An Excursion with the Boltzmann Equation at Low Speeds: Variance Reduced DSMC

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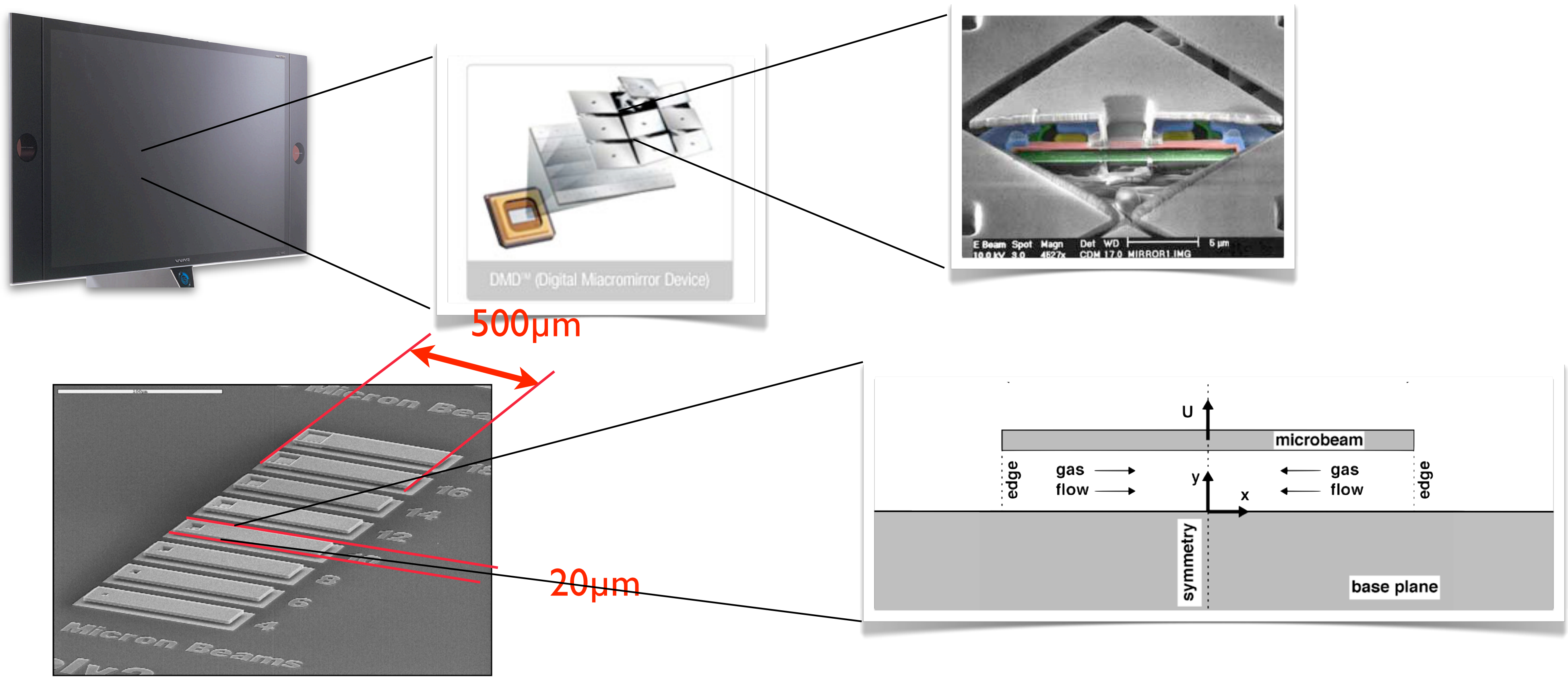
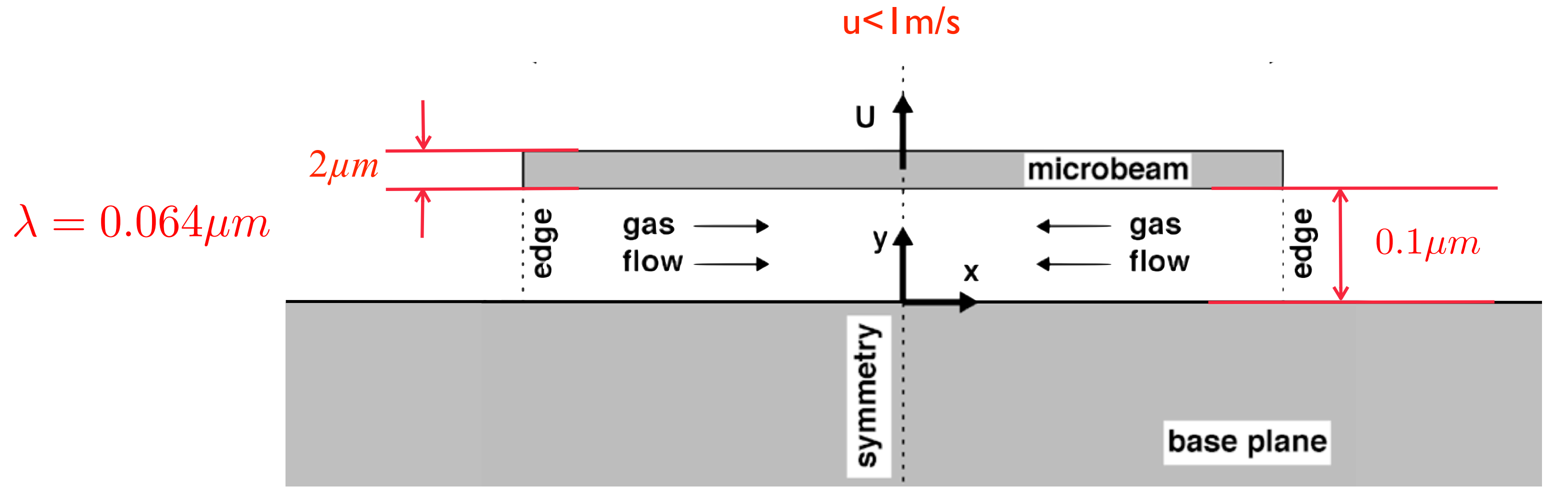
Application: Simulation of gases in MEMS/NEMS



How to calculate gas damping?

Application: Simulation of Gases in MEMS/NEMS



$$Kn = \frac{\lambda}{L} \not\ll 1$$

Navier-Stokes gas description does not hold!

[Gallis, 2004]

* figure not to scale

Kinetic Gas Flows

3 +3 +1 Dimensions

- Need detailed description distribution $f(\boldsymbol{x},\boldsymbol{c},t)$

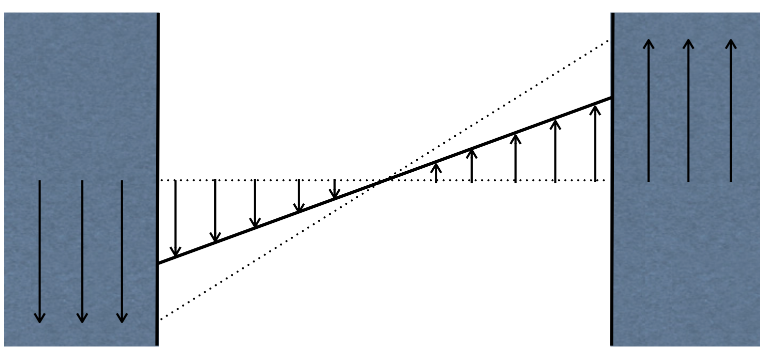
- The Boltzmann Equation (BE) [Boltzmann, 1871]

$$\frac{\partial f}{\partial t} + \boldsymbol{c}\cdot\frac{\partial f}{\partial \boldsymbol{x}} = \frac{1}{2}\int\int\int (\delta_1' + \delta_2' - \delta_1 - \delta_2)\, f_1 f_2 c_r \sigma d\Omega d\boldsymbol{c}_1 d\boldsymbol{c}_2$$

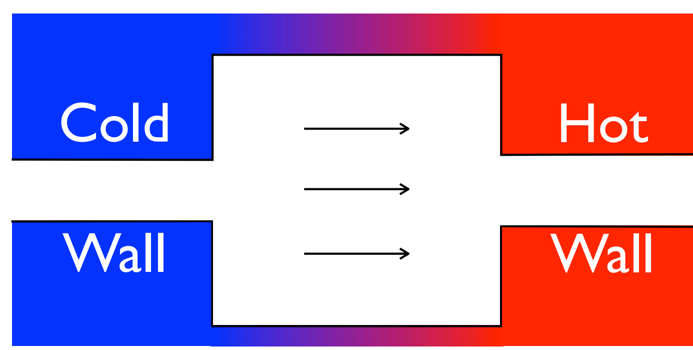
$$f = f(\boldsymbol{x},\boldsymbol{c},t) \qquad f_1 = f(\boldsymbol{x},\boldsymbol{c}_1,t) \quad f' = f(\boldsymbol{x},c',t) \quad f_1' = f(\boldsymbol{x},\boldsymbol{c}_1',t)$$

- Flow differs fundamentally from NS. For example:

Slip at wall

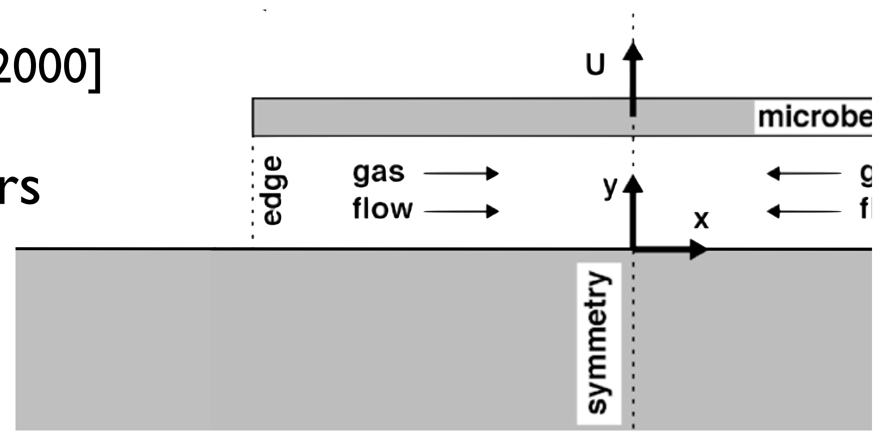


Temperature-flow coupling



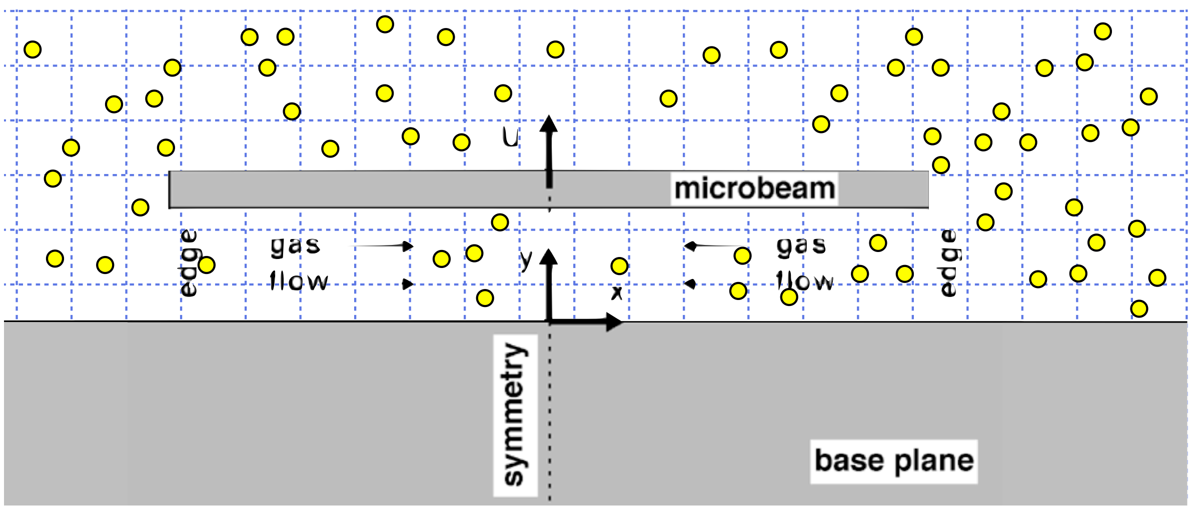
Solving Kinetic Flows

1. Direct numerical solution of the Boltzmann Equation
2. Direct Simulation Monte Carlo (DSMC) [Bird, 1963]
   - Simple & Fast
   - Accurate
     - [Wagner, 1992 & Hadjiconstantinou, 2000]
   - Used extensively for the last 40 years



