PECOS

Predictive Engineering and Computational Sciences

Application of the Metropolis-Hastings Algorithm for the Calibration of DSMC Parameters

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The University of Texas at Austin

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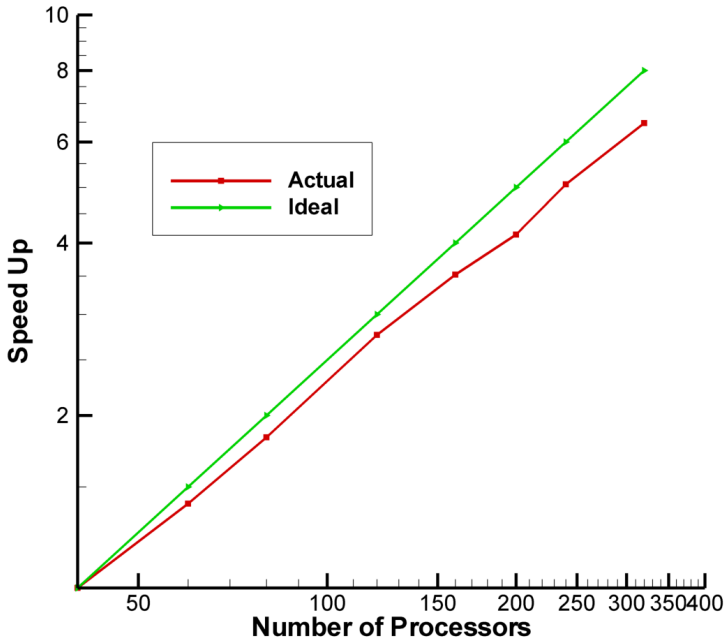
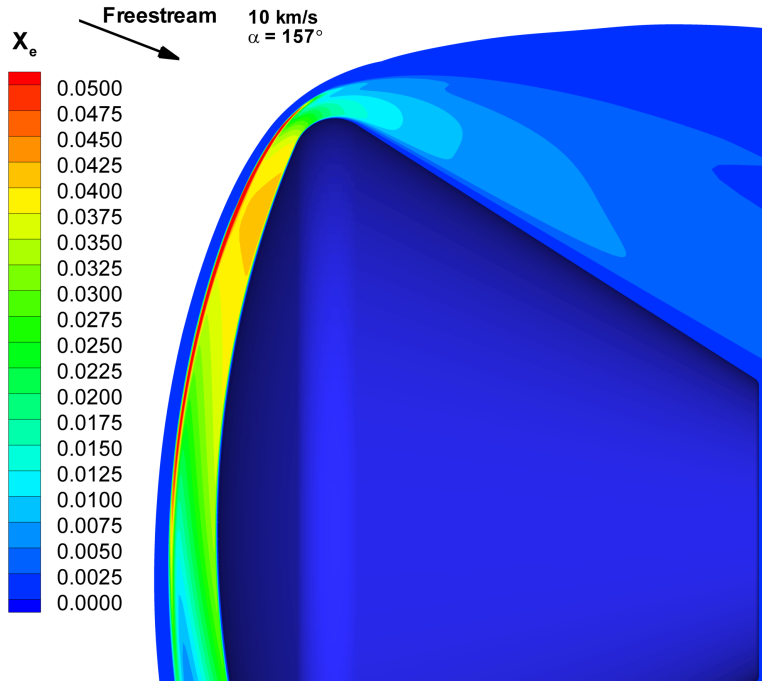
Previous PECOS Work - DPLR

Worked with DPLR from April 2008 - November 2008

- Visited NASA Ames for two weeks in July 2008 to learn DPLR.
- Helped get DPLR up and running on TACC Lonestar system.
- Presented poster for Fall 2008 PECOS review meeting.





Previous PECOS Work - DAC

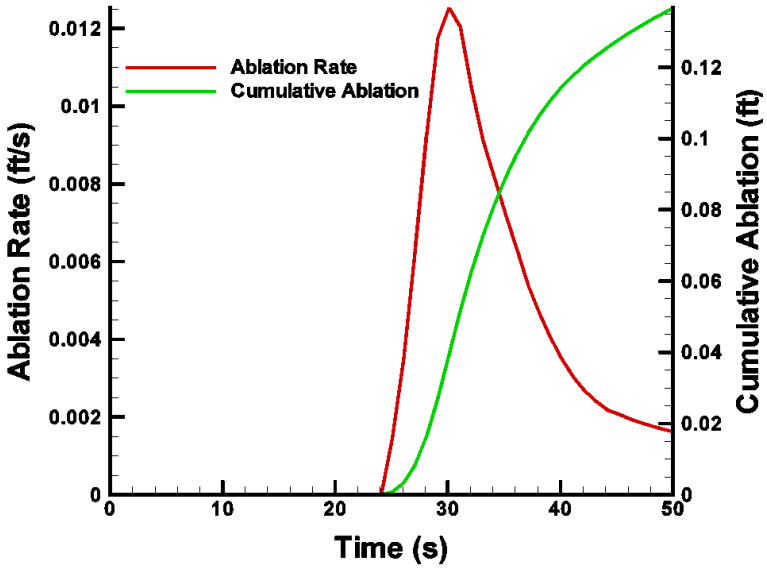
Worked with NASA's DSMC Analysis Code (DAC) from December 2008 - March 2009

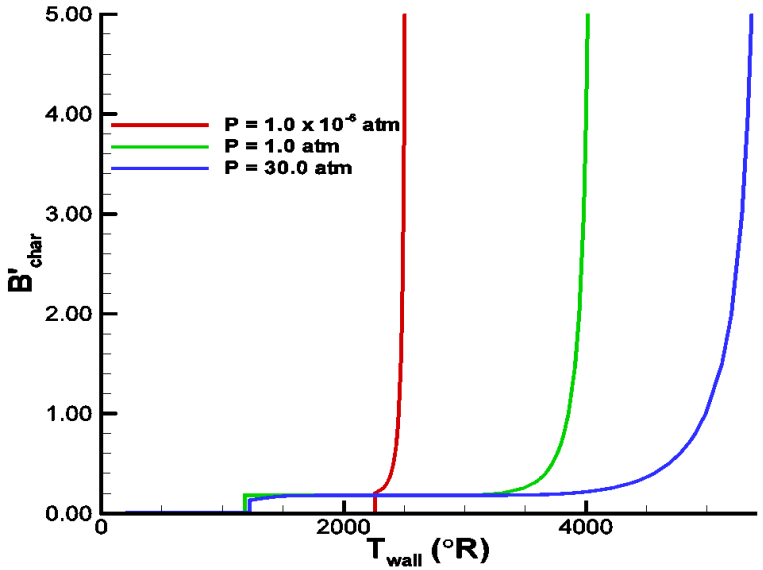
- Studied implementation of high-temperature air chemistry in DSMC.
- Learned about efficient parallel implementation of the DSMC method.
- Concluded that integration of DAC with MCMC would be difficult.
- Decided to incorporate concepts from DAC into a new DSMC code written specifically for integration with MCMC.

