Approaches for Emulating the Boltzmann Equation When Particle Simulation Becomes Inefficient

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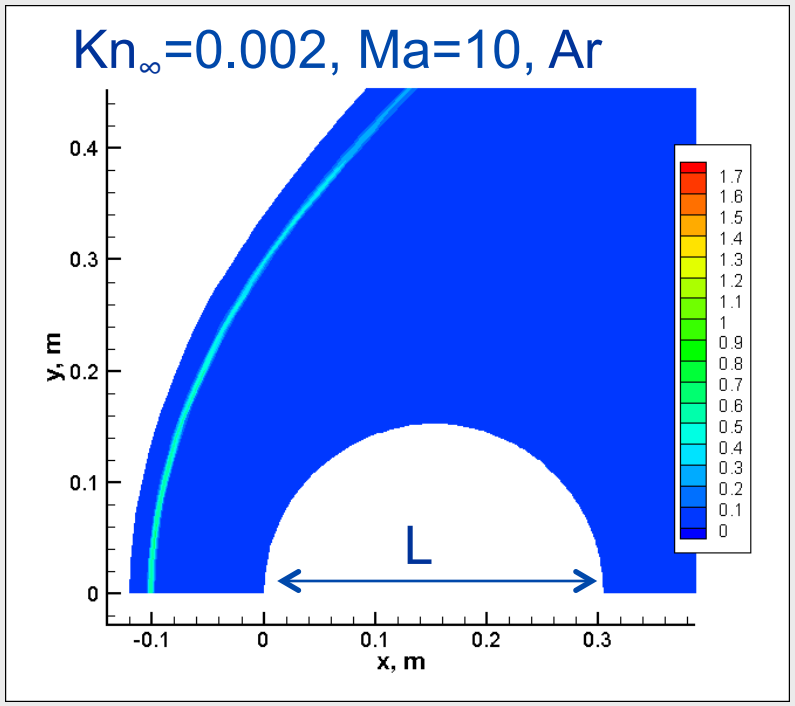
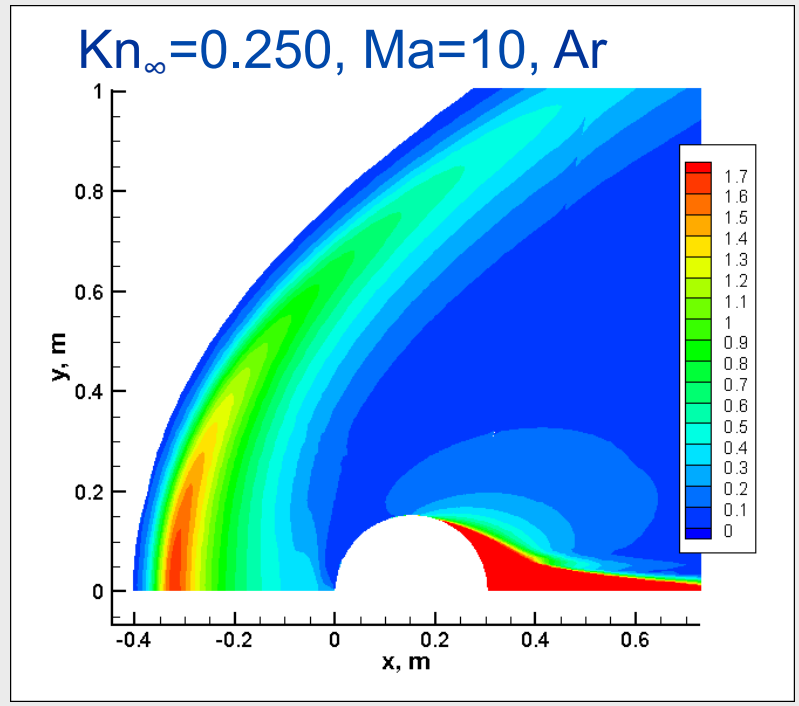
Overview

- 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?

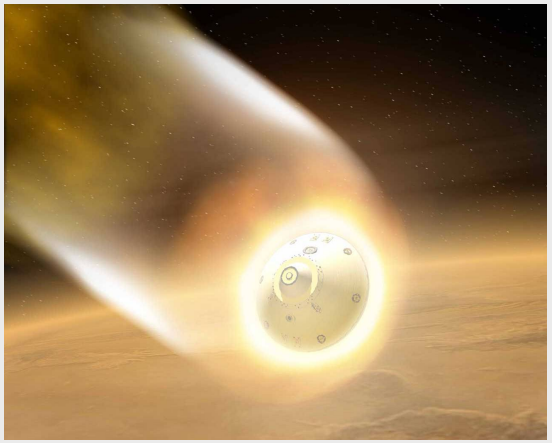




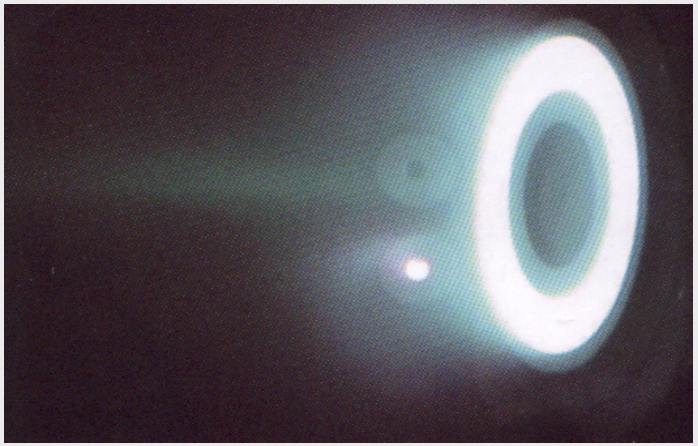
Continuum flow regime:
- small $Kn_\infty = \lambda / L \sim 1 / (\rho L)$
- high density and/or large L
- many collisions
- thermodynamic equilibrium

