldsymbol{c})$$

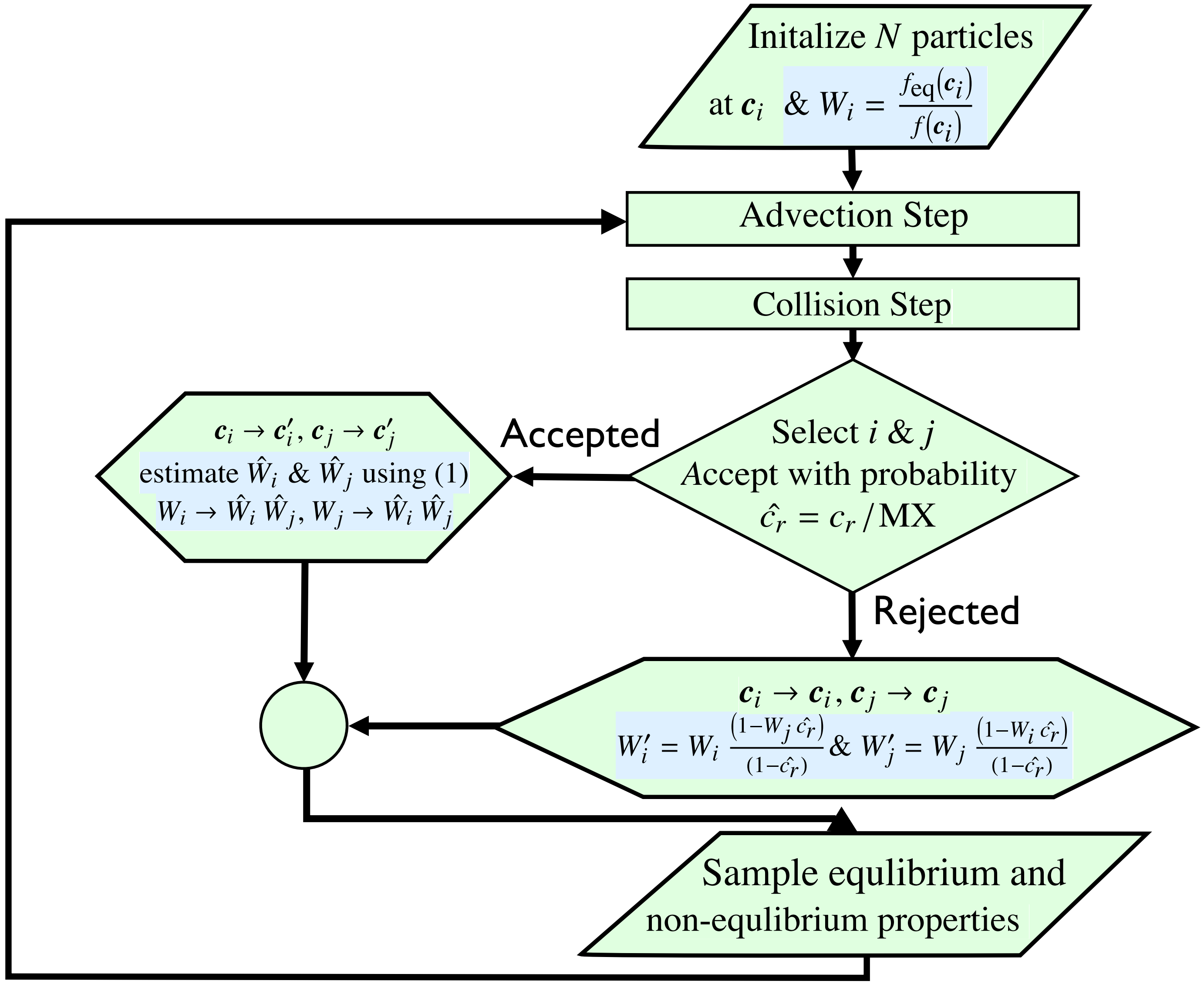
- **Implementation:**
  - For accepted particles

$$W_i \to \hat{W}_i = \frac{1}{\| S_i \|} \sum_{j \in S_i} W_j$$

(average weights within a sphere of radius ε in velocity space)

