PECOS

Predictive Engineering and Computational Sciences

Bayesian Inference for the Calibration of DSMC Parameters

James Strand

The University of Texas at Austin

October 5-6, 2010

Previous PECOS Work

- April 2008 - November 2008: DPLR
- December 2008 - March 2009: DAC
- June 2009 - September 2009: Chaleur (summer at Sandia labs)

Motivation

Benefits of the current work include:

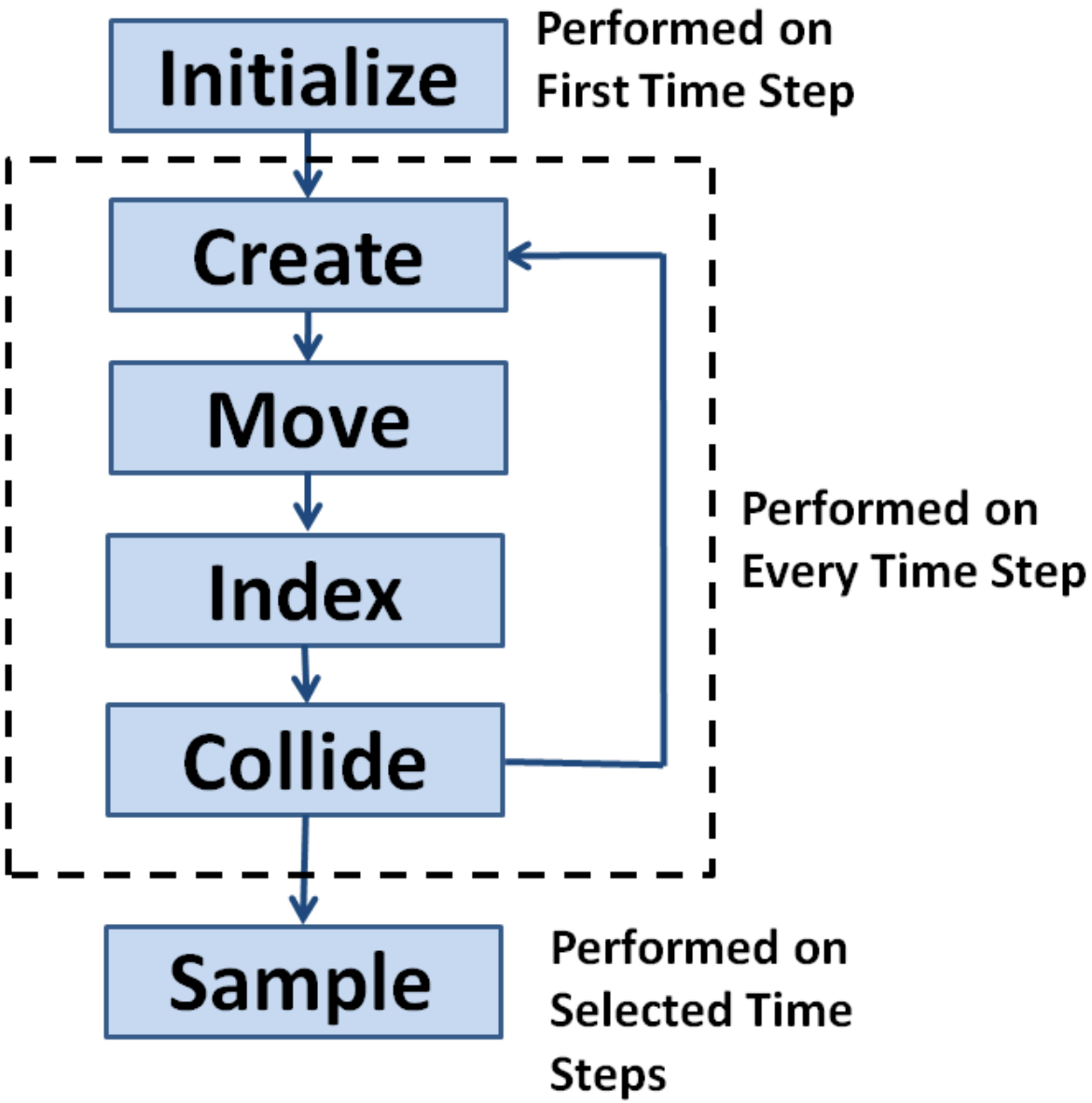
- Bayesian statistical methods will be introduced to a field where they have seen little if any prior use.
- Calibrated parameters obtained from this work will be of use to the DSMC community.
- DSMC will provide PECOS with useful insight about the shock-tube problem, and about re-entry flowfields in general.

