Direct Molecular Simulation of Hypersonic Flows

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ME Dept. Seminar, University of Kentucky (11/29/12)
We are nearing the point where we can directly simulate high-speed (thermochemical) nonequilibrium flows with atomistic simulations.

Flows consist of many collisions, but each involving only 2-6 atoms.

Collisions can be modeled with quantum mechanics by physicists and chemists.

“Atomistic fluid dynamics”

Large-scale computing and the nature of dilute gases enables such direct simulation of practical flows.
Outline

• The Direct Simulation Monte Carlo (DSMC) particle method

• All-atom Molecular Dynamics (MD) simulation of shock waves

• Spatial and temporal scales relevant to dilute gases
• DSMC vs. CFD (collision models vs. continuum models)

• Direct Molecular Simulation (DMS)
  – no DSMC collision models, simply embed MD collisions directly

• GPU acceleration of DMS

• Future potential of DMS

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Direct Simulation Monte Carlo (DSMC)

Google: “DSMC Bird”
Look for the: “Visual Wind-Tunnel Program”
For $Kn = \frac{\lambda}{L} > 0.01$ continuum modeling (Navier-Stokes) becomes inaccurate.

$Kn \sim 0.01$ (large $\lambda$)

$Kn \sim 0.01$ (small $L$)

$\Delta t \sim 1$ mean-collision-time

$\Delta x \sim 1$ mean-free-path ($\lambda$)

Stochastic collisions within $\Delta x$

Approx. 50 molecules per cell

Diffuse reflection from surfaces

$Kn \sim 0.01$ (small $L$)

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Thermochemical Nonequilibrium

Finite-Rate Energy Exchange
- Translational
- Rotational
- Vibrational
- Electronic
- Chemical

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1. Quantum mechanical (QM) energy calculations
2. Fit a potential energy surface (PES)
3. Integrate atomic trajectories on PES

Trajectory calculations simply integrate:
\[ \ddot{r}_i = \frac{m_i}{r_i} \]

Analytical function that inputs atomic positions and returns atomic forces
All-Atom Molecular Dynamics for Shock Waves

- Pure MD, millions of atoms, millions of timesteps, millions of collisions (~128 core CPUs for ~4 days)
- No adjustable parameters, ex. LJ-potential for Argon, Helium, Xenon, and nitrogen (vibrational ground state) are non-negotiable
- Can use freely-available LAMMPS MD code from Sandia

FIG. 3. Comparison between MD and DSMC temperature and density profiles for (a) $M_1=1.55$, (b) $M_1=5$, (c) $M_1=9$; (d) reciprocal shock thickness.

FIG. 6. Perpendicular vdf for $M_1=9$ (DSMC is the solid line, MD are circles). (a) $\rho_a=0.148$ (DSMC) and $\rho_a=0.144$ (MD), (b) $\rho_a=0.330$ (DSMC) and $\rho_a=0.348$ (MD), (c) $\rho_a=0.540$ (DSMC) and $\rho_a=0.561$ (MD), and (d) $\rho_a=0.743$ (DSMC) and $\rho_a=0.762$ (MD).
Xenon-Helium and Argon-Helium Mixtures


Figure 3: Species normalized density profiles obtained with MD and compared to the experimental measurements of Gmurczyk and co-workers.\textsuperscript{19} $\lambda_1$ values are listed in Tab. 2 for each case.

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Xenon-Helium and Argon-Helium Mixtures

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Diatomic Nitrogen


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Vibrational Nonequilibrium (In Progress)

- High energy collisions are sensitive to the PES (repulsive wall)

- Validate with Millikan and White experimental data for near-equilibrium (T~Tv)

- Collaboration with Minnesota Dept. of Chemistry to develop accurate PES for air species (dissociation)
Vibrational Nonequilibrium (In Progress)

- All-atom simulations
- 5 million atoms
- Rotation and vibrational energies are post-processed
- EDTD-MD and Trajectory-DSMC are very promising for arbitrary PES

Graph showing normalized temperatures as a function of distance.

