

# A Distributional Monte Carlo Method for the Boltzmann Equation

Aihua W Wood

Air Force Institute of Technology  
Department of Mathematics and Statistics

AFOSR Aug 2015



# Collaborators

- Christopher Schrock - AFIT/AFRL
- Alexander Alekseenko - CSUN
- Truong Nguyen - CSUN

# Outline

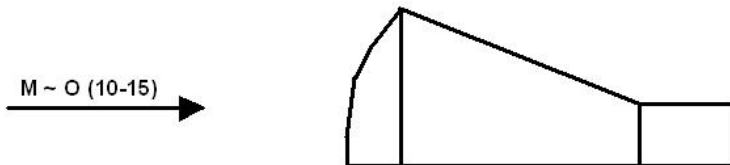
- Background
  - ▶ Kinetic Theory
  - ▶ Boltzmann Equation
  - ▶ Direct Simulation Monte Carlo
- Kernel Density Estimation
- Distributional Monte Carlo
  - ▶ DMC-KDE
  - ▶ DMC-BGK
- A Fast Solver for the Boltzmann Equation

# Background

- The Direct Simulation Monte Carlo (DSMC) method is popular for treatment of flows with continuum break down
- Such flows are important in hypersonic aerodynamics and micro-scale flows
- DSMC has limitations due to its nonphysical representation of the velocity distribution function (point measure)
- We seek to develop distributional methods for stronger convergence and reduced variances

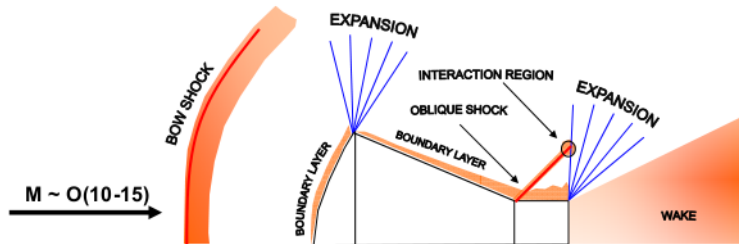
# Blunt Body Example

- Two ways to physically describe a gas
  - ▶ Macroscopic  $\rightarrow$  Continuum Fluid Equations
  - ▶ Microscopic  $\rightarrow$  Kinetic Theory
- Consider the hypersonic flow field around a blunt body



# Why Kinetic Theory?

- Regions where continuous equations may be invalid:



- Large portions of the flow field may be in local thermodynamic equilibrium, but the non-equilibrium effects of the small regions ripple throughout the domain
- Microscopic representation of flow field is required to accurately capture the physics

# The Kinetic Description of Gas

- Gas consists of particles that most of the time do not interact.
  - Each particle is associated with a velocity and a position.
  - The state of gas is described using the *molecular velocity distribution function*  $f(t, \vec{x}, \vec{v})$ .
- ⇒  $f(t, \vec{x}, \vec{v})d\vec{x}d\vec{v}$  gives the number of molecules contained in a box of size  $d\vec{x} \times d\vec{v}$  of the physical space

# Macroscopic Considerations

- Most thermodynamic quantities can be written as expectation values (weak form) of bounded and continuous functions, or moments of the velocity distribution function; e.g. density, bulk-velocity, temperature, stress-tensor, and energy flux.
- The availability of the velocity distribution values (strong form) may facility faster and more accurate deterministic solutions



# Relaxation Process

- As molecules collide and exchange energy, distribution of their velocities approaches the Maxwellian equilibrium distribution

$$f_M(\vec{v}) = \frac{n}{(2\pi RT)^{3/2}} \exp\left(-\frac{|\vec{v} - \vec{u}(t, \vec{x})|^2}{2RT}\right)$$

- The gas is **in the state of continuum** if its velocity distribution approaches the Maxwellian distribution.
- The Maxwellian distribution is defined by density  $n$ , bulk velocity  $\vec{u}$ , and temperature  $T$ .

# Boltzmann Equation

- Governing equation of Kinetic Theory
- Describes the evolution of particle energy PDF
- For unexcited monatomic gas, may examine velocity PDF

$$\frac{\partial}{\partial t} f(\vec{r}, \vec{c}, t) + \vec{c} \cdot \frac{\partial}{\partial \vec{r}} f(\vec{r}, \vec{c}, t) + \vec{F} \cdot \frac{\partial}{\partial \vec{c}} f(\vec{r}, \vec{c}, t) = J[f](\vec{r}, \vec{c}, t)$$

where  $f(\vec{r}, \vec{c}, t)$  is the probability of finding a particle of gas at time  $t$ , at point  $\vec{r}$ , moving with velocity  $\vec{c}$ .

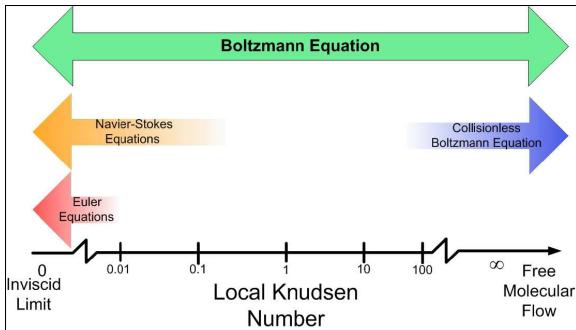
# Relation to Continuum Eqs.

- Taking appropriate moments of the BE yields conservation equations for mass, momentum, and energy
- Hilbert expansion:  $f = f_M(1 + \Phi + \Phi^2 + \dots)$ 
  - ▶ For  $f = f_M$ ,  $\rightarrow$  Euler Equations
  - ▶ Including 1<sup>st</sup> perturbation  $\rightarrow$  Navier-Stokes Equations
  - ▶ Higher order terms yield Burnett, Super Burnett, etc.