DSMC Overview

A "splitting" method for the BE



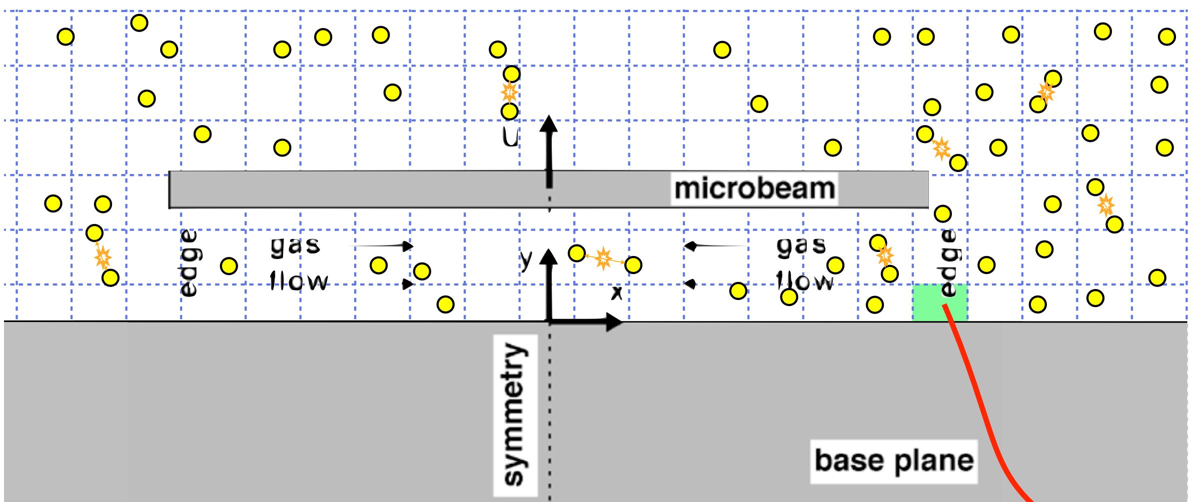
❶ Initialize domain with sample particles

❷ Advect particles

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

DSMC Overview

A "splitting" method for the BE



1. Initialize domain with sample particles
2. Advect particles
3. Collide in cell

(steps 2–3: Δt)

4. Sample cell properties:

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

$$\frac{\partial f}{\partial t} = \frac{1}{2} \int \int \int \left(\delta_1' + \delta_2' - \delta_1 - \delta_2\right) f_1 f_2 c_r \sigma d\Omega d\boldsymbol{c}_1 d\boldsymbol{c}_2$$

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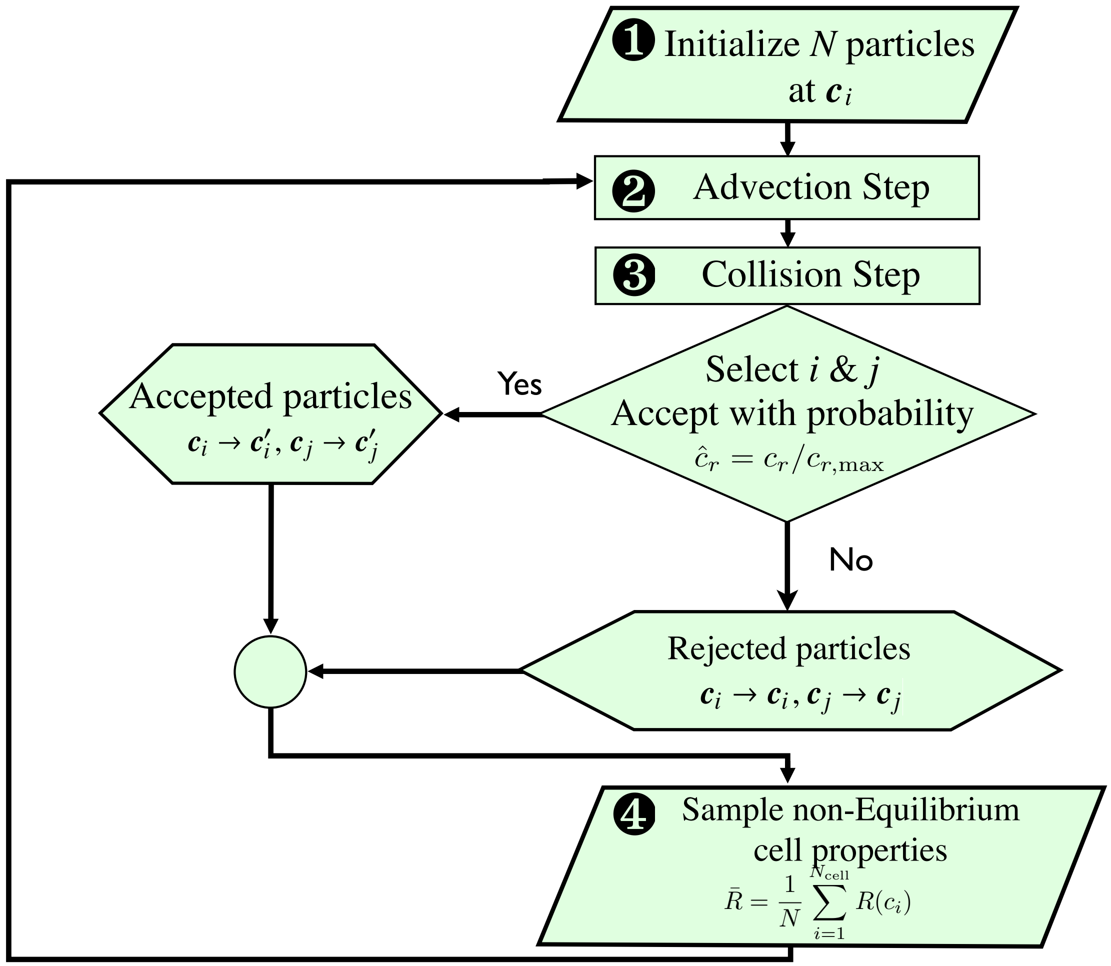
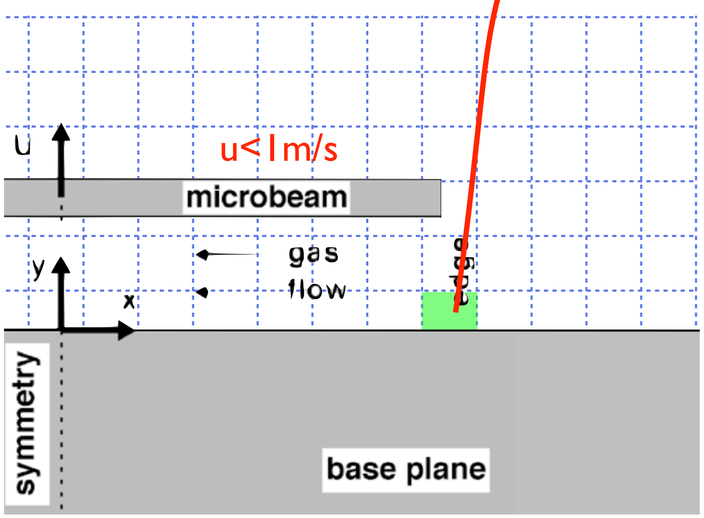
DSMC Summary



[Bird, 1994]

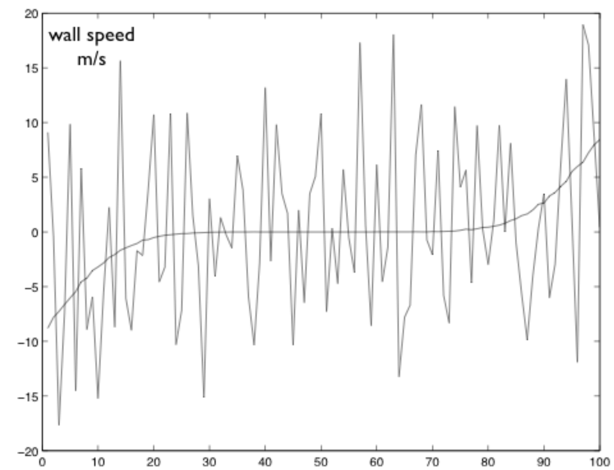
DSMC Disadvantage



Average cell property

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

Uncertainty in property



$$\sigma\left\{\bar{R}\right\} \simeq \frac{\sigma_R}{\sqrt{N_{\text{samples}}}}$$

$\overline{u} = O(1\, m/s)$

SD=O(300m/s)

$$\text{as } \bar{u} \rightarrow 0 \Rightarrow N_{\text{Samples}} \rightarrow \infty$$

DSMC becomes impractical for low-signal flows!

[Hadjiconstantinou et al, 2003]

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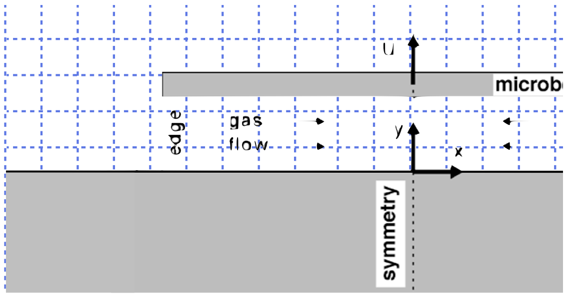
Previous Work



- Direct numerical BE solution [Sone, 1989], BGK CI or Linearized-BE
- Variance Reduced
  - Particle Methods:
    - Full BE [Baker et. al., 2006]
    - Linearized-BE [Koch et. al., 2005,2008]
  - Numerical DG solvers using VR MC evaluation of CI [Baker et. al., 2007]

- LVDSMC [Homolle et. al., 2007]
  - Particle method
  - Based on Hilbert formulation of CI
  - Complex models challenging [Wagner, 2009]
  - Boundary conditions challenging
  - Runs well despite complexity

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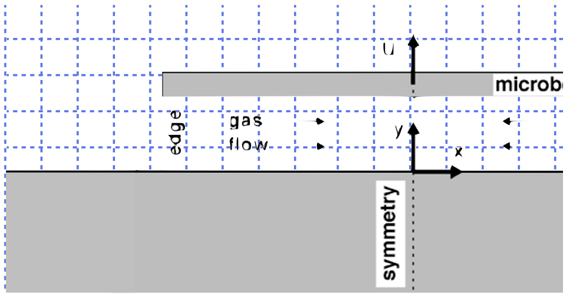
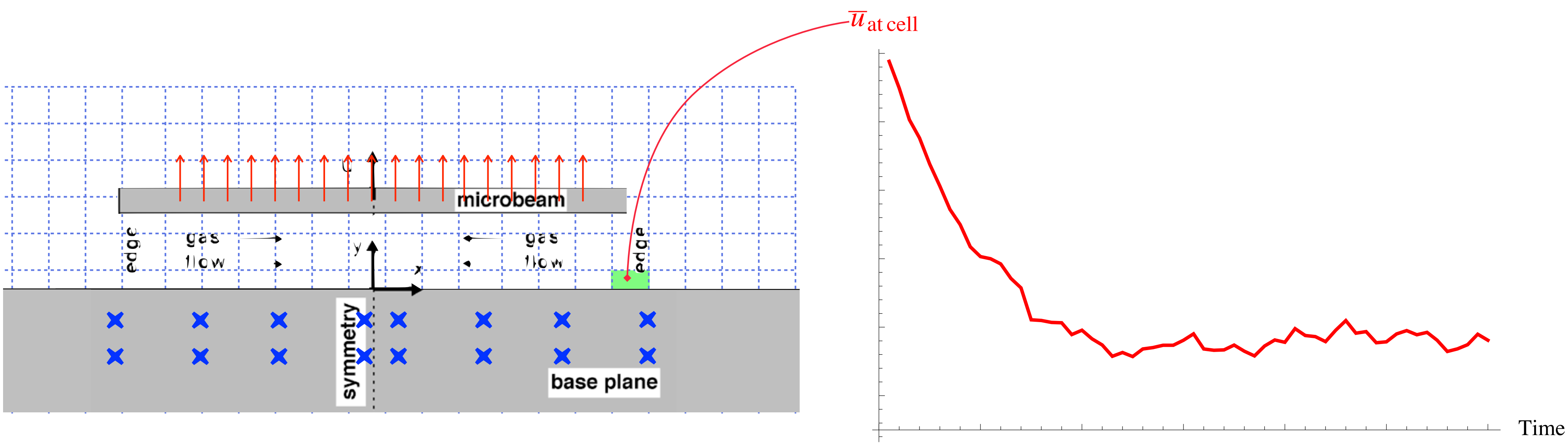
Thesis Goal