Previous PECOS Work - Chaleur

Worked with Chaleur from April 2009 - September 2009

- Worked with Ben Blackwell for three months at Sandia Labs.
- Assisted with automation of the verification test suite for Chaleur.
- Integrated Chaleur with ACE equilibrium thermochemistry code in order to eliminate need for input thermochemistry tables for Chaleur.
- Presented poster for Fall 2009 PECOS review meeting.





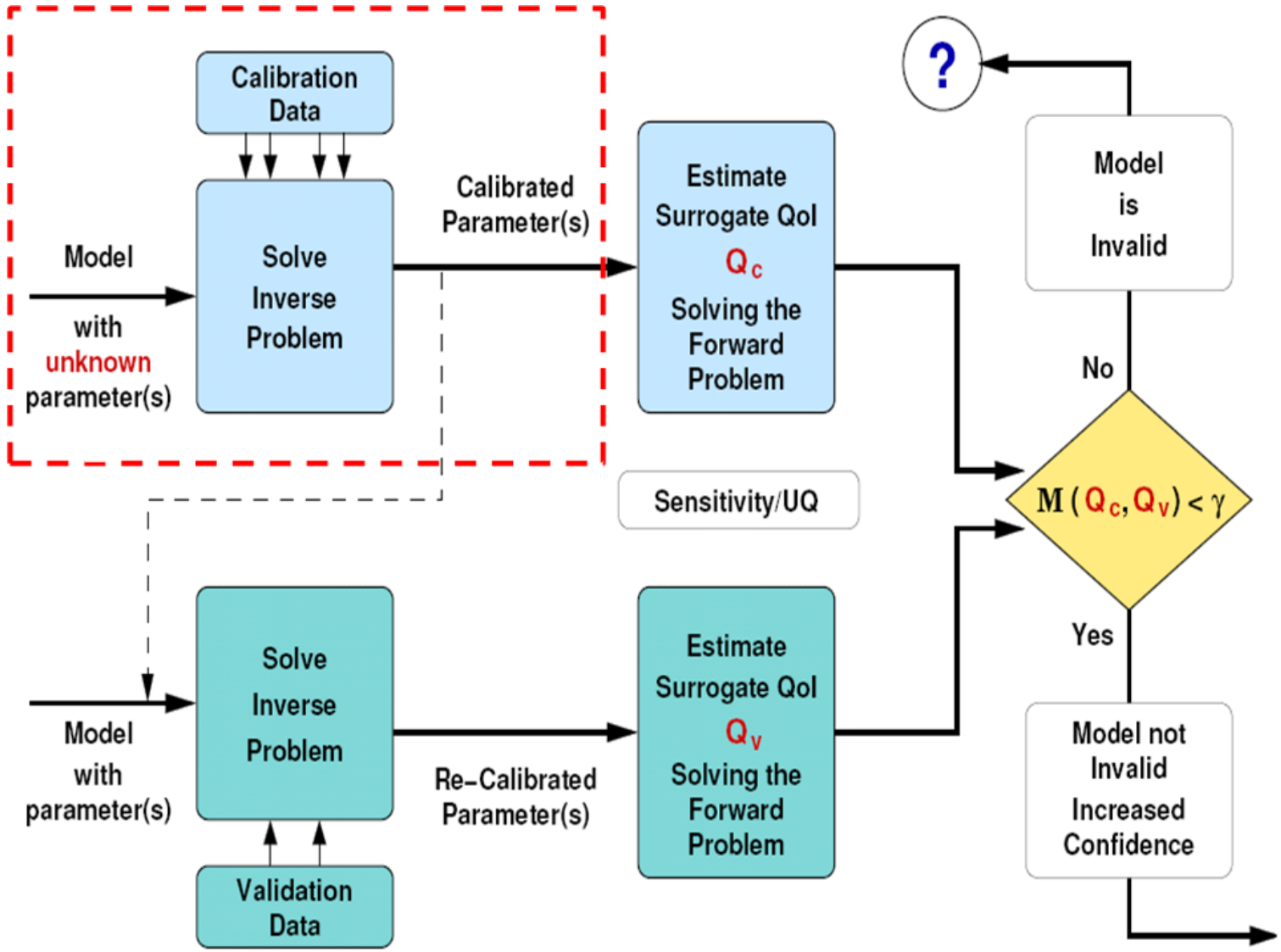
DSMC and MCMC

We are currently interested in only the calibration part of the calibration/validation cycle.

- Current goal is not to validate or invalidate the model.
- The DSMC model for high temperature air chemistry involves many parameters whose precise values are not known.
- Solving the inverse problem with MCMC 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 would be of great use to the DSMC community.

In the future, a verified code employing a properly validated DSMC model might be used to generate auxiliary data for the shock tube group.