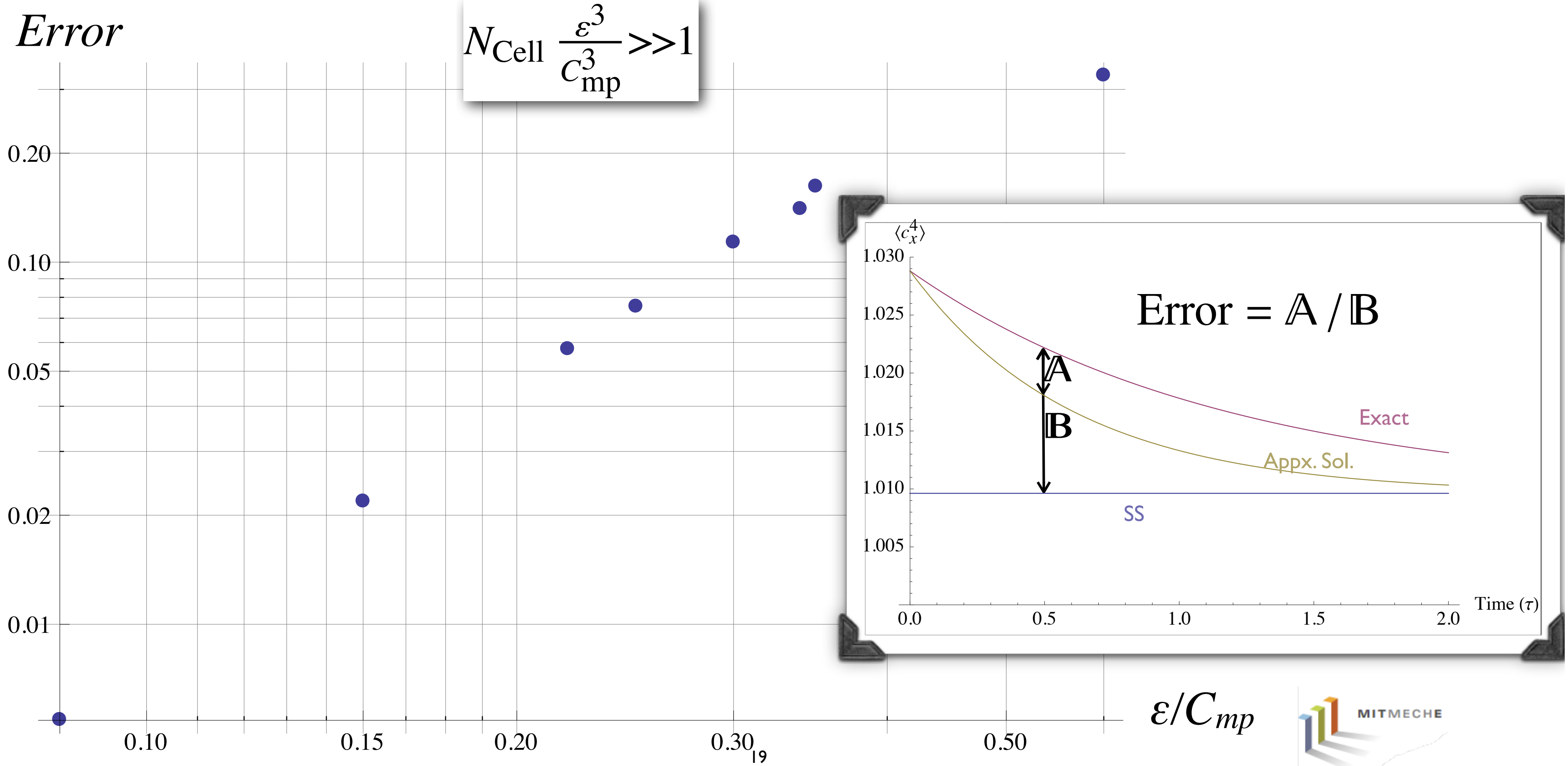
Final Algorithm

$$\hat{W}_i = \frac{1}{\| S_i \|} \sum_{j \in S_i} W_j \qquad (1)$$

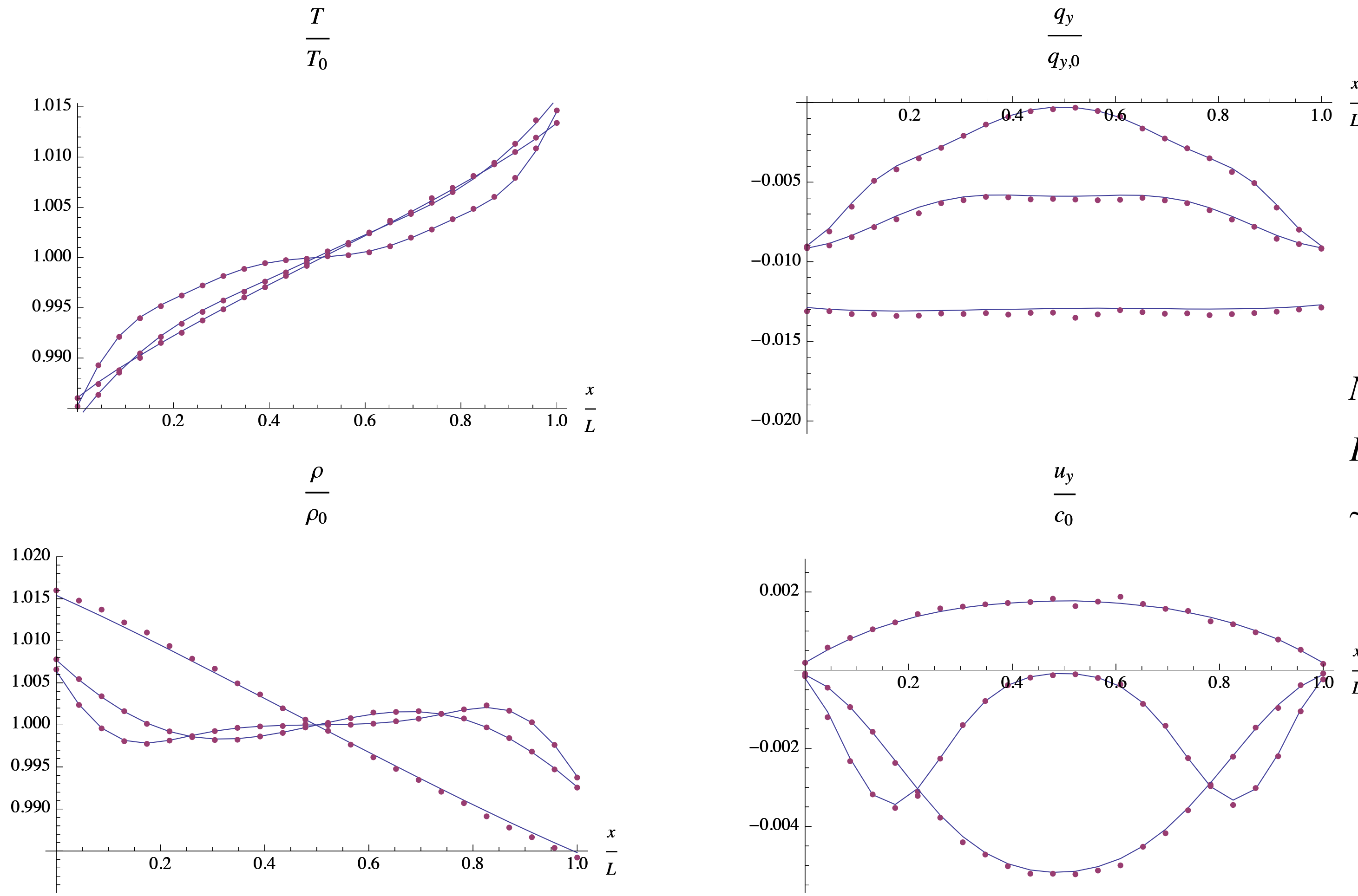


Results: Bias (error) vs. ε in 0D

$$N_{\mathrm{Cell}} \frac{\varepsilon^3}{C_{\mathrm{mp}}^3} >> 1$$



Results: 1D Transient Couette Flow

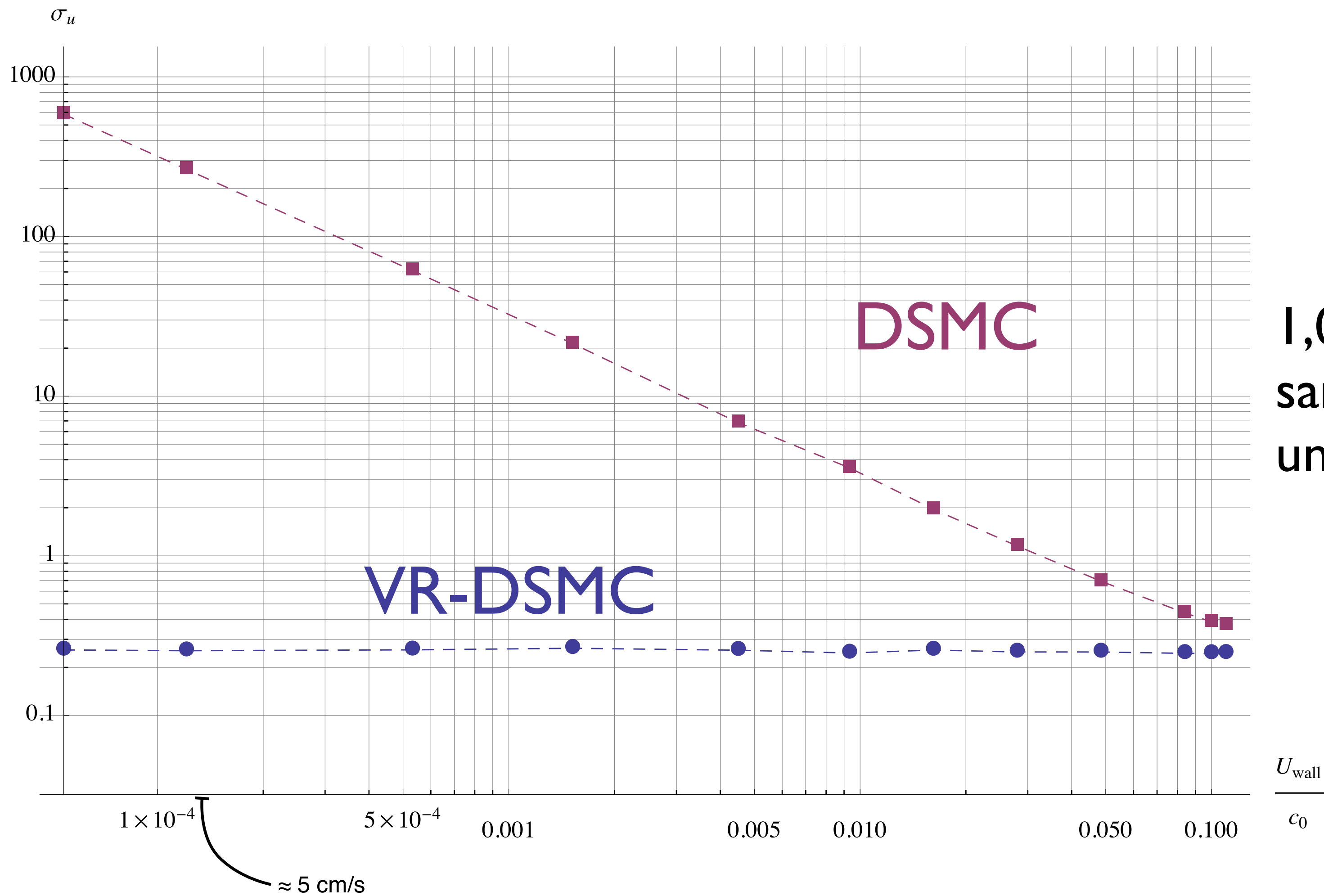


