Kinetic Particle Methods – Beyond Number of Time Steps, Cell Size, and Particles per Cell

Deborah A. Levin

Department of Aerospace Engineering
The Pennsylvania State University, University Park, PA

Institute for Computational and Experimental Research in Mathematics, (ICERM)
Brown University
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Hypersonic flows are characterized by spatial regions with both sub and supersonic flow in various degrees of thermochemical non-equilibrium and multiple length scales.

Navier-Stokes (NS) based continuum techniques encounter physical challenges in rarefied regions and are unable to capture the non-equilibrium phenomena.

An accurate modeling of such flows requires a kinetic consideration.

Kinetic methods, such as DSMC, are accurate but can be expensive, especially when applied to high density, low Kn flows.

DSMC is a relatively mature approach to solving the Boltzmann equ. What’s new?
Outline of Presentation

• Extensions of DSMC to low Kn-number flows, i.e., ES-BGK. Where will it work?

• Development of the best possible collision models using advanced chemistry approaches.

• New grids and multiple time-step considerations for plasma flows.
Objective of the Work

• To develop a basic computational framework based on the ellipsoidal statistical Bhatnagar-Gross-Krook (ES-BGK) model of the Boltzmann equation, capable of solving polyatomic multi-species gas flows. The framework is developed on the DSMC code, SMILE.

• The new particle-based method must have the following features –
  – Be more efficient than DSMC in modeling relatively high density flows,
  – be able to account for the non-equilibrium phenomena which characterize a transition Knudsen number regime out of range for NS solutions, and
  – give good agreement with both NS and DSMC for near-equilibrium flows.

• Start with flows where chemical reactions are not important.
Simplifications of Kinetic Equations

**Boltzmann equation** (spatially non-uniform case):

\[
\frac{\partial}{\partial t}(nf) + \vec{v} \cdot \frac{\partial}{\partial \vec{r}}(nf) + \vec{F} \cdot \frac{\partial}{\partial \vec{v}}(nf) = \left[ \frac{\partial}{\partial t}(nf) \right]_{\text{collisions}}
\]

\[\left[ \frac{\partial}{\partial t}(nf) \right]_{\text{collisions}} = \int \int n^2 \left( f^* f_1^* - ff_1 \right) \nu_r \sigma d\Omega d\vec{v}\]

**BGK collision model** (much simpler):

\[\left[ \frac{\partial}{\partial t}(nf) \right]_{\text{collisions}} = n\nu \left( f_e - f \right) \quad \nu = Pr \frac{nkT}{\mu}\]

**ES-BGK collision model** (still simple):

\[\left[ \frac{\partial}{\partial t}(nf) \right]_{\text{collisions}} = n\nu \left( f_{\text{ellipsoidal}} - f \right)\]

A fraction of particles in a cell is randomly selected. New velocities are assigned from a Maxwellian/ES distribution function.
Solution of BGK/ES-BGK Equation by Statistical Method

- A fraction of particles in a cell randomly selected. New velocities according to the Maxwellian/ES distribution function assigned.

- The velocities of particles, not selected, remain unchanged.

- Internal modes are relaxed to equilibrium at appropriate rates.

- The relaxation frequency for rotational equilibrium:
  \[ \nu_R = \frac{F_{\text{coll}}}{Z_R} \]

- Rotational collision number:
  \[ Z_R = \frac{3}{5Z_R^\infty} \cdot \frac{1}{1 + (\pi^{1/2}/2)(T^*/Teq)^{1/2} + (\pi + \pi^2/4)(T^*/Teq)} \]

- Number of particles selected for relaxation:
  \[ N_C = N(1 - \exp(-\nu \Delta t)) \]
## Two Simple Test Cases DSMC vs BGK

<table>
<thead>
<tr>
<th>Freestream Parameters</th>
<th>Case 1: High M</th>
<th>Case 2: Low M</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sphere diameter (m)</td>
<td>0.05</td>
<td>0.3048</td>
</tr>
<tr>
<td>Mach number – M</td>
<td>14.56</td>
<td>9.13</td>
</tr>
<tr>
<td>Static Temperature (K)</td>
<td>200</td>
<td>200</td>
</tr>
<tr>
<td>Static Pressure (kPa)</td>
<td>2.577</td>
<td>1.222</td>
</tr>
<tr>
<td>Velocity (m/s)</td>
<td>4200</td>
<td>2634.5</td>
</tr>
<tr>
<td>Density (/m^3)</td>
<td>4.34x10^{-4}</td>
<td>2.06x10^{-5}</td>
</tr>
<tr>
<td>Knudsen number</td>
<td>1.28x10^{-3}</td>
<td>8.9x10^{-3}</td>
</tr>
</tbody>
</table>
The shock width obtained using the ES-BGK method appears much thicker DSMC method.
Case I : Stagnation Line Profiles

Similar shock structures and close temperature values for ES-BGK and DSMC solutions.
Case I : Stagnation Line Profiles

The stagnation line number density and rotational temperature profiles for the ES-BGK and DSMC methods show less deviation. But the translational temperature exhibits a considerable difference, in the region where the shock is more thicker.
Case I : Velocity PDF Inside Shock

A strong departure from the equilibrium (Maxwellian distribution) can be observed from the bi-modal nature of the x-component velocity distribution inside the shock region.