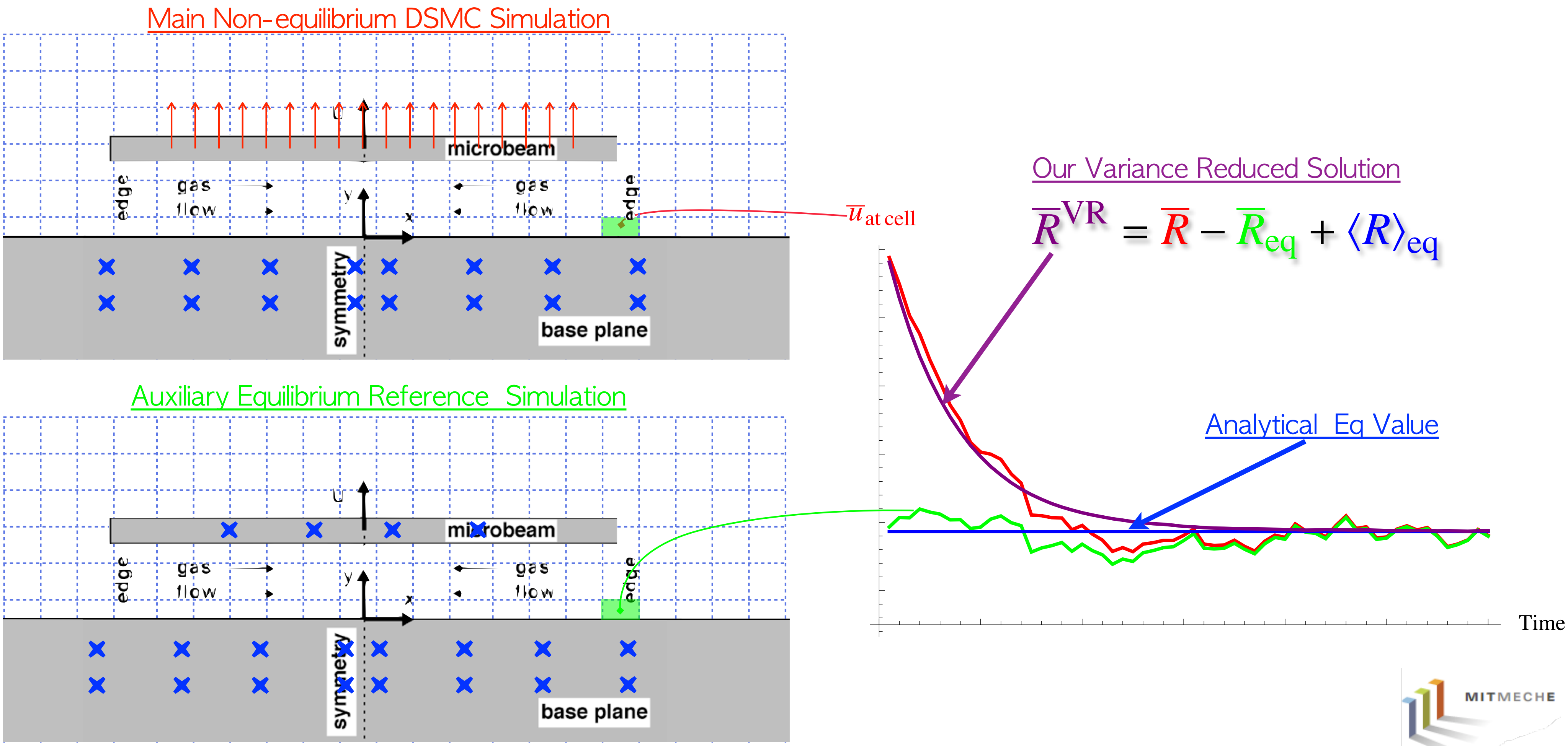
Solve low-signal kinetic flows using a method that is:

- Simple to implement
- Practical
- Can be easily extended to complex collision models , geometries and boundary conditions
- Preferably directly based on DSMC

Basic Thesis Approach (1)

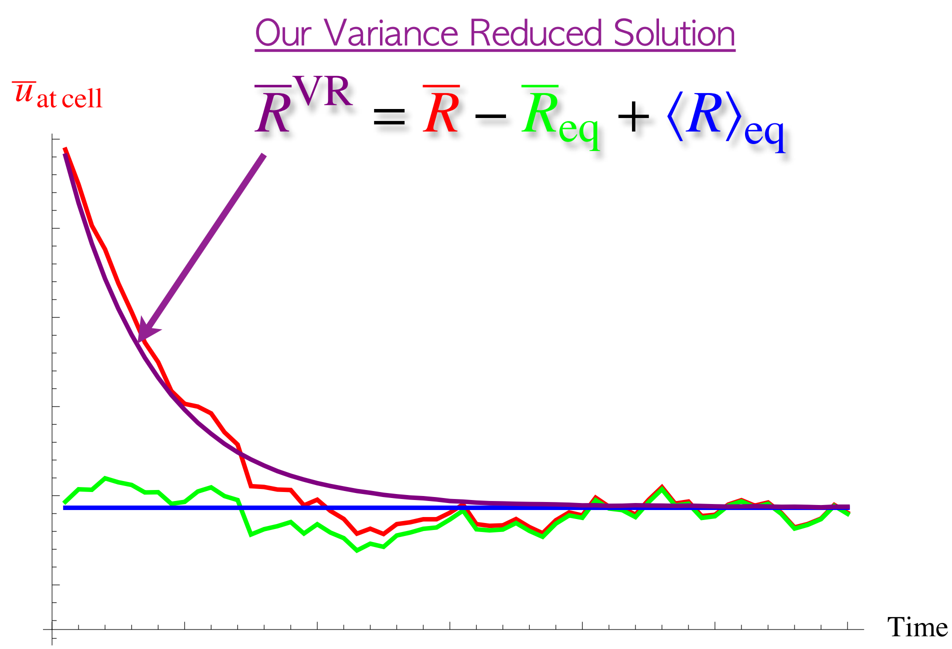


Basic Thesis Approach (2)



Basic Thesis Approach (3)

- Non-equilibrium and Equilibrium simulations have to stay correlated
  - Simulations share initial conditions and random variables
  - Basic challenge of this work
- Inspiration: [Ottinger et. al., 1997] polymer modeling
  - Short times and no boundaries



Basic Thesis Approach (4)

- Importance Weights. For each particle i

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

- Non-equilibrium property

$$\langle R \rangle = \int R(\boldsymbol{c}) f(\boldsymbol{c}) d\boldsymbol{c} \simeq \overline{R} = \frac{1}{N} \sum_{i=1}^{N_{\text{cell}}} R(\boldsymbol{c}_i)$$

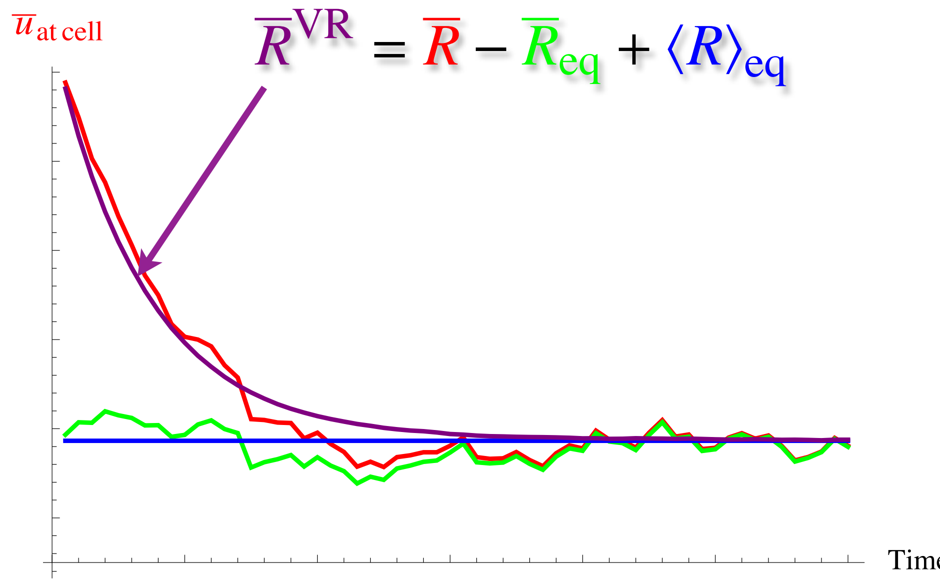
- Equilibrium property

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

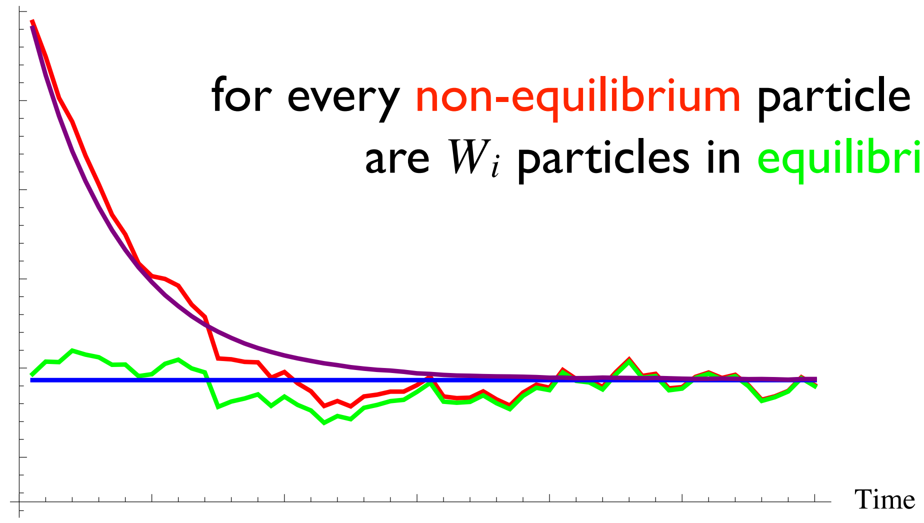
$$\simeq \overline{R_{\text{eq}}} = \frac{1}{N} \sum_{i=1}^{N_{\text{cell}}} W_i R(\boldsymbol{c}_i)$$

Our Variance Reduced Solution

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



Magnitude of Variance Reduction



for every non-equilibrium particle at $\boldsymbol{c}_i$ there are W_i particles in equilibrium

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

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

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

We need to choose eq reference state such that

$$\| W_i - 1 \| \ll 1 \Rightarrow \sigma^2 \{\overline{R}^{\text{VR}}\} \ll \sigma^2 \{\overline{R}\}$$

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VRDSMC Version 1.0

❶ Initialization and collisions with boundary

Distributions are explicitly known $W_i = \frac{f_{eq}(\boldsymbol{c}_i)}{f(\boldsymbol{c}_i)}$

❷ Advection Step

❸ Collisions Step: Particle-particle interaction

"accepted" term

$$\left[\frac{\partial f_{eq}}{\partial t}\right]_{\text{Collision}} = \frac{c_{r,max}}{2}\int\int\int\left(\delta_1' + \delta_2' - \frac{\delta_1}{W_2} - \frac{\delta_2}{W_1}\right) W_1 W_2 f_1 f_2 \frac{c_r}{c_{r,max}} \sigma d\Omega d\boldsymbol{c}_1 d\boldsymbol{c}_2 + \frac{c_{r,max}}{2}\int\int\int\left(-\delta_1 - \delta_2 + \frac{\delta_1}{W_2} + \frac{\delta_2}{W_1}\right)\frac{\frac{c_r}{c_{r,max}}}{\left(1 - \frac{c_r}{c_{r,max}}\right)} W_1 W_2 f_1 f_2 \sigma \left(1 - \frac{c_r}{c_{r,max}}\right) d\Omega d\boldsymbol{c}_1 d\boldsymbol{c}_2$$

