Molecular Gas Dynamic Simulations (MGDS) group:
(1 postdoctoral researcher, 2 PhD students, 2 Masters students)

- Directly incorporate advances in computational chemistry into macroscopic gas-dynamic models and simulations

- Research focuses on:
  - Gas-Phase collisions/reactions
    - AFOSR Young Investigator Program
  - Gas-Surface collisions/reactions
    - AFOSR – Aerothermodynamics
  - Large-scale Monte Carlo Simulation
    - NASA MSI - UMN
  - Hybrid DSMC-CFD Simulation
    - NASA
  - Continuum CFD Simulation
    - AFOSR – MURI Fundamental Processes in High-T Gas-Surface Interactions
The direct simulation Monte Carlo (DSMC) method

1. Decouples movement and collision processes
   - move particles significantly towards next collision
   - $\Delta t \leq \tau_c$ (mean-collision-time), typically $\Delta t \approx \frac{1}{5}\tau_c$

2. Treats collisions in a statistical (Monte Carlo) manner
   - randomly select collision pairs within the same cell (allow nearby particles to collide)
   - $\Delta x \leq \lambda$ (mean-free-path), typically $\Delta x \approx 0.5\lambda$
   - simulating real number density not required (use particle weights): $n = N_{p-cell}W_p$

$N_{p-cell} \approx 20$
Basic DSMC Algorithm

- Initialize system with particles
- Loop over time steps
  - Create particles at open boundaries
  - Move all the particles
  - Process any interactions of particle & boundaries
  - Sort particles into cells
  - Sample statistical values
  - Select and execute random collisions

Example: Flow past a sphere
Hypersonic Flow over a Planetary Probe
Cut-Cell Algorithms

- Cartesian flow field grids require non-trivial cut-cell algorithms for embedding complex geometry
- However, once written/debugged/verified, such treatment is very general, robust, and natural for DSMC
Rarefied Flow over MIR-Space Station
Air Flow over Nanoparticles

- Characterization of nanoparticle pollutants
- Low speed, complex geometry
- DSMC in transition regime
DSMC compared to CFD

- Boltzmann Equation:
  \[ \frac{\partial n f}{\partial t} + \mathbf{c} \cdot \nabla n f = \Delta [n f]_{\text{collisions}} \]

- Collision Rate and Transport Properties:
  In each DSMC cell, particles are randomly paired up and collided with the following probability:

  \[ P_{\text{collision}} \approx \frac{(C_{cc} g \Delta t) W_p}{V_{cell}}, \text{ where } [C_{cc} = \text{collision cross-section}] \text{ and } [g = \text{relative speed}] \]

  \[ VHS \text{ model: } C_{cc} = \frac{\pi d_{ref}^2}{g^{2z}} \rightarrow \mu = \mu_{ref} \left( \frac{T}{T_{ref}} \right)^\omega, \text{ where } \omega = \frac{1}{2} + \zeta \]

  \[ \begin{cases} 
    \mu, \kappa = \text{fcn}(T^\omega, \text{species}) \\
    D = \text{fcn}(T^\omega, \text{species})
  \end{cases} \]
Vibrational relaxation time, $\tau_{vib}$, is rewritten as a probability of vibrational energy exchange for individual collisions, $p(g)$:

The average probability is:

$$\bar{P} = \frac{1}{\tau_{vib} \nu}, \text{ where } \nu \text{ is the collision rate, and } \tau_{vib} = \frac{1}{p} \exp[A T_{tra}^{-1/3} + B]$$

(Millikan and White rates with Park’s high-T correction are used)

The probability for a given collision is then:

$$p(g) = \frac{1}{Z_o} g^\alpha \exp\left(-\frac{g^*}{g}\right), \text{ such that } \bar{P} = \int_0^\infty p(g) f(g) dg$$