(Location: x = -0.009 for ES-BGK and x = -0.0075 for DSMC)
Case II Mach 9: Comparison of Translational Temperature Contours

- Translational temperature profiles are similar, but thickness of the shock is wider in ES vs. DSMC.
- The width of the DSMC shock is about 0.015 m while the ES-BGK shock width is around 0.02 m.
Case II: Rotational Temperature Contours

- Rotational temperatures are in better agreement.
ES-BGK method predicts reasonably accurate shock and temperature profiles, as compared to DSMC.
Case II: Stagnation Line Profiles

- Difference in the stagnation line number density and rotational temperature is less.
- But the translational temperature shows considerable deviation, due to the difference in the shock width.
Case II: Velocity PDF inside Shock

- Departure from Maxwellian distribution is seen at $x=0.13$ (for DSMC) and $x=0.125$ (for ES-BGK), in the center of the shock.
- Both ES-BGK and DSMC predict the bi-modal nature of the x-component velocity distribution.
Does BGK Always Work this Well?

- Shock-shock interactions measured in a pure N₂ flow at Hypervelocity Expansion Tunnel (HET) facility of J. Austin, U. of Illinois.
- Double wedge configuration
- “High enthalpy case”: M=7.14, T_{static}=710 K, P_{static} = 0.78 kPa, \( v=3812 \text{ m/s, density= 0.0037 kg/m}^3 \), Kn=4.8 \( \times 10^{-4} \)

- DSMC numerical parameters:
  - Total number of time-steps (NSTEP) 100,000
  - Time step (TAU), s 1.0 \( \times 10^{-9} \)
  - Number of molecules in one simulated particle (PFnum), 1.0 \( \times 10^{13} \)
  - Number of cells, 450 \( \times 400 \)
  - Cell size, m 2.0 \( \times 10^{-4} \)
  - Grid Adaptation (NPG) 20

- Very, long calculations, 64 processors, many days. Can we do better?
• DSMC resolves experimentally observed complex shock structures,
• In BGK, an oblique shock, bow shock and triple point can be seen, but, there is no separation region.
Comparison of DSMC vs Schlieren Shock-Shock Interactions

High enthalpy case

Low enthalpy case
Comparison of DSMC vs Measured High-Enthalpy Case Heat Fluxes

- Unsteadiness is a challenging in comparison,
- VHS parameters gave largest change
- Also considered role of $N_2$ dissociation, accommodation coefficients, $Z_r$, $Z_v$ relaxation.
• Flow structure predicted by NS not better, not easier,
• Heat transfer poorly predicted.
The Quest for Equilibrium Breakdown

- A gas in equilibrium is the one that does not show any temporal variation in the distribution of energy states and composition.

- Maxwellian distribution corresponds to the equilibrium state.

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Kn = \frac{\lambda}{L}
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P = \frac{u}{\rho} \frac{d\rho}{dx} = M \frac{\sqrt{\pi \gamma}}{8} \frac{\lambda}{\rho} \frac{d\rho}{dx}
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Kn_{GLL} = \frac{\lambda}{Q} \frac{dQ}{dx}
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(Q could be \( \rho, T \) or \( v \))

Problem for statistical methods

- Camberos et al. and Alexeenko et al. have used entropy generation as the continuum breakdown parameter. Entropy generation parameter makes use of “gradients of the distribution function” that makes the parameter noisy for particle methods.
Potential Equilibrium Breakdown Approach

The K-S parameter provides a quantitative measure of the difference between the computed and theoretical cumulative distribution functions.

Data is sorted into different velocity bins. Size and number of velocity bins are selected to cover entire velocity spectrum and minimize statistical scatter.