$\Rightarrow$

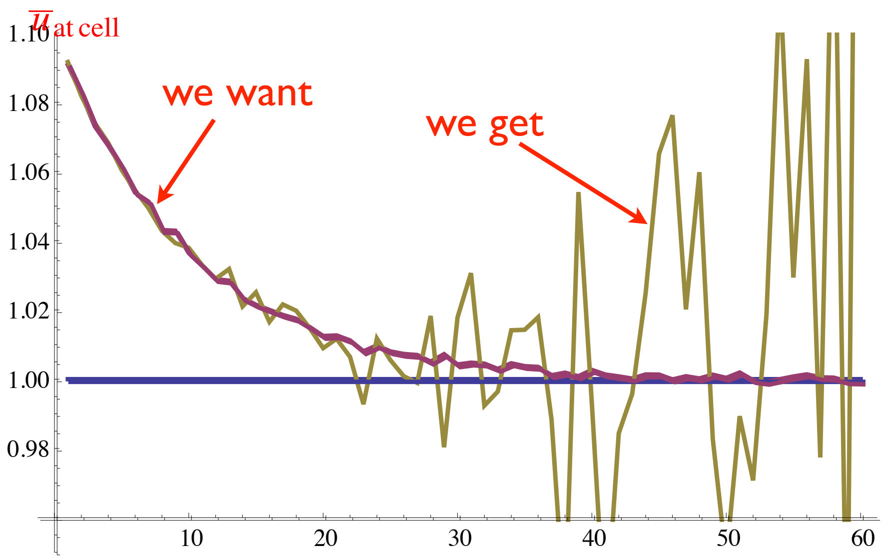
$W_i \to W_i W_j, W_j \to W_i W_j$

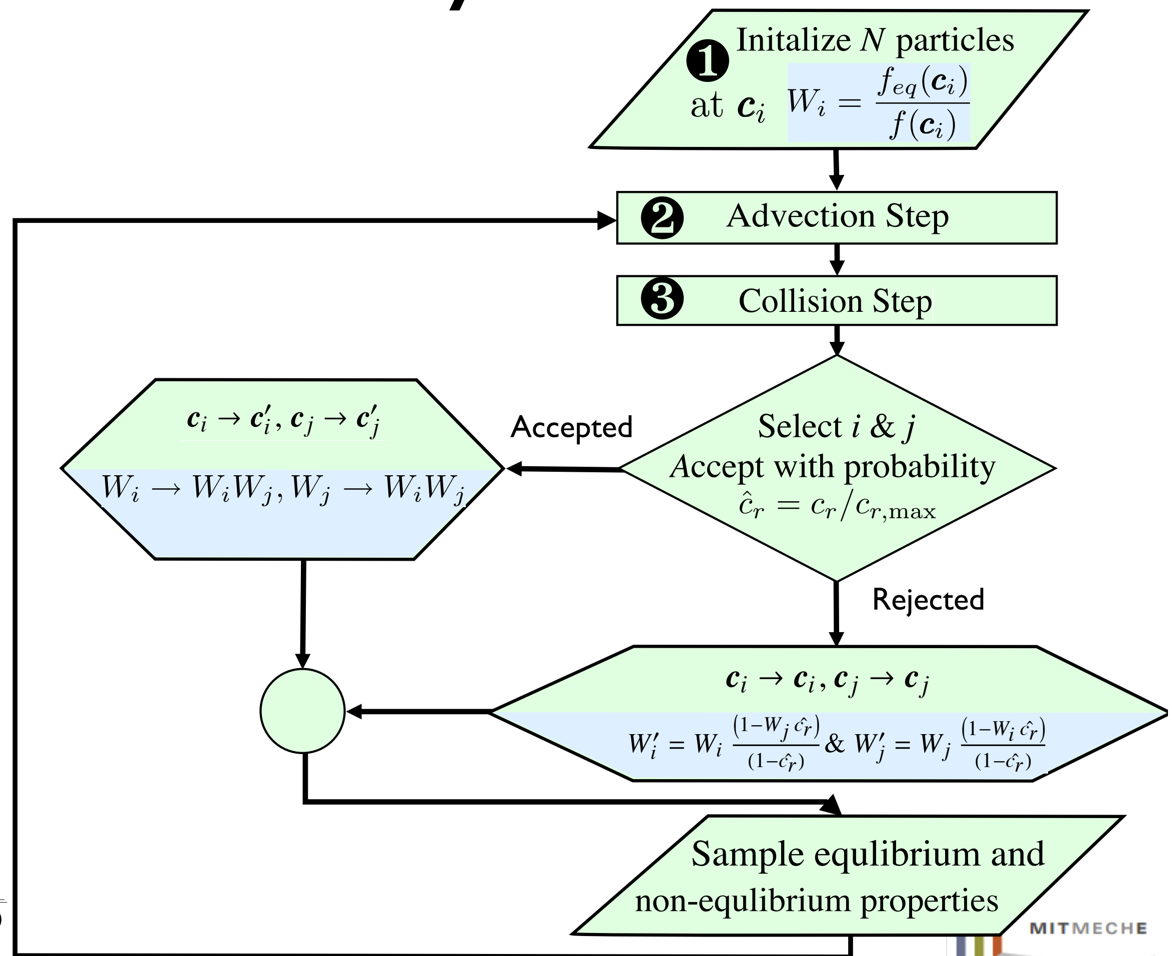
$W_i' = W_i \frac{(1-W_j \hat{c_r})}{(1-\hat{c_r})}$ & $W_j' = W_j \frac{(1-W_i \hat{c_r})}{(1-\hat{c_r})}$

"rejected" term

Algorithm Summary V1.0

- Major Problem:
  - Weights are unstable
    as $t \to 0 \Rightarrow \sigma^2 \{W_i\} \to \infty$
  - No Variance Reduction!





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Stability: Kernel Density Estimation

- KDE reconstructs a distribution using N samples and Kernels K with characteristic width ε.

$$\hat{f}(c) = \frac{1}{N}\sum_{i=1}^{N} K(c - c_i) \simeq f(c)$$

$$\hat{f}(c) = \int K(c - c')f(c')dc'$$

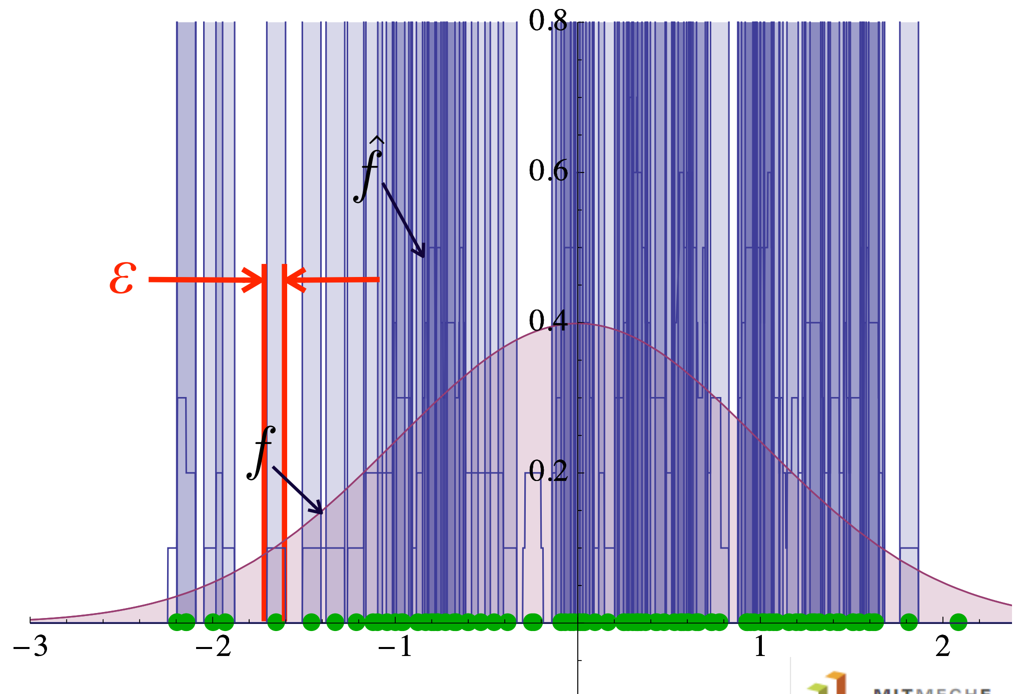
- Bias vs. Noise Tradeoff

$$\varepsilon \text{ large } \Rightarrow \text{ large } \left|\hat{f} - f\right| \text{ and smooth } \hat{f}$$

$$\varepsilon \text{ small } \Rightarrow \text{ small } \left|\hat{f} - f\right| \text{ but noisy } \hat{f}$$

- Exact in the limit

$$\lim_{\varepsilon \to 0, N \to \infty} \hat{f} = f$$



[Scott, 1992]

Stability: Smoothing Step

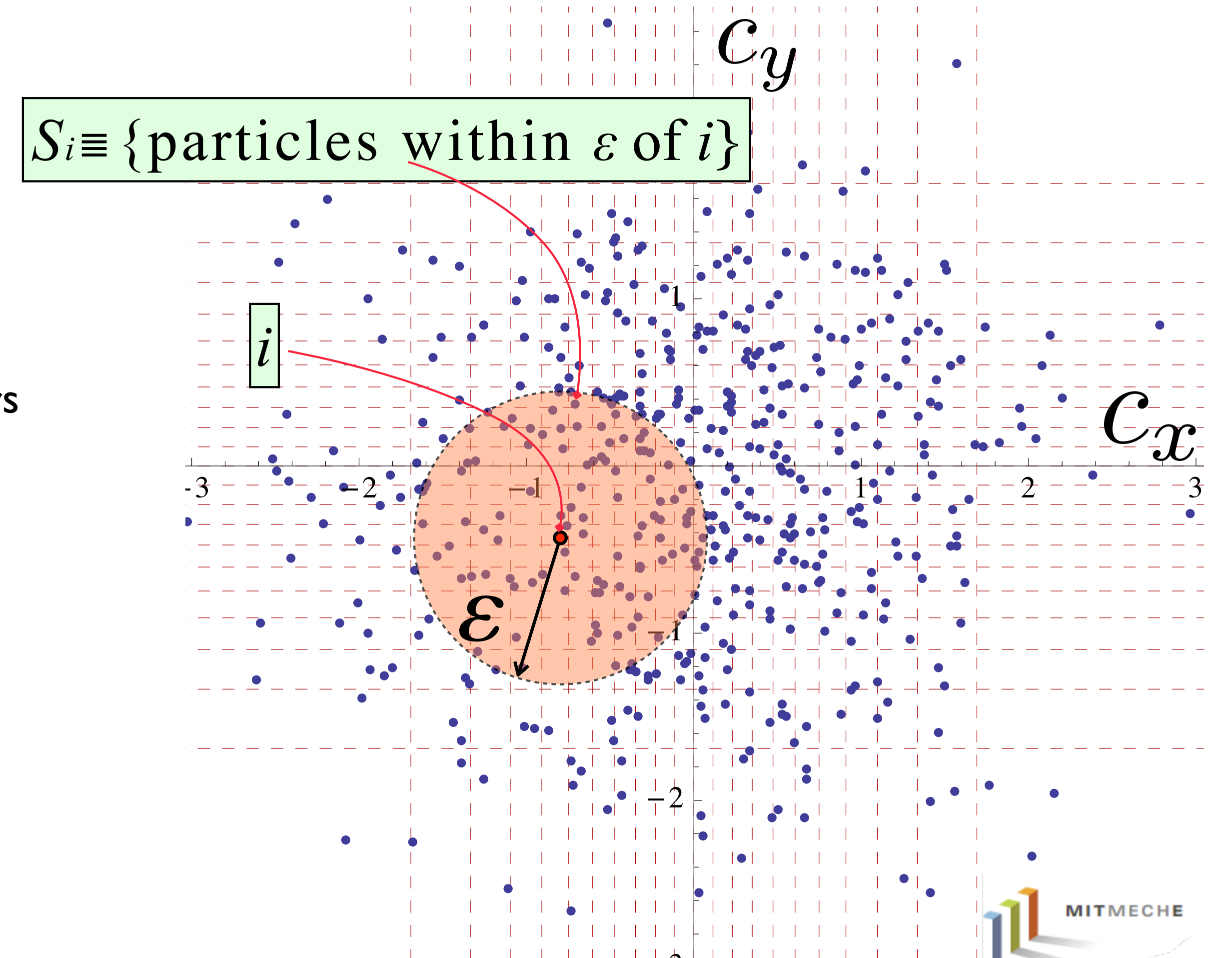
Requires finding all nearest neighbour within ε of each particle i

- Use $\hat{W}_i$ instead of W_i since

$$W_i \simeq \hat{W}_i = \frac{\hat{f}_{\text{eq}}(\boldsymbol{c}_i)}{\hat{f}(\boldsymbol{c}_i)}$$

- Requires finding all nearest neighbors within ε of each particle i

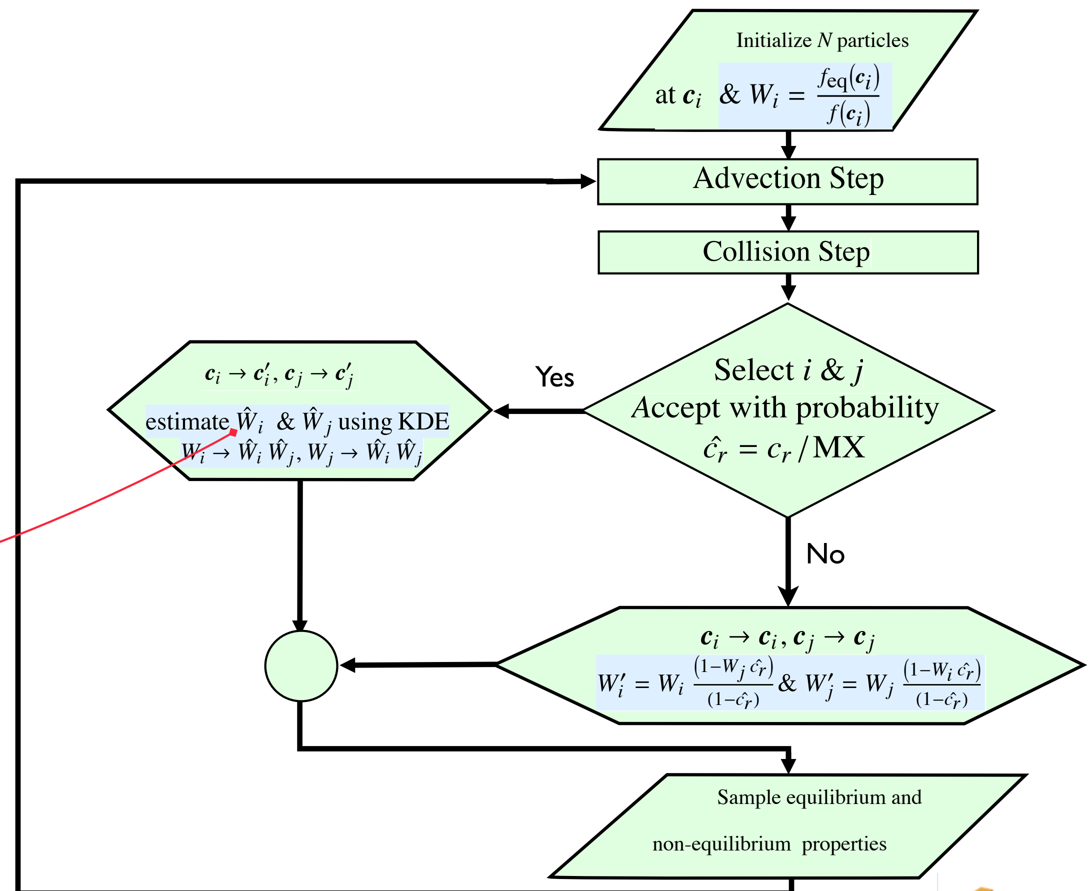
Giving $$\hat{W}_i = \frac{1}{\| S_i \|} \sum_{j \in S_i} W_j$$



Algorithm Summary V2.0

- Best performance when applying only on particles accepted for collision

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



[Al-Mohssen et. al, 2008]

Bias-Variance Tradeoff

- KDE is the <u>only</u> approximation that we introduce in this work.
- As $\varepsilon \to 0 \Rightarrow$ bias $\to 0 \Rightarrow$ solution is identical to DSMC
- If we hold $\overline{\| S_i \|}$ constant, $\varepsilon \downarrow \Rightarrow N_{\text{cell}} \uparrow$ and
    - $N_{cell} \propto \dfrac{1}{\varepsilon^3}$