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Combined Event-Driven / Time-Driven MD


Pure MD wastes a lot of time.

Event Driven

Time Driven

ME Dept. Seminar, University of Kentucky (11/29/12)
Combined Event-Driven / Time-Driven MD


- ED/TD MD algorithm detects and advances simulation to impending interactions, while accurately integrating each interaction using conventional Time-Driven (TD) MD.
- Multi-body interactions are also detected and simulated.
- Recently extended to polyatomic molecules including chemical reactions.
- For example, the time of an impending collision is:

\[ \theta_{ij} = \frac{\left( -v_{ij} \cdot r_{ij} \right) \pm \sqrt{(v_{ij} \cdot r_{ij})^2 - v_{ij} \cdot v_{ij}(r_{ij} \cdot r_{ij} - r_c^2)}}{(v_{ij} \cdot v_{ij})} \]

- Pure MD shocks: ~128 cores for 4 days
- ED/TD MD shocks: 1 core for 10 days (~50x faster - *exactly* the same result)
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Direct Simulation of Practical Flows

Molecular Dynamics

• Simulate every atom in real system
  – Thousands – Millions per $\lambda^3$
• Femtosecond ($10^{-15}$ s) timesteps

Vol $\sim \lambda^3$
Direct Simulation of Practical Flows

Molecular Dynamics
- Simulate every atom in real system
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Event-Driven Time-Driven MD
- Simulate every atom in real system
  - Thousands – Millions per $\lambda^3$
- Timesteps $\sim \tau_c$ (mean-coll-time)

Vol $\sim \lambda^3$

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• However, one can obtain precisely the same statistics with far fewer molecules. This is what DSMC does.

• Without all atoms and PES, collisions are chosen randomly within a cell (a very good assumption for dilute gases).
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):
     $$n = N_{p\text{-cell}} W_p$$
     $$N_{p\text{-cell}} \approx 20$$

$\Delta t \leq \tau_c$ (mean-collision-time), typically $\Delta t \approx \frac{1}{5} \tau_c$

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$$N_{p\text{-cell}} \approx 20$$
Direct Simulation Monte Carlo (DSMC)

There are two fundamental modeling requirements (assumptions) in DSMC:

A) **During one time step, how many of the (~20) particles in a certain cell should undergo a collision? How many should transfer internal energy? How many should chemically react?**
   - Collision rate directly related to viscosity, thermal conductivity, diffusion coefficients
   - Rotational/Vibrational “collision numbers” \((Z_{\text{rot}}, Z_{\text{vib}})\) determine rates of rotational/vibrational excitation/relaxation
   - Steric factors coupled with reaction activation energies determines rates of reaction

B) **For particles selected for the above types of collisions, what are the post-collision properties?**
   - Most widely used is the Borgnakke-Larsen model (relax towards equilibrium)
DSMC compared to CFD

- **Boltzmann Equation:**
  \[
  \frac{\partial f}{\partial t} + \mathbf{c} \cdot \nabla f = \Delta [nf]_{\text{collisions}} \quad f(x, c, t) \quad c(v_x, v_y, v_z) \quad x(x, y, z)
  \]

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

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

  MD potential ($\psi$) \quad $C_{cc} = fcn(g^\zeta, \text{species})$ \quad \[\mu, \kappa = fcn(T^\omega, \text{species})\]

  \[D = fcn(T^\omega, \text{species})\]
DSMC compared to CFD

- **Boltzmann Equation:**
  \[
  \frac{\partial n_f}{\partial t} + \mathbf{c} \cdot \nabla n_f = \Delta [n_f] \text{collisions} \quad f(x, \mathbf{c}, t) \quad \mathbf{c}(v_x, v_y, v_z) \quad \mathbf{x}(x, y, z)
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  \[
  C_{cc} = \text{fcn}(g^\zeta, \text{species})
  \]