The velocity PDF is then computed

$$f(u_i) = \frac{N_i}{N_{total} \delta u}$$

The Maxwellian PDF is calculated at the local temperature

$$M(u_i) = \frac{1}{\sqrt{\pi u_m}} e^{-u_i^2/u_m^2}$$

The K-S parameter is then obtained as follows:

$$D_n = \max_{1 \leq i \leq n} \left( C(u_i) - A(u_i) \right)$$
Comparison of Temperature Contours in Ar - Mach 10

- Hybrid method is compared with the benchmark DSMC method. Three cases of switching criteria are shown, 0.01, 0.05 and 0.25.
- The agreement is good for switching criterion of 0.01 and slowly distorts for higher switching switching criteria.
The range of values shows the large flow gradients in the flow due to the shock.
Role of Quasi-classical trajectory methods in improvement of:

• Total collision cross section
• Chemical reaction cross section
• Chemical relaxation

Particularly important for hypervelocity, non-thermal collisions of anything other than $N_2 + N_2$. 
Introduction

- The Jovian moon Io, the most geologically active body in our solar system, has a unique atmosphere
- Contributions to the Ionian atmosphere are complex and numerous
  - Dissociation of volcanically expelled SO$_2$
  - Sublimation of SO$_2$ surface frosts
- Io's rarefied atmosphere makes DSMC the computational method of choice
- There is a lack of reliable SO$_2$ dissociation data at very high collision energies – needed for planetary models (Goldstein et al, U of Texas, Austin
- Therefore, collisions between SO$_2$ and O are simulated to develop reaction and collision models for the Ionian atmosphere
- Two PESs considered: Murrell and ReaxFF
Methodology: Governing Equations

- Hamilton equations – MD/QCT
  \[ \dot{p}_{i,j} = -\frac{\partial V}{\partial r_{i,j}}, \dot{r}_{i,j} = -\frac{p_{i,j}}{m_i} \]

- Murrell and ReaxFF define system potential \( V \) differently

- Possible reaction paths
  - \( \text{SO}_2 + \text{O} \rightarrow \text{SO} + 2\text{O} \)
  - \( \text{SO}_2 + \text{O} \rightarrow \text{S} + 3\text{O} \)
  - \( \text{SO}_2 + \text{O} \rightarrow \text{S} + \text{O} + \text{O}_2 \)
  - \( \text{SO}_2 + \text{O} \rightarrow \text{SO} + \text{O}_2 \)
  - \( \text{SO}_2 + \text{O} \rightarrow \text{SO}_3 \) Not modeled by Murrell PES

- Each case is defined by relative velocity and \( \text{SO}_2 \) internal energy

- Collision velocities studied: 1-80 km/s (1.06 x 10\(^{-20}\) – 6.80 x 10\(^{-17}\) J)

- \( \text{SO}_2 \) internal energies studied: 0.5 x 10\(^{-19}\) – 8.0 x 10\(^{-19}\) J

- 10,000 trajectories run for each case

- Impact parameters and \( \text{SO}_2 \) orientation are defined by initial coordinates and momenta, which are determined through microcanonical sampling
Methodology: Potential Energy

- Murrell
  - \[ V = V_{MOL} + V_{INT} \]
    - \( V_{MOL} \): Murrell\(^1\) 3-body molecular potential
    - \( V_{INT} \): Lennard-Jones 6-12 potential
    - Defined entirely by internuclear distances

- ReaxFF\(^2\)
  - \( V \) is a complex potential that includes many terms
    - Bond order
    - Under/over-coordination penalty
    - Valence angle energy
    - Torsion energy
    - Conjugation effects
    - van der Waals interactions
    - Coulomb interactions
  - Parameters were fit to DFT computations on \( \text{SO}_2 + \text{O} \) system

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Comparing Murrell and ReaxFF Potentials

- Steeper inner-wall for Murrell potential (LHS)
- Larger atomization target for Murrell potential (RHS)
Reaction Cross Sections: $\text{SO}_2 + \text{O} \rightarrow \text{SO} + 2\text{O}$

\[
\sigma_{r,MD} = \pi b_{\text{max}}^2 \frac{N_r}{N_T}
\]

- TCE cross section increases much more rapidly than the two computed methods
- ReaxFF predicts more dissociation than Murrell PES at lower velocities
- Both models predict increasing cross section with increasing velocity until reaching maxima, then decreasing with higher velocities
Total Cross Sections used in DSMC

- Total cross section data is fit to the VHS cross section of Bird

\[
\sigma_{VHS} = \sigma_{ref} \left( \frac{2kT_{ref}}{\mu_{SO_2, O}} v_{rel}^2 \right)^{\omega_{AB} - 1/2} \Gamma \left( 5 / 2 - \omega_{AB} \right)
\]

- ReaxFF and Murrell cross sections are greater than Bird VHS cross sections

- Murrell and ReaxFF curve-fits are accurate to within 10% of all computed data points