# The Spectrum

Metric of Validity of Continuum and Equilibrium Hypotheses:

$$Kn = \frac{\lambda}{L}$$



# Problem with Hilbert's 6th Problem?

- Hilbert called to develop “mathematically the limiting processes ... which lead from the atomistic view to the laws of motion of continua”
- Contemporary research interpretation: passage from the kinetic theory of Boltzmann to the continuum theory of Euler as the Knudsen number  $K_n \rightarrow 0$ .
- References:
  - ▶ “From Boltzmann to Euler,” M. Slemrod, Computers and Math with Appl, 2012
  - ▶ “Hilbert’s 6th Problem,” Gorban and Karlin, Bulletins of Am Math Soc., (2014)
  - ▶ “The Problem with Hilbert’s 6th Problem,” M. Slemrod, Math Model. Nat. Phenom. (2015)
  - ▶ “Famous Fluid Equations are Incomplete,” Mathematical Physics Review, Quanta Mag., Jul 21, 2015

# Direct Simulation Monte Carlo

- Developed by Bird c.1963, consistency with BE established in 1980s, applicable to dilute gases
- Stochastic simulation of a fraction of the particles, with each representing  $N/N_{sim}$  actual particles
- Uncoupling of molecular convection and collisions over small time steps
- Representative collision pairs selected and collisions computed
- Molecules convected along their velocity vector
- Simulation evolved multiple times to reduce statistical scatter

# Uncoupling Principle

- Boltzmann Equation in absence of external forces:

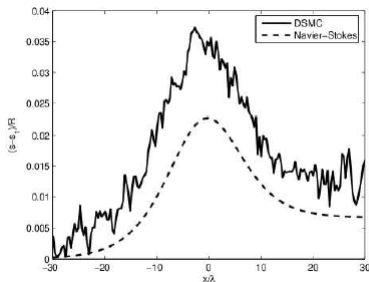
$$\frac{\partial}{\partial t}[f] = -Df + Jf$$

- The uncoupling of convection and collision over  $\Delta t$

$$f = (1 - \Delta t D)(1 + \Delta t J)f_0 + \mathcal{O}(\Delta t^2)$$

# Challenges with DSMC

- Significant Variation in Solution (Scatter)



- Error Estimation
- Computational Expense



# DSMC Representation of the VDF

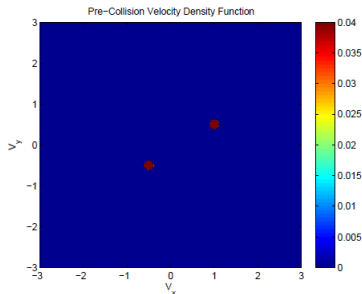
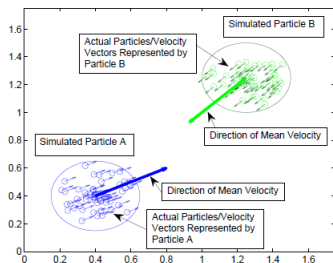
- As each simulated particle has a single velocity, within a given cell the VDF is represented as a point measure approximation

$$f(\vec{v}) = \frac{1}{N_p} \sum_i^{N_p} \delta(\vec{v} - \vec{v}_i)$$

- The assumption  $W = N/N_p = O(10^8)$  particles each possess the same velocity is nonphysical
- In regions of low density this assumption exaggerates the effect of collisions and increases the fluctuations in the solution
- Assumption limits DSMC to weak converge

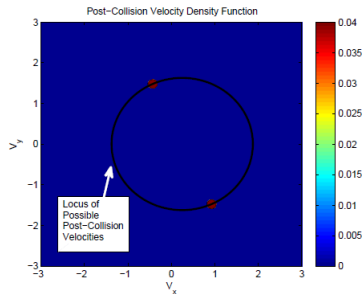
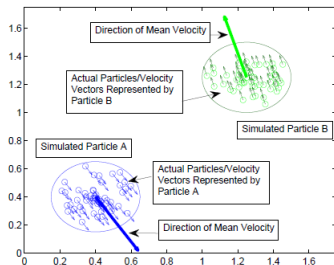
# A DSMC 2-D Example

## Pre-collision Illustration



# DSMC Simulated Collision

## Post-collision Illustration

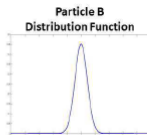
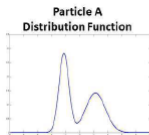


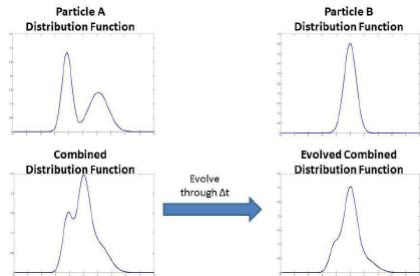
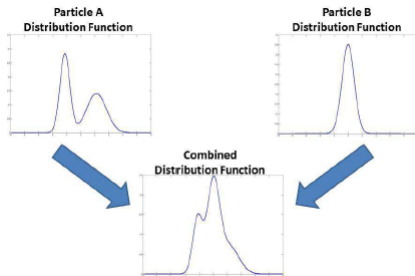
# Distributional Monte Carlo

- As each simulated particle represents a large number of actual particles, allow each particles velocity to be distributed and possess its own VDF,  $f_i$
- Overall VDF given by

$$f(\vec{c}) = \frac{1}{N_p} \sum_{i=1}^{N_p} f_i(\vec{c})$$

- Treat collisions between particle pairs as a space homogeneous relaxation of the combined 2W actual particles they represent