  MD potential \((\psi)\) \(\times\) \[
  \{\mu, \kappa = \text{fcn}(T^\omega, \text{species})
  \]

  \[
  D = \text{fcn}(T^\omega, \text{species})
  \]

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DSMC compared to CFD

- Boltzmann energy distribution functions:

\[ f(e_{\text{ROT}}) \]

Boltzmann energy distributions

\[ e_{\text{ROT}}, e_{\text{VIB}} \rightarrow T_{\text{ROT}}, T_{\text{VIB}} \]

- Internal Energy Exchange and Dissociation:

\[ P_{\text{vib-rot-trans}} \approx \text{fcn}(g, e_{\text{rot}}, e_{\text{vib}}, Z_{\text{rot}}, Z_{\text{vib}}, \text{species}) \]

\[ \frac{\partial E_{\text{rot}}}{\partial t}, \frac{\partial E_{\text{vib}}}{\partial t} = \text{fcn}(T, T_{\text{rot}}, T_{\text{vib}}, \tau_{\text{rot}}, \tau_{\text{vib}}, \text{species}) \]

\[ P_{\text{dissociation}} = \text{fcn}(e_{\text{coll}}, E_{\text{ref-diss}}, p_{\text{steric}}, \text{species}) \]

\[ k_{\text{dissociation}} = \text{fcn}(T, T_{\text{vib}}, T_{\text{ref}}, \text{species}) \]
DSMC compared to CFD

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Boltzmann energy distributions

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Argon is accurately modeled by the Lennard-Jones potential:

\[ \psi(r_{ij}) = 4\epsilon \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^{6} \right] \]

where \( \epsilon/k = 119.18 \text{ K} \) and \( \sigma = 4.42 \text{ Å} \)

Scattering angle computed by integrating potential and is a function of relative speed (g) and impact parameter (b):

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

Collision cross-section obtained by integrating the scatter angle over all impact parameters and is function of relative speed (in this case):

\[ Q^{(2)*}(g^*) = 3 \int_{0}^{\infty} (1 - \cos^2 \chi) b^* db^* \]

Interatomic Potential to Viscosity (Argon)

- At high relative speed a power-law model for the collision cross-section is valid.

Variable-Hard-Sphere model in DSMC: \( Q_{VHS}^{(2)} = \frac{Q_{HS}^{(2)}}{g^{2\xi}} \)

- At low relative speeds the VHS model is less valid

- Upon integration of \( Q^{(2)}(g^*) \) using Chapman-Enskog theory:

\[
\Omega^{(2,2)*} = \frac{1}{3T^{*4}} \int_0^\infty \exp\left(-g^{*2}/T^{*}\right)g^{*7}Q^{(2)}(g^*)dg^*
\]

- DSMC-VHS collision model parameter:

\[
\mu_{VHS} \approx \mu_{REF}\left(\frac{T}{T_{REF}}\right)^\omega, \text{ where } \omega = \frac{1}{2} + \xi
\]

\( \omega \approx 0.66 \) for high T

\( \omega \approx 0.8 \) for low T
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For real gases, DSMC attempts to model the true cross-section (and also employs probabilistic models for post-collision properties).

However, an alternative is to integrate collisions directly within DSMC ("Trajectory-based DSMC") [only ~100x slower than DSMC].

Carefully match the HS cross-section with the impact parameter variation used for the collision calculations.

Simply make the HS cross-section conservatively large, and it will be the PES that determines the collision rate (and also post-collision states).

Predicting multibody collision rates is interesting (needed for recombination reactions).
Trajectory-DSMC vs. Pure MD

Exactly equal to pure MD.

There are no DSMC models that can get this level of agreement.

Exactly equal to pure MD.
Rotational level distribution functions within shock wave.

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Trajectory-DSMC vs. Pure MD

- Rotational level distribution functions within shock wave.