- ReaxFF > Murrell for velocities < 14 km/s
2D DSMC Counter-flow Simulation

- 60 locations of out-flowing SO$_2$ at thermal temperature of 500 K at 10 km/s distributed evenly along the surface
- Incident O comes in at 10 km/s
- Overall number density: $1.5 \times 10^{18}$ molecule/m$^3$
- Both VHS cross section curve fits are explored

Oxygen (O)

Sulfur Dioxide (SO$_2$)
Reactions turned off, to examine effect of non-reactive cross section

- Bird/Ozawa VHS cross section << Murrell or ReaxFF, allowing more O penetration
- Therefore, less O near surface for Murrell, ReaxFF models
2D DSMC Simulation - No Reactions (2/2)

- More O penetration to the surface for Bird/Ozawa VHS/Grillo TCE
- **Significant differences between models highlight importance of model selection**
2D DSMC Simulation: \( \text{SO}_2 + \text{O} \rightarrow \text{SO} + 2\text{O} \)

Comparison of SO mole fractions

- More reactive activity for the Bird/Ozawa VHS/Grillo TCE model
- Slightly more dissociation for Murrell than ReaxFF
Low Density, Plasmas, and Propellants of the Future
Ion Engines

- Usually the life time of the satellite is dependent on the life time of the thruster system on board
- Satellite missions require high efficiency thruster systems
- Electric propulsion devices have higher specific impulse ($O(1-3)$) than chemical.
- Future interplanetary missions could use hybrid chemical-electric means of thrusters
- Involves physical challenges
  - *Disparate length scales*
  - *Disparate time scales*
  - *Disparate density scales*
Adaptive Mesh Refinement (AMR)

- Used in various scientific branches from astrophysics to biology especially when there is a multi-scale characteristics inherent to the problem.

<table>
<thead>
<tr>
<th>Parent-Children Connectivity</th>
<th>Active</th>
<th>Deactive</th>
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<tbody>
<tr>
<td>Active Cells List</td>
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<table>
<thead>
<tr>
<th>Number of Cells</th>
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<tbody>
<tr>
<td>AMR</td>
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<tr>
<td>Uniform</td>
</tr>
<tr>
<td>3% stretching</td>
</tr>
<tr>
<td>8% stretching</td>
</tr>
</tbody>
</table>
Species Specific Timestep

- $O(2-3)$ difference in velocity and number density between ions and neutrals in usual operating conditions.
- Serikov* devised an algorithm
  \[ N_{\text{max}} = N_i \times N_n \times \max(W_i, W_n) \times g_{\text{max}} \times \sigma_T^{\text{max}} \times F_{\text{NUM}} \times \Delta t / V_c \]
- Basic idea is to extrapolate the impact of collisions between fast and slow species during the short interval of the faster species.

Timestep Algorithm

- The algorithm is repeated for $N_{\text{max}}$ times;
  1) Select a pair of particles $A_i^s$ and $A_n^r$
  2) Calculate relative velocity $g_{in}^{sr} = |c_i^s - c_n^r|$ and call a random number $R (0<R<1)$. If $R > \frac{g_{in}^{sr} \sigma_i (g_{in}^{sr})}{\max \sigma_{max}^{sr}}$, no collision occurs, return to Step 1. If not proceed to Step 3.
  3) Replace
     - $c_i^s$ by $c_i'^s$ with probability $W_i / \max \{W_i, W_n\} \times \max \{\tau_i, \tau_n\} / \tau_n$
     - $c_n^r$ by $c_n'^r$ with probability $W_i / \max \{W_i, W_n\} \times \max \{\tau_i, \tau_n\} / \tau_i$
Cross-Sections

- Xe is used in the simulations. Cross-sections used between neutrals and ions;

\[ \sigma_{nn} = \frac{2.117 \times 10^{-18}}{v_{rel}^{0.24}} \text{m}^2 \quad \sigma_{ni} = \frac{6.416 \times 10^{-16}}{v_{rel}} \text{m}^2 \]

- The major mechanism for depositing energy from ions to neutrals is the Charge Exchange (CEX) reactions;

\[ Xe_{slow} + Xe_{fast}^- \Rightarrow Xe_{fast} + Xe_{slow}^+ \]

- The CEX cross-section used;

\[ \sigma_{CEX} = (-0.8821 + \log(v_{rel}) + 15.1262) \times 10^{-20} \text{m}^2 \]
1 Thruster

- Case 1A results
- Top figure shows the number density distribution for the neutrals
- Bottom figure shows the number density for the ions. A radial Gaussian profile is given at the thruster exit which is observed in experiments
Distribution functions

- 2 cells are tagged in the domain in order to investigate the fractions of CEX ions and neutrals. The figure shows the location of cells in the computational domain.