DSMC and MCMC

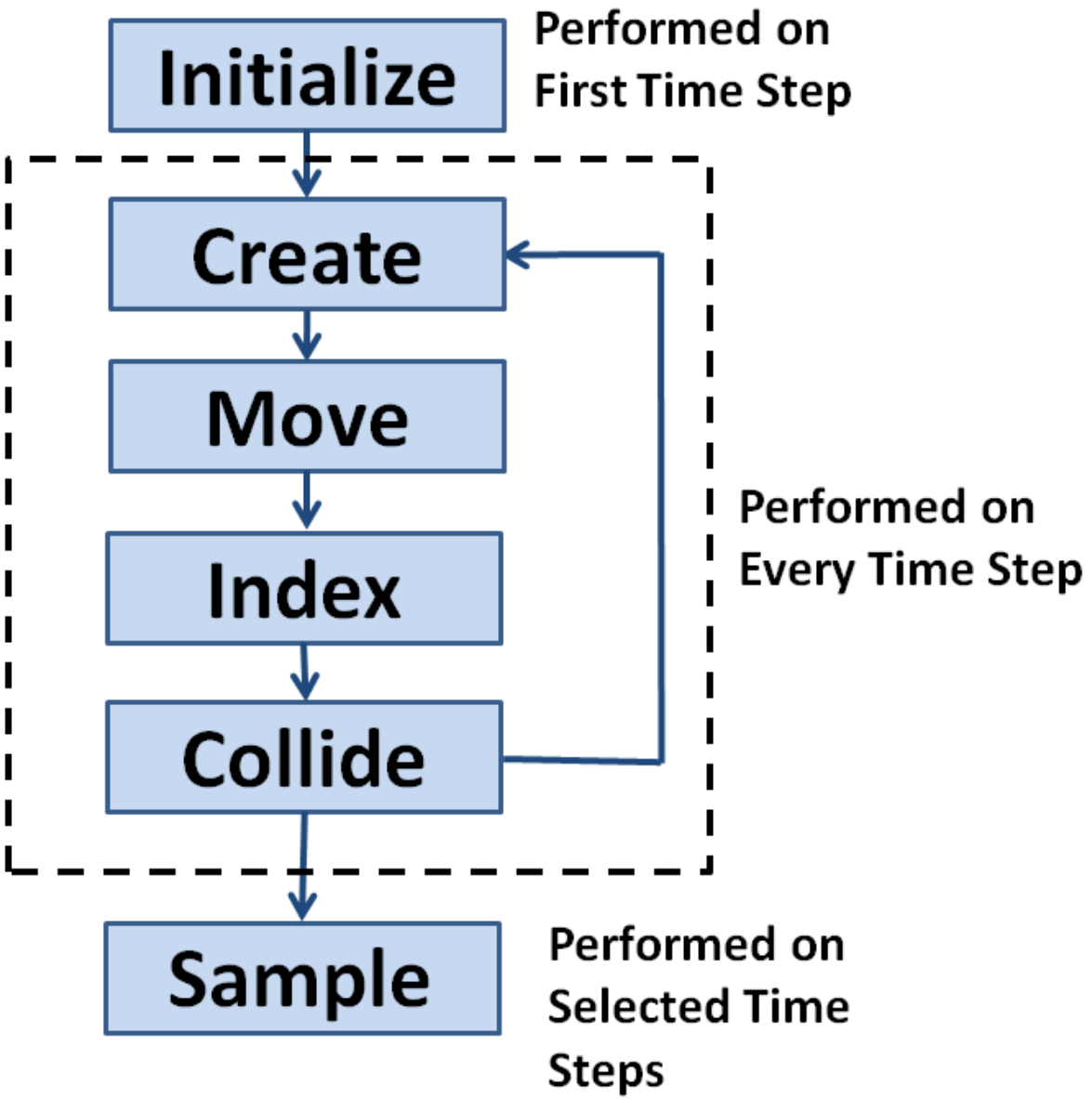


Introduction: DSMC Method

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

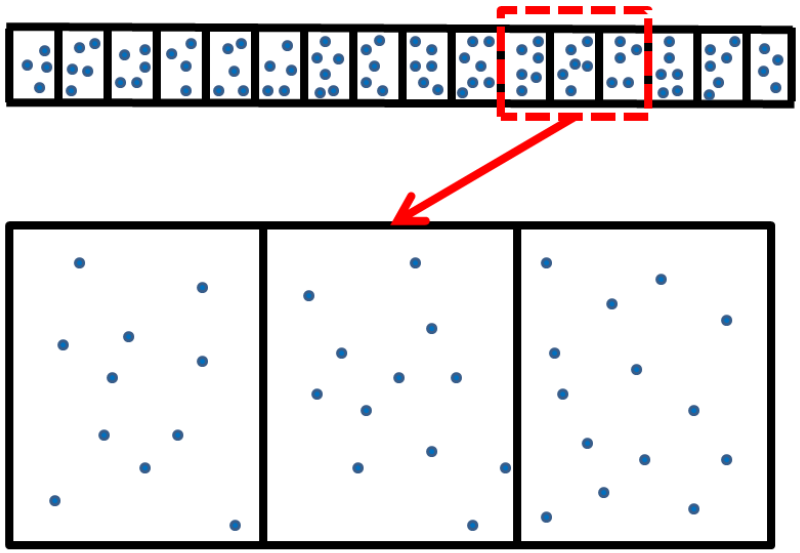
- Simulated particles represent large numbers of real particles.
- Particles move and undergo collisions with other particles.
- Can be used in highly non-equilibrium flowfields (such as strong shock waves).
- Can model thermochemistry on a more detailed level than most CFD codes.

Introduction: DSMC Method



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.

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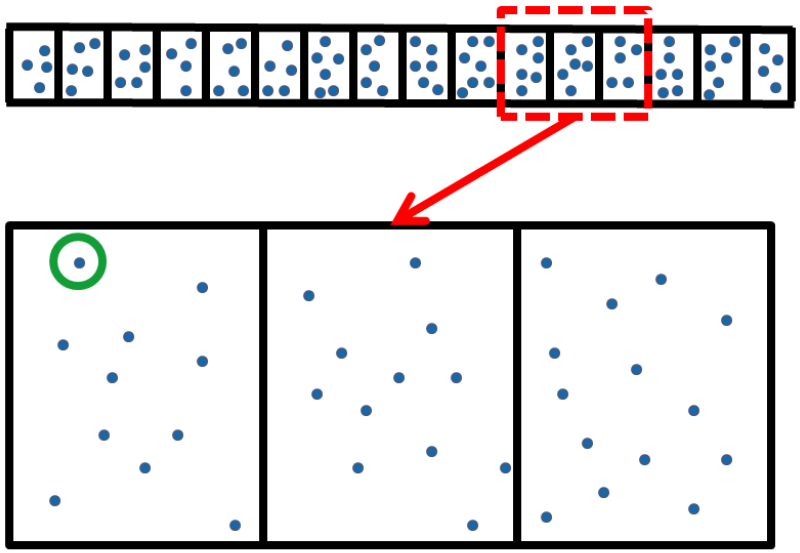