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

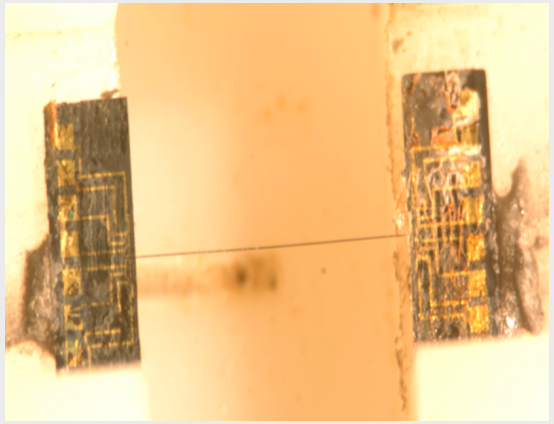
Nonequilibrium Systems



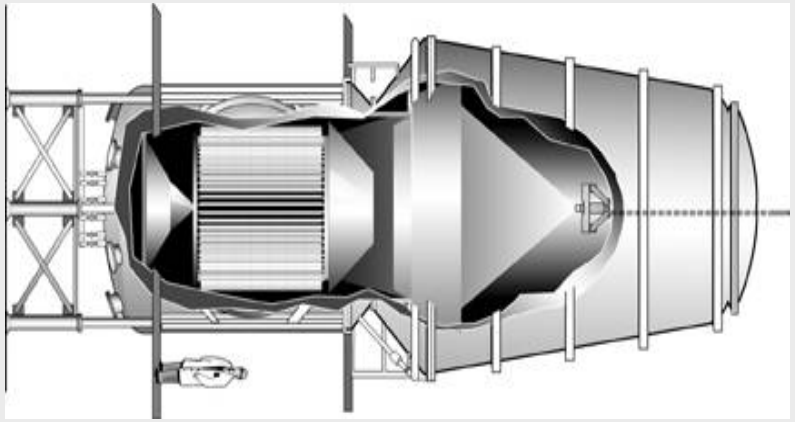
Hypersonic Vehicles



Spacecraft Propulsion

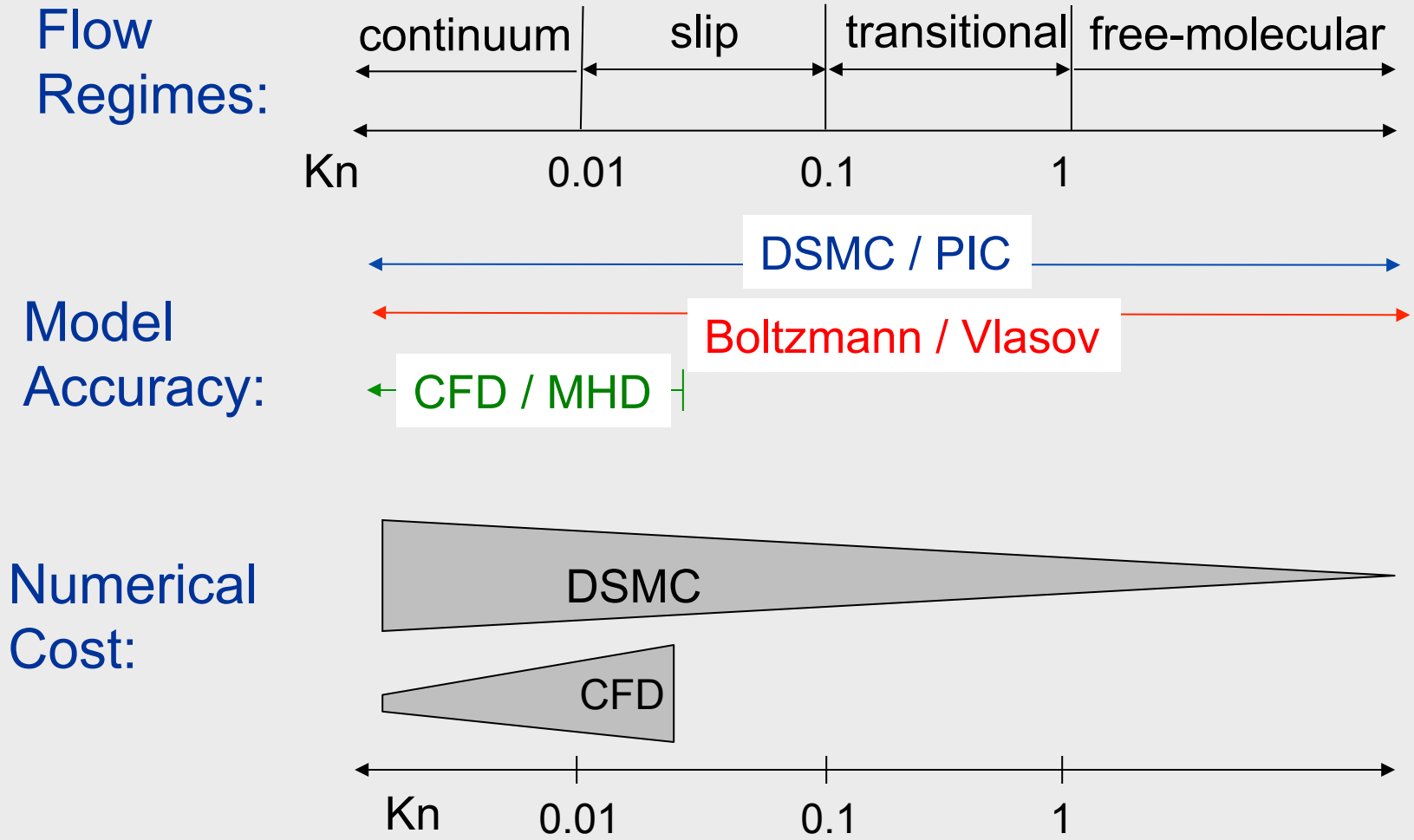


Micro-scale Gas Flows



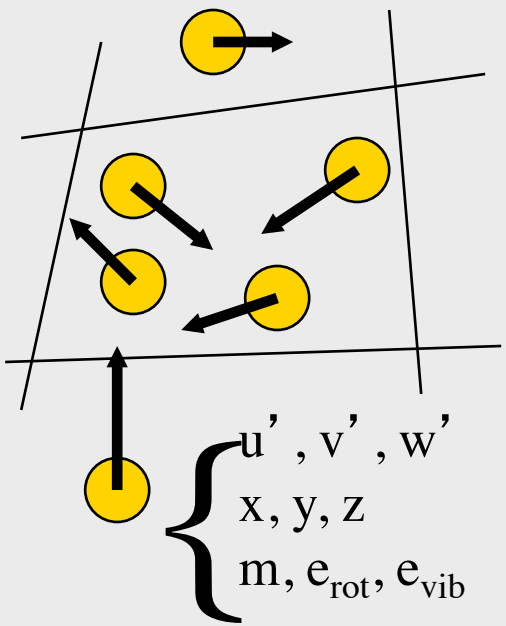
Vacuum Systems

Computational Modeling of Nonequilibrium Flow



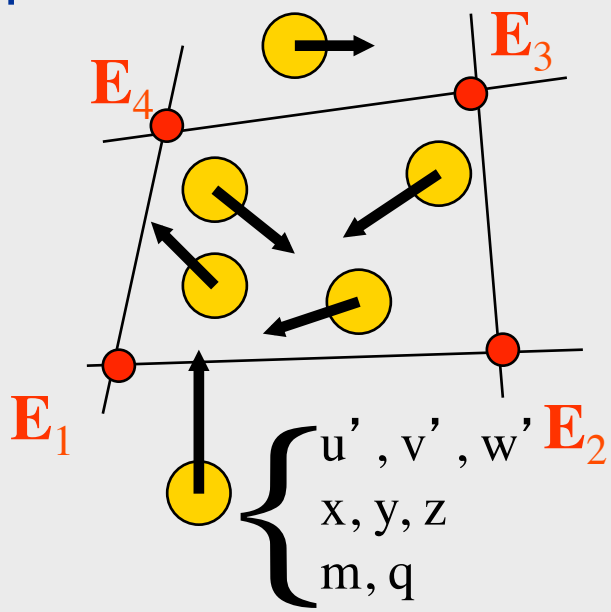
Direct Simulation Monte Carlo Method (DSMC)

- 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

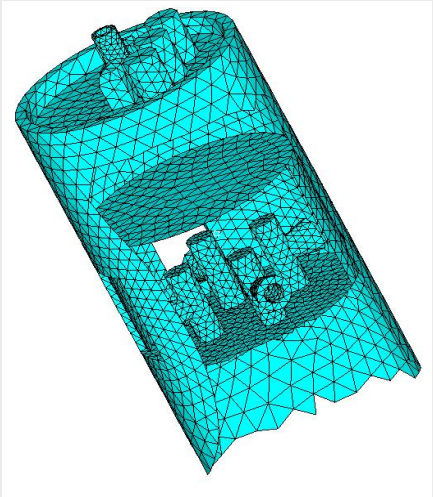


Particle In Cell (PIC)

- 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



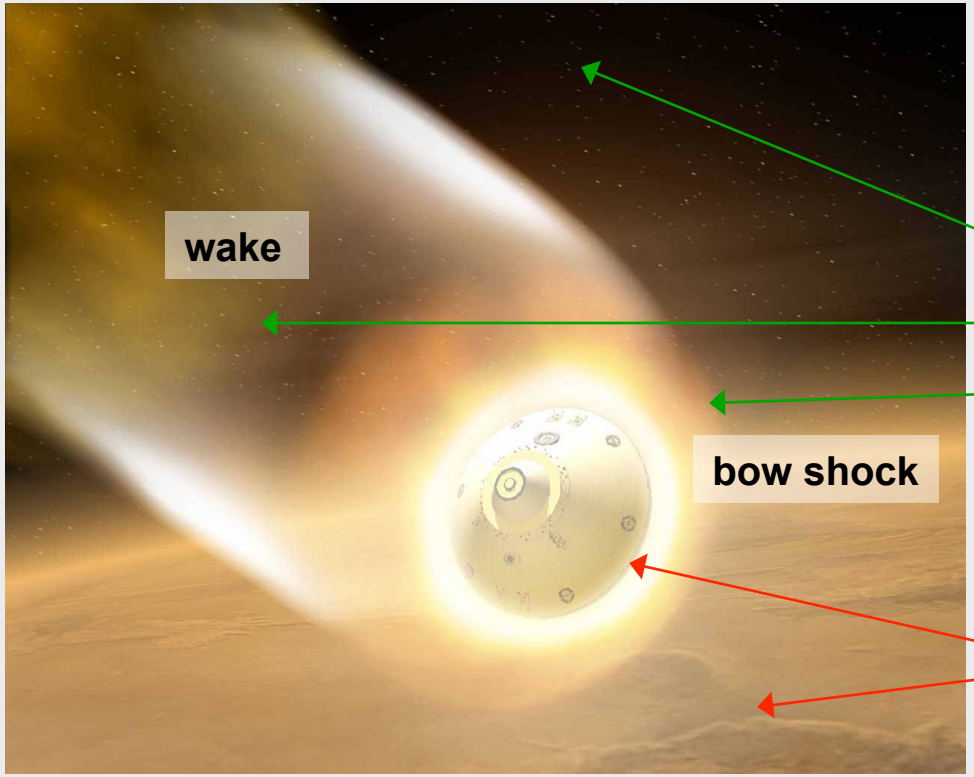
Particle Methods: Strengths and Inefficiencies