Introduction: DSMC

Direct Simulation Monte Carlo (DSMC) is a particle based simulation technique.

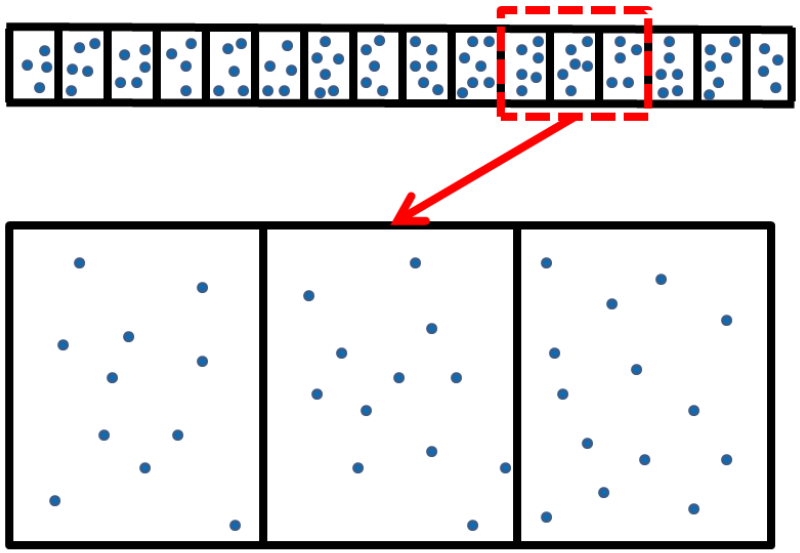
- Simulated particles represent large numbers of real particles.
- Particles move and undergo collisions with other particles.
- Can be used in highly non-equilibrium flowfields (such as strong shock waves).
- Can model thermochemistry on a more detailed level than most CFD codes.

Introduction: DSMC



DSMC Collisions

DSMC collisions are performed statistically. Pairs of molecules are randomly selected from within a cell, a collision probability is calculated for each selected pair, and a random number draw determines whether or not the pair actually collides.



$$P_{collision} = \frac{\sigma_T c_r}{(\sigma_T c_r)_{max}}$$

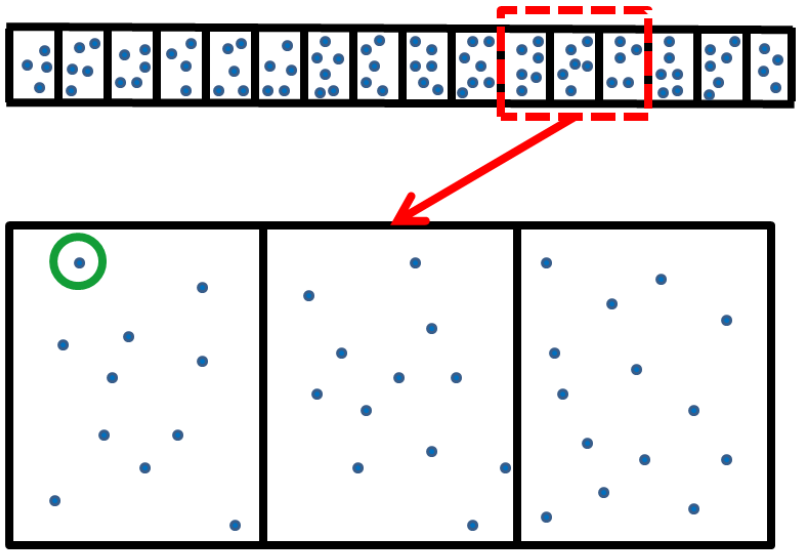
σ_T = Total collision cross section.

c_r = Relative speed between the two selected particles.

$(\sigma_T c_r)_{max}$ = Estimated maximum value of $\sigma_T c_r$ for the cell.