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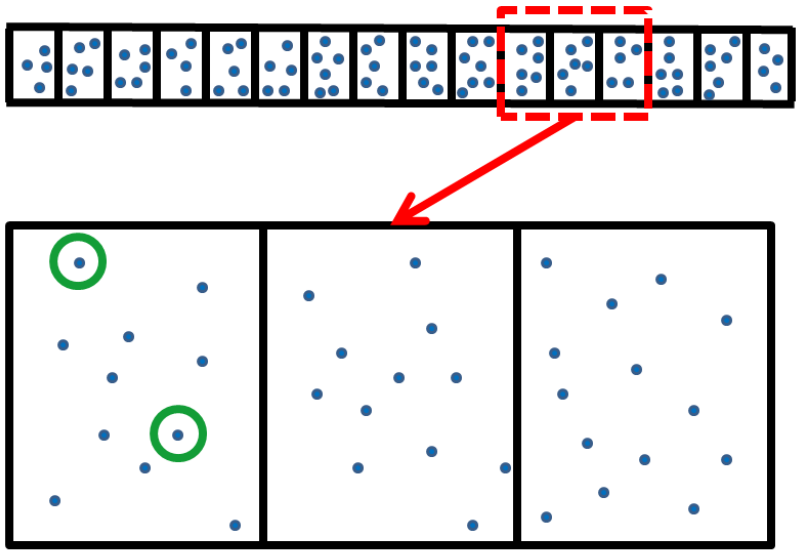

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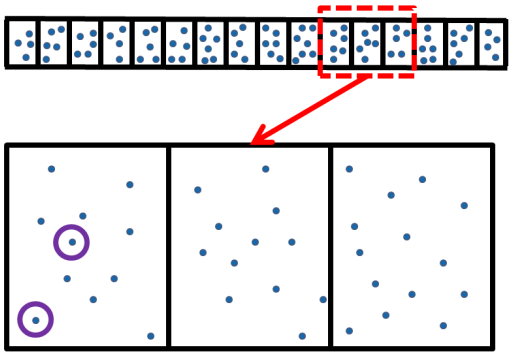
DSMC Collisions

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.

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

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

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V_c = Cell volume.

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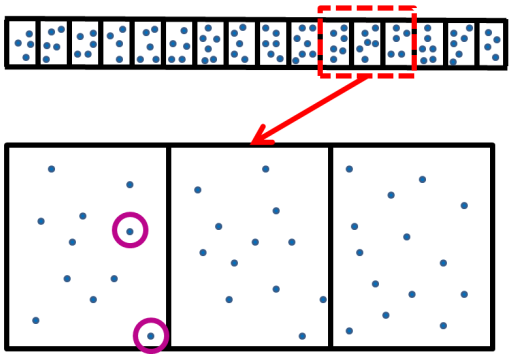

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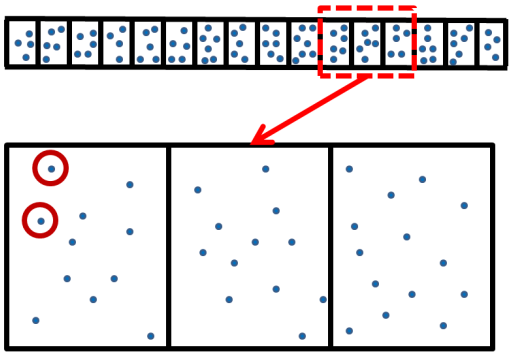

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Hard-Sphere Model

The hard-sphere collision model is the simplest model used in DSMC. In most collision models σ_T is a function of the relative speed between the two molecules. For hard spheres, σ_T is independent of the relative speed.

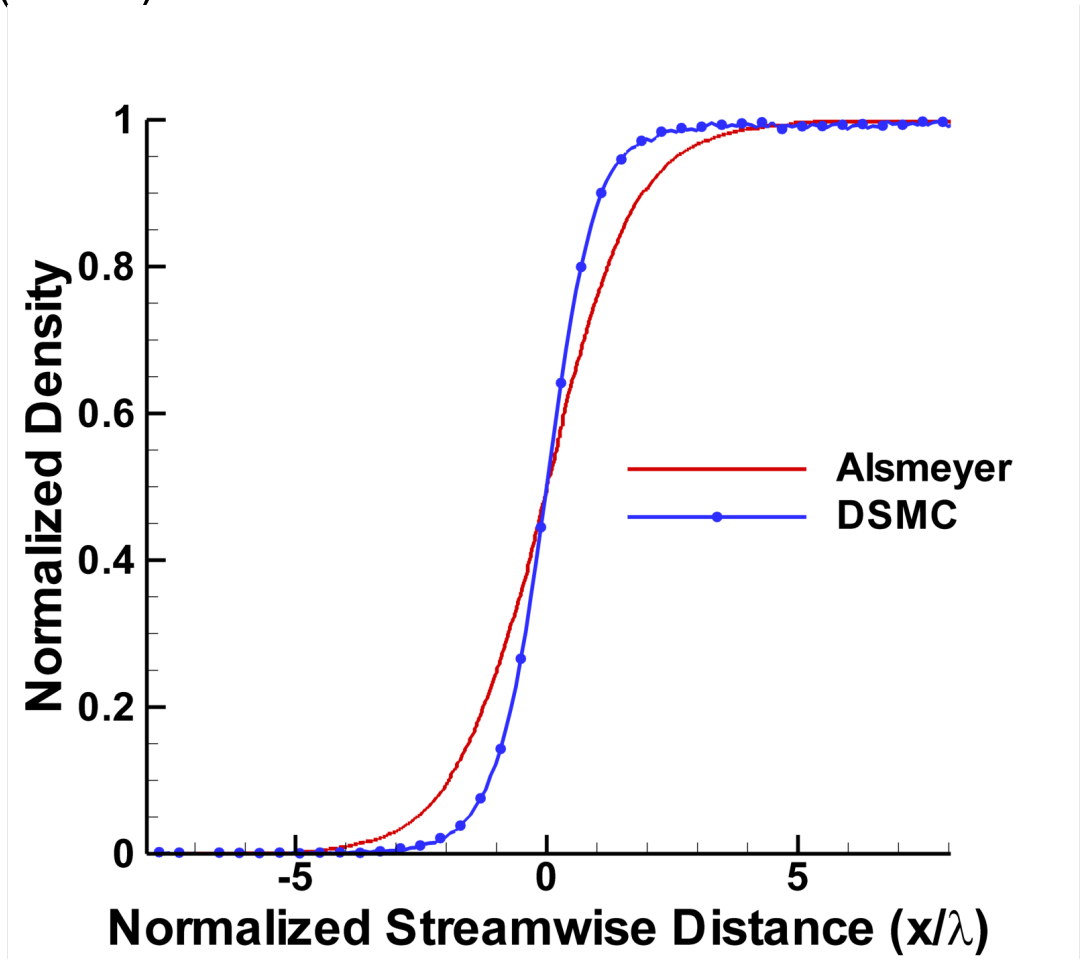
For a monatomic gas:

$$\sigma_T = \pi d_{HS}$$

Thus, for a given species, there is only one parameter to calibrate, the hard-sphere diameter d_{HS}.