# Kernel Density Estimation (KDE)

- Process for estimating PDF from discrete samples

$$\hat{f}(x; h) = \frac{1}{Nh} \sum_{i=1}^N K\left(\frac{x - X_i}{h}\right)$$

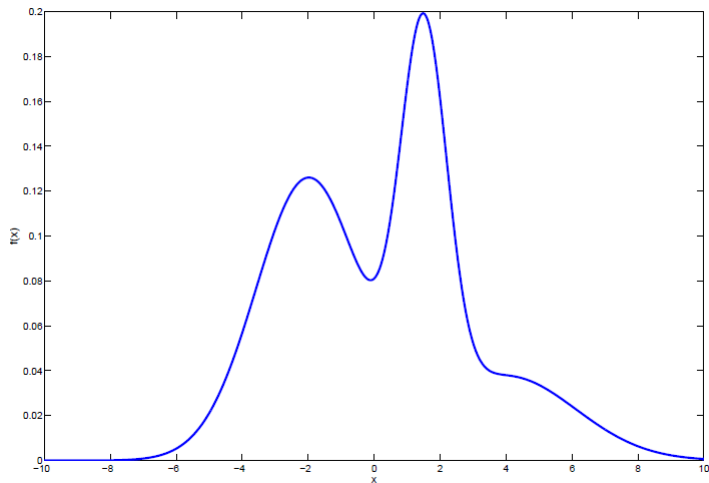
- The  $L^2$  kernel function satisfying

$$\int K(x) dx = 1, \quad \int xK(x) dx = 0$$

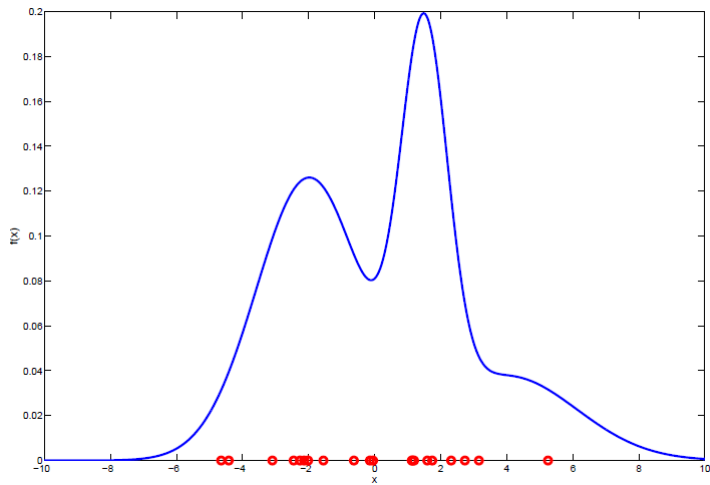
- Examples of kernel functions

$$K(x) = \begin{cases} \frac{1}{2} & |x| \leq 1 \\ 0 & |x| > 1 \end{cases}, \quad K(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right)$$

# KDE Simulation 1/4

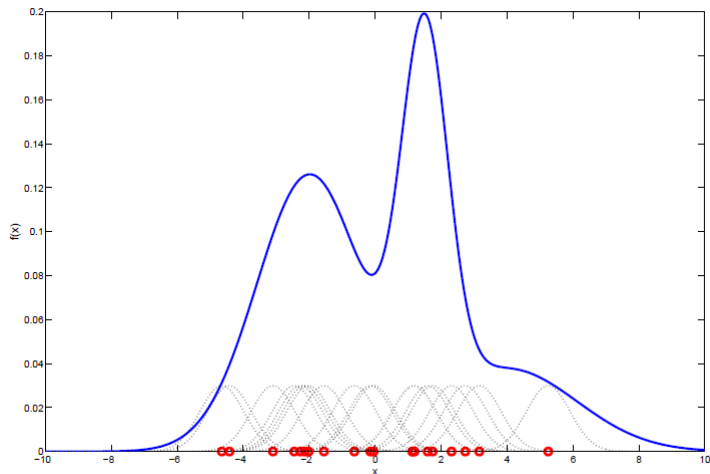


## KDE Simulation 2/4

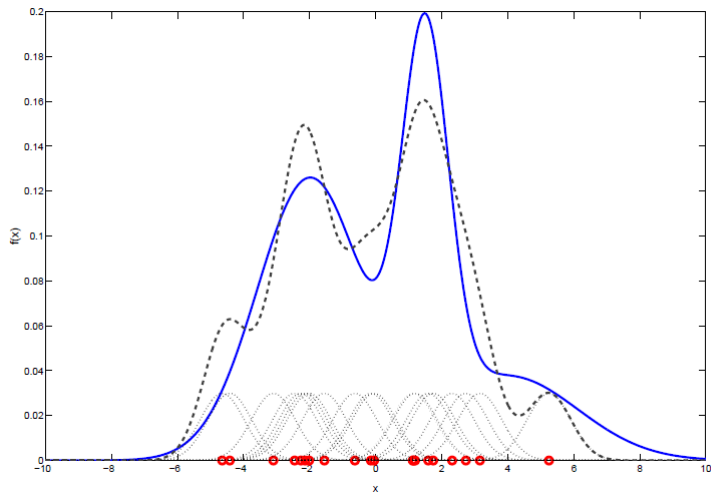




# KDE Simulation 3/4



# KDE Simulation 4/4



# DMC-KDE

- Particle VDFs are of fixed functional form

$$f = \frac{1}{N_p} \sum_{i=1}^{N_p} f_i$$
$$f_i(\vec{v}) = \frac{1}{h^3} K\left(\frac{\vec{v} - \vec{v}_i}{h}\right)$$