- 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

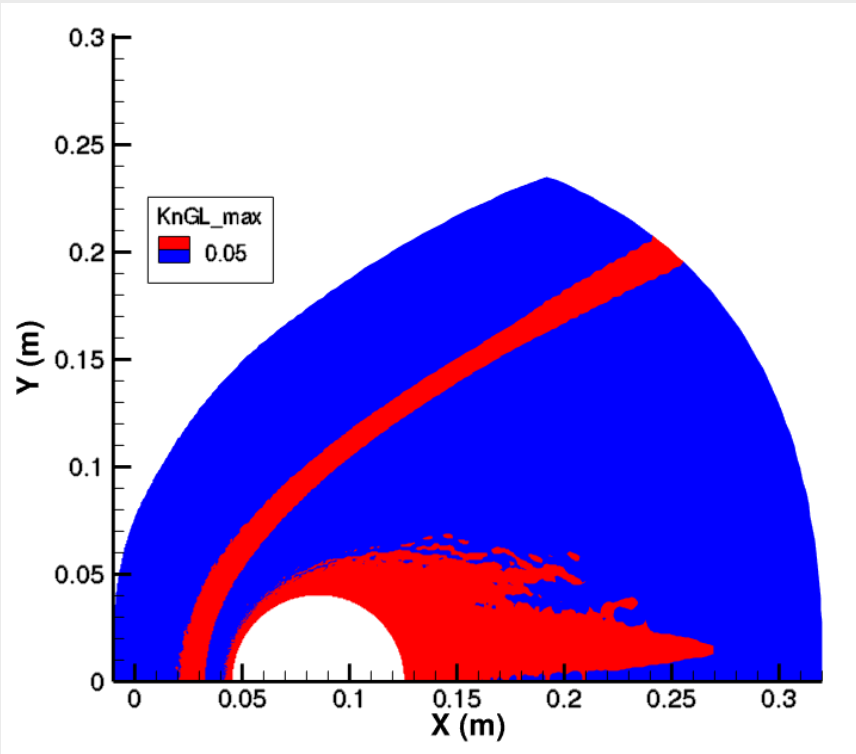


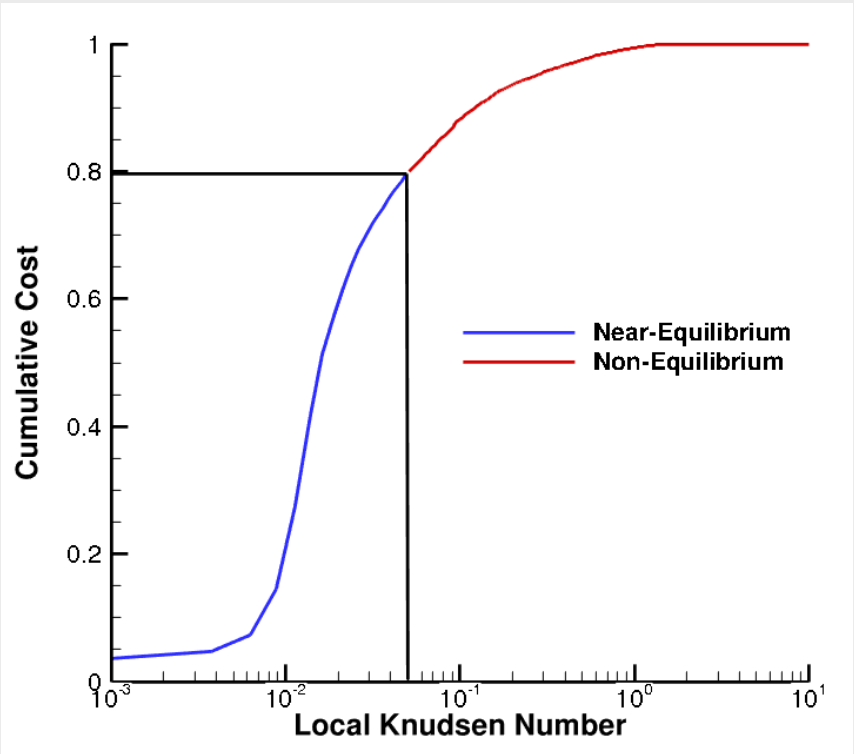
Rarefied DSMC approach:
based on kinetic theory
high altitude, low density
small length scales

Continuum CFD approach:
solve NS equations
low altitude
long length scales

Particle Inefficiency: 1. Highly Collisional Regions

Mach 10, Kn_∞=0.01





80% of DSMC calculation spent in near-equilibrium regions

Hybrid Particle-Continuum Methods

- 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)

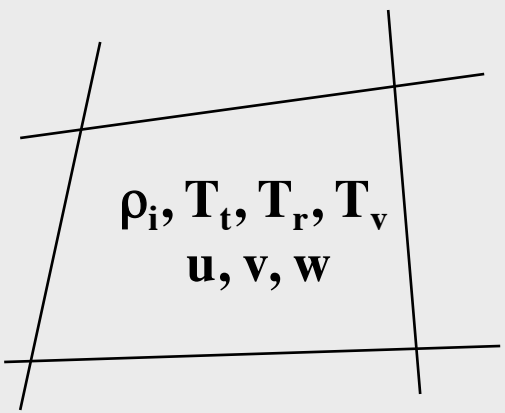
Continuum
Martin, Scalabrin, and Boyd
J Phys D, **341**, 2012

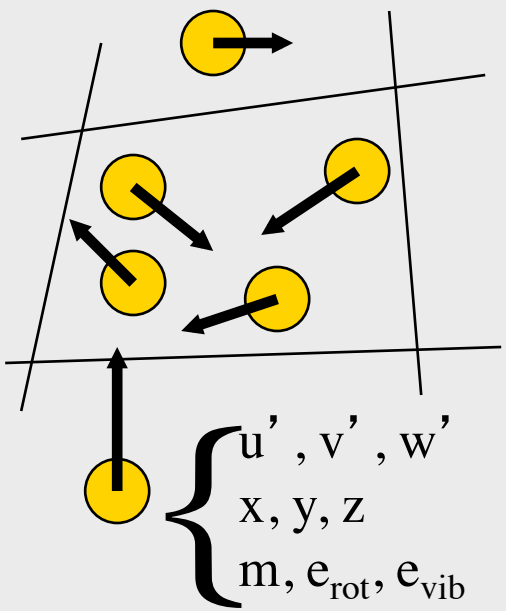
Particle
Dietrich and Boyd
J Comp Phys, **126**, 1996

NS solver (LeMANS) ↔ interface ↔ DSMC (MONACO)

- 2D/3D unstructured mesh
- modified Steger-Warming flux-vector splitting, parallel
- point-implicit time integration
- many physical models

- 2D/3D unstructured mesh
- parallel, domain decomposition
- many physical models





Continuum Breakdown

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

$$Kn_{GL-Q} = \lambda \left| \frac{\nabla Q}{Q} \right|$$

$$Kn_{GL} = \max(Kn_{GL-\rho}, Kn_{GL-V}, Kn_{GL-T})$$

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

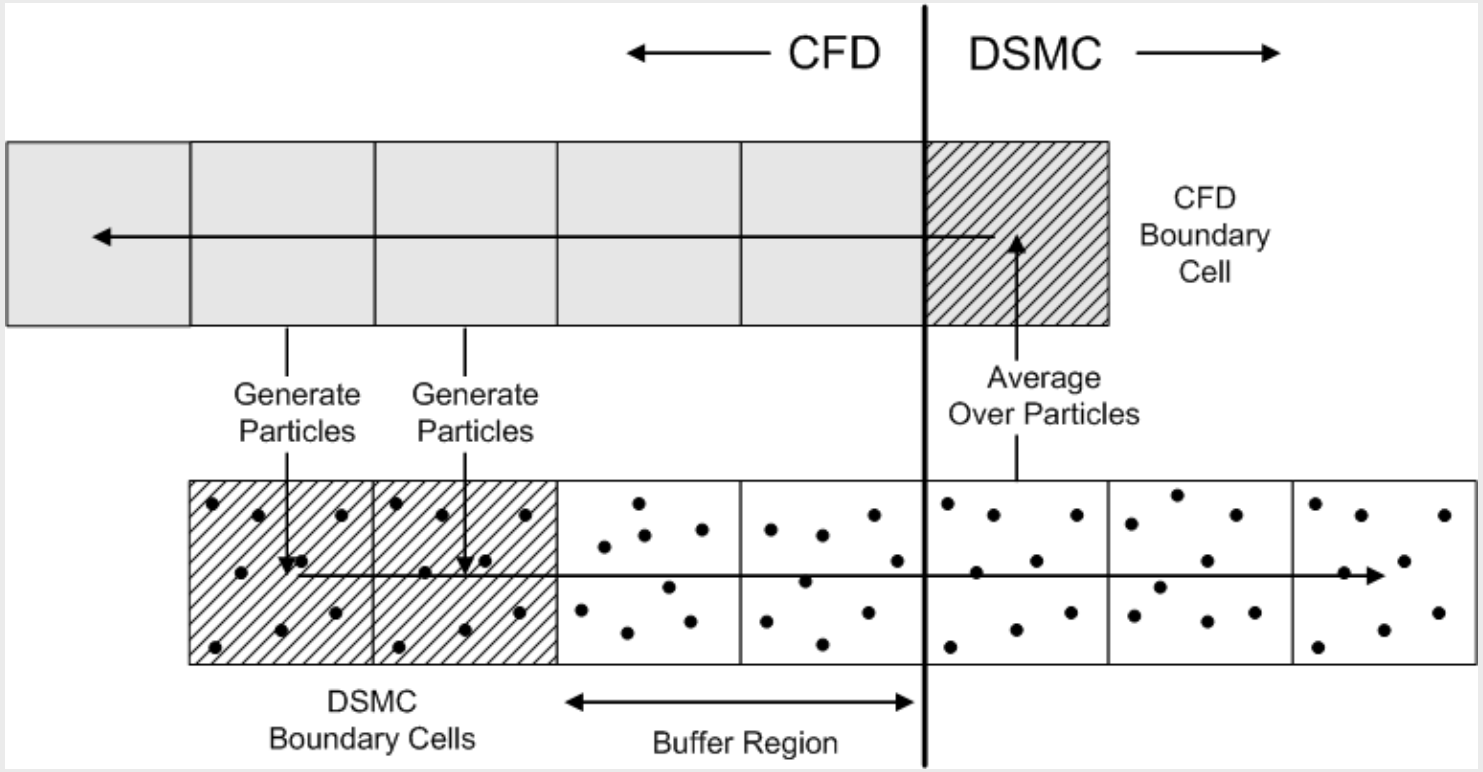
$$\left| \frac{DSMC_{SOL'N} - CFD_{SOL'N}}{DSMC_{SOL'N}} \right| < 5\%$$