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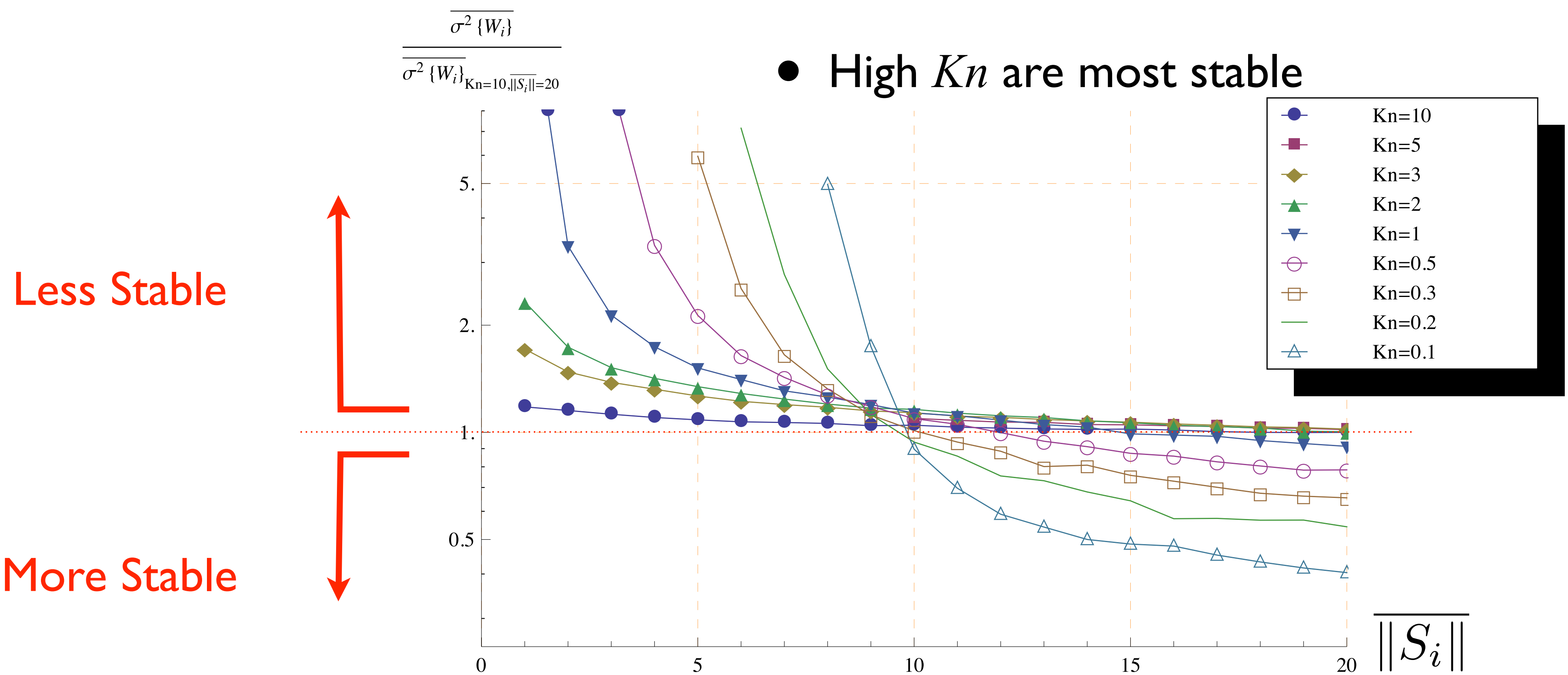
Stability Effectiveness

- Stability increases with $\overline{\| S_i \|}$
- High Kn are most stable



Local Reference States (1)

- In this work we chose a Maxwell-Boltzmann(MB) f_{MB} reference state with the free parameters

$$f_{\mathrm{MB}}(\boldsymbol{c}_i; \overline{n}_{\mathrm{VR}}, \overline{\boldsymbol{u}_{\mathrm{VR}}}, \overline{T_{\mathrm{VR}}})$$

- KDE introduces bias regardless of MB reference state

- We discovered that using local reference states introduces the substantially bias without affecting stability

⇒Collisions more accurate with local reference state $f_{MB,loc}$

- Advection mixes particles across cells

⇒need global reference state $f_{eq,0}$

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Local Reference States (2)

- We readily can go from a global to a local reference state

$$W_i' = \frac{f_{MB,loc}(\boldsymbol{c}_i)}{f_{eq}(\boldsymbol{c}_i)} W_i$$

global samples $f_{eq,0}$

$$\{\boldsymbol{c}_i, W_i\}$$

local samples $f_{MB,loc}$

$$\{\boldsymbol{c}_i, W_i'\}$$

$$W_i = \frac{f_{eq}(\boldsymbol{c}_i)}{f_{MB,loc}(\boldsymbol{c}_i)} W_i'$$

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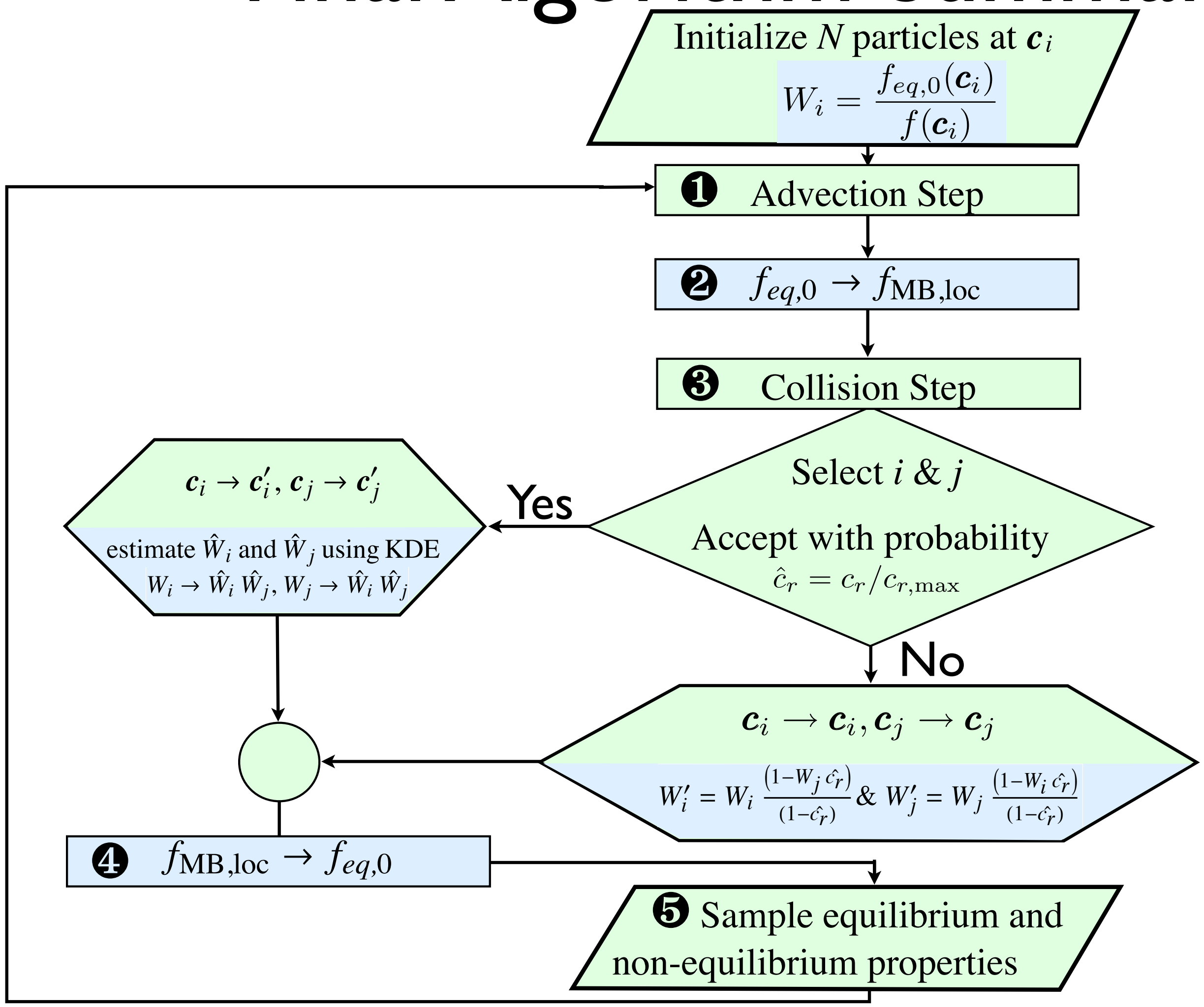
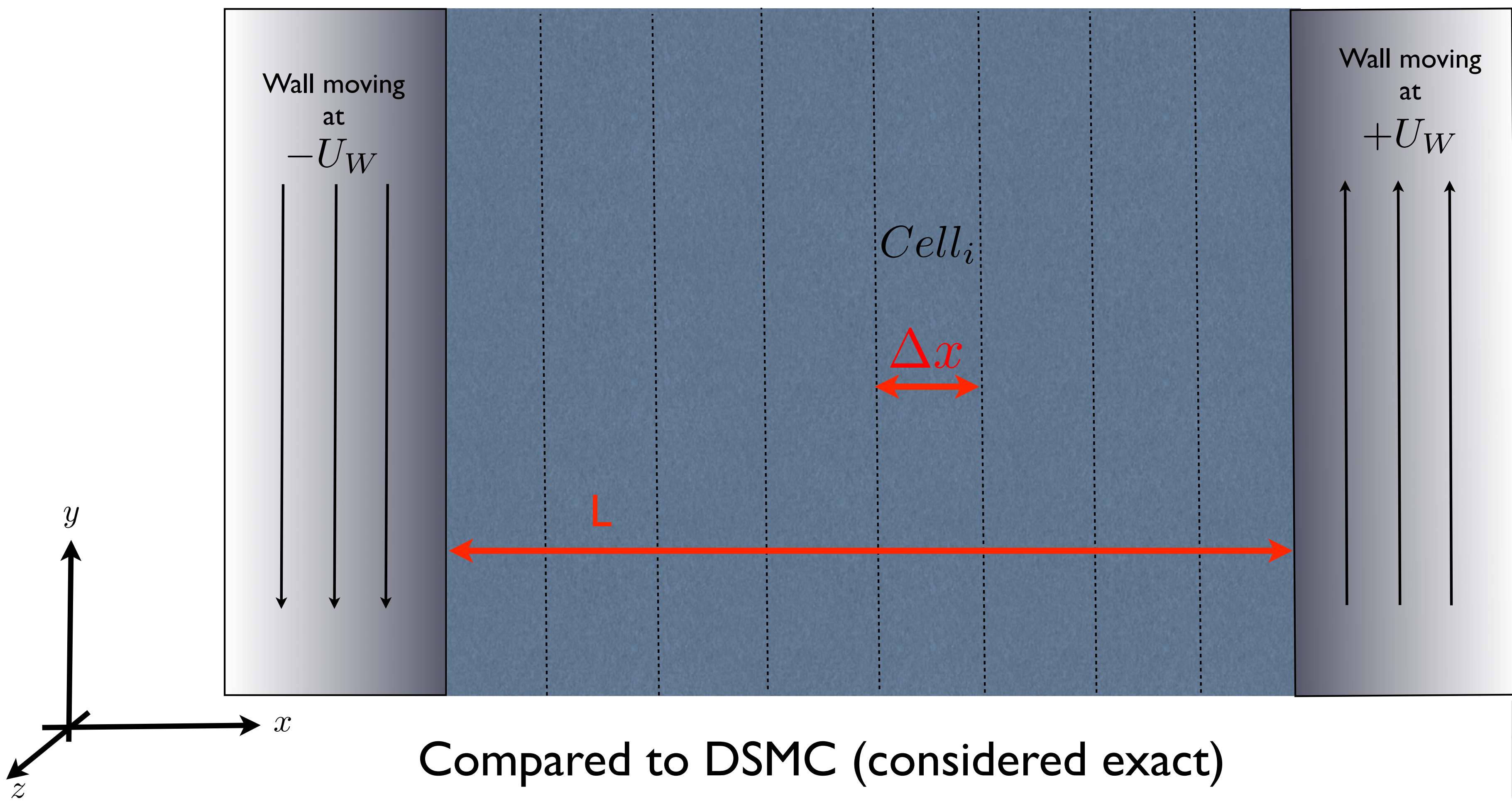
Final Algorithm Summary



1D Verification

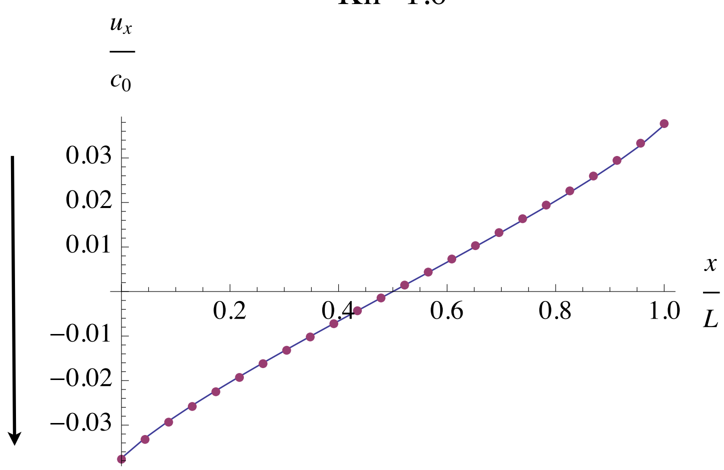


Compared to DSMC (considered exact)