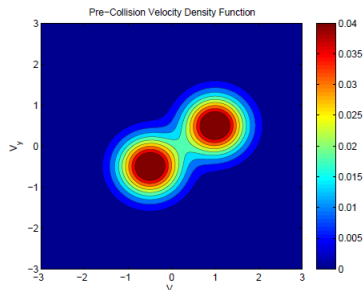
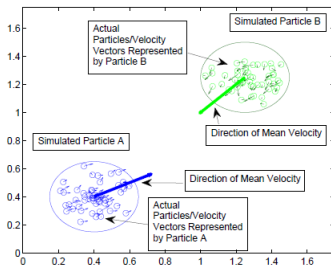
- Mean velocity allowed to vary, but kernel function/bandwidth fixed
- On the basis of physical reasoning we choose a Gaussian kernel for  $K$

$$K(\vec{x}) = (2\pi)^{-3/2} \exp\left(-\frac{\|\vec{x}\|^2}{2}\right)$$
$$h = \left[\frac{32}{3\sqrt{2}N_p}\right]^{\frac{1}{5}} \sigma_{est}$$

- Choosing  $h(N_p)$  s.t.  $\lim_{N_p \rightarrow \infty} h(N_p) = 0$

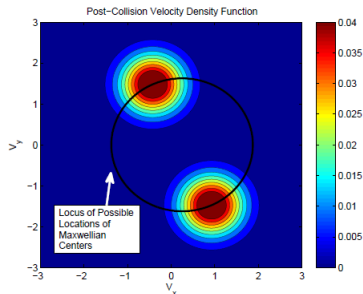
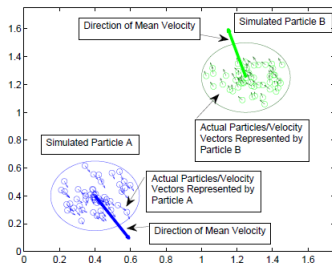
# A DMC-KDE 2-D Example

- Pre-collision: actual particles represented by one simulated particle no longer possess the same velocity, but are in translational equilibrium as a collection



# DMC-KDE Simulated Collision

- Post-collision mean velocities determined using same stochastic rules as Nanbus method



# Convergence of DMC-KDE

- Preserves Weak Convergence in  $L^1$  (probability measure)

$$\lim_{\Delta t \rightarrow 0} \lim_{N \rightarrow \infty} \int_{\mathbb{R}^3} \phi(\vec{c}) \tilde{f}(\vec{c}) d\vec{c} = \int_{\mathbb{R}^3} \phi(\vec{c}) f(\vec{c}) d\vec{c}$$

- Strong convergence in  $L^\infty$

$$\lim_{\Delta t \rightarrow 0} \lim_{N_p \rightarrow \infty} \left\| \tilde{f} - f \right\|_\infty = 0$$

- Pointwise convergence for bounded solutions

$$\lim_{\Delta t \rightarrow 0} \lim_{N_p \rightarrow \infty} \tilde{f}(\vec{c}) = f(\vec{c})$$

for all  $\vec{c} \in \mathbb{R}^3$ .

# DMC-KDE Summary

- Analogous to applying a kernel density estimator to DSMC
- Distribution function is directly obtained
  - ▶ *Stochastic Solver vs. Stochastic Simulator*
  - ▶ *Cost of evaluating distribution function at  $M$  points is  $O(MN_p)$*
  - ▶ *Fast Gaussian Transform can be used to reduce to  $O(M + N_p)$*
- Strong convergence is achieved
- DMC-KDE employs fixed PDFs thus is not fully distributional

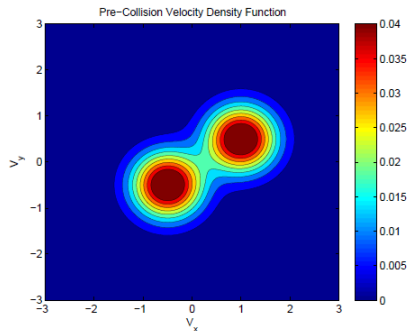
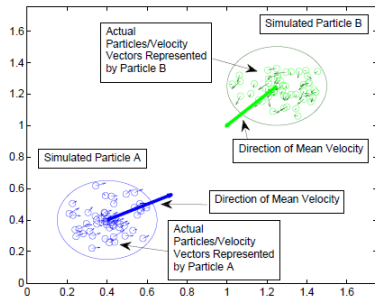
# Essence of DMC

- Seek a fully distributional method with collision selection criteria and collision modeling that fully incorporate non-singular particle velocity distributions
  - ▶ allow for non-Maxwellian particle distributions
- For *near-Maxwellian* distributions, the collision selection criteria from DMC-KDE provides fair approximations
- Treat collision interactions “distributionally”
  - ▶ apply space homogeneous relaxation process on the joint distribution function of the  $2W$  particles the two simulated particles represent
  - ▶ evolve as appropriate



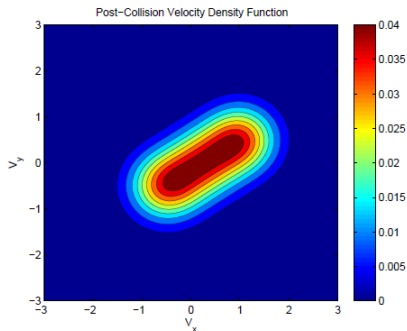
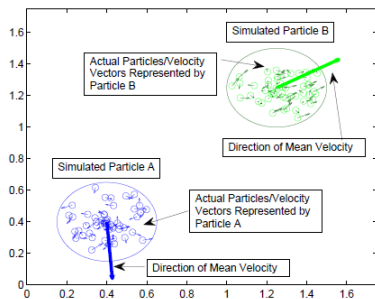
# A DMC 2-D Example

Each particle possesses a VDF



# DMC Simulated Collision

Collision interactions computed as a relaxation toward equilibrium (for the simulated pair)