1D Shock in Argon - Hard-Sphere Model

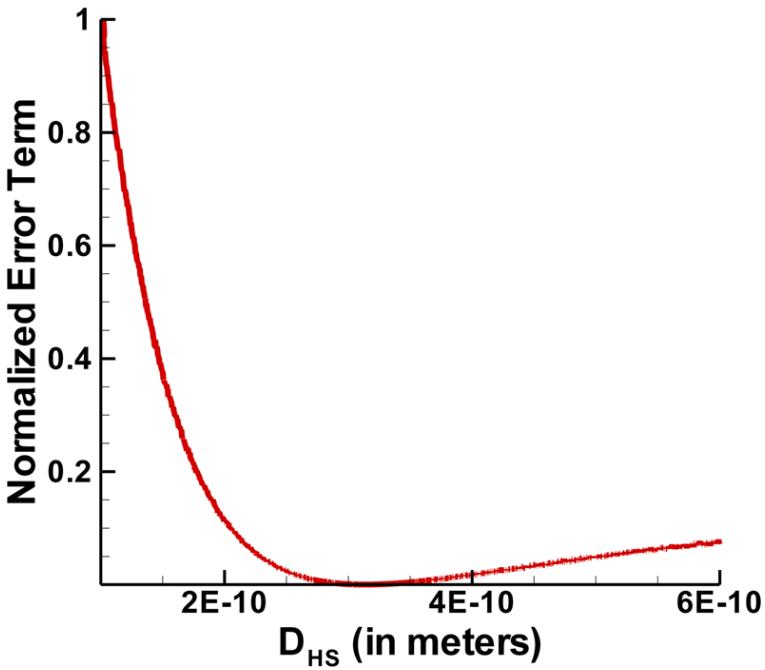
DSMC simulation of 1D shock in argon at Mach 3.38, using the hard sphere collision model, compared to experimental data from Alsmeyer (1976).

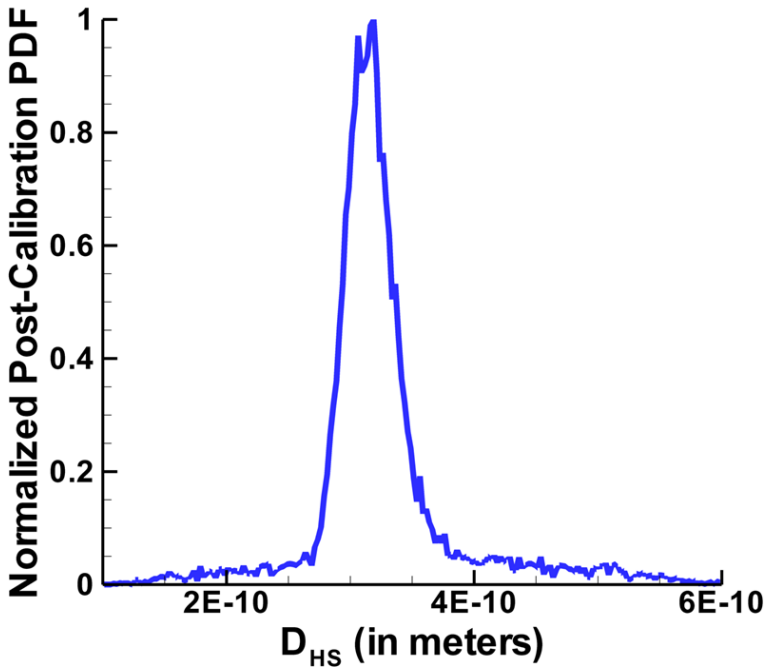


$$\tilde{\rho}_{error} = \tilde{\rho}_{Als} - \tilde{\rho}_{DSMC}$$
$$E = [\tilde{\rho}_{error}][\tilde{\rho}_{error}]^T$$
$$P = e^{-\frac{1}{2}\sigma E}$$

Hard-Sphere Diameter for Argon

- Parameter to be calibrated is d_{HS}, the hard-sphere diameter for argon.
- Brute force method used to explore the parameter space.
- Metropolis-Hastings algorithm used to solve inverse problem.
- Normalized density profiles from Alsmeyer(1976) used for calibration.





Variable Hard Sphere Model

The VHS method 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 method.