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

$$B = \max(\tau^*_{i,j}, q^*_i)$$

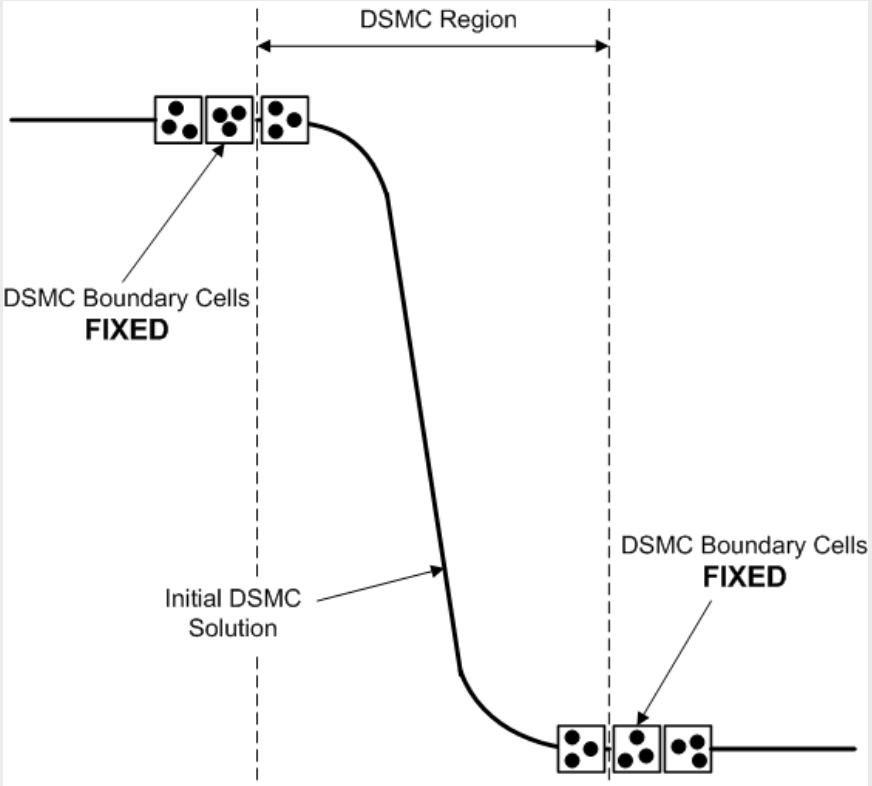
Hybrid Coupling Method

- 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

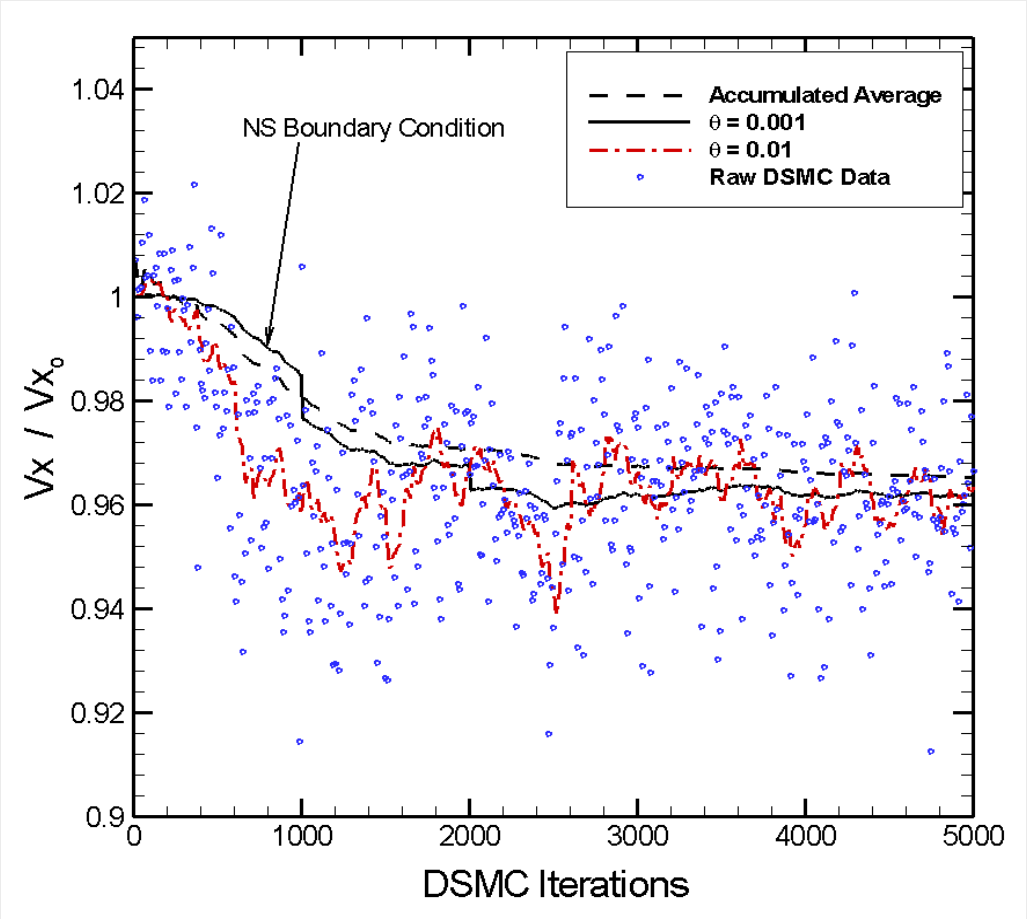
- Sub-relaxation technique (Sun and Boyd, 2005)

$$\overline{A_j} = (1-\theta)\overline{A_{j-1}} + \theta A_j$$

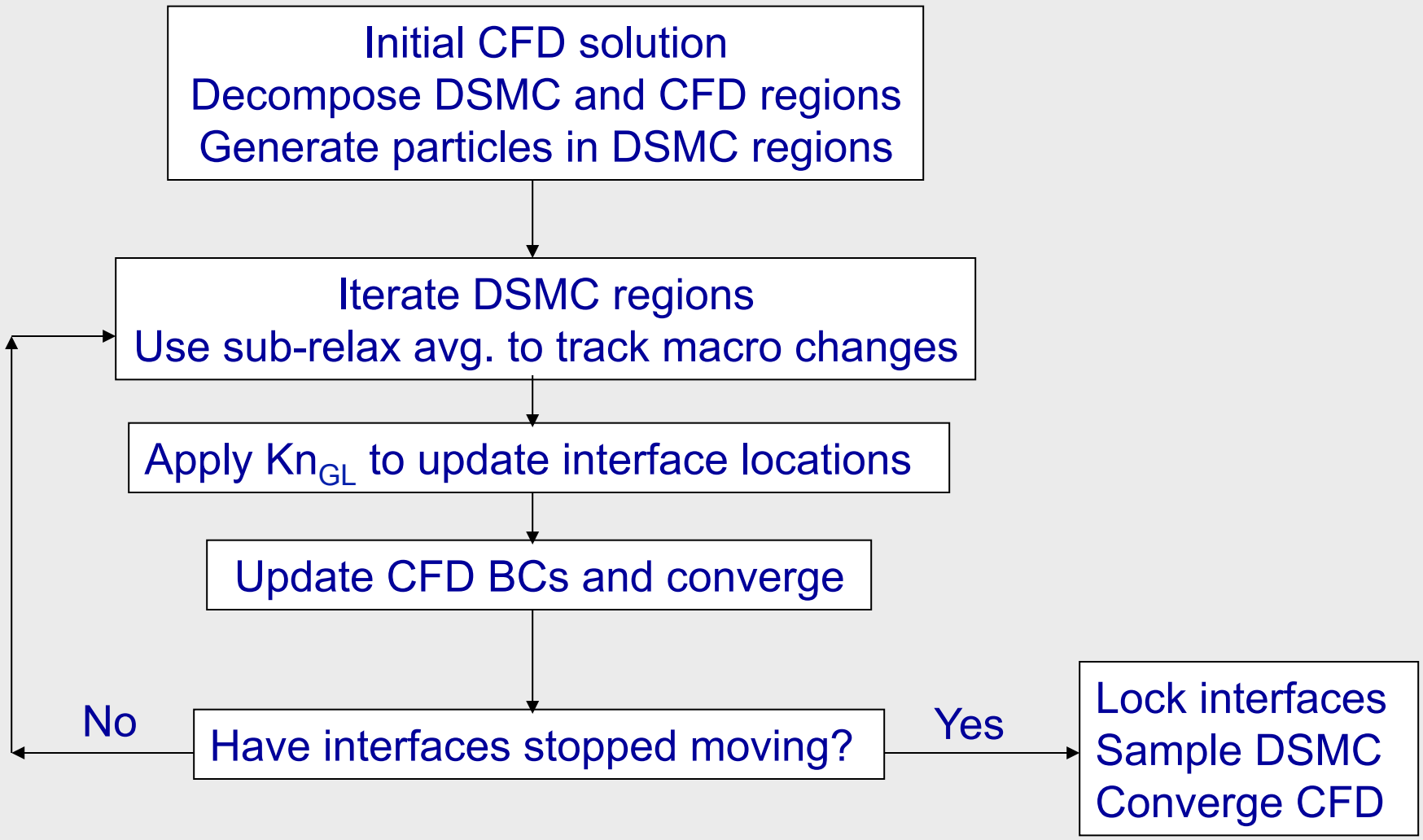
- History before time-step i is removed by

$$\overline{A_j}' = \overline{A_j} + \frac{(1-\theta)^{j-i}}{1-(1-\theta)^{j-i}}(\overline{A_j} - \overline{A_i}'),$$

