Approaches for Emulating the Boltzmann Equation When Particle Simulation Becomes Inefficient

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Overview

- Particle methods to emulate Boltzmann-like equations for nonequilibrium gas and plasma flow:
  - Direct Simulation Monte Carlo (DSMC)
  - Particle In Cell (PIC)
  - Strengths and inefficiencies

- Hybrid particle-continuum method:
  - Multi-scale, steady, hypersonic gas flow

- Deterministic solution of kinetic equations:
  - Multi-component, unsteady, plasma flow

- Final comments
What is Nonequilibrium?

Continuum flow regime:
- small $Kn_\infty = \frac{\lambda}{L} \sim \frac{1}{(\rho L)}$
- high density and/or large $L$
- many collisions
- thermodynamic equilibrium

Rarefied flow regime:
- large $Kn_\infty$
- low density and/or small $L$
- few collisions
- nonequilibrium

$Kn_\infty = 0.002$, $Ma = 10$, $Ar$

$Kn_\infty = 0.250$, $Ma = 10$, $Ar$
Nonequilibrium Systems

Hypersonic Vehicles

Spacecraft Propulsion

Micro-scale Gas Flows

Vacuum Systems
Computational Modeling of Nonequilibrium Flow

Flow Regimes:
- continuum
- slip
- transitional
- free-molecular

Kn
- 0.01
- 0.1
- 1

Model Accuracy:
- DSMC / PIC
- Boltzmann / Vlasov
- CFD / MHD

Numerical Cost:
- DSMC
- CFD
Direct Simulation Monte Carlo Method (DSMC)

- Particle method for nonequilibrium gas flows:
  - developed by Bird (1960s)
  - particles move/collide in physical space
  - particles possess molecular level properties, e.g. $u'$ (thermal velocity)
  - cell size $\Delta x \sim \lambda$, time step $\Delta t \sim \tau$
  - collisions handled statistically (not MD)
  - internal energy relaxation, chemistry
  - gas-surface interactions
Particle In Cell (PIC)

- Particle method for nonequilibrium plasma:
  - developed since the 1960s
  - charged particles move in physical space
  - particles possess molecular properties, e.g. $u'$ (thermal velocity)
  - cell size $\Delta x \sim \delta$, time step $\Delta t \sim 1/\omega$
  - self-consistent electric fields, $E$
  - may be combined with DSMC for collisional plasmas
Particle Methods: Strengths and Inefficiencies

• Strengths:
  – Results consistent with kinetic equations
  – Robust handling of complex geometry
  – Many advanced physical models

• Inefficiencies:
  – Processing of highly collisional regions
  – Resolution of low-probability populations and events
  – Low speed flows (statistical noise)
  – Explicit algorithm (small time step)
Hypersonic Flows

- Hypersonic vehicles encounter a variety of flow regimes:
  - continuum: modeled accurately and efficiently with CFD
  - rarefied: modeled accurately and efficiently with DSMC
Particle Inefficiency:  
1. Highly Collisional Regions

Mach 10, Kn_{\infty} = 0.01

80% of DSMC calculation spent in near-equilibrium regions
• Basic concepts:
  – numerical efficiency of continuum methods
  – physical accuracy of particle methods
  – goal: reproduce results from a full particle simulation at a fraction of the cost

• Challenges:
  – domain decomposition into continuum and particle regions (continuum breakdown)
  – communication of information between continuum and particle regions (coupling methods)
MPC Method  
(Modular Particle Continuum)

**Continuum**
Martin, Scalabrin, and Boyd  
J Phys D, **341**, 2012  
- 2D/3D unstructured mesh  
- modified Steger-Warming flux-vector splitting, parallel  
- point-implicit time integration  
- many physical models

**Particle**
Dietrich and Boyd  
J Comp Phys, **126**, 1996
- 2D/3D unstructured mesh  
- parallel, domain decomposition  
- many physical models

---

\[
\begin{align*}
\rho_i, T_t, T_r, T_v \\
u, v, w
\end{align*}
\]

\[
\{ u', v', w' \\
x, y, z \\
m, e_{\text{rot}}, e_{\text{vib}}
\]
Continuum Breakdown

