Progress and Future Prospects for Particle-Based Simulation of Hypersonic Flow

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Hypersonics into the 21st Century – Research Progress since 2001 and 
Future Directions in Aerothermodynamics

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The long term goals for particle-based simulation research include:

1) Capability for large-scale particle solutions of 3D hypersonic flows that completely overlap with continuum (CFD) solutions.
   - this involves computational efficiency research
   - ultimately involves hybrid particle-continuum capability

2) Developing new, increasingly accurate, reduced-order models for engineering design and analysis.

3) Incorporating ab initio based (quantum chemistry) collision models directly into particle simulations to improve our understanding of hypersonic flows at the most fundamental level.

4) Experimental validation of particle simulation predictions.

The paper presents progress towards these goals and future research directions.

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Challenges and Future Directions

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4) Experimental validation of particle simulation predictions.

The presentation focuses on the highlighted topics.

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Outline

Molecular Dynamics

Direct Simulation Monte Carlo (DSMC)

Progress on a hybrid DSMC-CFD method
  - the need for highly consistent molecular-continuum models (new ones)

Trajectory-based DSMC simulations

State-resolved DSMC simulations

New physics revealed by these approaches
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All-Atom Molecular Dynamics

- Pure MD: millions of atoms, millions of timesteps ($\Delta t_{MD} \sim 10^{-15}$s), millions of collisions, deterministic given boundary conditions
- No adjustable parameters: simple potentials for argon, helium, xenon, and nitrogen (vibrational ground state) are established
- Freely-available LAMMPS MD code from Sandia is used

Potential Energy Surface (PES)

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Pure Argon and Xe-He / Ar-He Mixtures

- Significant experimental data exists for normal shock waves and accurate (yet simple) PES for these interactions are well-established
- Step-by-step validation of MD simulations


Diatomic Nitrogen (no vibrational excitation)

- MD validation with experimental data from Robben and Talbot (1966)
- PES involved rigid rotor molecules interacting with a site-to-site Lenard-Jones (LJ) potential


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Direct Simulation Monte Carlo (DSMC)

Molecular Dynamics

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

Vol $\sim \lambda^3$
Direct Simulation Monte Carlo (DSMC)

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

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

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Direct Simulation Monte Carlo (DSMC)

- One can obtain precisely the same statistics with far fewer molecules
- Deterministic nature is lost, however, in dilute gases the pre-collision orientations (not energies) of molecules are completely random
  - this random nature can be readily verified by pure MD simulations

\[ \text{Vol} \sim \lambda^3 \]

Each simulated particle represents a large number of identical real particles.
Direct Simulation Monte Carlo (DSMC)


DSMC assumptions (very good ones…)

1) Move molecules for timesteps of $O(\tau_c)$
2) Simulate only a (statistically necessary) fraction of real molecules
3) Select possible collision pairs within cells of size $O(\lambda)$ and randomize their orientations
**Direct Simulation Monte Carlo (DSMC)**


**DSMC assumptions (very good ones…)**

1) Move molecules for timesteps of O(τ_c)

2) Simulate only a (statistically necessary) fraction of real molecules

3) Select possible collision pairs within cells of size O(λ) and randomize their orientations

**DSMC collision models**

4) How many collisions should occur during a given τ_c and within a given λ^3?

5) What are the outcomes of these collisions?

… trajectory-based DSMC and state-to-state DSMC have the potential to eliminate (4) and (5)…
Direct Simulation Monte Carlo (DSMC)

Typical DSMC collision models

viscosity/diffusion \((\mu, \kappa, D)\)  ---- total cross-section  ---- prob. of collision
rotation/vibration relaxation \((\tau_r, \tau_v)\)  ---- collision numbers \((Z_r, Z_v)\)  ---- prob. of inelastic collision
chemical reaction rates \(k(T,T_v)\)  ---- prob. of reaction \(P(E_{\text{coll}}, E_v, \text{steric factors})\)

+ equilibrium redistribution of trans-rot-vib energies (based on \(E_{\text{coll}}\)) and random scattering
DSMC solution for a planetary probe geometry
DSMC solution for MIR Space Station geometry
DSMC for reacting flow through porous material