$$j = \tfrac{1}{\theta} + i$$

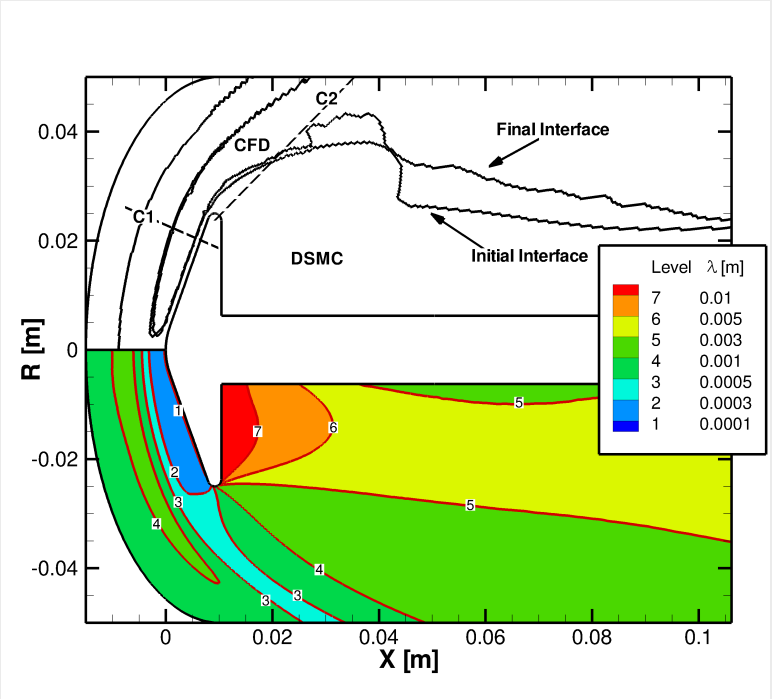


Hybrid CFD-DSMC Algorithm

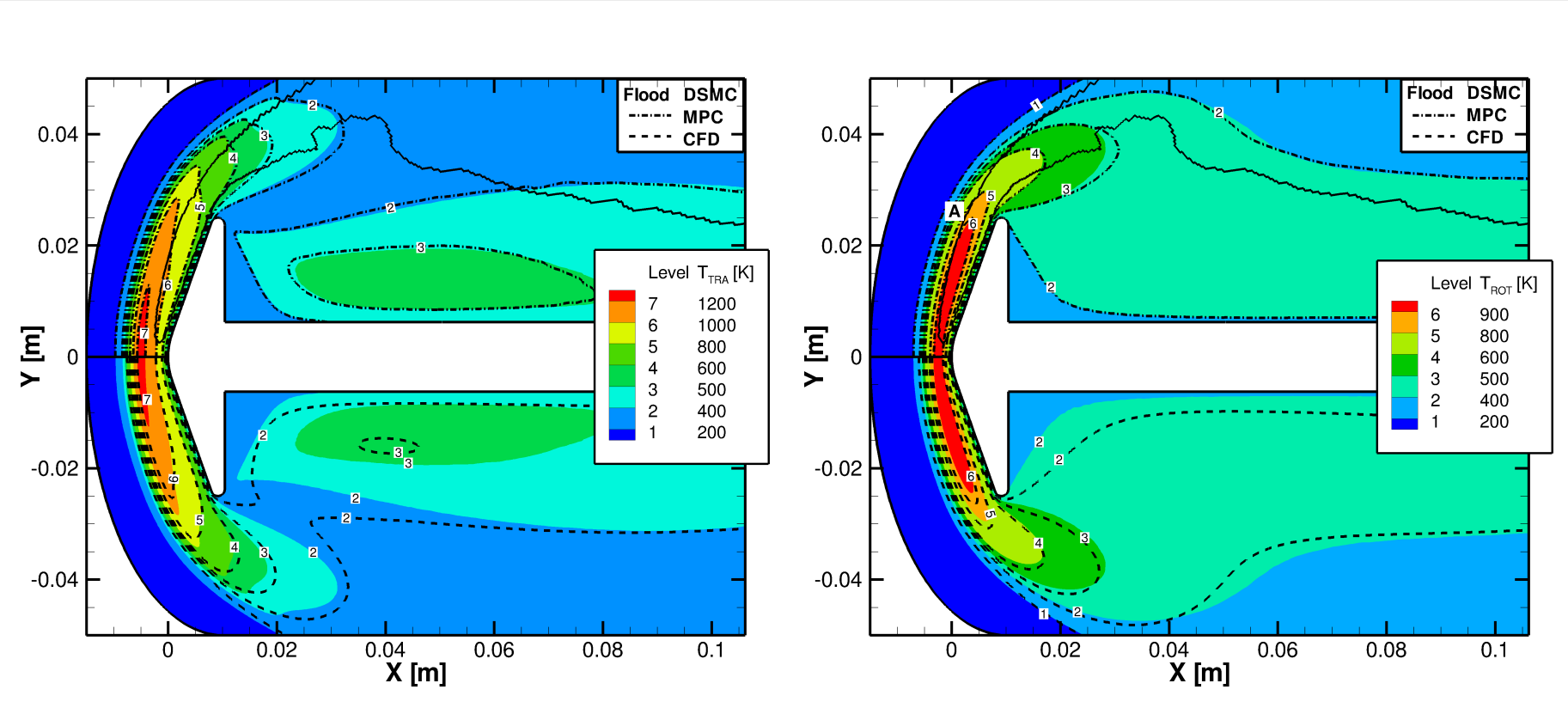


Example: Hypersonic Flow Over Planetary Probe

- 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



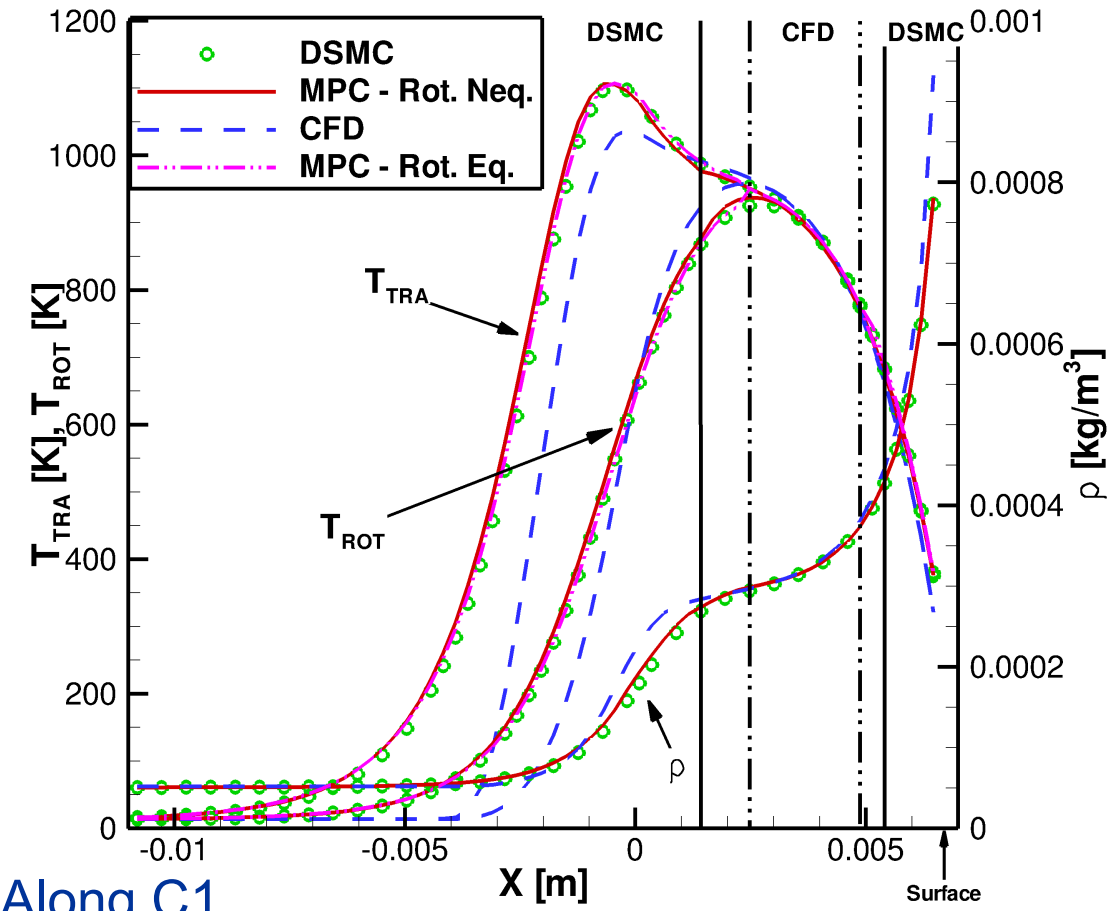
Temperature Contours



Translational

Rotational

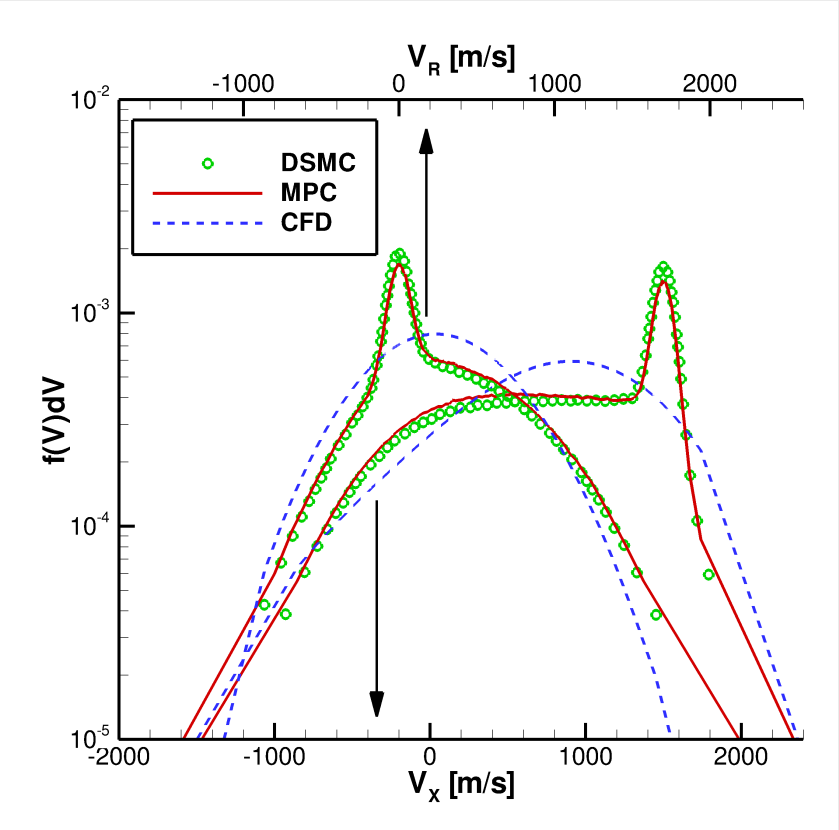
Flow Field Profiles

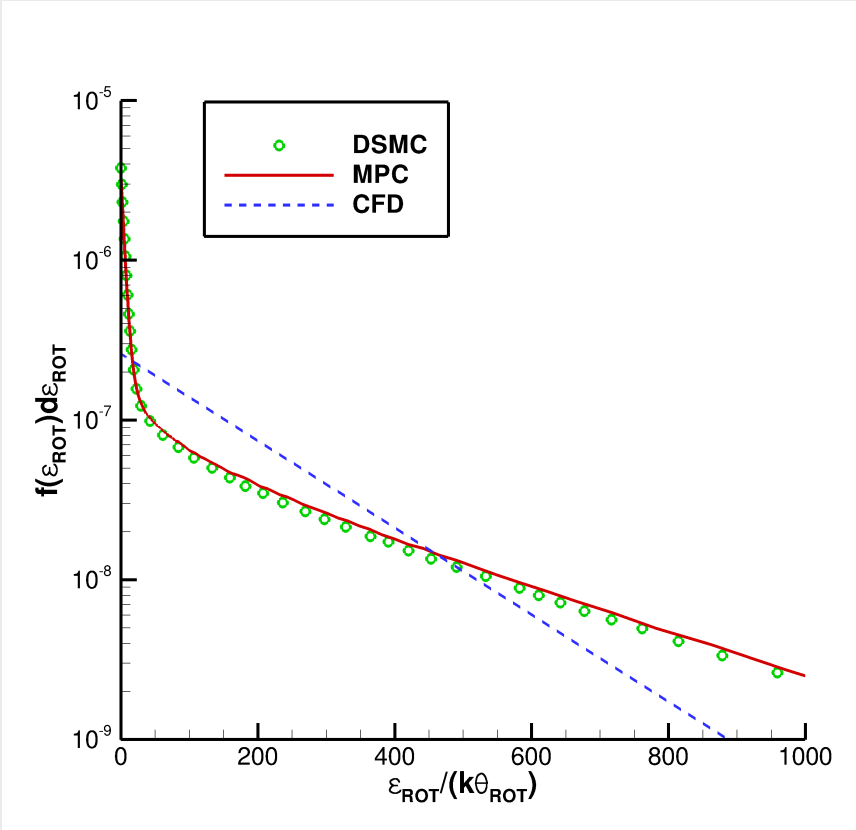


Along C1

Particle Distributions

Point A

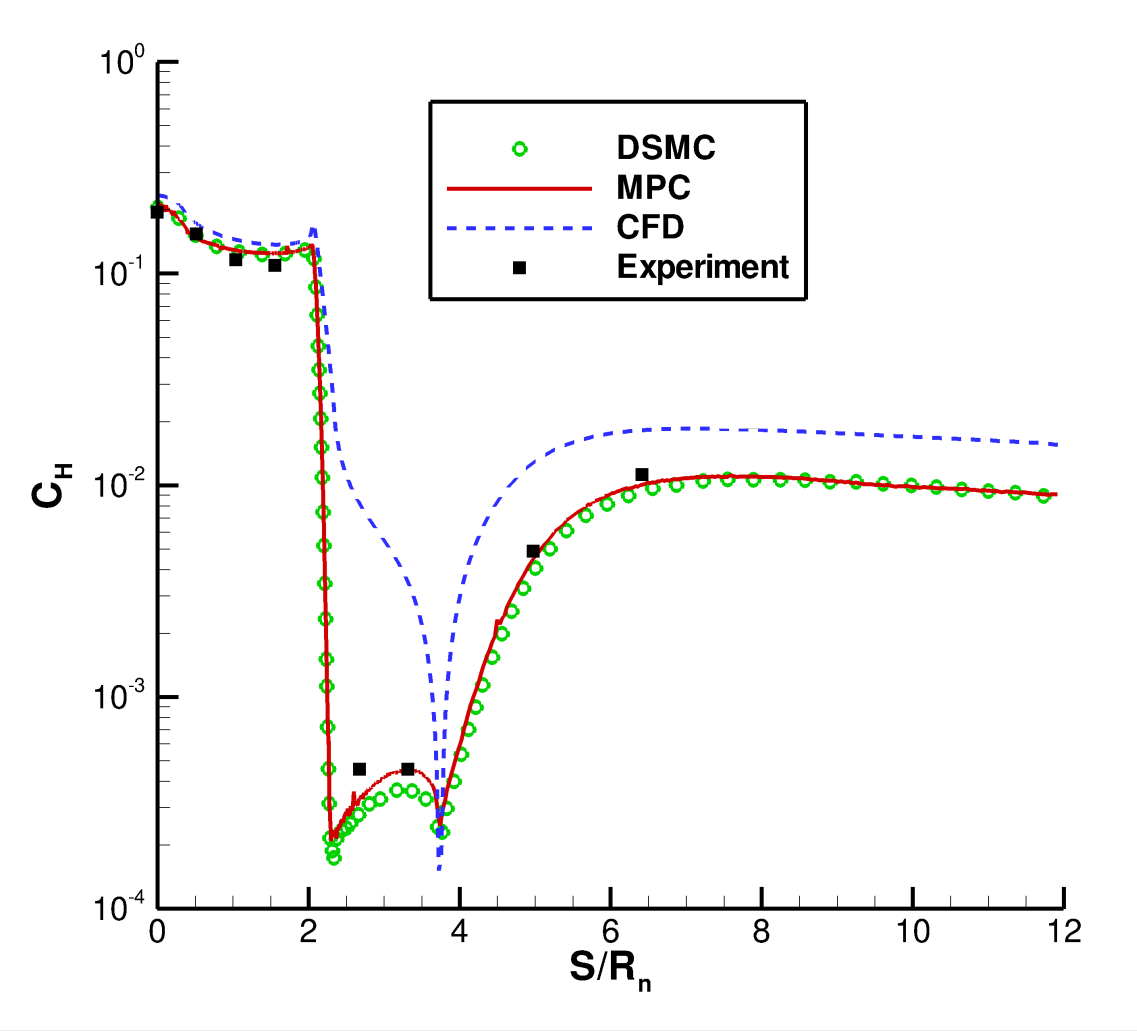




Velocities

Rotational Energy

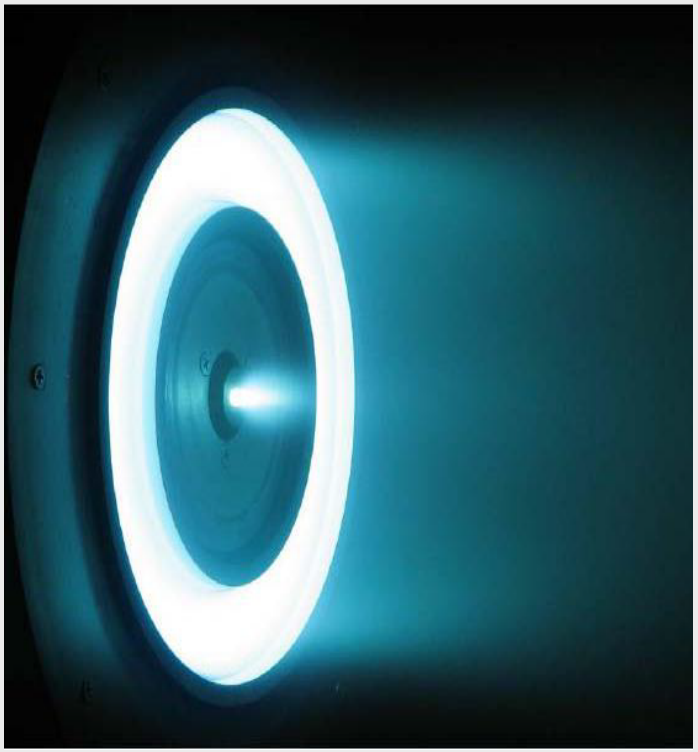