N_{Cell}=500

Kn=1.0

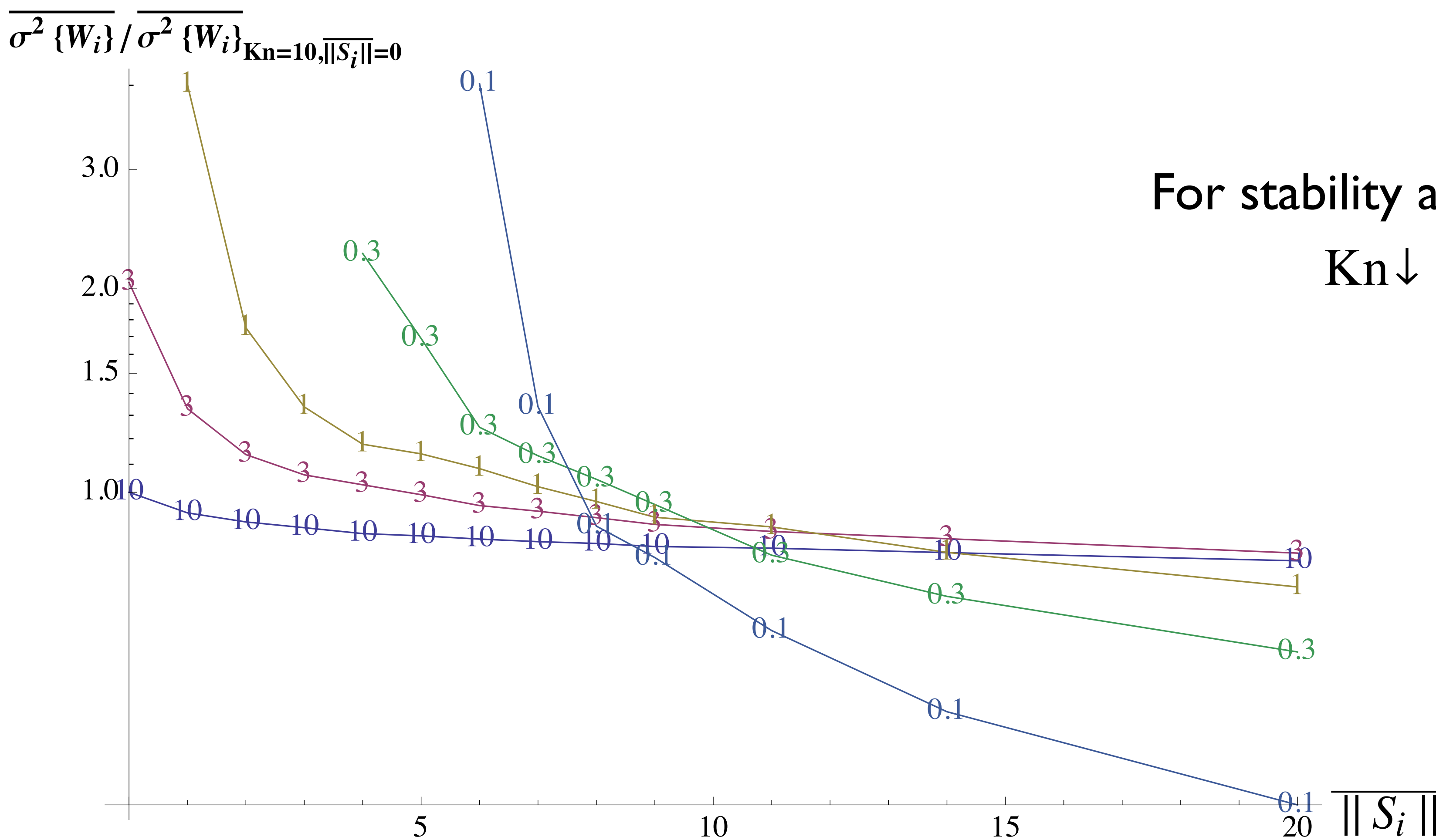
~1% **Relative** Error

Relative Sampling Uncertainty



1,000,000 less samples for the same uncertainty at 5cm/s!

Stability



For stability at a fixed ε

$\mathrm{Kn}\downarrow \;\Rightarrow\; \| S_i \| \uparrow$

$\Rightarrow\; N_{\mathrm{Cell}} \uparrow$

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* ε
  - *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}

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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:**

Candidates= $N_{Eff} N_{Cel} (N_{Cell} - 1) MX \sigma \Delta t / V_{Cell}$

- **if we choose particles of velocity classes c_i and c_j with weights W_i and W_j respectively there will be:**

$(N_{Eff})^2 W_i W_j \; C_{ij} \sigma \Delta t / V_{Cell}$ Collisions

- **to correctly account for this we use the following collision probabilities:**

$$P_i = \frac{W_j \, c_{\text{ij}}}{\text{MX}}$$

$$P_j = \frac{W_i \, c_{\text{ij}}}{\text{MX}}$$