- $Z_o$, $\alpha$, and $g^*$ are determined to reproduce curve-fit data when integrated over an equilibrium velocity distribution
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(Millikan and White rates with Park’s high-T correction are used)

- The probability for a given collision is then:
  \[ p(g) = \frac{1}{Z_o} g^\alpha \exp \left( -\frac{g^*}{g} \right), \text{ such that } \overline{P} = \int_0^\infty p(g) f(g) dg \]

- $Z_o$, $\alpha$, and $g^*$ are determined to reproduce curve-fit data when integrated over an equilibrium velocity distribution.

\[
\begin{align*}
P_{\text{vib-rot-trans}} &\approx fcn(g, e_{\text{rot}}, e_{\text{vib}}, Z_{\text{rot}}, Z_{\text{vib}}, \text{species}) & \quad \frac{\partial E_{\text{rot}}}{\partial t}, \frac{\partial E_{\text{vib}}}{\partial t} = fcn(T, T_{\text{rot}}, T_{\text{vib}}, \tau_{\text{rot}}, \tau_{\text{vib}}, \text{species}) \\
P_{\text{dissociation}} &\approx fcn(e_{\text{coll}}, E_{\text{ref-diss}}, p_{\text{steric}}, \text{species}) & \quad k_{\text{dissociation}} = fcn(T, T_{\text{vib}}, T_{\text{ref}}, \text{species})
\end{align*}
\]
Collision-cross sections can be determined using computational chemistry (interatomic potentials):

\[
\chi(g^*, b^*) = \pi - 2b^* \int_{r_{ij,m}}^{\infty} \frac{dr_i^* / r_{ij}^*}{\sqrt{1 - \frac{b^2}{r_{ij}^2} - \frac{\psi(r_{ij}^*)}{g^*}}}
\]

At high temperatures (>300 K for Argon), the DSMC-VHS collision assumption is valid:

\[
Q(2)^*(g^*) = 3 \int_0^{\infty} (1 - \cos^2 \chi) b^* db^*
\]

Many DSMC collision models exist, extremely careful and expensive experiments are required to test their accuracy (very limited data)…

As MD potentials increase in sophistication and physical accuracy, MD could potentially be used to better-inform DSMC collision models.
Molecular Dynamics (MD) Simulation of Shocks

- Normal shocks involve highly non-equilibrium flow and are stringent tests for collision models, they are symmetrical and contain a feasible number of atoms (40 mean-free-paths, typically between 500,000 and 1 million atoms)

“LAMMPS”
open-source
MD code
(Sandia National Laboratory, USA)
Combined Event-Driven / Time-Driven MD

- Event-Driven (ED) MD literature
  1. Efficient detection of impending collisions (neighbor lists, scales with $O(N)$ or better).
  2. Data structures for efficient sequencing of events (heaps, binary trees, scaling with $O(N)$).
  3. Collision detection algorithms for non-spherical (hard) particles.

Near perfect agreement between MD and DSMC for density, temperature, and velocity distribution functions (all Mach numbers)

- DSMC-VHS power-law assumption is very accurate if $\omega$ chosen properly ($\omega=0.7$)
- Consistent with LJ collision cross-section theory and reported values of $\omega$

Helium(98.5%) – Xenon(1.5%) Mixture

- Mach 3.61, T=300K, $\rho = 0.5$ kg/m$^3$ – simulation (dilute conditions)

  ~420,000 atoms
  5 days on 128 CPUs or
  5 days on 2 CPUs
  (accelerated method)

- Clear species separation measured experimentally due to mass disparity

- Experiment by Gmurczyk et al., 1979
Helium - Argon Mixtures

Mach 1.58
T=162 K
\( \rho = 0.1 \text{ kg/m}^3 \)
- simulated under dilute conditions
\( \sim 680,000 \) atoms

Experiments by Harnett and Muntz, 1972

Parallel/Perpendicular Temperatures (left)
Avg. species velocities (right)
Nitrogen Shock Waves (Rotational Excitation)

- Mach 7, T=28K, $\rho = 0.1 \text{ kg/m}^3$ – simulation (dilute conditions)
- MD models atoms only; harmonic oscillator potential for intra-molecular and LJ for inter-molecular interactions (no dissociation possible)

- Experiment by Alsmeyer, 1977
- Density and rotational temperature profiles
- As good or better agreement than existing DSMC models
Collisions involving vibrational energy exchange will require Potential Energy Surfaces (PES) computed from Quantum Mechanics methods.