- Investigate diffusion of O and N into real TPS microstructure, diffusion of CO, CO2, CN (products) out of the microstructure, including gas-fiber reactions
- Flow within fibers usually lies in transition regime (Kn>=0.01 based on fiber diameter)
- Actual microstructure can be imaged by tomography, triangulated by a marching-cube technique, and imbedded with DSMC using advanced “cutcell” algorithms
- Solution involves ~1.5Million surface triangles and ~200M particles on ~120 cores
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Hybrid DSMC-CFD Motivation

- Aerothermodynamics of non-equilibrium hypersonic flows
  - accurate particle simulation in localized regions of non-equilibrium flow (shock, sharp leading edge, 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
Rotational/Vibrational Nonequilibrium Flows

Stagnation line profile:

- Goal is to exactly reproduce full DSMC results despite only simulating a portion of the flow with DSMC
- Gradients predicted by CFD are sharper
- Most important feature is that the hybrid simulation correctly shifts the $T_{VIB}$ profile in the continuum region of the shock layer
- Through hybrid DSMC-CFD coupling, the solution converges, in agreement with pure DSMC


MPC Research Progression


Consistent Physical Modeling for Hybrid Methods

- For many advanced physical models, a molecular model simply doesn’t integrate (analytically) to match the functional form of existing continuum models
- Continuum models are curve-fit to match experimental data (Ex. Blottner viscosity model, equilibrium constant and backwards reaction rates, etc.)

\[ P_{\text{VIB}} = f(g), \ g = \text{relative velocity of collision pair} \]
- accurate for non-Boltzmann distributions (desirable for DSMC), but no analytical match to CFD (\( \tau_V \))

\[ P_{\text{VIB}} = f(T), \ T = \text{cell average temperature} \]
- inaccurate for non-Boltzmann distributions, however, analytically matches CFD (\( \tau_V \))
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Trajectory Based DSMC ("CTC-DSMC")

- Number of *trajectories* selected using a conservative hard-sphere cross-section

\[ \text{Vol} \sim \lambda^3 \]
Trajectory Based DSMC ("CTC-DSMC")

- Number of trajectories selected using a conservative hard-sphere cross-section
- If trajectories initialized with \(0 < b < b_{\text{max}}\), where \(b_{\text{max}}\) equals the hard-sphere cross-section, then the PES determines the collision rate (finite deflection angle)
- Also, the PES determines the post collision states

Only modeling input is the PES.

\[\text{Vol} \sim \lambda^3\]

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Trajectory-DSMC vs. Pure MD

- We can now directly verify CTC-DSMC with pure MD (crucial advancement)
- We aim for *exact* agreement (so far, so good)

Norman and Schwartzentruber
“GPU-accelerated Classical Trajectory Calculation DSMC applied to shock waves”,

Research on 3-body collisions:

Norman and Schwartzentruber
3D CTC-DSMC is possible…

- 22 million particle DSMC-CTC calculation
- Trajectories replace the collision models in the Molecular Gas Dynamic Simulator (MGDS) code
- Number of trajectories is far larger than number of collisions using the DSMC-VHS model
- LJ potential accurately determines true collision rate in agreement with known value
CTC-DSMC for Rotating/Vibrating N₂

- All-atom simulation (each trajectory integrates the motion of 4 N atoms)
- Simulation operates only atom positions and velocities
- No rotational or vibrational energies are defined (post-processed only)
- No Zₐ, Zₐ, σₐ, or Borgnakke-Larsen collision models
- Essentially automates the trajectories required to converge state-to-state cross-sections

Mach 15, ρ=1.5x10⁻⁴ kg/m³

Ling-Rigby + Harmonic Oscillator for N₂
State-to-State DSMC Models

- If a PES is validated to be accurate and state-resolved cross-sections can be converged, then a state-to-state model should give exactly the same result as CTC-DSMC.
- However, a state-to-state model would be much more efficient (possibly as efficient as standard DSMC models) and would be the preferred approach.