- Gradient-length Knudsen number, $K_{n_{GL}}$ (Boyd, et al.)
  - related to Chapman-Enskog (CE) expansion terms

\[
K_{n_{GL-Q}} = \frac{\lambda \nabla Q}{Q}
\]

\[
K_{n_{GL}} = \max(K_{n_{GL-\rho}}, K_{n_{GL-V}}, K_{n_{GL-T}})
\]

- for regions in the flow field where $K_{n_{GL}} < 0.05$

\[
\left| \frac{DSMC_{SOL'N} - CFD_{SOL'N}}{DSMC_{SOL'N}} \right| < 5\%
\]

- Similarly, Garcia and Alder proposed using non-dimensionalized shear stress and heat flux:

\[
B = \max(\tau_{i,j}^*, q_i^*)
\]
Hybrid Coupling Method

- State-based coupling
  - use existing CFD and DSMC boundary procedures
DSMC Boundary Conditions

• Generate particles in the interior and boundary of DSMC domain

• Use the Chapman-Enskog distribution based on local CFD information

Velocity profile through a normal shock
CFD Boundary Conditions

- Average DSMC data communicated to CFD has large fluctuations
- Sub-relaxation technique (Sun and Boyd, 2005)
  \[
  \bar{A}_j = (1 - \theta) \bar{A}_{j-1} + \theta A_j
  \]
- History before time-step \( i \) is removed by
  \[
  \bar{A}_j' = \bar{A}_j + \frac{(1 - \theta)^{j-i}}{1 - (1 - \theta)^{j-i}} (\bar{A}_j - \bar{A}_i'),
  \]
  \[
  j = \frac{1}{\theta} + i
  \]
Hybrid CFD-DSMC Algorithm

- Initial CFD solution
- Decompose DSMC and CFD regions
- Generate particles in DSMC regions

Iterate DSMC regions
- Use sub-relax avg. to track macro changes
- Apply $K_{GL}$ to update interface locations

Update CFD BCs and converge
- Have interfaces stopped moving?

No

Yes
- Lock interfaces
- Sample DSMC
- Converge CFD
Example: Hypersonic Flow Over Planetary Probe

- Nitrogen flow over sting-mounted planetary probe:
  - conditions correspond to experimental study in the CNRS expansion tunnel
  - $Kn=0.01$, $T=13.6$ K, $M=20$

- Simulations:
  - full DSMC
  - full CFD (Navier-Stokes)
  - MPC simulation initialized by CFD solution
Temperature Contours

Translational

Rotational
Flow Field Profiles

Along C1
Particle Distributions

Point A

Velocities

Rotational Energy
Surface Heating
• Optimum use of hybrid methods:
  – Low Kn with important pockets of high-Kn flow
  – Speedup of 30 over DSMC in our best 2D case

• Further improvement of current methodology:
  – Less conservative breakdown parameters
  – Additional physical phenomena (e.g. gas mixtures, chemistry)

• Unsteady flows:
  – relatively few studies
  – main challenges: DSMC cost and fluctuations
Hall Thruster Discharge Plasma

• Partially magnetized plasma in Hall thrusters includes complex mechanisms:
  – Dynamic interaction between acceleration and ionization (Breathing mode)
  – Wall interactions (Near-wall sheath, SEE, sputtering)
  – Multi-dimensional physics

• All species (ion, neutral atoms, electrons) follow a non-Maxwellian VDF
Particle Inefficiency:
2. Resolving Rare Populations

Deterministic scheme resolves tail using fewer resources
Hall Thruster Computational Modeling

- **Fluid model (a)**
  - Near-equilibrium assumed
  - Numerically efficient

- **Particle method (b)**
  - Statistical noise (macro-particles)
  - Easy to implement even in high-dimensional flows

- **Direct Kinetic method (c)**
  - Good resolution of VDF
  - A large number of grid points required

\[ Kn \ll 1 \text{ (collisional)} \]
\[ Kn \approx 1 \]

\[ VDF: \text{Number of particles in } [v, v+dv] \]
Hall Thruster Simulation

• 1D Hybrid-kinetic simulation
  – Ions: (1) DK solver and (2) PIC solver
  – Atoms, electrons: Fluid approach [1, 2]
  – Quasi-neutral plasma