# DMC Strong Convergence

If  $f \in L^\infty$  is a solution of the space homogeneous BE at  $t = t^k$ , then  $\check{f}^k$  of DMC converges in  $L^\infty$  to  $f^k$ :

$$\lim_{N_p \rightarrow \infty} \|\check{f} - f\| = 0.$$

# A DMC Bhatnagar-Gross-Krook Approximation

- To facilitate numerical demonstration of the DMC framework, a scheme employing the BGK approximation was developed
- Distribution computed using space homogeneous BGK equation
- Deterministic collision modeling facilitated by distributed velocities
  - ▶ Point measure based SPM (e.g. DSMC) could not sample all possible outcomes
- Potential drastic effects on variance w/ removal of one stochastic element

**Theorem:** Let  $f$  be the solution of Boltzmann equation with smooth initial data  $f_0$ ,  $\hat{f}$  the DMC solution. Then  $\|\hat{f} - f\|_{L^1} \rightarrow 0$ , as  $N_{sim} \rightarrow 0$ ,  $\Delta t \rightarrow 0$

# The Bobylev-Krook-Wu Solution

- First known closed form solution to the space homogeneous BE
- Specific to Maxwell molecule
- Spherically symmetric solution

$$f(\vec{v}, t) = \frac{1}{(1\pi\tau(t))^{-3/2}} \exp\left(-\frac{\|\vec{v}\|^2}{2\tau(t)}\right) \left[1 + \frac{1 - \tau(t)}{\tau(t)} \left(\frac{\|\vec{v}\|^2}{2\tau} - \frac{3}{2}\right)\right]$$

where,

$$\tau(t) = 1 - \theta e^{-\lambda t}$$

$$\theta \in \left[0, \frac{2}{5}\right]$$

$$\lambda = \frac{\pi}{2} \int_0^{2\pi} B(\theta) (1 - \cos(\theta)^2) d\theta$$

- Present work utilizes  $\theta = \frac{2}{5}, \lambda = \frac{1}{6}$ .

# Normalized Moments

- Bobylev solution

$$z_n(t) = \left(1 - \frac{2}{5}e^{-\lambda t}\right)^{n-1} \left[1 + \frac{2}{5}(n-1)e^{-\lambda t}\right]$$

- DSMC:

$$z_n(t) = \frac{1}{N_p(2n+1)!!} \sum_{i=1}^{N_p} \tilde{c}_i^{2n}(t)$$

- DMC-KDE:

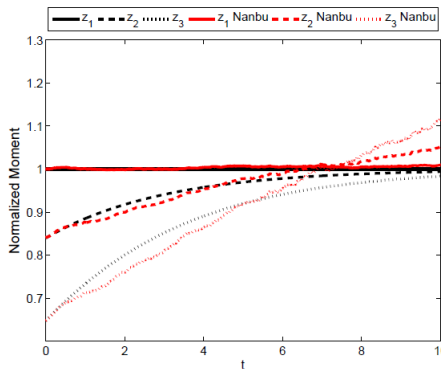
$$z_n(t) = \frac{1}{N_p(2n+1)!!} \sum_{i=1}^{N_p} \tilde{c}_i^{2n}(t) + c_n h^{2n}$$

- DMC-BGK moments computed using simple quadrature

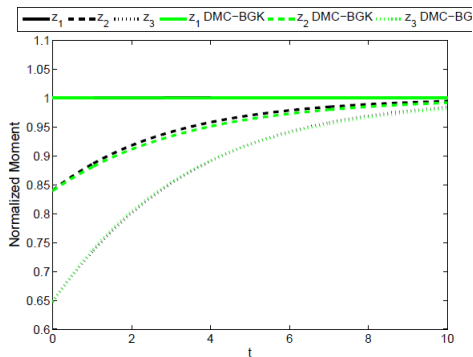
# Normalized Moments Compared

- 100 simulated particles, 600 run ensemble,  $\Delta v = 2/3$

Nanbu DSMC



DMC-BGK



# Total Variation

- Total variation:

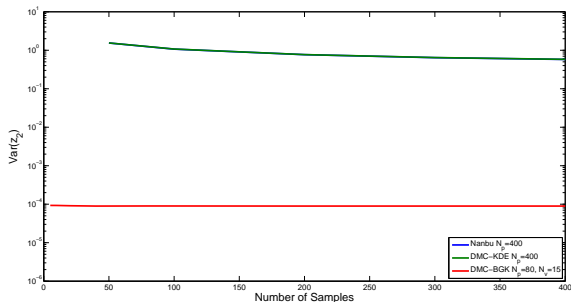
$$V(z_n) = \int_0^{10} |z'_n(t)| dt$$

- Compared to Nanbu-DSMC and DMC-KDE, DMC-BGK shows
  - 1 marked reduction of variance
  - 2 superior energy conservation



# Variation of Second NM

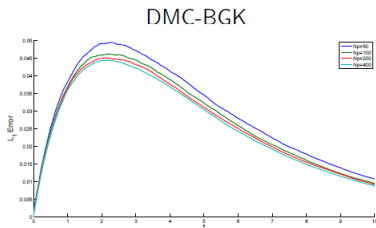
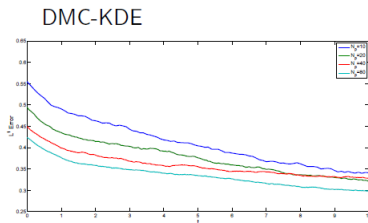
- Nanbu-DSMC/DMC-KDE/DMC-BGK



- Four orders of magnitude reduction in total variation obtained for  $z_1$  through  $z_4$