Treatment of low-lying electronic levels (oxygen) a difficult problem. Collaboration with Don Truhlar’s group (UMN-Chemistry).

ED/TD MD simulations would produce large database of collision outcomes. However, would inherently contain the most dominant transitions that actually occur in the shock layer.

Potentially:
- Enable model reduction
- Provide a baseline solution
Non-Equilibrium Flows (Hypersonics and MEMS)

- Wide variation in the Knudsen number
  \[ Kn = \frac{\lambda}{l_c} \]
  - Range of altitudes, extreme compression/expansion regions
  - Thin shock waves, boundary layers, and sharp leading edges
  - Interactions between such phenomena
Modular Particle-Continuum (MPC) - Motivation

- Aerothermodynamics of non-equilibrium hypersonic flows
  - accurate particle simulation in localized regions of non-equilibrium flow (shock, boundary layer, and wake regions)
  - efficient continuum simulation in near-equilibrium regions
- a hybrid particle-continuum algorithm enables the separation of disparate length and time scales
Continuum Breakdown

- Continuum breakdown parameter:
  - Gradient-Length Knudsen Number

\[ Kn_{GL} = \max \left( \frac{\lambda}{Q} |\nabla Q| \right) \]

\[ Q = \rho, |V|, T \]

- Cutoff Value
  - \( Kn_{GL} > 0.05 \) (DSMC)
  - \( Kn_{GL} < 0.05 \) (CFD)
  - empirically determined based on database of DSMC and CFD results

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Domain Decomposition and Mesh Refinement

- Begin with a NS solution on a mesh designed for NS equations
- Continuum breakdown parameter sets up initial particle regions (shock, wake)
- Particle mesh refined down to $\lambda$ (modular - separate meshes)
- Larger continuum cells and larger implicit time-steps are responsible for most of computational speedup (DSMC-cost $\sim$ 3xCFD-cost per cell per timestep)
Information Transfer

- **State-based coupling**
  - Chapman-Enskog distribution of particles in DSMC boundary cells (initially, entire particle region filled with particles corresponding to NS solution)
  - Use averaging techniques to provide macro-properties for NS boundary cells
  - Information transfer involves updating the standard boundary conditions in both particle and continuum regions
Controlling Statistical Scatter in DSMC Averages

- Sub-relaxation average:
  \[
  \overline{A_j} = (1 - \theta) \overline{A_{j-1}} + \theta A_j
  \]

- Occasionally corrected to reduce the time-lag
  \[
  \overline{A_j}' = \overline{A_j} + \frac{(1 - \theta)^{j-i}}{1 - (1 - \theta)^{j-i}} (\overline{A_j} - \overline{A_i}'),
  \]
  \[
  j = \frac{1}{\theta} + i
  \]

- Statistical scatter controlled very well for hypersonic steady-state flows
MPC Simulation of a 2D Cylinder

- **PROBLEM SETUP:**
  1. Obtain initial NS solution.
  2. Apply $\text{Kn}_{GL}$ and setup DSMC mesh.
  3. Fill with particles consistent with initial NS solution (Chapman-Enskog vdfs).
  4. Simulate particle regions using the DSMC method. The solution should progress towards the correct non-equilibrium solution.
  5. Transfer this information into continuum regions and update the NS solution.