DSMC Collisions

DSMC collisions are performed statistically. Pairs of molecules are randomly selected from within a cell, a collision probability is calculated for each selected pair, and a random number draw determines whether or not the pair actually collides.



$$P_{collision} = \frac{\sigma_T c_r}{(\sigma_T c_r)_{max}}$$

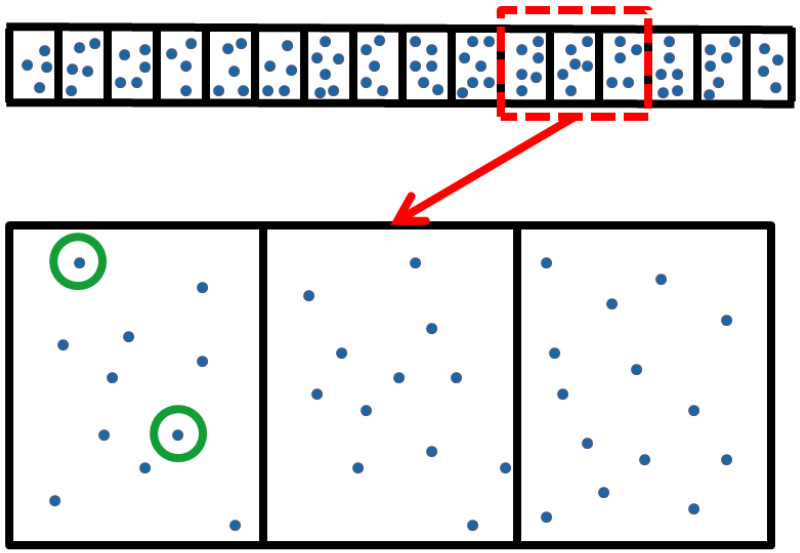
σ_T = Total collision cross section.

c_r = Relative speed between the two selected particles.

$(\sigma_T c_r)_{max}$ = Estimated maximum value of $\sigma_T c_r$ for the cell.

DSMC Collisions

DSMC collisions are performed statistically. Pairs of molecules are randomly selected from within a cell, a collision probability is calculated for each selected pair, and a random number draw determines whether or not the pair actually collides.



$$P_{collision} = \frac{\sigma_T c_r}{(\sigma_T c_r)_{max}}$$

σ_T = Total collision cross section.

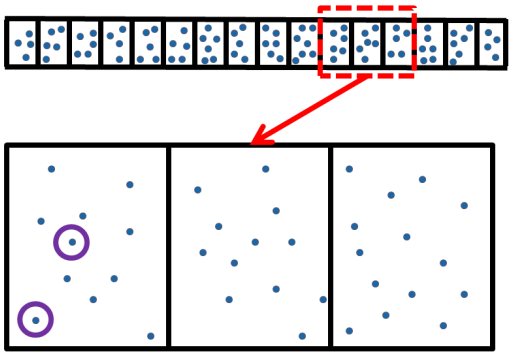
c_r = Relative speed between the two selected particles.

$(\sigma_T c_r)_{max}$ = Estimated maximum value of $\sigma_T c_r$ for the cell.

DSMC Collisions

If the pair does not collide, their velocities are left unchanged and a new pair is selected. If the pair does collide, the velocities of both colliding particles are immediately adjusted to their calculated post-collision values, and then a new pair is selected. The number of selections in a given cell is a function of the overall simulation properties and of the properties within that cell at that time step.

$$N_{selected} = \frac{1}{2} N \overline{N} F_N (\sigma_T c_r)_{max} \Delta t / V_c$$



N = Number of simulation particles in the cell.

$\overline{N}$ = Moving average of the number of simulation particles in the cell.

F_N = Number of real particles represented by each simulation particle.

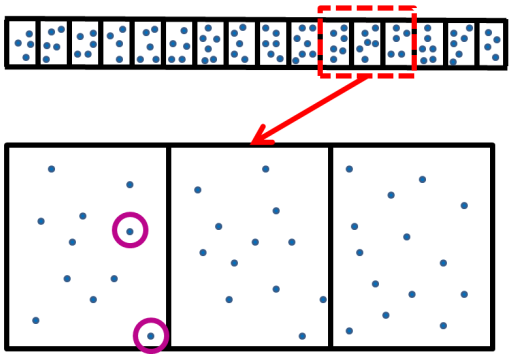
Δt = Simulation time step.

V_c = Cell volume.

DSMC Collisions

If the pair does not collide, their velocities are left unchanged and a new pair is selected. If the pair does collide, the velocities of both colliding particles are immediately adjusted to their calculated post-collision values, and then a new pair is selected. The number of selections in a given cell is a function of the overall simulation properties and of the properties within that cell at that time step.

$$N_{selected} = \frac{1}{2} N \overline{N} F_N (\sigma_T c_r)_{max} \Delta t / V_c$$



N = Number of simulation particles in the cell.

$\overline{N}$ = Moving average of the number of simulation particles in the cell.

F_N = Number of real particles represented by each simulation particle.