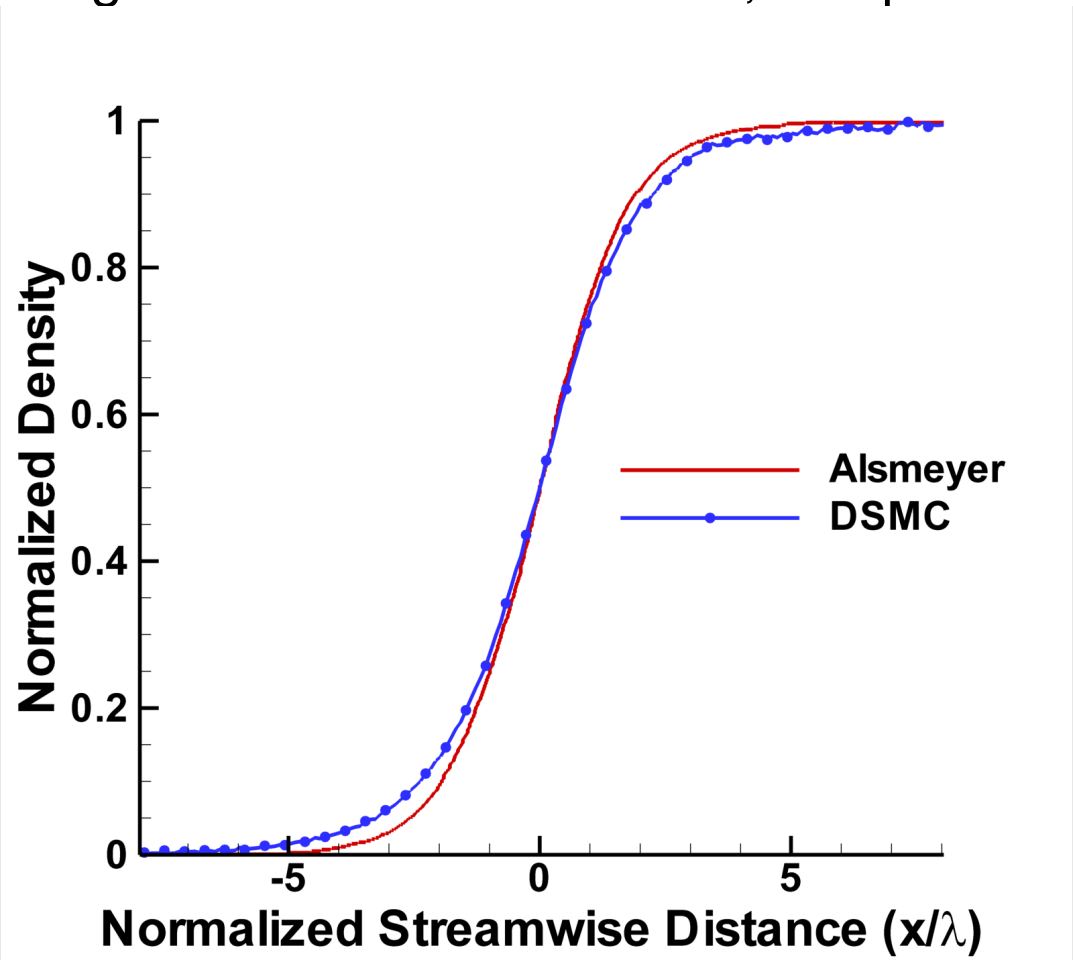
$$\sigma_T = \pi d_{VHS} = \pi d_{ref} \left(\frac{c_{r,ref}}{c_r} \right)^{(\omega - \frac{1}{2})}$$

The above formulation is good for bringing out the underlying physics, since ω is the temperature-viscosity exponent, and d_{ref} will have values which are of the same order as the hard sphere diameter. However, for MCMC purposes, there are only two relevant parameters here, d_{ref} and ω.

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

1D Shock in Argon - VHS Model

DSMC simulation of 1D shock in argon at moderate Mach numbers, now using the VHS collision model, compared to data from Alsmeyer (1976).



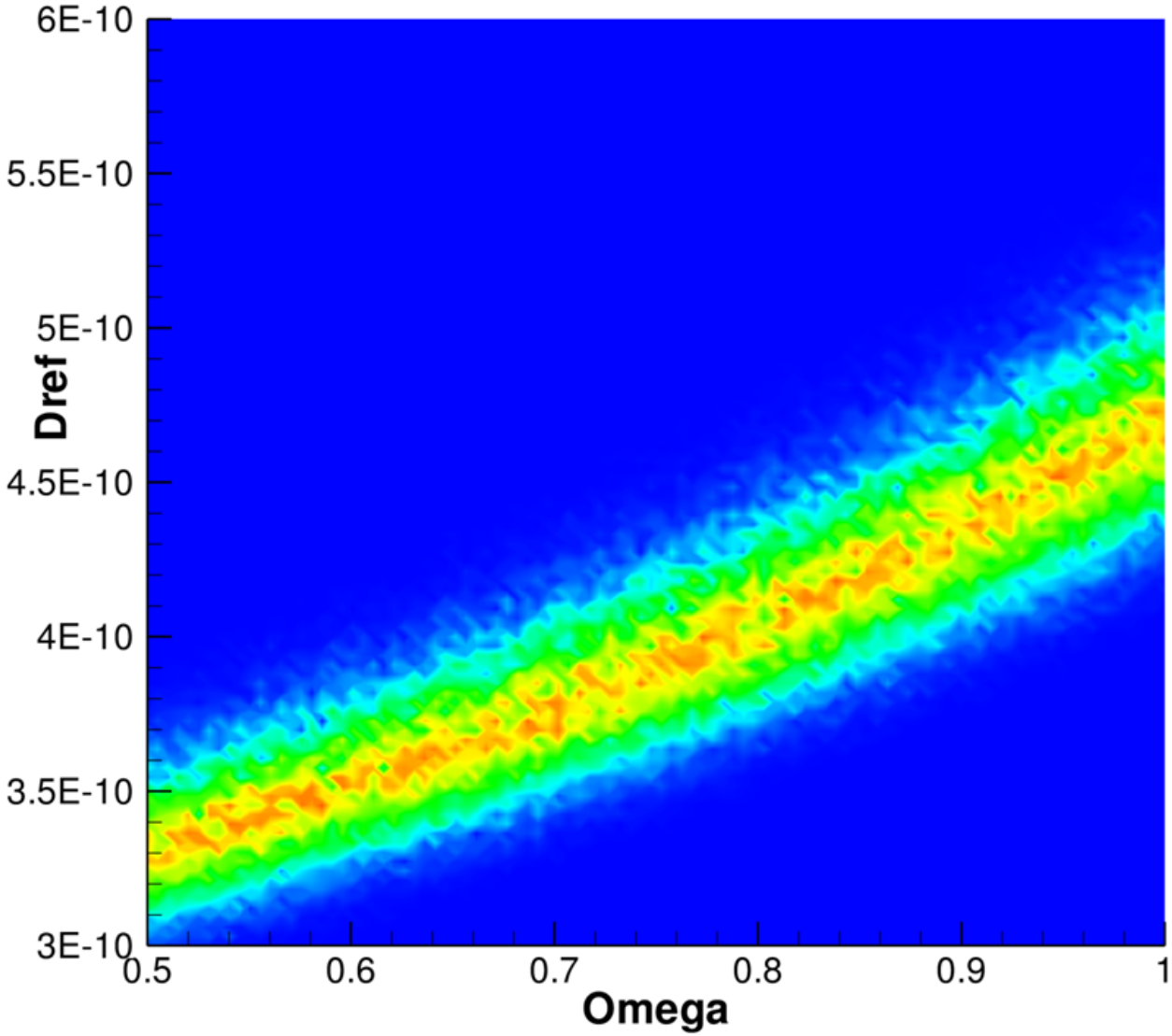
$$\tilde{\rho}_{error} = \tilde{\rho}_{Als} - \tilde{\rho}_{DSMC}$$
$$E = [\tilde{\rho}_{error}][\tilde{\rho}_{error}]^T$$
$$P = e^{-\frac{1}{2}\sigma E}$$