Surface Heating



Final Comments for Hybrid Particle-Continuum Methods

- 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

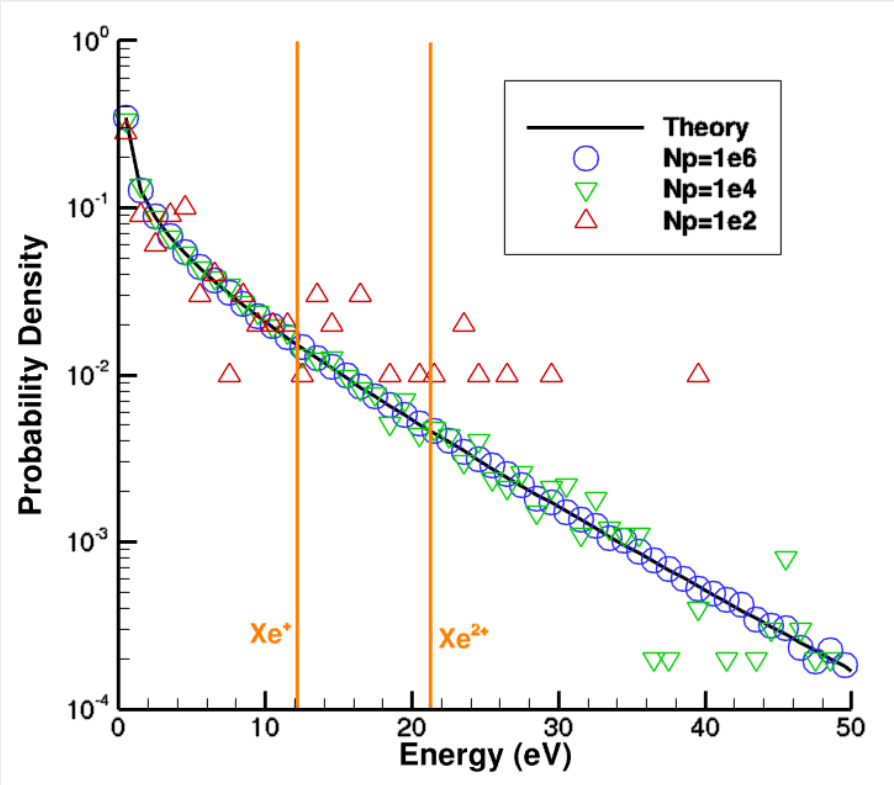


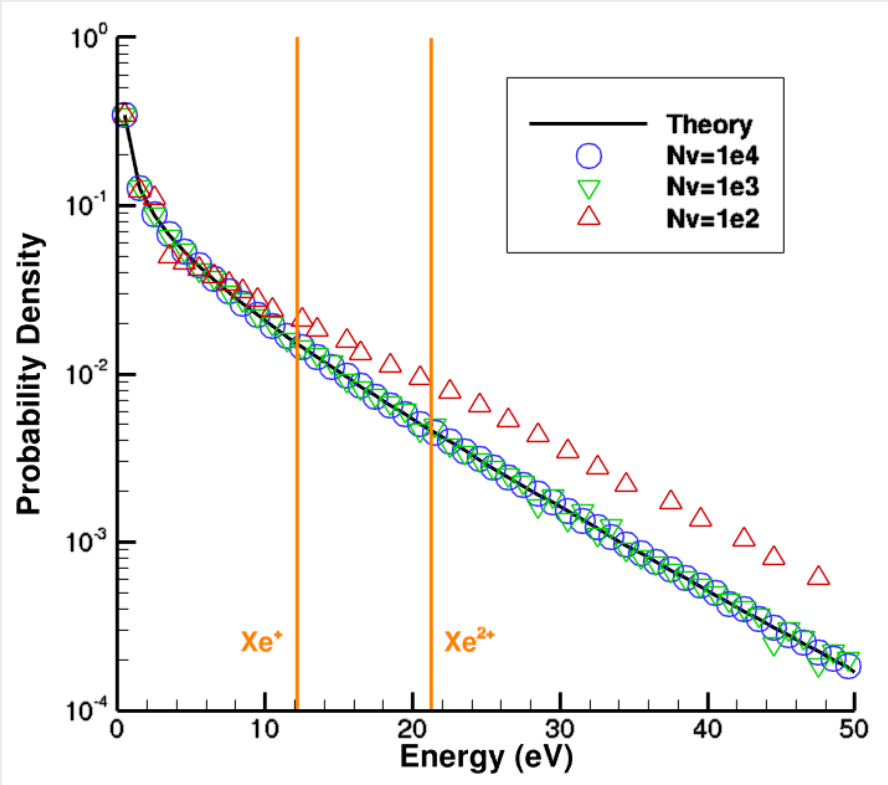
6kW Hall Thruster (University of Michigan)

- 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

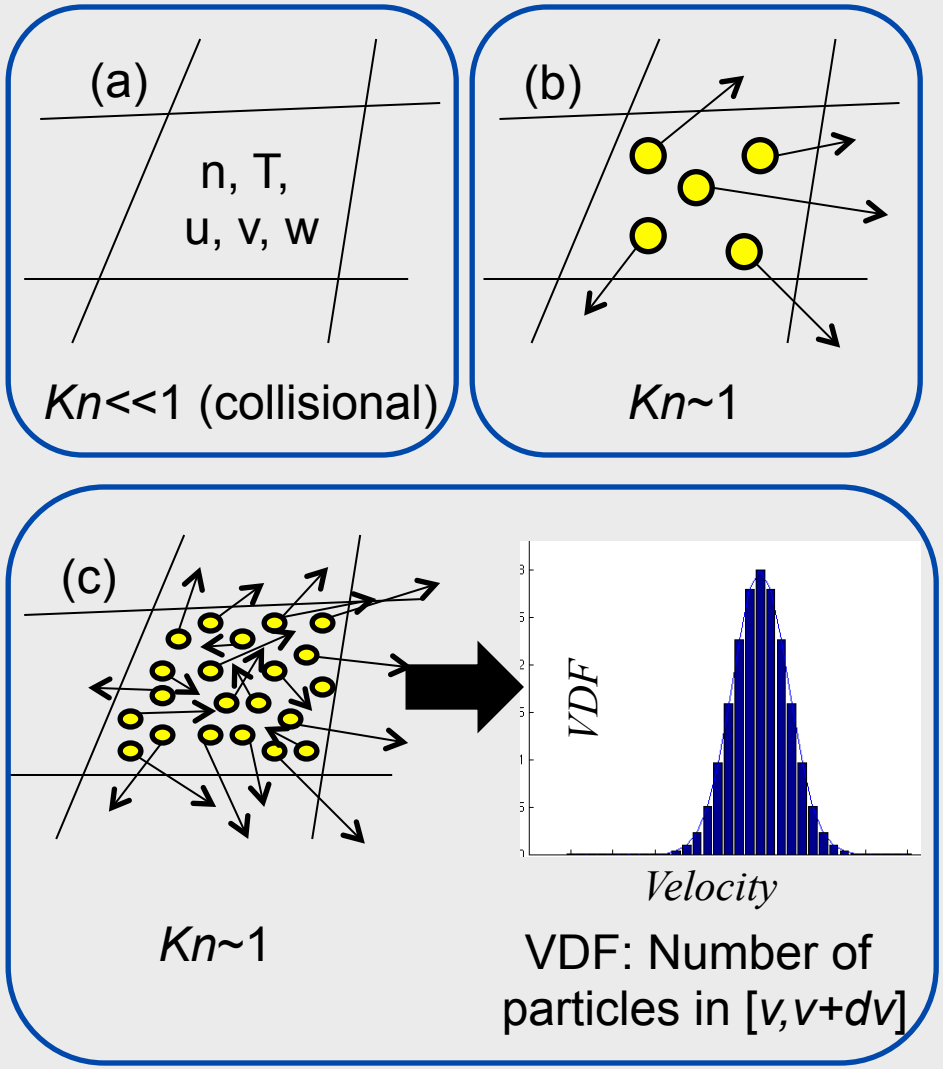
Particle Electrons, Te=10 eV **Deterministic**





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

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

	Hybrid-DK	Hybrid-PIC	Measured
Id	3.59 A	3.94 A	4.5 A
η	0.74	0.69	0.5
Thrust	88.7 mN	90.8 mN	83 mN