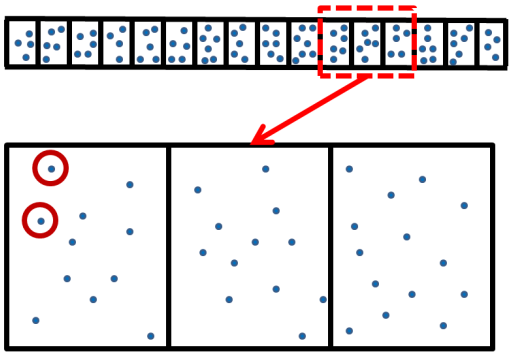
Δt = Simulation time step.

V_c = Cell volume.

DSMC Collisions

If the pair does not collide, their velocities are left unchanged and a new pair is selected. If the pair does collide, the velocities of both colliding particles are immediately adjusted to their calculated post-collision values, and then a new pair is selected. The number of selections in a given cell is a function of the overall simulation properties and of the properties within that cell at that time step.

$$N_{selected} = \frac{1}{2} N \overline{N} F_N (\sigma_T c_r)_{max} \Delta t / V_c$$



N = Number of simulation particles in the cell.

$\overline{N}$ = Moving average of the number of simulation particles in the cell.

F_N = Number of real particles represented by each simulation particle.

Δt = Simulation time step.

V_c = Cell volume.

DSMC Parameters

The DSMC model includes many parameters related to gas dynamics at the molecular level, such as:

- Elastic collision cross-sections.
- Vibrational and rotational excitation probabilities.
- Reaction cross-sections.
- Sticking coefficents and catalytic efficiencies for gas-surface interactions.
- ...etc.

DSMC Parameters

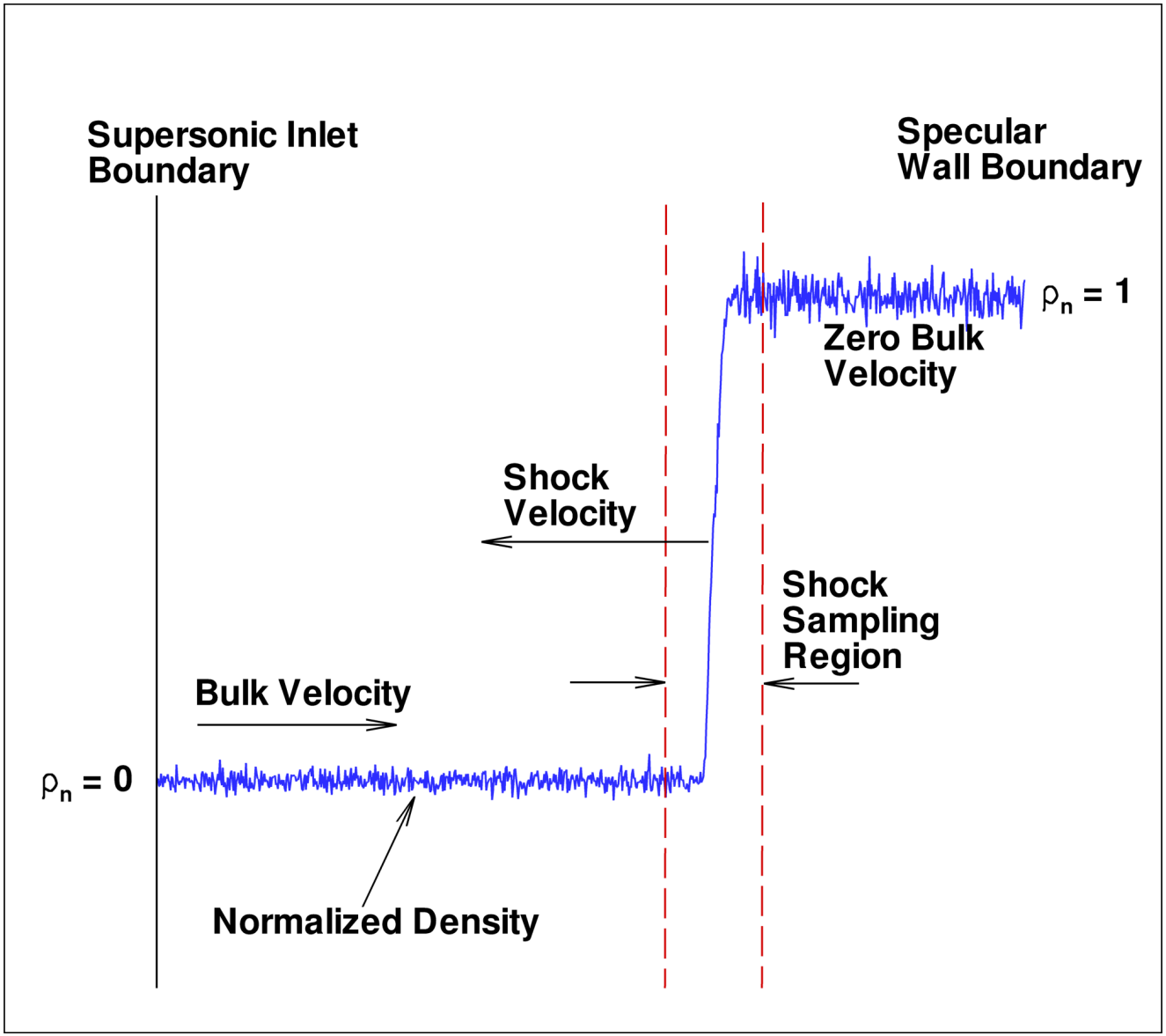
- In many cases the precise values of some of these parameters are not known.
- Parameter values often cannot be directly measured, instead they must be inferred from experimental results.
- By necessity, parameters must often be used in regimes far from where their values were determined.
- More precise values for important parameters would lead to better predictive capability for DSMC.