# $L^1$ Error Compared

- 100 run ensemble,  $\Delta v = 2/3$



# DMC Summary

- DMC provides 1<sup>st</sup> stochastic particle method utilizing distributed velocities
  - ▶ No restriction on method of computing collision outcomes
- DMC-KDE turns a Boltzmann simulator into a Boltzmann solver
  - ▶ Strong convergence
  - ▶ Direct computation/visualization of distribution function
  - ▶ No variance reduction
- DMC-BGK employs a deterministic method for collision outcomes
  - ▶ Hybrid stochastic-deterministic method
  - ▶ Substantial improvement in accuracy and variance reduction

# Solving the Boltzmann Collision Integral

Development of a fast deterministic solver for the Boltzmann equation

# Challenges in solving the Boltzmann Equation numerically

- Direct numerical evaluation takes  $O(N^{\frac{11}{3}})$  operations each time step, where  $N$  is the number of velocity points.
- **A 2 GHz processor will use about 50 seconds if  $N = 10^3$  and about  $1.59E+3$  years if  $N = 10^6$ .**
- **Approaches to solving the Boltzmann equation:**
  - ▶ Use HPCs.
  - ▶ Use efficient numerical techniques (velocity discretization, integration, and methods for massive parallelization.)
  - ▶ Approximations to the Boltzmann equation must be used when appropriate.
  - ▶ Fastness must balance numerical errors.

# Galerkin discretization in velocity variable

- Choose a rectangular region  $K$  and chop it uniformly into little cells  $K_j$ .
- The Galerkin approximation to the solution of the Boltzmann equation on each cell  $K_j$  is of the form

$$f(t, \vec{x}, \vec{v})|_{K_j} = \sum_{i=1}^s f_{i;j}(t, \vec{x}) \phi_i^j(\vec{v}).$$

- Substituting this into  $J[f]$  and hit the result by a basis function and integrate over  $K_j$ :

$$\frac{\partial}{\partial t} f_{i;j}(t, \vec{x}) + \vec{v}_i^j \cdot \vec{\nabla}_x f_{i;j}(t, \vec{x}) = I_{\phi_i^j}$$

# Galerkin projection of the collision operator

- where:

$$I_{\phi_i^j} = \int_3 \int_3 f(t, \vec{x}, \vec{v}) f(t, \vec{x}, \vec{v}_1) A(\vec{v}, \vec{v}_1; \phi_i^j) d\vec{v}_1 d\vec{v},$$

- and the term

$$A(\vec{v}, \vec{v}_1; \phi_i^j) = \frac{|\vec{g}|}{2} \int_0^{2\pi} \int_0^{b_*} (\phi_i^j(\vec{v}') + \phi_i^j(\vec{v}'_1) - \phi_i^j(\vec{v}) - \phi_i^j(\vec{v}_1)) b db d\varepsilon. \quad (1)$$

- $A(\vec{v}, \vec{v}_1; \phi_i^j)$  is independent of time and can be **precomputed**.

# Properties of the collision kernel

- **Theorem 1.** Let operator  $A(\vec{v}, \vec{v}_1; \phi_i^j)$  be defined by (1) with all gas particle having the same mass and potential of the particle interaction being spherically symmetric. Then  $A(\vec{v}, \vec{v}_1; \phi_i^j)$  is symmetric with respect to  $\vec{v}$  and  $\vec{v}_1$ , that is

$$A(\vec{v}, \vec{v}_1; \phi_i^j) = A(\vec{v}_1, \vec{v}; \phi_i^j) \quad \forall \vec{v}, \vec{v}_1 \in \mathbb{R}^3$$

Also,

$$A(\vec{v}, \vec{v}; \phi_i^j) = 0 \quad \forall \vec{v} \in \mathbb{R}^3$$

- **Theorem 2.** Let operator  $A(\vec{v}, \vec{v}_1; \phi_i^j)$  be defined by (1) and let potential of molecular interaction be dependent only on the distance between the particles. Then  $\forall \vec{\xi} \in \mathbb{R}^3$ ,

$$A(\vec{v} + \vec{\xi}, \vec{v}_1 + \vec{\xi}; \phi_i^j(\vec{u} - \vec{\xi})) = A(\vec{v}, \vec{v}_1; \phi_i^j)$$

I.e,  $A(\vec{v}, \vec{v}_1; \phi)$  is invariant with respect to a shift.



# Derivation of the methods

1. Approximate  $f(t, \vec{x}, \vec{v})$  as a sum of Maxwellian distributions.

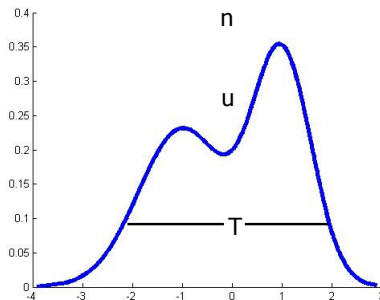
$$f(t, \vec{x}, \vec{v}) = \sum_{i=1}^p f_M(t, \vec{x}, \vec{v}).$$

The density estimation of solutions  $f(t, \vec{x}, \vec{v})$  can be done by applying Expectation Maximization Algorithm (EMA).

# Derivation of the methods

1. Approximate  $f(t, \vec{x}, \vec{v})$  as a sum of Maxwellian distributions.

$$f(t, \vec{x}, \vec{v}) = \sum_{i=1}^p f_M(t, \vec{x}, \vec{v}).$$

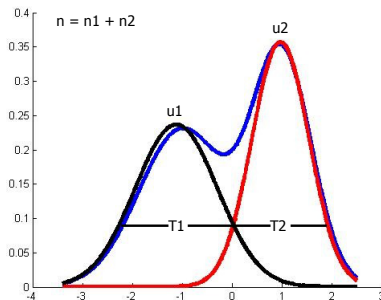


The density estimation of solutions  $f(t, \vec{x}, \vec{v})$  can be done by applying Expectation Maximization Algorithm (EMA).