Isp	1810 s	1850 s	1600 s

[1] Boeuf et al., J. Appl. Phys, **84**, 3541 (1998).
[2] Koo et al., Phys. Plasmas., **13**, 033501 (2006).

Direct Kinetic (DK) Simulation

Ion kinetic eq. (1D):

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

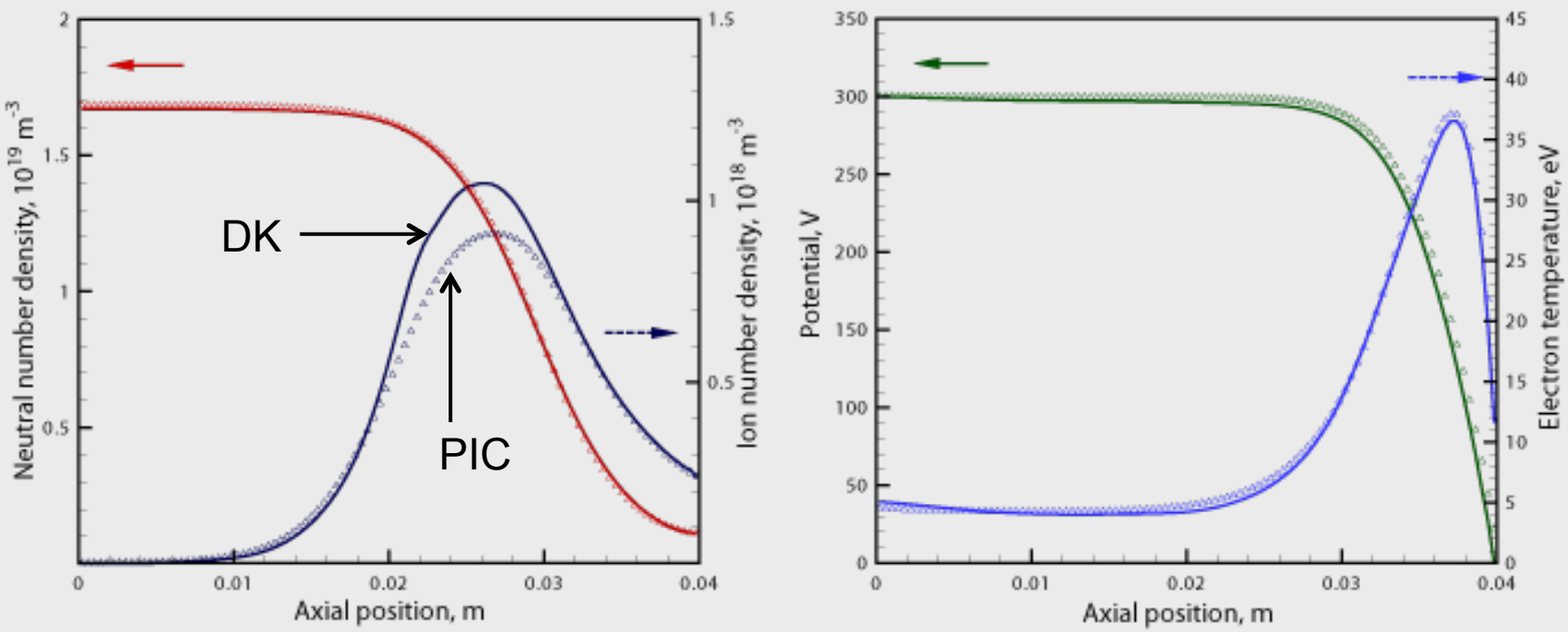
- Ionization + charge exchange collisions
- Dimensionally split (2nd-order in time)
- Finite Volume method using flux reconstruction (2nd-order in space): Conservative, positivity preserving
- Adaptive time step: based on *CFL condition*

$$\max\left(\frac{v\Delta t}{\Delta x}, \frac{a\Delta t}{\Delta v}\right) \leq 1$$