Solving the inverse problem via Bayesian inference would allow multiple types and sets of data (potentially from NASA EAST, CUBRC, plasma torches, etc.) to be used simultaneously in order to provide the best possible parameters for the given model. If done properly, this could be of great use to the DSMC community.

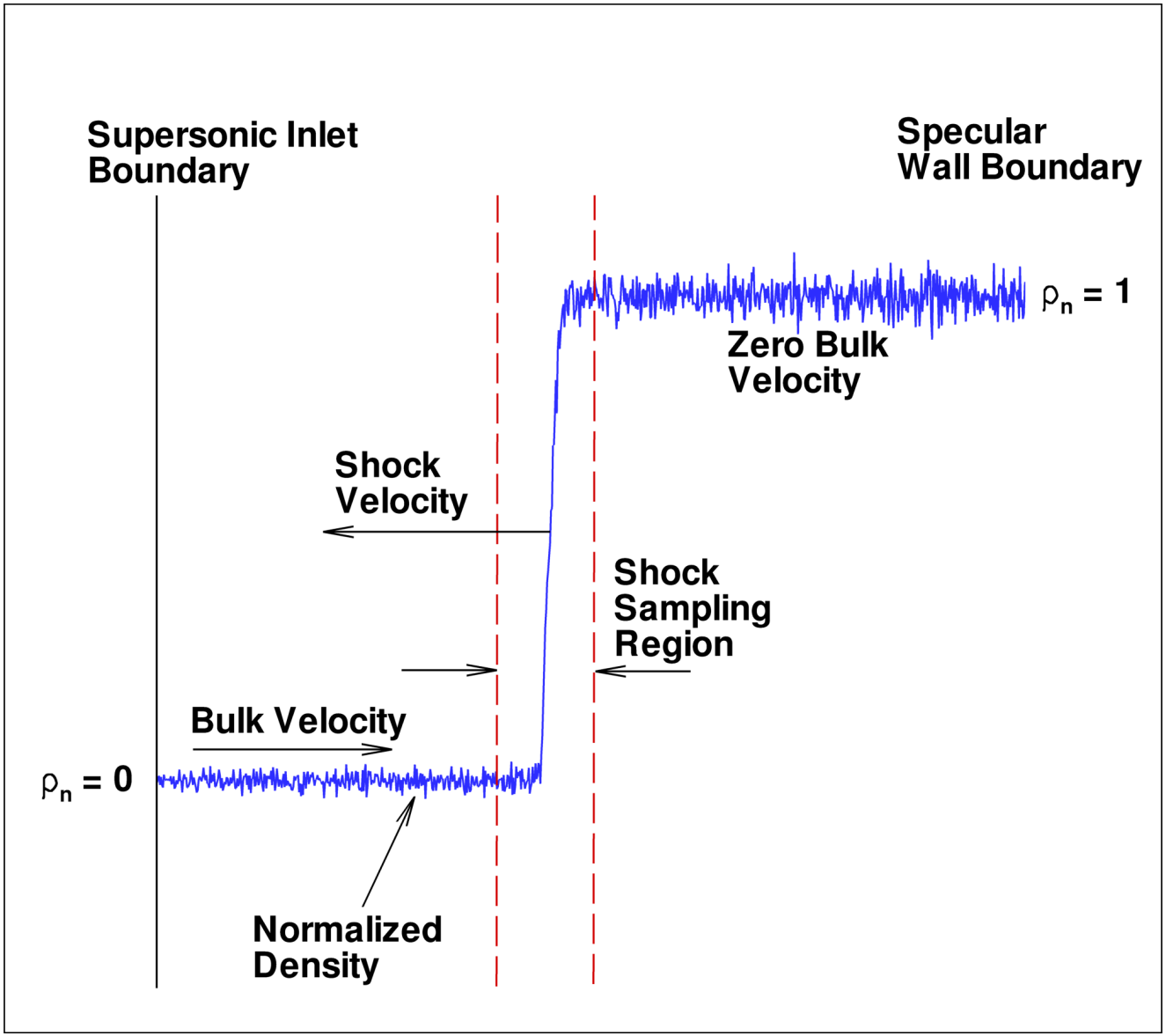
1D Shock Simulation

- Base flow is a 1D, unsteady shock, moving through the computational domain.
- A set of sample cells moves with the shock. These sample cells continuously collect data on the shock profile.
- This method allows for a smooth solution in an unsteady flow without the computational cost of ensemble averaging or using excessively large numbers of particles.
- No prior knowledge of the post-shock conditions is required.

1D Shock Simulation