## Derivation of the methods

1. Approximate  $f(t, \vec{x}, \vec{v})$  as a sum of Maxwellian distributions.

$$f(t, \vec{x}, \vec{v}) = \sum_{i=1}^p f_M(t, \vec{x}, \vec{v}).$$



The density estimation of solutions  $f(t, \vec{x}, \vec{v})$  can be done by applying Expectation Maximization Algorithm (EMA).

# Derivation of the methods (cont.)

## 2. Rewrite DG projection of the B.C.I in convolution form.

Using the invariant property of  $A(\vec{v}_1, \vec{v}; \phi_i^j)$  with respect to a shift, we can re-write the collision integral as:

$$I_i(\vec{\xi}) = \int_3 \int_3 f(t, \vec{x}, \vec{v} - \vec{\xi}) f(t, \vec{x}, \vec{v}_1 - \vec{\xi}) A(\vec{v}_1, \vec{v}; \phi_i^c) d\vec{v} d\vec{v}_1.$$

where  $\vec{\xi} = \vec{\xi}^j$  is the vector that connects the centers of the element  $K_c$  (cell in the center) and the element  $K_j$ .

## Derivation of the methods (cont.)

3. Replacing the density estimation expression of  $f(t, \vec{x}, \vec{v})$  into the formulation of  $I_i(\vec{\xi})$ , we obtain:

$$\begin{aligned}
 I_i(\vec{\xi}) &= \frac{8}{\omega_i \Delta \vec{v}} \int_3 \int_3 \left( \sum_{i'=1}^P f_{M_{i'}}(t, \vec{x}, \vec{v} - \vec{\xi}) \right) \left( \sum_{i''=1}^P f_{M_{i''}}(t, \vec{x}, \vec{v}_1 - \vec{\xi}) \right) A(\vec{v}_1, \vec{v}; \phi_i^c) d\vec{v} d\vec{v}_1 \\
 &= \frac{8}{\omega_i \Delta \vec{v}} \sum_{\substack{i' \neq i'' \\ i', i''=1}}^P \int_3 \int_3 f_{M_{i'}}(t, \vec{x}, \vec{v} - \vec{\xi}) f_{M_{i''}}(t, \vec{x}, \vec{v}_1 - \vec{\xi}) A(\vec{v}_1, \vec{v}; \phi_i^c) d\vec{v} d\vec{v}_1 \\
 &= \frac{8}{\omega_i \Delta \vec{v}} \sum_{\substack{i' \neq i'' \\ i', i''=1}}^P (I_{i' i''}(\vec{\xi})),
 \end{aligned}$$

where  $I_{i' i''}(\vec{\xi}) = \int_3 \int_3 f_{M_{i'}}(t, \vec{x}, \vec{v} - \vec{\xi}) f_{M_{i''}}(t, \vec{x}, \vec{v}_1 - \vec{\xi}) A(\vec{v}_1, \vec{v}; \phi_i^c) d\vec{v} d\vec{v}_1$ .

# Derivation of the methods (cont.)

## 4. Diagonalization of $A(\vec{v}, \vec{v}_1; \phi_i^c)$ .

- In the discrete velocity space, kernel  $A(\vec{v}, \vec{v}_1; \phi_i^c)$  can be represented by an  $N \times N$  symmetric matrix. Thus we can compute its Eigen-Decomposition using available software such as LAPACK and/or PROPACK:

$$A(\vec{v}, \vec{v}_1; \phi_i^c) = \sum_{k=1}^N \lambda_k \Psi_k(\vec{v}) \Psi_k^T(\vec{v}_1) + \varepsilon_{DG}$$

# Derivation of the methods (cont.)

## 4. Diagonalization of $A(\vec{v}, \vec{v}_1; \phi_i^c)$ .

- In the discrete velocity space, kernel  $A(\vec{v}, \vec{v}_1; \phi_i^c)$  can be represented by an  $N \times N$  symmetric matrix. Thus we can compute its Eigen-Decomposition using available software such as LAPACK and/or PROPACK:

$$A(\vec{v}, \vec{v}_1; \phi_i^c) = \sum_{k=1}^N \lambda_k \Psi_k(\vec{v}) \Psi_k^T(\vec{v}_1) + \varepsilon_{DG}$$

- We can further approximate  $A(\vec{v}, \vec{v}_1; \phi_i^c)$  using M-pairs of eigenvalues and eigenvectors:

$$A(\vec{v}, \vec{v}_1; \phi_i^c) = \sum_{k=1}^M \lambda_k \Psi_k(\vec{v}) \Psi_k^T(\vec{v}_1) + \varepsilon_{DG} + \varepsilon_{truncation}$$

where  $\varepsilon_{truncation} = O\left(\sqrt{\frac{\sum_{i=M+1}^N |\lambda_i|^2}{\sum_{i=1}^N |\lambda_i|^2}}\right)$

# Derivation of the methods (cont.)

5. Substituting the Eigen-Decomposition of  $A(\vec{v}, \vec{v}_1; \phi_i^c)$  into  $I_i^{i' i''}$ :

$$\begin{aligned} I_i^{i' i''}(\vec{\xi}) &= \int_3 \int_3 f_{M_{i'}}(t, \vec{v} - \vec{\xi}) f_{M_{i''}}(t, \vec{v}_1 - \vec{\xi}) \left( \sum_{k=1}^M \lambda_k \Psi_k(\vec{v}) \Psi_k(\vec{v}_1) \right) d\vec{v} d\vec{v}_1 \\ &= \sum_{k=1}^M \lambda_k \left( \int_3 f_{M_{i'}}(t, \vec{v} - \vec{\xi}) \Psi_k(\vec{v}) d\vec{v} \right) \left( \int_3 f_{M_{i''}}(t, \vec{v}_1 - \vec{\xi}) \Psi_k(\vec{v}_1) d\vec{v}_1 \right). \end{aligned}$$