N$_2$ at 70 km
Mach 3, 6, 12
$\text{Kn}_D = 0.01$
$\text{Tw} = 300, 500, 1000K$
**Progression of MPC Solution**

- DSMC regions progress towards correct non-equilibrium solution
- Overlap regions facilitate the movement of interfaces

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**Shock Region**

- Increasing time

**Wake Region**

- Increasing time

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Mixed Continuum and Non-Equilibrium Flow

- Shock interior
  - Highly non-equilibrium
- MPC particles reproduce full DSMC distribution
Mixed Continuum and Non-Equilibrium Flow

- Post shock region
  - Near equilibrium
- Navier-Stokes equations accurately model the flow
Mixed Continuum and Non-Equilibrium Flow

- Post shock continuum region
  - Near equilibrium
- Navier-Stokes equations accurately model the flow
Mixed Continuum and Non-Equilibrium Flow

- Rapidly expanding wake region
  - Highly non-equilibrium
  - Significant velocity slip
- MPC particles reproduce full DSMC results
Planetary Probe - High Density

- Axi-symmetric
- 70 degree blunted cone (15cm diameter)
- Mach 16 flow of $N_2$
- 2 order of magnitude in $\lambda$
- $Kn_D = 0.001$

- Experiment performed in LENS facility at CUBRC

- Top - Full DSMC
- Bottom - Solution in particle regions of a hybrid simulation

- Shock wave not simulated using DSMC

(10 times faster than DSMC)
Planetary Probe - High Density

- Fore-body Flow
- NS (and hybrid) agrees very well with DSMC except for shock interior
- Previously determined that modeling the shock with DSMC is not necessary to predict the remainder of the flow and surface properties
Planetary Probe - High Density

- **Heating Rates**

- \( s = \) distance along the capsule surface starting at stagnation point

- Hybrid results in excellent agreement with full DSMC simulation

- All simulations agree in compressed fore-body region

- NS (no-slip) typically over predicts heating rates especially in rarefied wake region
Hollow Cylinder-Flare

- Axi-symmetric
- Mach 12 flow of $N_2$
- Shock-shock, shock-boundary layer interactions
- Re-circulating flow at cylinder-flare juncture
- Experiment performed in LENS facility at CUBRC (Run #11)

- Top - Full DSMC
- Bottom - Solution in particle regions of a hybrid simulation

(1.4 times faster than DSMC)
Hollow Cylinder-Flare

- Interface locations and mesh refinement

- Final interface lies closer to cylinder wall due to slip velocity at the wall

- The loosely-coupled hybrid method is able to automatically move interfaces and accommodate this

- Flow properties are extracted at several stations along geometry
Hollow Cylinder-Flare

- Cut 2 - rarefied flow above cylinder
- DSMC and hybrid shock lies closer to cylinder wall
- Region of thermal non-equilibrium next to the wall (temperature jump)
- Note the portion of flow in thermal equilibrium which is accurately modeled by NS equations
- Particle regions provide significantly new boundary conditions for continuum regions
Rotational/Vibrational Non-Equilibrium

- Modularity allows for rapid incorporation (with confidence) of advanced physical models
- Both DSMC and CFD codes already contain such models (i.e. CFD multi-temperature)
- Only the statistical scatter and information transfer for new physical parameters need be addressed
- Agreement between DSMC and NS models for near-continuum flows currently an issue
Hybrid DSMC-CFD Conclusions

1. Statistical scatter can be controlled for hypersonic steady-state flows

2. Loose-coupling combined with mesh refinement enables both temporal and spatial-scale decoupling

3. Localized non-equilibrium regions are present and are well detected by $Kn_{GL}$ continuum breakdown parameter and cutoff value (>0.05)

4. Such a Modular Particle-Continuum (MPC) method is able to accurately reproduce full DSMC flowfield, surface properties, and velocity distribution functions, using less computational resources

5. Challenges remain for 3D complex geometry and especially for consistent advanced physical models
QUESTIONS?

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