1D Shock Simulation



Parallelism

DSMC:

- DSMC code is MPI parallel, with dynamic load rebalancing periodically during each run.
- Allows very fast simulation of small problems.
- Super-linear speed-up due to better cache use.
- Simulations which took 20 minutes on 1 processor take less than 20 seconds on 64 processors.
- Faster DSMC simulations allow for much longer MCMC chains to be run in a practical amount of time.

MCMC:

- Any given chain must be run in sequence.
- MCMC can be parallelized by running multiple chains simultaneously.

Preliminary Results - Variable Hard Sphere Model

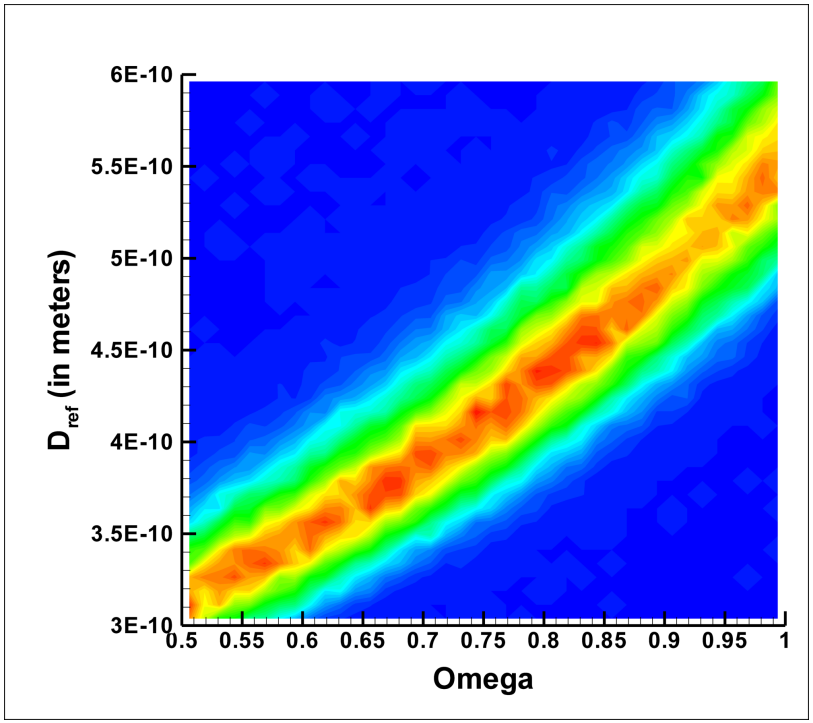
The VHS model has two parameters, d_{ref} and ω. This allows the collision cross-section to be dependent on relative speed, which is more physically realistic than the hard sphere model.