Steady state shear flow

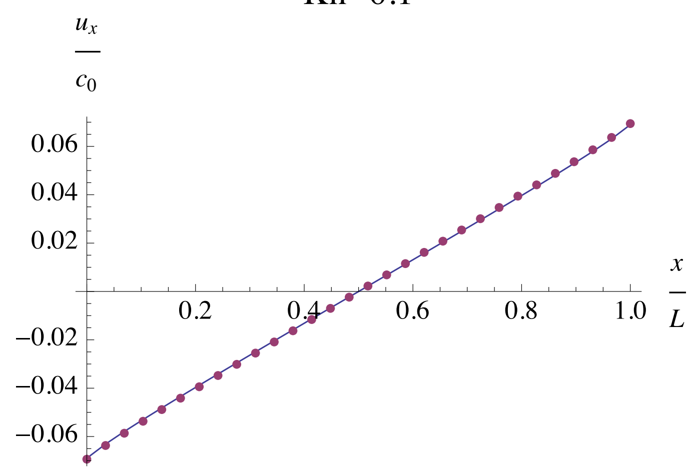
Global Reference State

Kn=1.0



N_{Cell}=500

Kn=0.1



N_{Cell}=50,000

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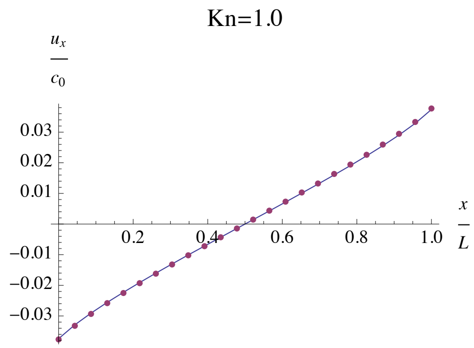
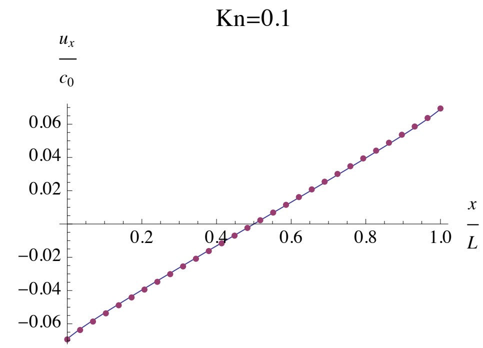
Steady state shear flow

Global Reference State

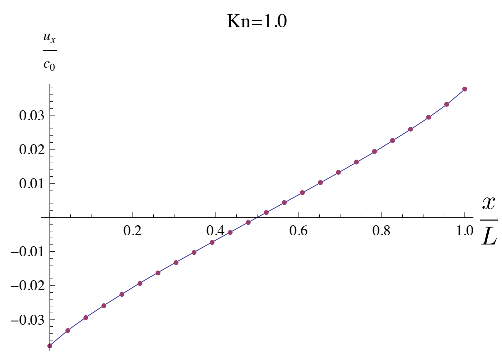


N_{Cell}=500

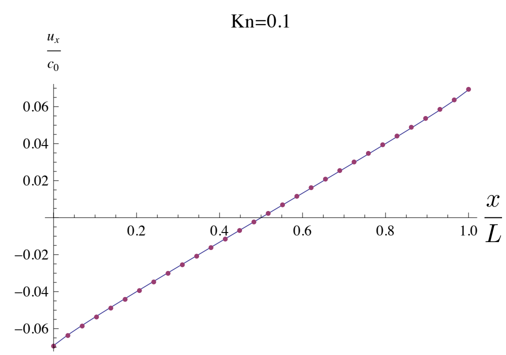


N_{Cell}=50,000

Local Reference State



N_{Cell}=200



N_{Cell}=3,000

>15x advantage

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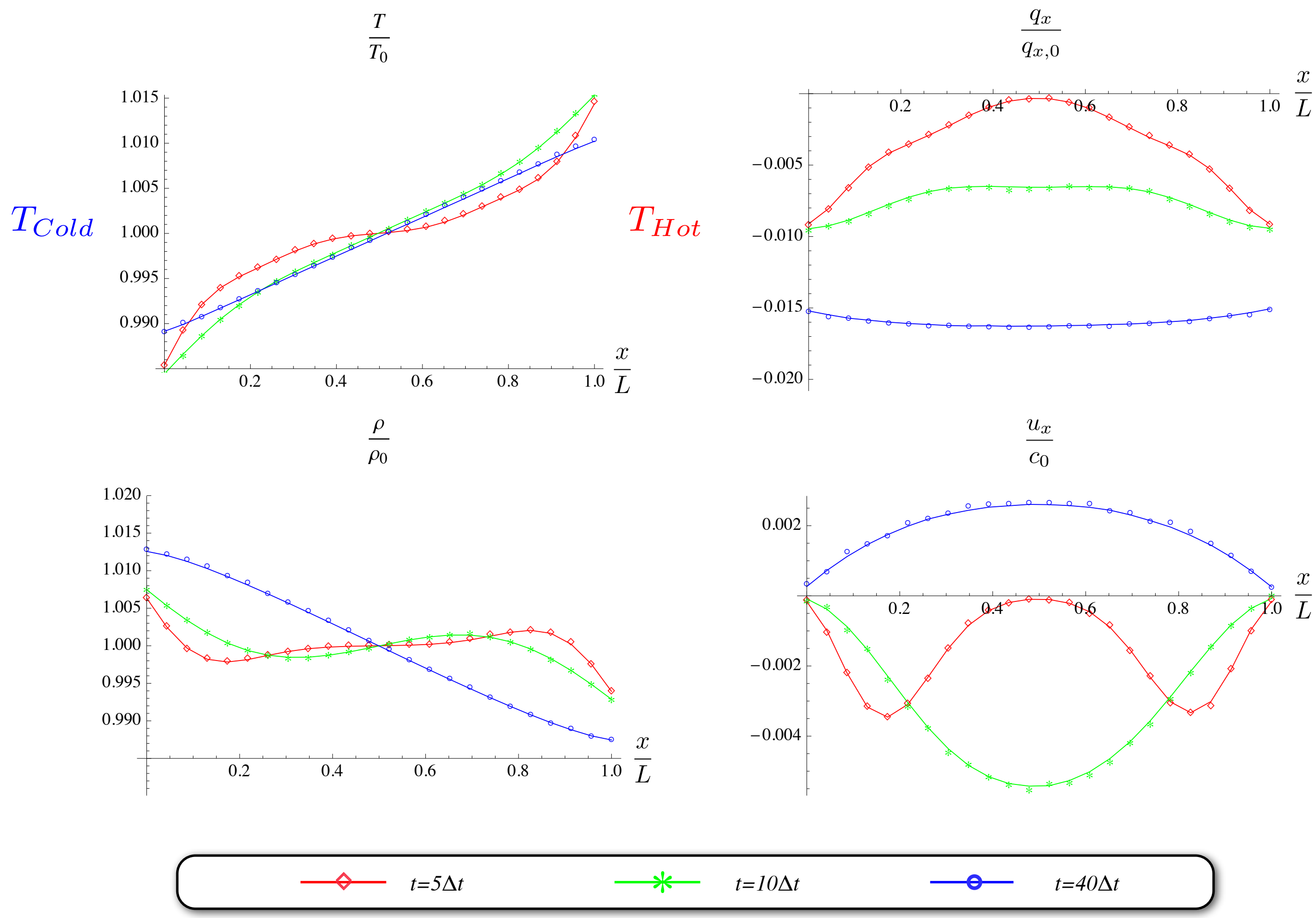
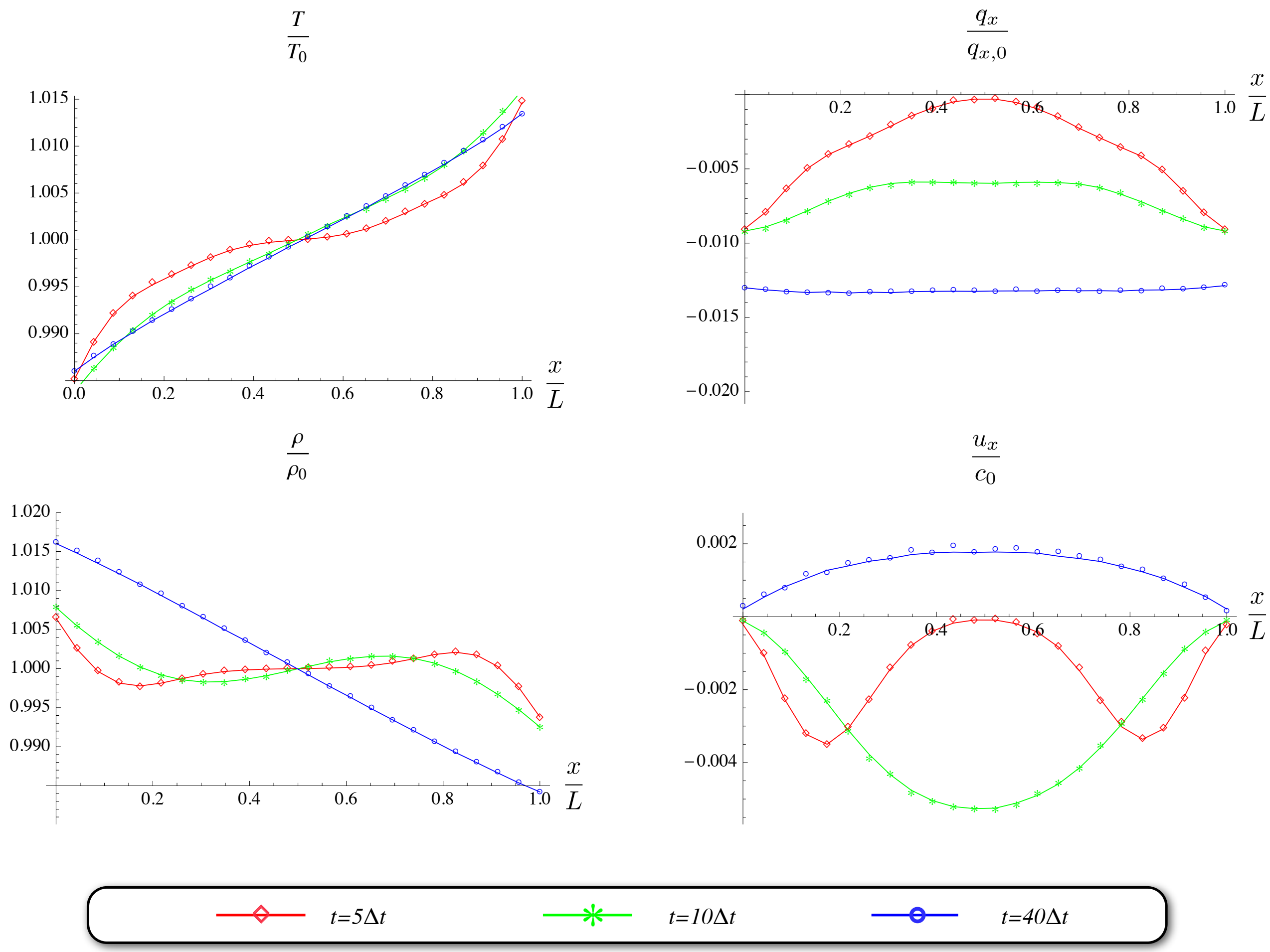
Transient Results Kn=10



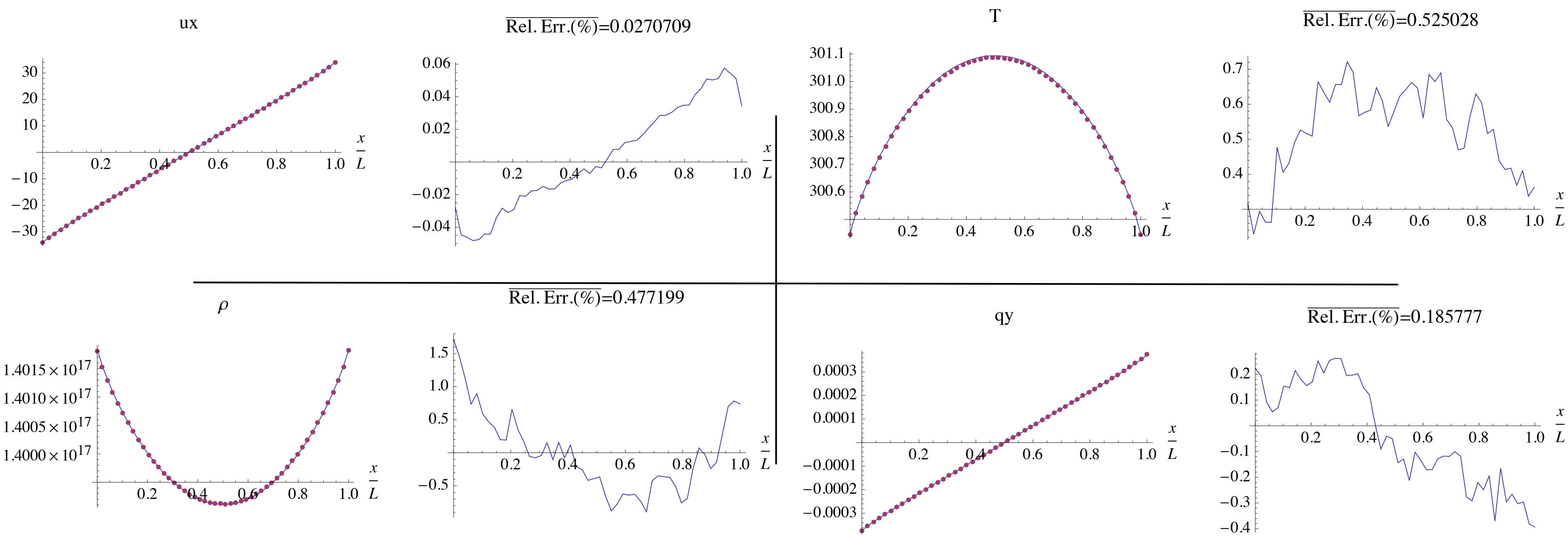
[Manela, 2007]