VHS Parameters for Argon

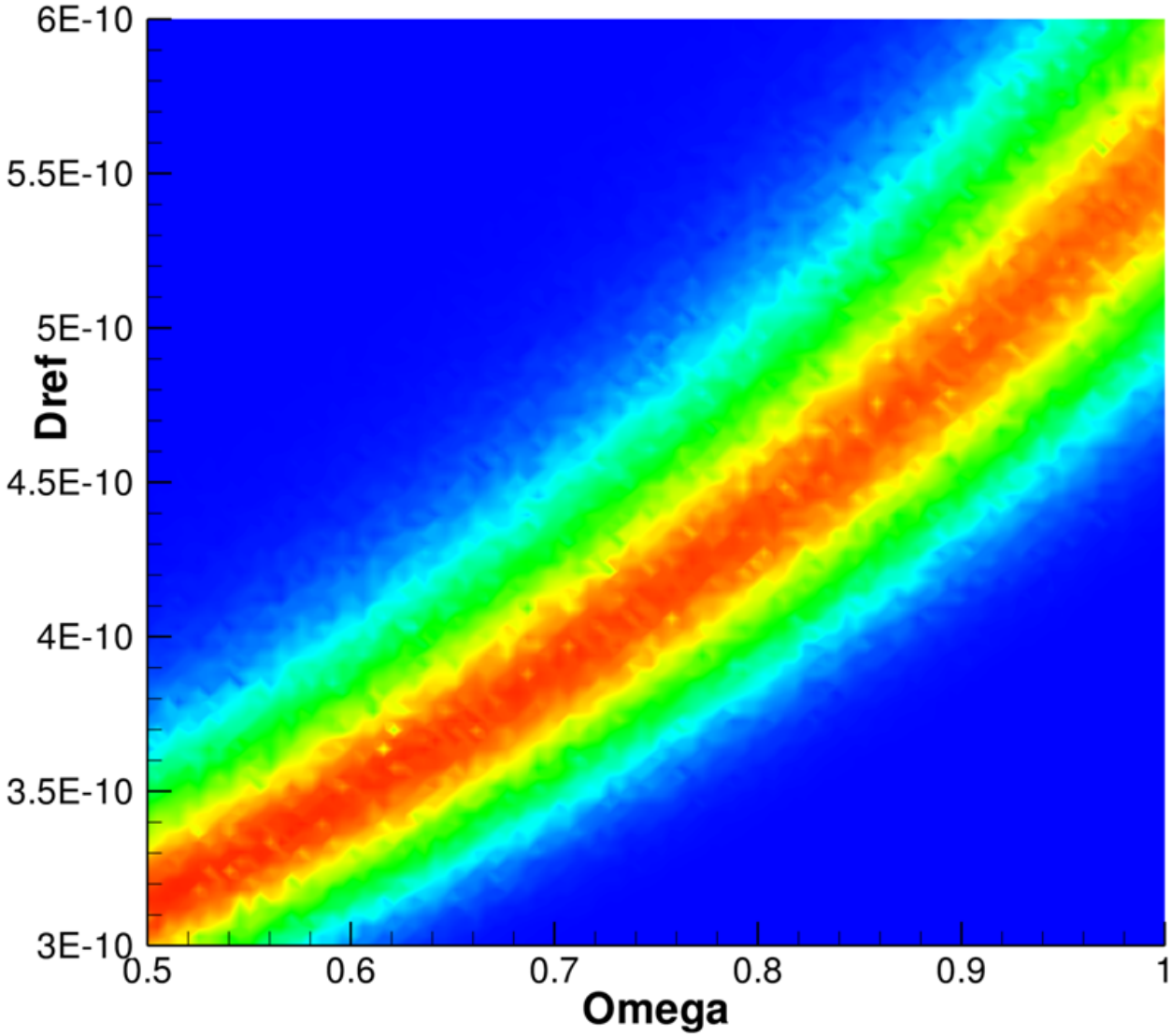
DSMC simulation of 1D shock in argon at moderate Mach numbers, now using the VHS collision model.

- Parameters to be calibrated are d_{ref} and ω, the reference diameter and the temperature-viscosity exponent for argon.
- Brute force method used to explore the parameter space.
- Normalized density profiles from Alsmeyer(1976) used for calibration.

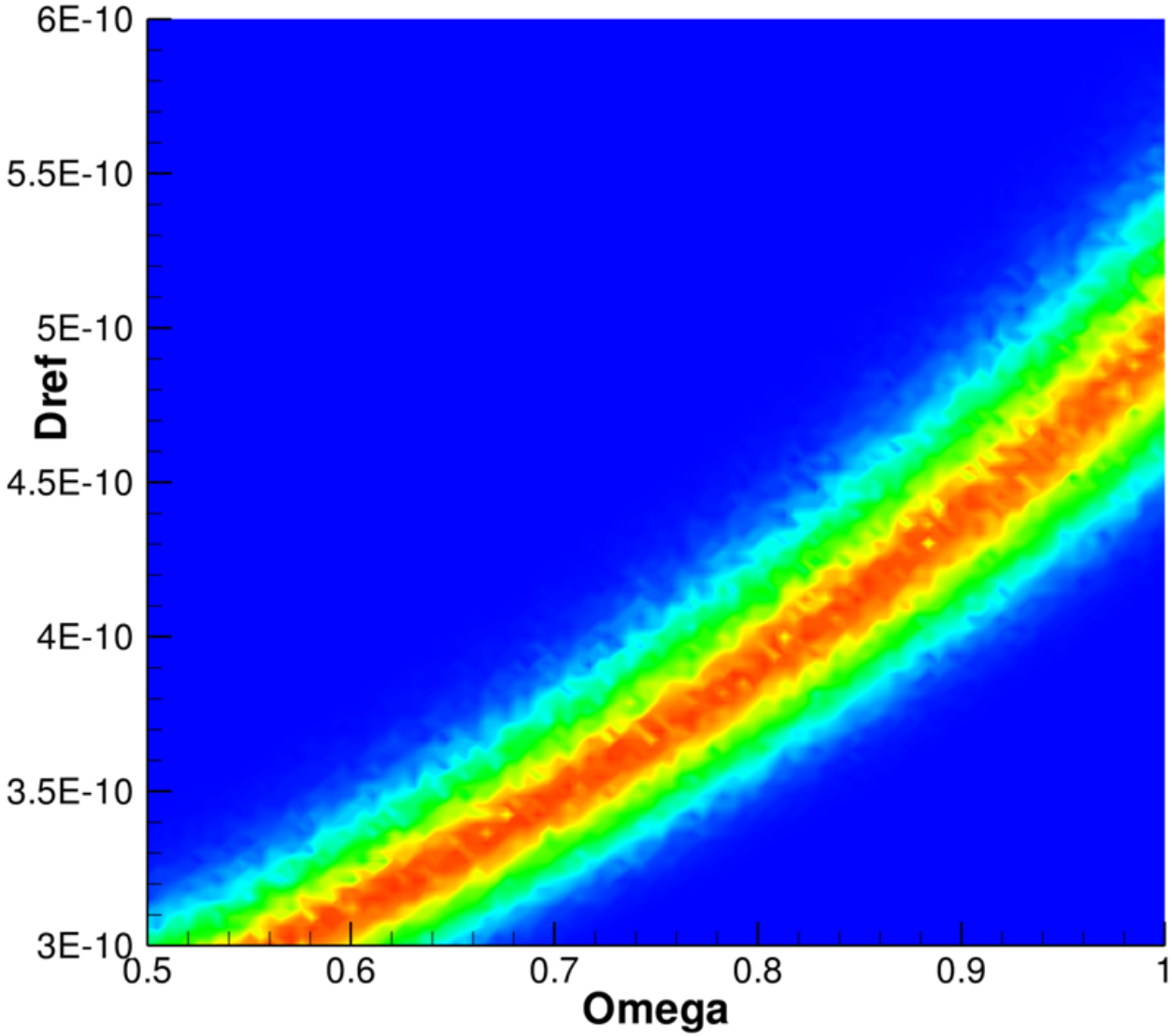
Uniform Sample of the Parameter Space: Mach 1.76