Computational Parameters

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

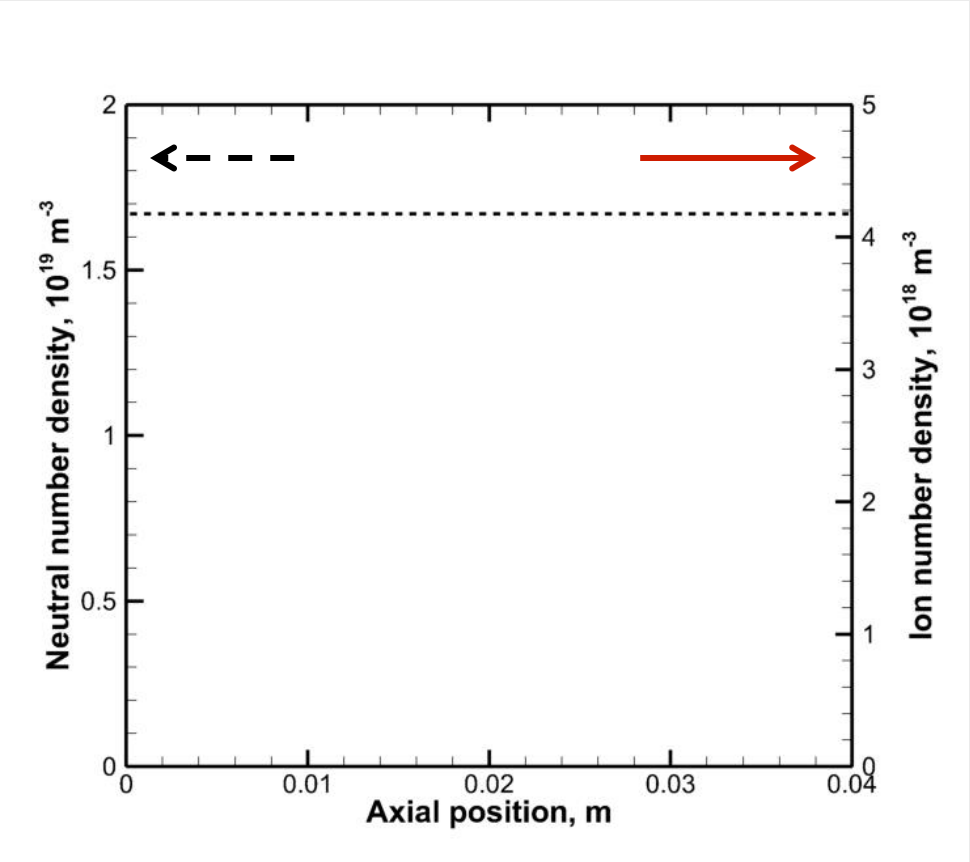
Time Averaged Results



- 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



Anode

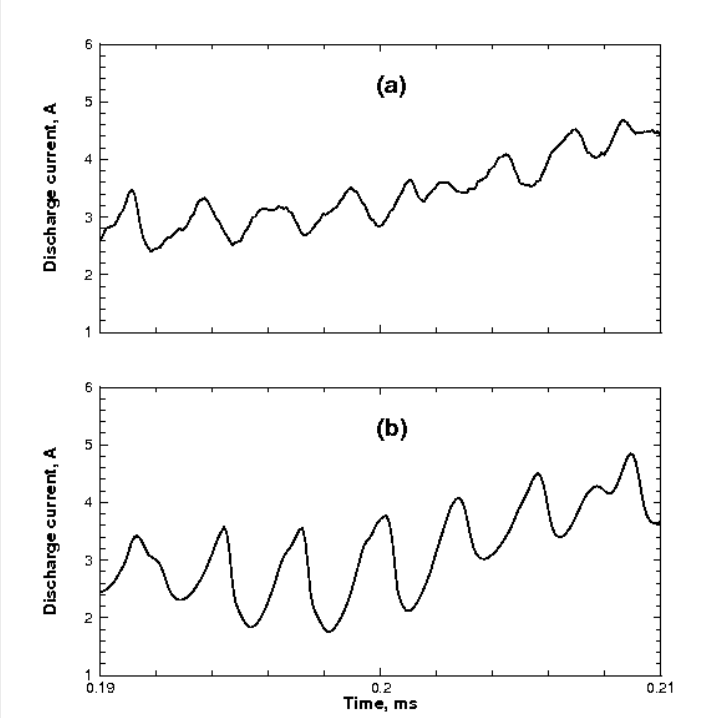
Channel Exit

High-Frequency Oscillations

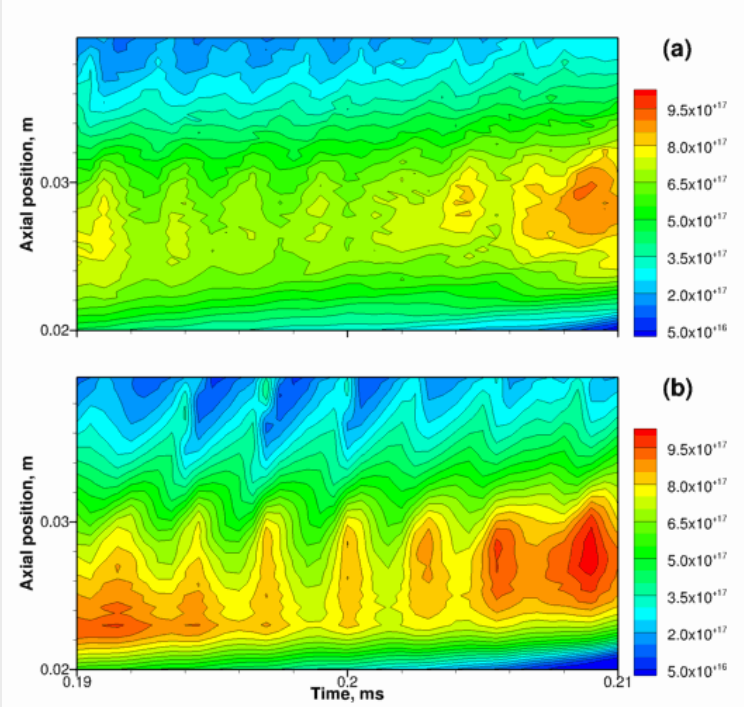
- High-frequency oscillations captured well in DK simulation
  - Transit-time oscillations ~300 kHz due to ionization
  - These oscillations correspond to ion acoustic speed

(a) Hybrid-PIC

(b) Hybrid-DK



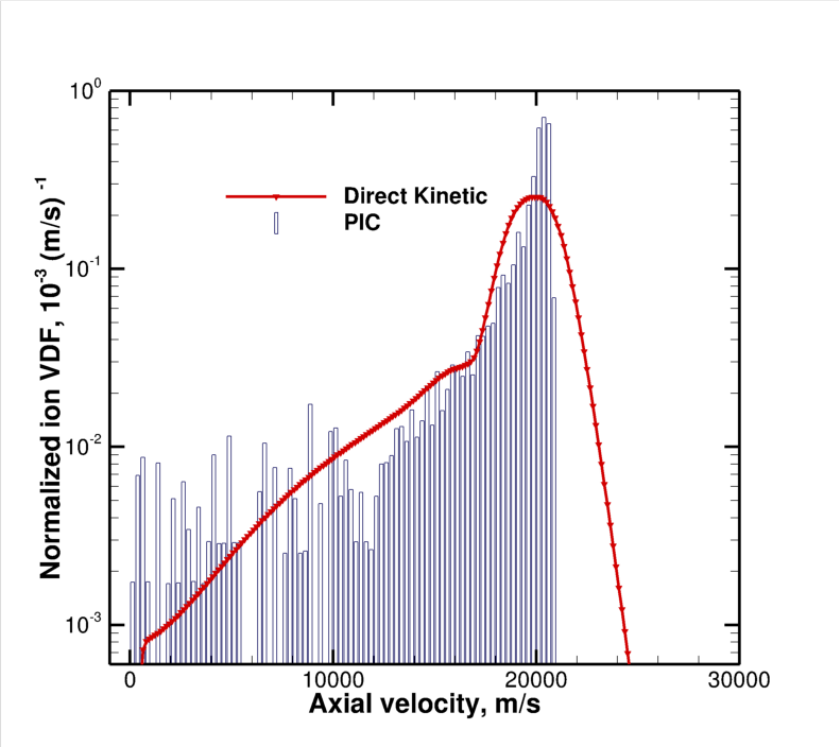
Discharge current



Plasma density

Instantaneous Ion VDF

- 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