- Instead of performing trajectories on the fly (CTC-DSMC), many individual trajectory calculations (classical or quasi-classical) are performed:

\[
\sigma_T(E_{tr}) = 2\pi \int bdb = \pi b_{max}^2 P(E_{tr}, v, J)
\]

\[
P(E_{tr}, v, J) = \frac{1}{(2\pi)^3 b_{max}^2} \int_{b=0}^{b_{max}} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} \int_{R=\rho^-}^{\rho^+} \int_{\eta=0}^{2\pi} p(E_{tr}, b, \theta, \phi, R, \eta) b \sin \theta db d\theta d\phi dR(d\nu dJ)
\]

- By integrating over trajectories corresponding to all possible pre- and post-collision states, one can obtain the total cross-section(s) [\(\sim\)collision rate] as well as state-transition probabilities.
- There are 9390 ro-vib states for \(N_2\) (\(1 < v < 60\) and \(2 < J < 279\)) …….
Likely there are many model simplifications that can be made accurately.
For example, although the total cross section generally depends on \((E_{tr}, \nu, J)\), the \(J\) dependence is weak, reducing 9390 sets of cross-sections to 60

\[
\sigma_T(E_{tr}, \nu) = f(a_{\nu}, E_{tr}),
\]

where \(a_{\nu}\) are curve-fit coefficients specific to a vibrational state \(\nu\).


Jaffe, Schwenke, Chaban, “Theoretical Analysis of N2 Collisional Dissociation and Rotation-Vibration Energy Transfer”, AIAA Paper 2009-1569
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Pure MD relaxation, shock, and expansion simulations clearly show that rotational relaxation rates ($\tau_R$ and $Z_R$) depend strongly on the **degree of nonequilibrium and the direction** to the equilibrium state.

[Compressing flows = fast excitation]  [Expanding flows = slow de-excitation]

**“Directional” Dependence of Rotational Relaxation**

- $T_{\text{inf}}$
- $100$ K
- $300$ K
- $1000$ K
- $2000$ K
A New Rotational Model for DSMC and CFD

- A simple phenomenological model, easy to implement and computationally efficient (called the NDD model), reproduces pure MD for a range of compressing and expanding flows
- Parameterized for nitrogen

\[ p_{rot}^{NDD}(\varepsilon_t, \varepsilon_r) = \min\{C_nC_a \, \tilde{p}_{rot}(\varepsilon_t, \varepsilon_r), \frac{1}{2} \} \]

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

- In the continuum limit the model integrates to the following (for use in CFD):

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

Rotation-Vibration Coupling at High Temperature

- A number of studies (based on computational chemistry) predict that $\tau_V$ and $\tau_R$ approach one another at high temperatures.
- Indicating that rotation should be considered in addition to vibration.

![Graph showing the relationship between $Z = \tau_V / (\tau_c KT)$ and $T_t$]

- Pure Molecular Dynamics relaxations.
- State-resolved DSMC relaxations.
Pure MD simulations predict very interesting physics that no current model can reproduce; at high temperatures rot-vib exchange becomes important.

Pure MD simulations suggest an intrinsic coupling that can only be modeled using $\tau_R$, $\tau_V$, and $\tau_{R-V}$.

PES ranging from HO to AHO reduce the temperature at which this occurs.
Preliminary MD of a Dissociating N₂ Shock Wave

- We now use a Morse-type potential that allows for dissociation.
- We plan to enable CTC-DSMC to handle dissociation for larger calculations.
- We plan to use new PES: [NASA Ames N3] and [Minnesota N4,O4,N2O2].
Progress and Future Directions

- Combined, DSMC and CFD provide a highly consistent multi-scale modeling framework for all hypersonic flight regimes

- Already nearing a complete overlap between DSMC and CFD for 3D (steady) flows, however, ultimately hybrid methods are required

- Hybrid methods are already quite capable, however, the remaining challenge is formulating highly consistent chemistry models for DSMC and CFD

- Direct molecular simulation (MD / Trajectory-DSMC) is possible and state-to-state models are being developed; all in an effort to replace DSMC collision models and directly link computational chemistry to aerothermodynamics.

- Future research should use all tools at our disposal in a consistent manner (quantum chemistry, MD, state-to-state, DSMC, CFD, etc.) to understand hypersonic flows at the most fundamental level

- Develop accurate, reduced-order models to design the next generation of Air Force vehicles
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Pure MD wastes a lot of time.

\[ \theta_{ij} = \frac{(\mathbf{v}_{ij} \cdot \mathbf{r}_{ij}) \pm \sqrt{(\mathbf{v}_{ij} \cdot \mathbf{r}_{ij})^2 - \mathbf{v}_{ij} \cdot \mathbf{v}_{ij} (\mathbf{r}_{ij} \cdot \mathbf{r}_{ij} - r_c^2) / (\mathbf{v}_{ij} \cdot \mathbf{v}_{ij})}}{\mathbf{v}_{ij} \cdot \mathbf{v}_{ij}} \]

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