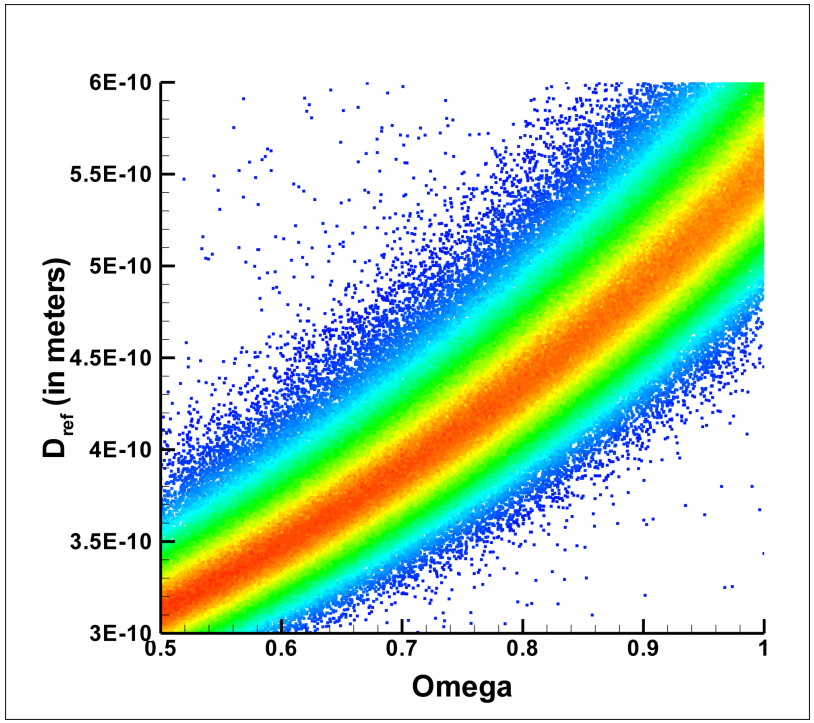
$$\sigma_T = \pi d_{VHS} = \pi d_{ref} \left(\frac{c_{r,ref}}{c_r} \right)^{(\omega - \frac{1}{2})}$$

$$c_{r,ref} = f(d_{ref}, \omega).$$

1D Shock in Argon - VHS Model

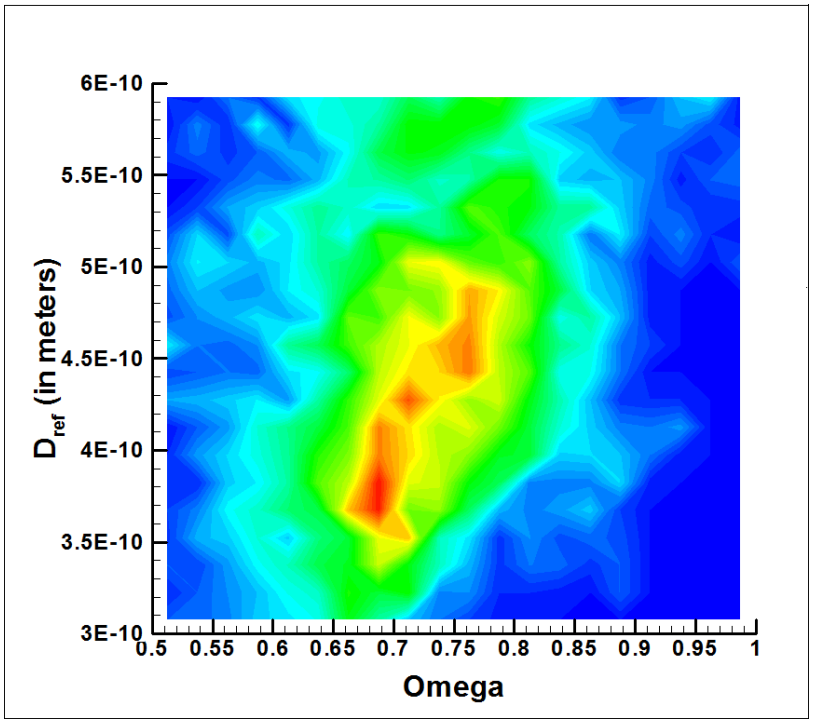
DSMC simulation of 1D shock in argon at Mach 3.38, using the VHS collision model, compared to data from Alsmeyer (1976). Parameters to be calibrated are d_{ref} and ω, the reference diameter and the temperature-viscosity exponent for argon.