Exactly equal to pure MD.
Direct Simulation of Practical Flows

- Example trajectory embedded within a DMS calculation
- Long-lived collision that would likely be involved in a multibody collision
The Direct Simulation Monte Carlo (DSMC) particle method

All-atom Molecular Dynamics (MD) simulation of shock waves

Spatial and temporal scales relevant to dilute gases

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Future potential of DMS

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Trajectory-DSMC using GPUs

- >99% CPU time spent integrating collisions (DSMC move/sort/geom <1%). Thus perfectly suited for **GPU acceleration** (CPU handles move/sort/geom)
- Trajectory-DSMC ~100x more expensive than DSMC, but 2 weeks of GPU coding has found speed-up of 30x per GPU!

<table>
<thead>
<tr>
<th></th>
<th>~10^6 molecules</th>
<th>~4×10^6 molecules</th>
</tr>
</thead>
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<tr>
<td></td>
<td>avg.time DMSstep (s)</td>
<td>speedup</td>
</tr>
<tr>
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<td>1</td>
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<tr>
<td>CPU (OMP)</td>
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<td>11.52</td>
</tr>
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<td>1 GPU+CPU(OMP)</td>
<td>7.79</td>
<td>47.91</td>
</tr>
<tr>
<td>2 GPU+CPU(OMP)</td>
<td>5.17</td>
<td>72.27</td>
</tr>
<tr>
<td><strong>4 GPU+CPU(OMP)</strong></td>
<td><strong>3.69</strong></td>
<td><strong>101.23</strong></td>
</tr>
</tbody>
</table>

Table 1. Parallel scaling for GPU accelerated DMS simulations. OMP = OpenMP. The speedup/GPU is calculated as (speedup-11.5)/(# of GPUs)

- Condor Cluster (AFRL) = 164 GPUs (164 million particle simulation)
- Titan Cluster (DOE) = 18,688 GPUs !! (18 billion particles…)

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A New Rotational Nonequilibrium Model

- Current DSMC codes use either $Z_{\text{rot}} = 5 =$ constant or $Z_{\text{rot}}(T)$ – Parker
- Parker model fit to single experimental data set (experiments vary widely)
Our results clearly show that the rotational relaxation rate strongly depends on the **degree** of nonequilibrium and the **direction** to nonequilibrium.
Our results clearly show that the rotational relaxation rate strongly depends on the degree of nonequilibrium and the direction to nonequilibrium.
New Model Results

Atomistic shock wave simulations led directly to new DSMC and CFD models for rotation.

\[ Z_{\text{rot}}(T_t, T_r) = \frac{Z_r^\infty}{1 + \frac{T_r^*}{T_t}} \left( \frac{T_r}{T_t} \right)^n \]

\[ \tilde{p}_{\text{rot}}(\varepsilon_t, \varepsilon_r) = \frac{\Gamma(\frac{\zeta_t}{2})\Gamma(\frac{\zeta_r}{2})}{\Gamma(\frac{\zeta_t}{2} + n)\Gamma(\frac{\zeta_r}{2} - n)Z_r^\infty} \left[ 1 + \left( \frac{\zeta_t}{2} + n - 1 \right) \frac{k_B T^*}{\varepsilon_t} \right] \left( \frac{\varepsilon_t}{\varepsilon_r} \right)^n \]

Shock: \( T_1 = 300 \text{K}, M_1 = 7 \)
1) Pure Molecular Dynamics of normal shock waves is possible

2) MD simulations have been validated with all available experimental data for Ar, Ar-He, Xe-He, and N$_2$(rotation and vibration) shock waves

3) New internal energy relaxation physics were found for N$_2$ rotational excitation/relaxation (ground vibrational state)
   - weaker temperature dependence than prior models
   - strong dependence on direction and degree of nonequilibrium
   - new DSMC and CFD models formulated for rotation

4) Preliminary results show that trajectory-based DSMC exactly reproduces pure MD results at a cost $\sim$100x slower than DSMC. However, trajectory-DSMC is perfectly suited for GPU acceleration with realistic 30x/GPU speedup on existing architectures.

5) The capability exists to directly use QM collision routines from chemists and physicists for the simulation of 3D nonequilibrium flows over complex geometry.
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