• Operation condition (SPT-100)
  – Discharge voltage: 300 V
  – Discharge current: 4.5 A
  – Mass flow rate: 5.0 mg/s
  – Maximum magnetic field: 200 G

• Simulation Domain
  – Axial length: 4cm
  – Radius: 3cm (inner), 5cm (outer)

Thruster Performance

<table>
<thead>
<tr>
<th></th>
<th>Hybrid-DK</th>
<th>Hybrid-PIC</th>
<th>Measured</th>
</tr>
</thead>
<tbody>
<tr>
<td>( I_d )</td>
<td>3.59 A</td>
<td>3.94 A</td>
<td>4.5 A</td>
</tr>
<tr>
<td>( \eta )</td>
<td>0.74</td>
<td>0.69</td>
<td>0.5</td>
</tr>
<tr>
<td>Thrust</td>
<td>88.7 mN</td>
<td>90.8 mN</td>
<td>83 mN</td>
</tr>
<tr>
<td>( t_s p )</td>
<td>1810 s</td>
<td>1850 s</td>
<td>1600 s</td>
</tr>
</tbody>
</table>

Ion kinetic eq. (1D):

\[
\frac{\partial f}{\partial t} + v \cdot \frac{\partial f}{\partial x} + \frac{qE}{m} \cdot \frac{\partial f}{\partial v} = S
\]

- Ionization + charge exchange collisions
- Dimensionally split (2nd-order in time)
- Finite Volume method using flux reconstruction (2nd-order in space): Conservative, positivity preserving
- Adaptive time step: based on CFL condition

\[
\max \left( \frac{v \Delta t}{\Delta x}, \frac{a \Delta t}{\Delta v} \right) \leq 1
\]
## Computational Parameters

<table>
<thead>
<tr>
<th></th>
<th>Hybrid-DK</th>
<th>Hybrid-PIC</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Timestep</strong></td>
<td>1 ns</td>
<td>1 ns</td>
</tr>
<tr>
<td><strong>Grid size, dx</strong></td>
<td>0.4 mm</td>
<td>0.4 mm</td>
</tr>
<tr>
<td><strong>Velocity bin, dv</strong></td>
<td>250 m/s (total of 400 velocity bins)</td>
<td>-</td>
</tr>
<tr>
<td><strong>Number of particles</strong></td>
<td>-</td>
<td>300,000 (average = 3,000 per cell)</td>
</tr>
<tr>
<td><strong>Ionization</strong></td>
<td>Every time step</td>
<td>Depending on # of particles</td>
</tr>
<tr>
<td><strong>Atoms, Electrons</strong></td>
<td>Fluid</td>
<td>Fluid</td>
</tr>
<tr>
<td><strong>Computational time</strong></td>
<td>1.6 hours</td>
<td>3.6 hours</td>
</tr>
</tbody>
</table>
Time Averaged Results

- Good agreement between DK and PIC simulations
- PIC simulation yields lower ion number density due to the treatment of ionization
Plasma Oscillations

- Breathing mode
  - Observed experimentally
  - Low frequency: ~20 kHz
  - Ions are generated inside the channel and accelerated out of the channel exit
  - Neutral atoms are depleted and resupplied
High-Frequency Oscillations

- High-frequency oscillations captured well in DK simulation
  - Transit-time oscillations ~300 kHz due to ionization
  - These oscillations correspond to ion acoustic speed

(a) Hybrid-PIC

(b) Hybrid-DK

Discharge current

Plasma density
Instantaneous ion VDFs show the largest difference.

Observations:
- DK: Ionization is captured well (low-velocity components). High-velocity components due to negative E field inside the channel.
- PIC: Beam is captured well. Empty bins in low-velocity components.

Normalized instantaneous ion VDFs at channel exit of SPT-100.
Final Comments for DK Method

• DK works well for specific situations:
  – Unsteady flow, simple collision mechanisms
  – Non-linear plasma waves (reduced grid heating)

• Extend to multi-dimensions:
  – Spatially: straightforward
  – Velocity: coordinate transformation, mesh adaption

• Extend to multi-components:
  – Atoms: straightforward (already done!)
  – Electrons:
    – effective use of velocity mesh
    – interaction with other plasma components