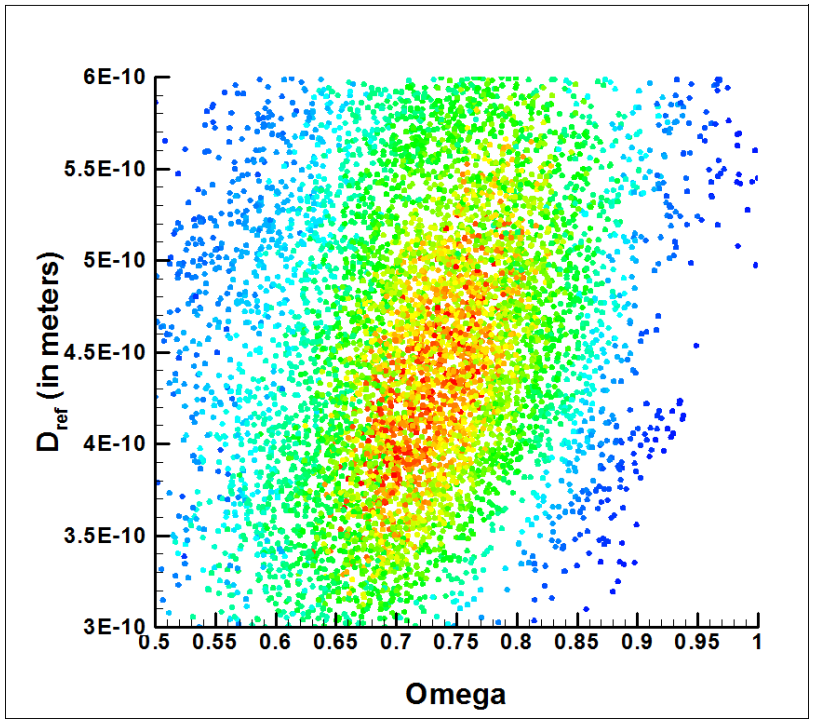




VHS Model - Second Calibration

DSMC simulation of 1D shock in argon at Mach 9, using the VHS collision model, compared to molecular dynamics simulation data from Valentini and Schwartzentruber (2009). Once again calibrating d_{ref} and ω.





Recent Work - Multiple Species

- DSMC code improved to include ability to simulate flows with multiple species.
- Each species has its own molecular properties (mass, reference diameter, characteristic vibrational temperature, etc.).
- Detailed comparison performed between our DSMC code and standard DSMC implementation, using a Helium-Xenon shock as a test case.
- Care was taken to implement in a way that simplifies the future inclusion of dissociation, recombination, exchange, and ionization reactions.

Recent Work - Rotational Excitation

- Rotation is assumed to be fully excited.
- Particles have either zero degrees of freedom (monatomic species) or two degrees of freedom (diatomic species).
- Each particle has its own value of rotational energy, and this variable is continuously distributed (rotation is not considered quantized).
- Some fraction of collisions are considered inelastic, and in some of these collisions rotational energy is redistributed between the two particles and between the translational and rotational modes. The redistribution is based on the Larsen-Borgnakke model.
- The parameter relevant to rotational excitation is Z_R, the rotational collision number.
- Z_R may be treated as a constant. It could also be collision partner dependent, temperature dependent, or both.

Recent Work - Vibrational Excitation

- Vibration is not assumed to be fully excited, and vibrational levels are quantized.
- Each particle has its own vibrational level, which is associated with a certain vibrational energy based on the simple harmonic oscillator model.
- As with rotation, in some fraction of collisions energy is redistributed between the two particles and between the translational and vibrational modes.
- The parameter relevant to vibrational excitation is Z_V, the vibrational collision number.
- Like with rotation, Z_V may be treated as a constant, or it can be collision partner dependent, temperature dependent, or both.

Project Status

Completed

- Write and test a DSMC code suitable for integration with MCMC and optimized for a 1D shock problem.
- Write and test basic MCMC code to examine interaction of DSMC with MCMC.
- Parallelize the DSMC code to allow for simulation of longer chains in a practical amount of time.
- Improve the DSMC code with support for multiple species along with rotational and vibrational excitation.

Project Status

Currently Underway

- Improve the DSMC code with support for realistic air chemistry, including dissociation, recombination, exchange, and ionization reactions.
- Improve the likelihood function to account for uncertainty in the experimental data.

Future Work

- Switch to QUESO for improved MCMC algorithm, diagnostics, etc.
- One-way couple DSMC code with HPCRad to enable simulation of EAST shock tube results.
- Perform sensitivity analysis to determine parameters to be calibrated.
- Calibrate those parameters based on the data available from the EAST facility, and provide the calibrated parameter PDFs to the DSMC community.