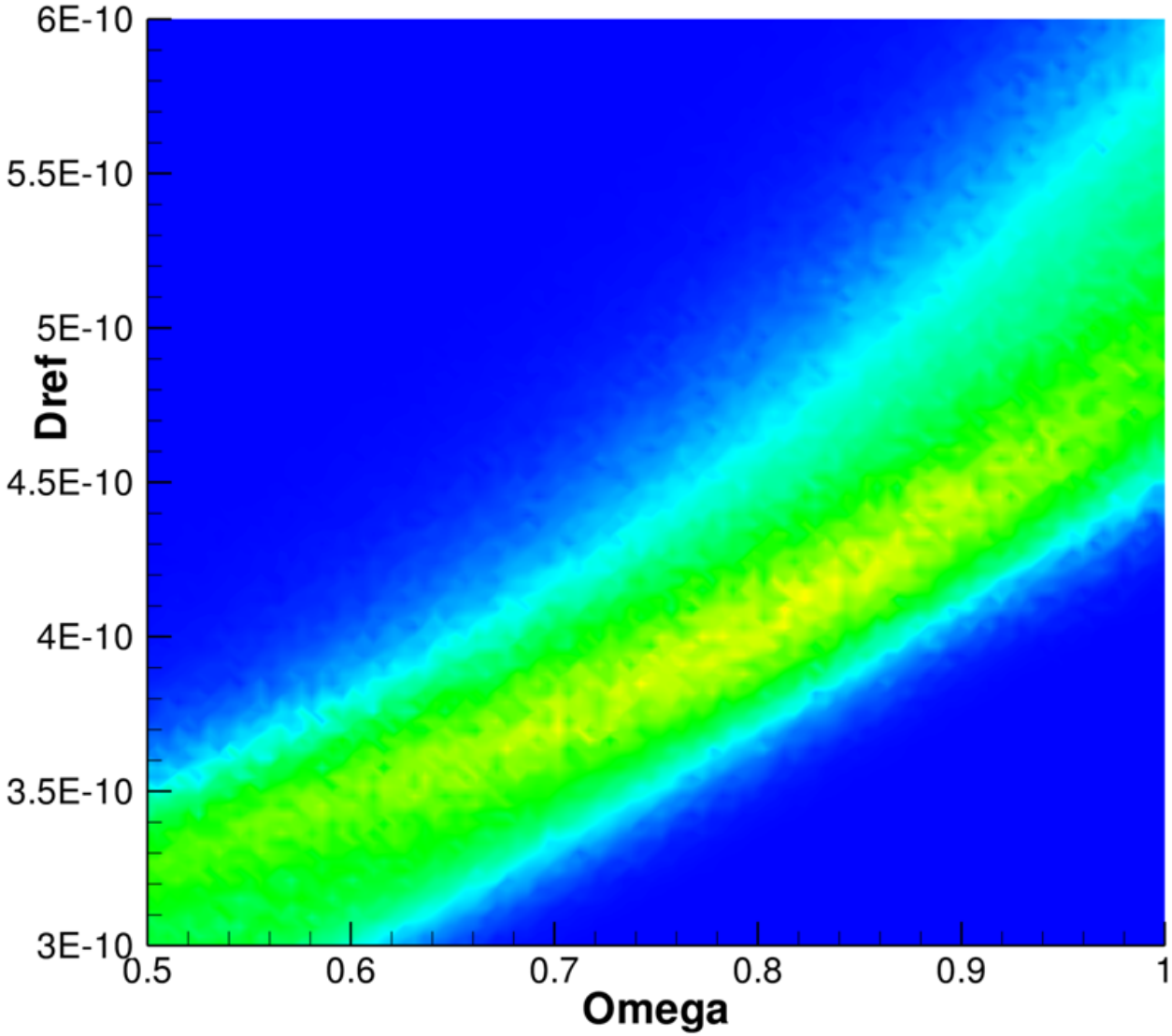
Uniform Sample of the Parameter Space: Mach 3.38



Uniform Sample of the Parameter Space: Mach 9.0



Uniform Sample of the Parameter Space: Combined



Current and Future Work

- Code currently being tested with multiple species, which will allow for calibration with helium-xenon shock data.
- Chemical reactions will be added, starting with simple reactions and moving towards high-temperature air chemistry.
- Chemistry introduces a host of new parameters which can be calibrated, and also makes available a great deal of additional experimental data.
- If necessary, code can be parallelized.
- Ultimately, would like to provide the DSMC community with calibrated values for parameters which are important for air chemistry, such as reaction and vibrational excitation cross sections.
- A DSMC code specifically designed to solve the shock tube problem might also provide useful insight for the PECOS shock tube group.