Transient Results Kn=1.0



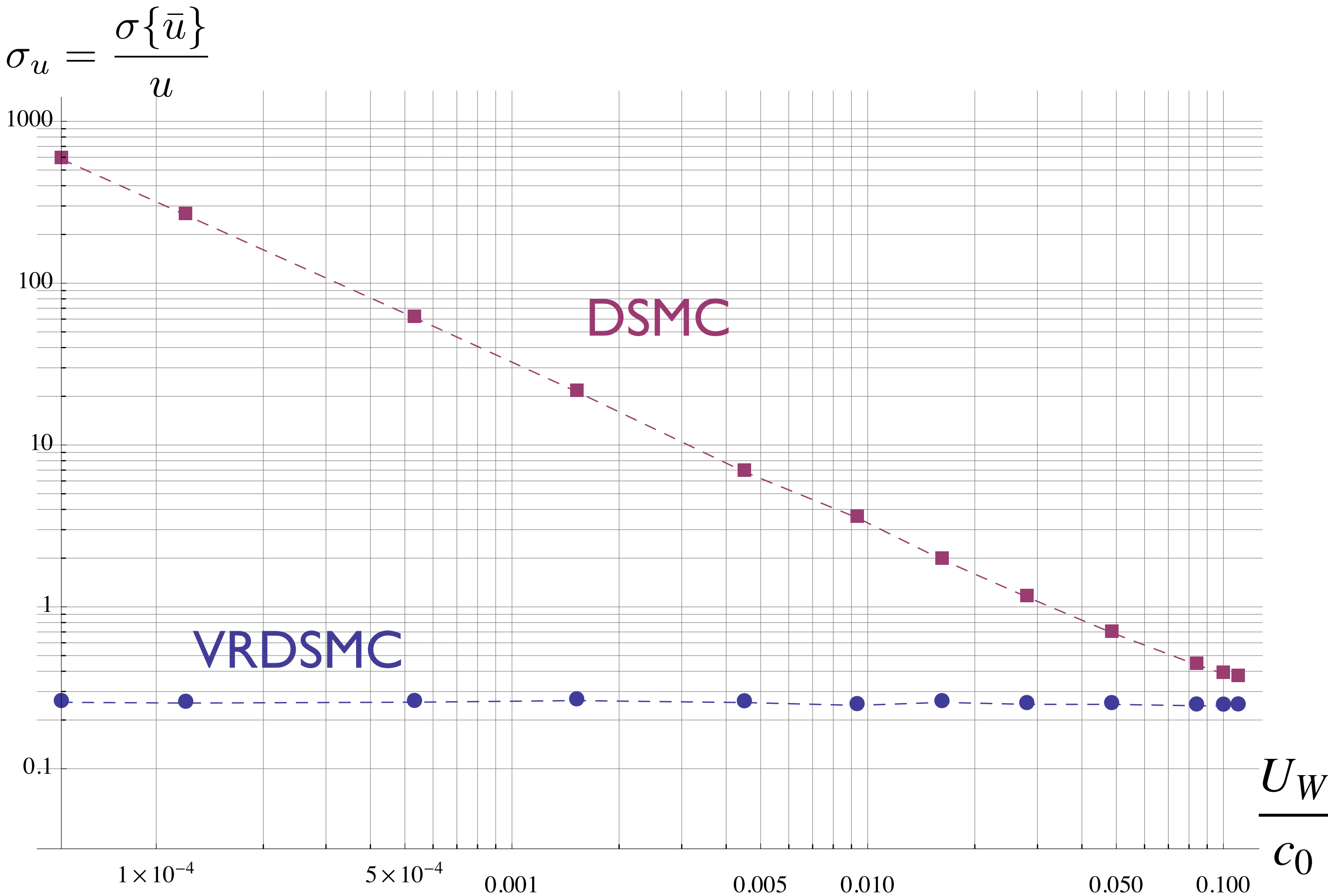
Stringent Coupled Verification Problem

Steady state shear flow



Kn=0.1 , *Ma=0.1*

VR Effectiveness



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

Conclusions

- Variance reduction using likelihood ratios is viable and exciting
  - Advantage: DSMC simulation is not perturbed
  - Should be considered for any low signal kinetic flow problem
- Small increase in computational cost
  - Cost $O(N_{Cell}\ Log(N_{Cell}))$ vs. $O(N_{Cell})$ for DSMC
  - Small extra cost related to minimum N_{cell}
- Different collisions models:
  - BGK [Landon, 2010]
- Looking Forward
  - 2D-3D problems--trivial
  - Complex collision models (Maxwell, VHS, etc.)
  - Chemistry

The End

Variance Reduction Approach

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

$$\downarrow$$

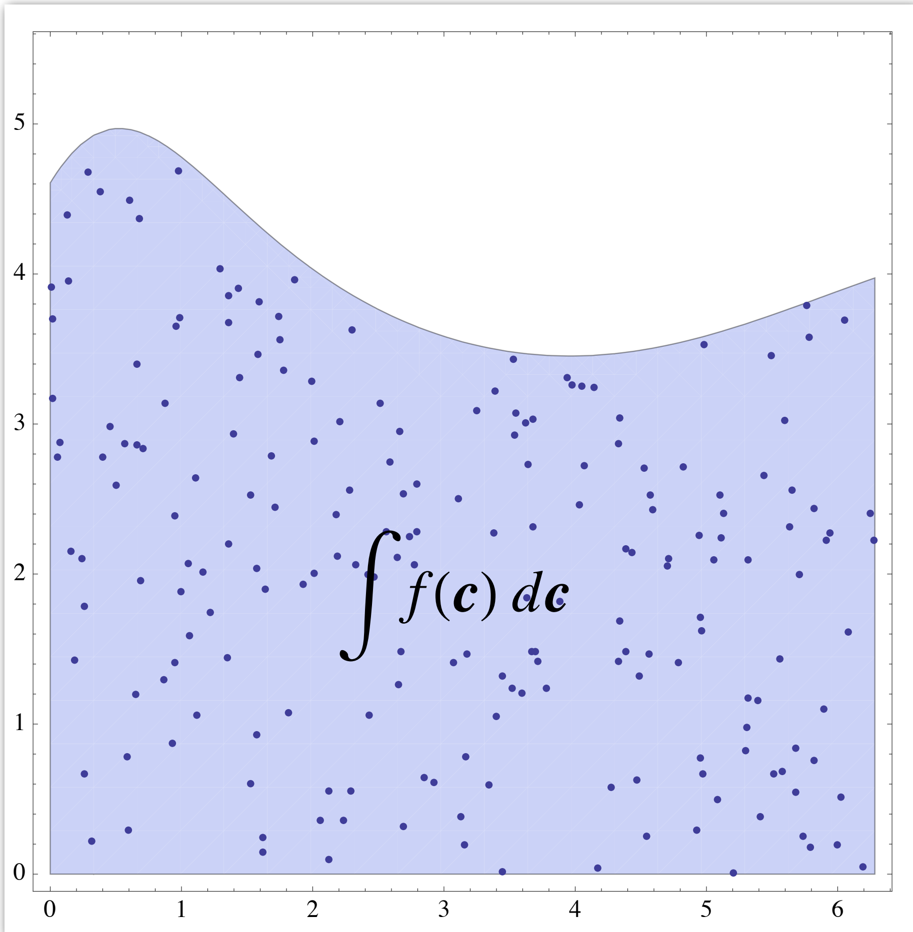
$$I = \int \{f(\boldsymbol{c}) - g(\boldsymbol{c})\}\, d\boldsymbol{c} \;+ \int g(\boldsymbol{c})\, d\boldsymbol{c} \qquad (2)$$