- Two locations at different downstream locations where the collision frequencies are different can help quantify the density and velocity distributions for each species.
Distribution Functions

- Left figure shows the neutral velocity along x direction for both cells. The distribution in Cell 2 shows the expansion characteristics.
- Right figure shows the ion velocity distribution that have undergone CEX reaction. Cell 1, being closer to the thruster exit and having higher collision frequency, shows a larger fraction of CEX ions compared to Cell 2.
3 Thruster – Case 1B

- Left figure shows the neutral velocity contours, 3 distinct plumes merge into a single one after about 3 diameters downstream.
- Right figure shows the ion number density contours on x-z plane, off-plane thruster start to interact at around 5 diameters.
3 Thruster – Line Plots

- Left figure shows the neutral number density distribution along the centerline of the middle thruster.
- Right figure shows the ion number density distribution along the centerline of the middle thruster.
Basic algorithm

- Computational particles are created at the domain boundaries.
- Particles are moved with prescribed time steps.
- Particles are then mapped to cells to perform calculations based on the governing equations.
- With Domain Decomposition
  - Once a particle crosses processor domain, it is stored to a communication list and then communicated to corresponding processor.
- Around 7000 lines of code is written excluding the open-source libraries being employed and 2300 lines are purely related to communication.
• A single thruster jet is introduced into the domain where there was only Cartesian mesh (no AMR).
• Particles are appended to the cell linked lists and basic calculations are performed.
• A good scalability is observed.
Naïve Domain Decomposition & AMR
Naïve Domain Decomposition & AMR

• With AMR employed, the scalability is diminished.
• Looking at the processor mapping, the load-balance is uneven (i.e. number of AMR cells each processor domain has).
• The volume to surface ratio is getting smaller. A 3D blocking can be employed to remedy this.
• The ultimate solution is to use graph partitioning software.
Load-Balanced Domain Decomposition with Parmetis

- A well-known graph partitioning library called Parmetis is used.
- Compared to naïve decomposition, even for a simple case with 3 thrusters, 11% speed-up was observed.
Futuristic Propellants – Dual Use

- Colloid thruster + Ion engines
- Notice the 10 order of magnitude drop in density!!!
Contributions from:

1. Neal Parsons, Ph.D student, QCT/MD
2. Varun Patil, MS student, BGK/DSMC
3. Burak Korkut, Ph.D student, Ion thrusters, AMR grids

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DSMC Method

Direct simulation Monte-Carlo (DSMC) method is a discrete particle simulation method that provides numerical approximation to the solution of the Boltzmann equation.

- Underlying assumption: uncoupling of particle motion and collisions.
- Free molecular motion model is deterministic.
- Probabilistic techniques are used for modeling particle collisions.
- Gas-surface interaction parameters implement the boundary conditions.

Constraints: DSMC method becomes prohibitively expensive for simulating high density flows.

Simplified methods based on Bhatnagar-Gross-Krook (BGK) model kinetic equation (*Physical Review*, 94, 1954, 511) have evolved to handle such flows.

BGK method differs from DSMC only in collision modeling.
Statistical BGK/ESBGK Method

- The Boltzmann equation:
  \[
  \frac{\partial}{\partial t} (nf) + \mathbf{u} \cdot \frac{\partial}{\partial \mathbf{r}} (nf) + \mathbf{F} \cdot \frac{\partial}{\partial \mathbf{u}} (nf) = \left[ \frac{\partial}{\partial t} (nf) \right]_{\text{collision}}
  \]

  \[
  \left[ \frac{\partial}{\partial t} (nf) \right]_{\text{collision}} = \int \int_0^{2\pi} \int_0^\infty n^2 (f^* f_1^* - ff_1) \nu r \sigma d\Omega d\nu
  \]

- In BGK model, a simplified form of the Boltzmann equation is solved.
  \[
  \left[ \frac{\partial}{\partial t} (nf) \right]_{\text{collision}} = n\nu (f_e - f)
  \]

- Flow is artificially relaxed to equilibrium with a rate depending on local flow properties.
  \[
  \nu = \text{Pr}. \frac{nkT}{\mu}
  \]

- ESBGK model evolved to correct the unphysical Prandtl number of unity in BGK model.
  \[
  \left[ \frac{\partial}{\partial t} (nf) \right]_{\text{collision}} = n\nu (f_e - f) \quad \Rightarrow \quad \left[ \frac{\partial}{\partial t} (nf) \right]_{\text{collision}} = n\nu (f_{\text{ellipsoidal}} - f)
  \]