## Derivation of the methods (cont.)

5. Substituting the Eigen-Decomposition of  $A(\vec{v}, \vec{v}_1; \phi_i^c)$  into  $I_i^{i' i''}$ :

$$\begin{aligned} I_i^{i' i''}(\xi) &= \int_3 \int_3 f_{M_{i'}}(t, \vec{v} - \vec{\xi}) f_{M_{i''}}(t, \vec{v}_1 - \vec{\xi}) \left( \sum_{k=1}^M \lambda_k \Psi_k(\vec{v}) \Psi_k(\vec{v}_1) \right) d\vec{v} d\vec{v}_1 \\ &= \sum_{k=1}^M \lambda_k \left( \int_3 f_{M_{i'}}(t, \vec{v} - \vec{\xi}) \Psi_k(\vec{v}) d\vec{v} \right) \left( \int_3 f_{M_{i''}}(t, \vec{v}_1 - \vec{\xi}) \Psi_k(\vec{v}_1) d\vec{v}_1 \right). \end{aligned}$$

Therefore,

$$I_{\phi_i}^{j} = \sum_{\substack{i' \neq i'' \\ i', i''=1}}^P \sum_{k=1}^N \lambda_k \left( \int_3 f_{M_{i'}}(t, \vec{v} - \vec{\xi}) \Psi_k(\vec{v}) d\vec{v} \right) \left( \int_3 f_{M_{i''}}(t, \vec{v}_1 - \vec{\xi}) \Psi_k(\vec{v}_1) d\vec{v}_1 \right). \quad (2)$$

## Derivation of the methods (cont.)

5. Substituting the Eigen-Decomposition of  $A(\vec{v}, \vec{v}_1; \phi_i^c)$  into  $I_i^{i' i''}$ :

$$\begin{aligned} I_i^{i' i''}(\vec{\xi}) &= \int_3 \int_3 f_{M_{i'}}(t, \vec{v} - \vec{\xi}) f_{M_{i''}}(t, \vec{v}_1 - \vec{\xi}) \left( \sum_{k=1}^M \lambda_k \Psi_k(\vec{v}) \Psi_k(\vec{v}_1) \right) d\vec{v} d\vec{v}_1 \\ &= \sum_{k=1}^M \lambda_k \left( \int_3 f_{M_{i'}}(t, \vec{v} - \vec{\xi}) \Psi_k(\vec{v}) d\vec{v} \right) \left( \int_3 f_{M_{i''}}(t, \vec{v}_1 - \vec{\xi}) \Psi_k(\vec{v}_1) d\vec{v}_1 \right). \end{aligned}$$

Therefore,

$$I_{\phi_i}^{j} = \sum_{\substack{i' \neq i'' \\ i', i''=1}}^p \sum_{k=1}^N \lambda_k \left( \int_3 f_{M_{i'}}(t, \vec{v} - \vec{\xi}) \Psi_k(\vec{v}) d\vec{v} \right) \left( \int_3 f_{M_{i''}}(t, \vec{v}_1 - \vec{\xi}) \Psi_k(\vec{v}_1) d\vec{v}_1 \right). \quad (2)$$

6. Goal: To compute the convolution integrals accurately!

## Pre-computed Ansatz: $F_k(\vec{\xi}, T)$

- To optimize the evaluation of (2), we design the following object:

$$F_k(\vec{\xi}, T) = \frac{1}{(\sqrt{\pi T})^3} \int_3 \exp\left(-\frac{|\vec{w} - \vec{\xi}|^2}{T}\right) \psi_k(\vec{w}) d\vec{w}.$$

- Therefore,

$$\int_3 f_M(t, \vec{v} - \vec{\xi}) \psi_k(\vec{v}) d\vec{v} = n F_k(\vec{\xi} + \vec{u}, T).$$

That is, to obtain the values of the convolution integrals, we just need to perform interpolations for  $F_k(\vec{\xi}, T)$ .

- The values of  $F_k(\vec{\xi}, T)$  can be computed accurately using adaptive quadrature with high Gauss order.

# Evaluating B.C.I takes $\mathcal{O}(N^2)$ flops each iteration

1. Perform DG interpolations of  $F_k(\vec{\xi}, T)$  at  $N$  different velocity points.

# Evaluating B.C.I takes $\mathcal{O}(N^2)$ flops each iteration

1. Perform DG interpolations of  $F_k(\vec{\xi}, T)$  at  $N$  different velocity points.  
 $\Rightarrow$  It takes  $O(N)$  operations for the DG interpolations.
2. These operations are repeated for each of the  $N$  eigenvectors used in relation (2).

# Evaluating B.C.I takes $\mathcal{O}(N^2)$ flops each iteration

1. Perform DG interpolations of  $F_k(\vec{\xi}, T)$  at  $N$  different velocity points.  
 $\Rightarrow$  It takes  $O(N)$  operations for the DG interpolations.
2. These operations are repeated for each of the  $N$  eigenvectors used in relation (2).

Overall, it takes  $O(N^2)$  operations.

**Note:** The time of performing the projection algorithm  $\ll$  the time of performing DG interpolations for  $N$  eigenvectors as  $N$  is large.

# Advantages & Disadvantages of the new method

## Advantages:

- Fast method of order  $O(N^2)$ , where  $N$  is the total number of velocity points.
- Can be implemented using parallelization.

## Disadvantages:

- Interpolation errors.
- Requires large storage  $O(MN^2)$ , where  $M$  is a fraction of  $N$ , to store the values of the pre-computed ansatz  $F_k$