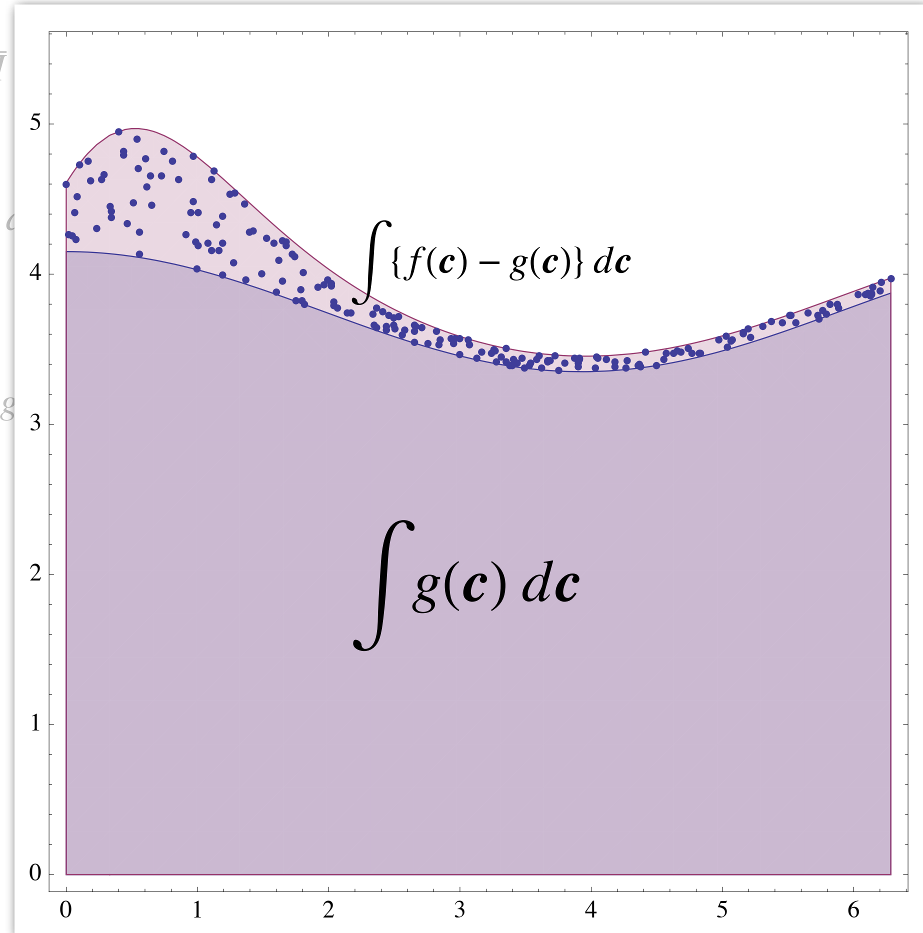
$$\downarrow$$

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

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

Variance Reduction Approach





Variance Reduction Approach

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

$$\downarrow$$

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

$$\downarrow$$

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

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

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

Simulate using deviational particles

Hadjiconstantinou, Baker, Homolle, Radtke

Variance Reduction Approach

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

↓

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

↓

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

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

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

Simulate using deviational particles

Hadjiconstantinou, Baker, Homolle, Radtke

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

Unmodified DSMC　　**Auxiliary** Weighted DSMC

My approach

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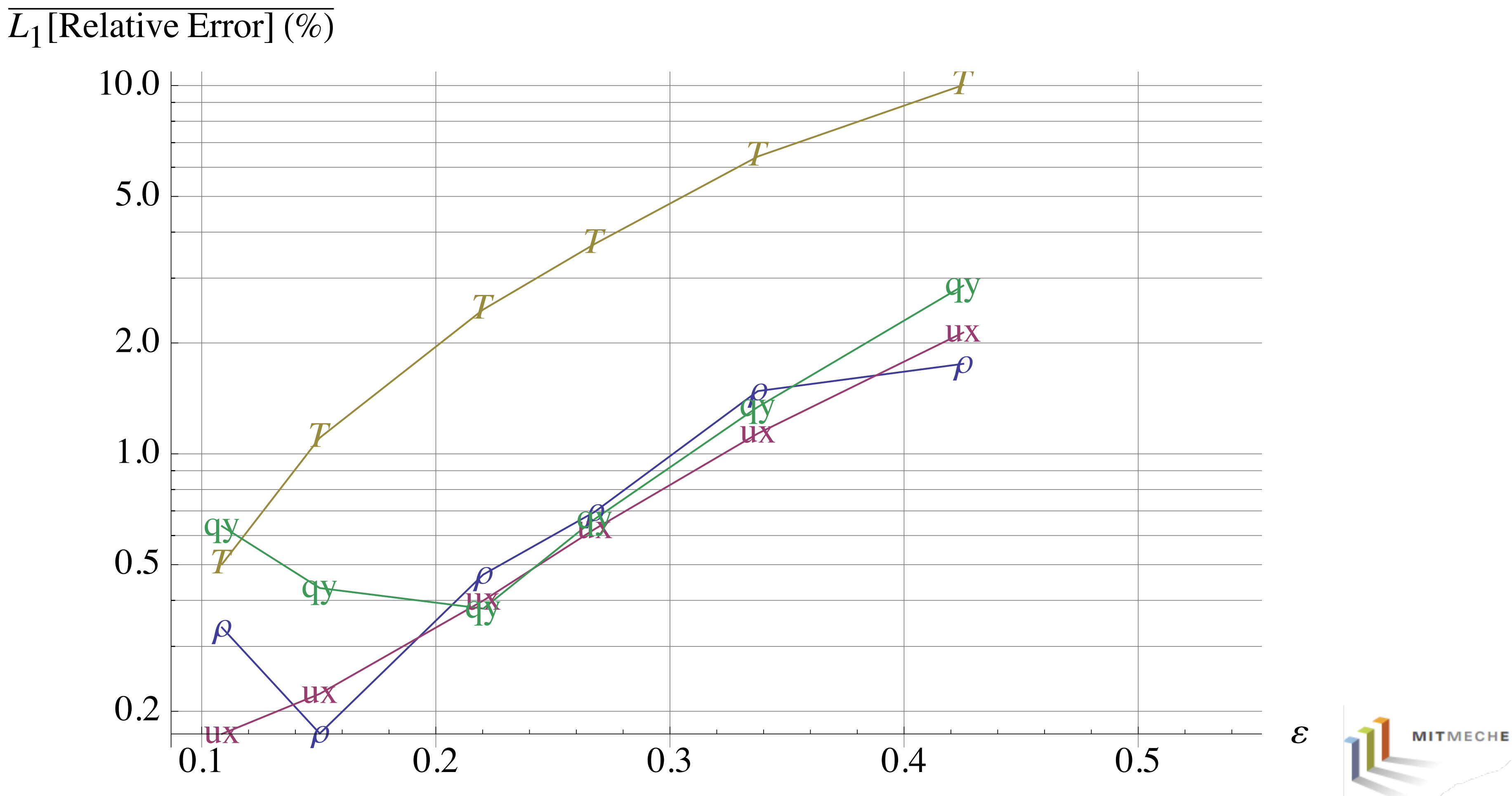
Reminder: KDE Bias (error) vs. ε in 1D



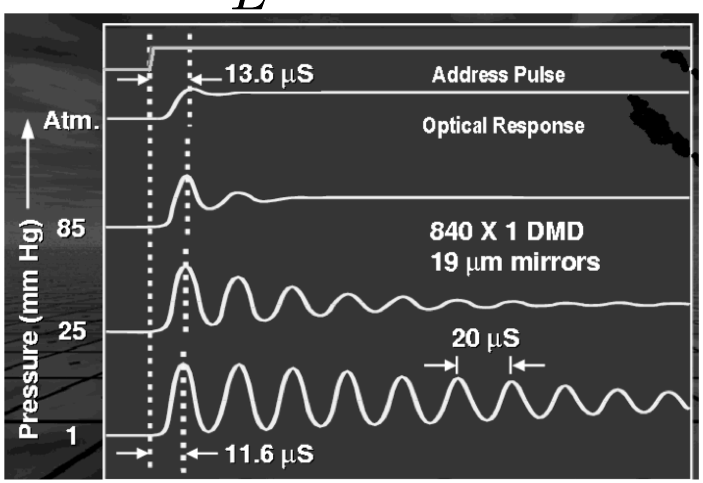
Calculating DMD gas speed

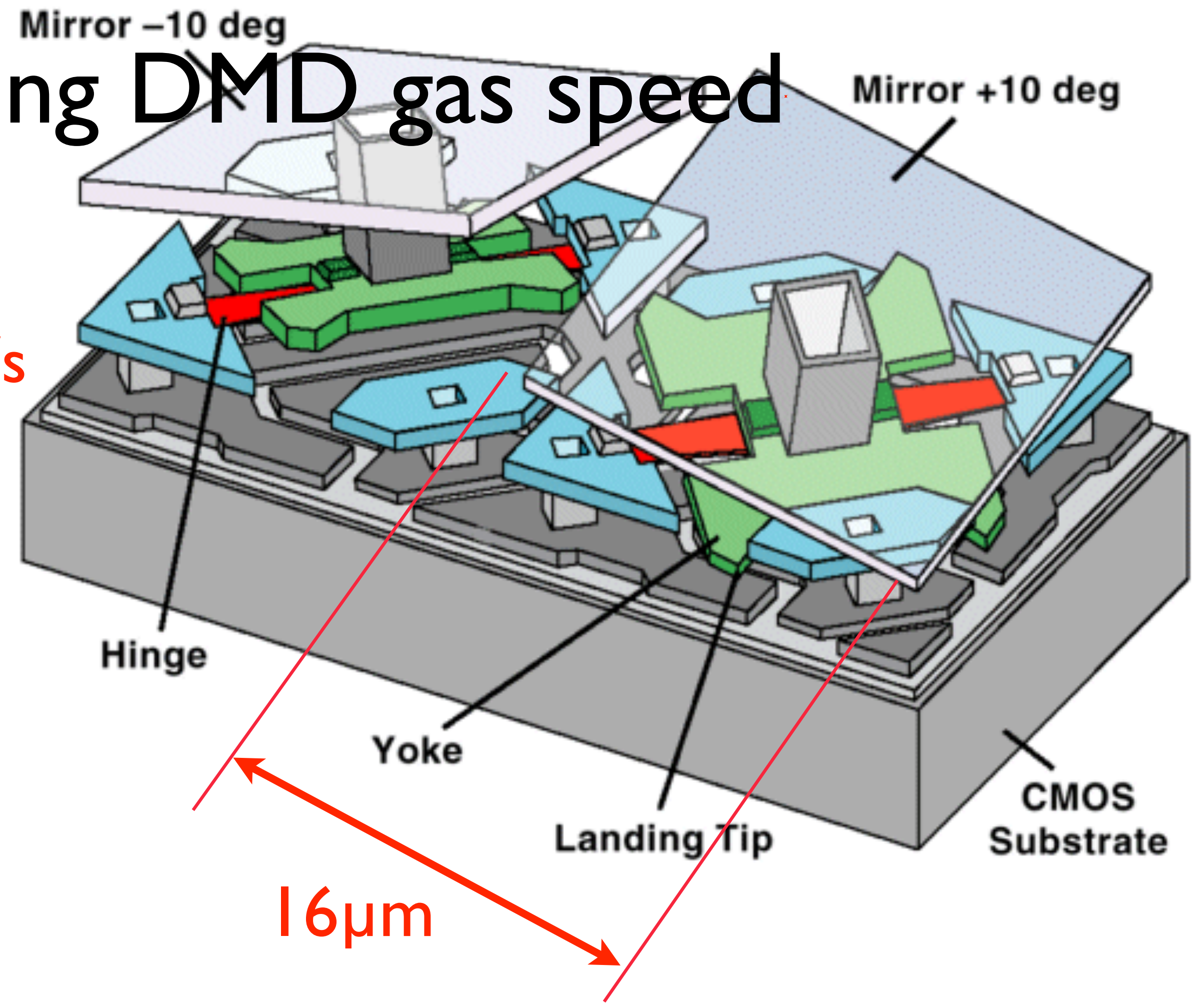
$$\tan(10) = \frac{x}{8\mu m} \rightarrow x \approx 1.4\mu m$$

charicteristic speed=0.1 m/s

$$\lambda \approx 30nm$$

$$\mathrm{Kn} = \frac{\lambda}{L} \Rightarrow \mathrm{Kn} \simeq 0.04 - 0.12$$





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Acceleration Methods for Rarefied Gas Solver

- Problem
  - To find SS solution of Flow ⇒ Need to integrate system for long time
  - Problem is faced in particle methods and traditional solvers
  - Most problematic for low Kn problems
- Approach
  - Re-formulate as a root finding problem over macroscopic properties
  - Needed to develop the concept of "maturing" to couple properties to consistent PDFs

- Publications/Conferences
  - Al-Mohssen, H. A., Hadjiconstantinou, NG, Kevrekidis, I.; Acceleration Methods for Coarse-Grained Numerical Solution of the Boltzmann Equation, J. Fluids Eng. 129, 908 2007
  - Al-Mohssen, H. A., Hadjiconstantinou, NG, Kevrekidis, I.; Acceleration Methods for course-grained Numerical Solution of the Boltzmann Equation, 4th International Conference on Nanochannels, Microchannels and Minichannels, June 19-21, 2006.
  - Al-Mohssen, H. A., Hadjiconstantinou, NG, Kevrekidis, I.; A coarse Newton approach for steady solutions of the Boltzmann Equation, Third MIT Conference on Computational Fluid and Solid Mechanics, June 14-17th, 2005.

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Acceleration Methods

Finding Steady State Solutions of Kinetic Flows

- Options for finding steady state solutions:
  1. Explicit time integration scheme
     - Stability condition limits us to relatively small time steps and $time_{SS} \approx \frac{\tau}{Kn^2}$
  2. Implicit scheme for finding steady state solutions
     - Convergence problems at low Kn
  3. New proposed method for finding SS solutions of multi-scale problems for small Kn

Problem Statement

We want to find the *steady state solution* of the BE. We are interested in the first few moments of f (velocity, temperature, etc.)

- Consider the x-direction flow velocities; denote the velocity in node j at a certain time t as $u_j(t)$
- Furthermore, let $\vec{u}(t)$ be the vector $\vec{u}(t) = \{u_1(t), u_2(t), ..., u_j(t), ..., u_n(t)\}^T$
- If we define $\vec{F}(\vec{u}) = \partial\vec{u}/\partial t$ then we are interested in finding $\vec{u}_{SS}$ such that $\vec{F}(\vec{u}_{SS}) = \vec{0}$

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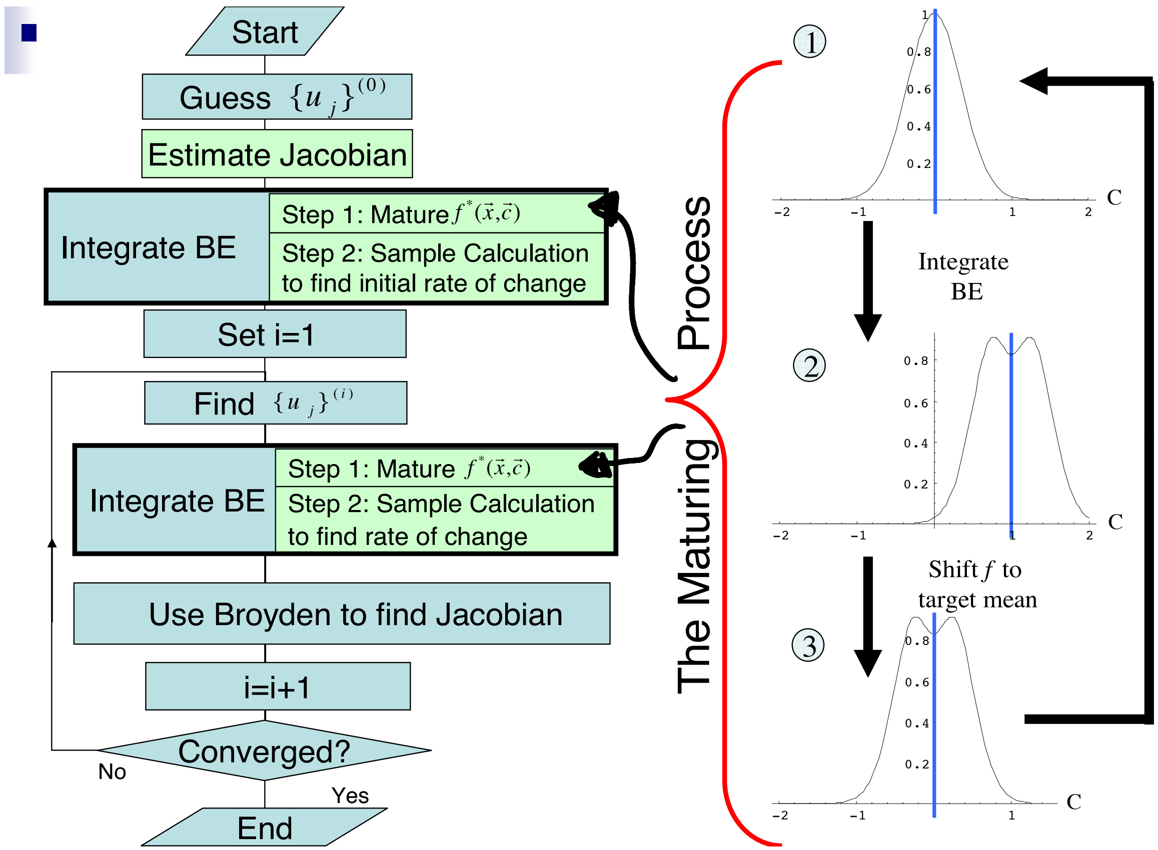
Acceleration Methods (2/3)



Coin-Flipping Stability