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Multiscale Methods for Dilute Fluids and Plasmas

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SIAM 6 July 2009

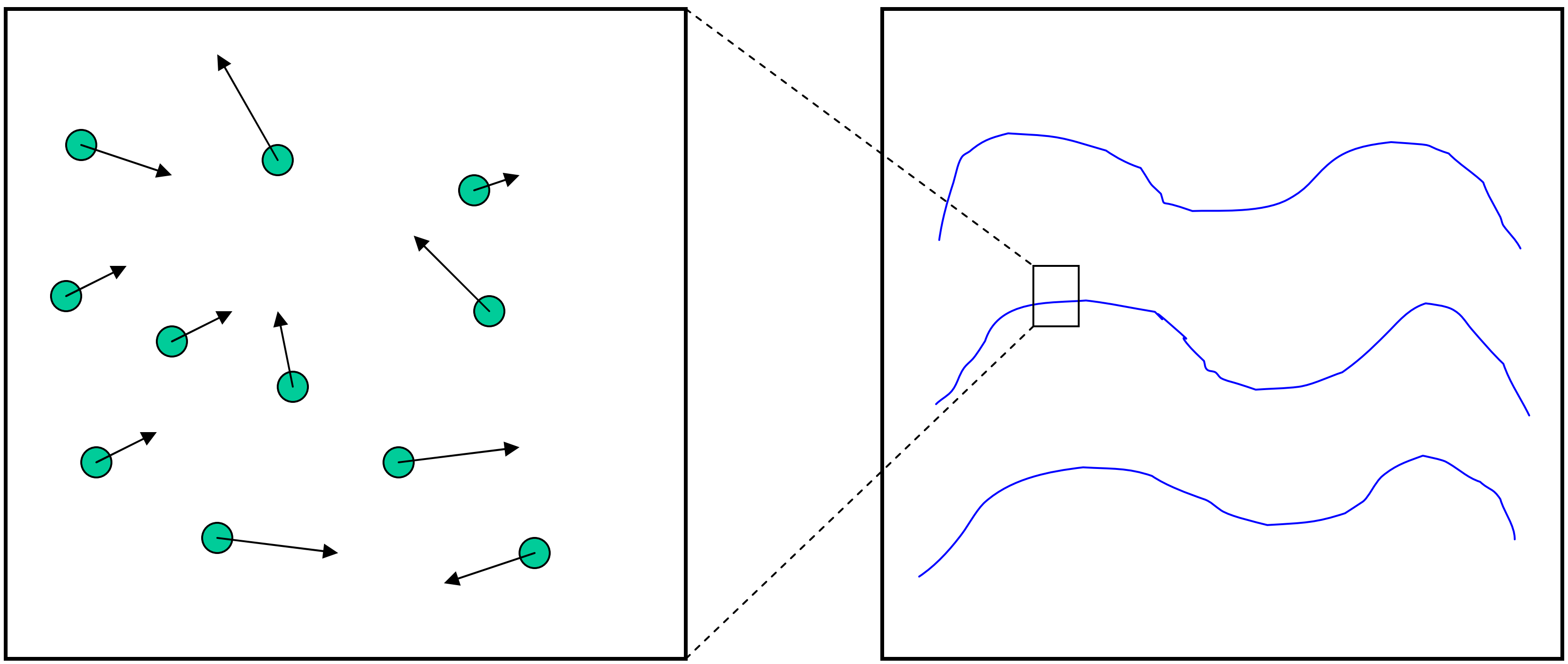
Outline

- Particle dynamics vs. continuum dynamics
  - when does the continuum description fail?
- Rarefied gas dynamics
  - Boltzmann equation
  - short range collisions
- Plasmas
  - Landau-Fokker-Planck equation
  - Coulomb collision - long-rang collisions
- Fluid dynamic (i.e., continuum) limit
- Numerical methods
  - Direct Simulation Monte Carlo (DSMC)
  - failure in fluid dynamic limit
- Multiscale numerical methods
  - robust in fluid dynamic limit

Gas Flow: Particle vs. Fluid

Particle description
- Discrete particles
- Motion by particle velocity
- Interact through collisions

Fluid (continuum) description
- Density, velocity, temperature
- Evolution following fluid eqtns (Euler or Navier-Stokes)



When does continuum description fail?

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Flow with Constant Density (Incompressible)

- Incompressible Euler equations (ρ=1)

$$\nabla \cdot u = 0$$

$$\partial_t u + u \cdot \nabla u + \nabla p = 0$$

- No need for particles

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Compressible Flow

- Compressible Euler equations
  - shock waves

$$\partial_t \rho + \nabla \cdot (\rho u) = 0$$

$$\rho(\partial_t u + u \cdot \nabla u) + \nabla p = 0$$

$$\partial_t E + \nabla \cdot (u(E + p)) = 0$$

  - E=total energy = $\rho(|u|^2/2 + e)$
- No need for particles
  - but need thermodynamics $p = p(\rho, e)$
  - entropy S is needed

Compressible Flow

"S= k log W"

- Compressible Euler equations
  - shock waves

$$\partial_t \rho + \nabla \cdot (\rho u) = 0$$

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Boltzmann's grave

When Does the Continuum Description Fail?

- Rarefied gases and plasmas
- Knudsen number Kn=ε
  - ε = (mean free path)/(characteristic distance)
  - measures significance of collisions
  - mean free path = distance traveled by a particle between collisions

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Rarefied vs. Continuum Flow: Knudsen number Kn

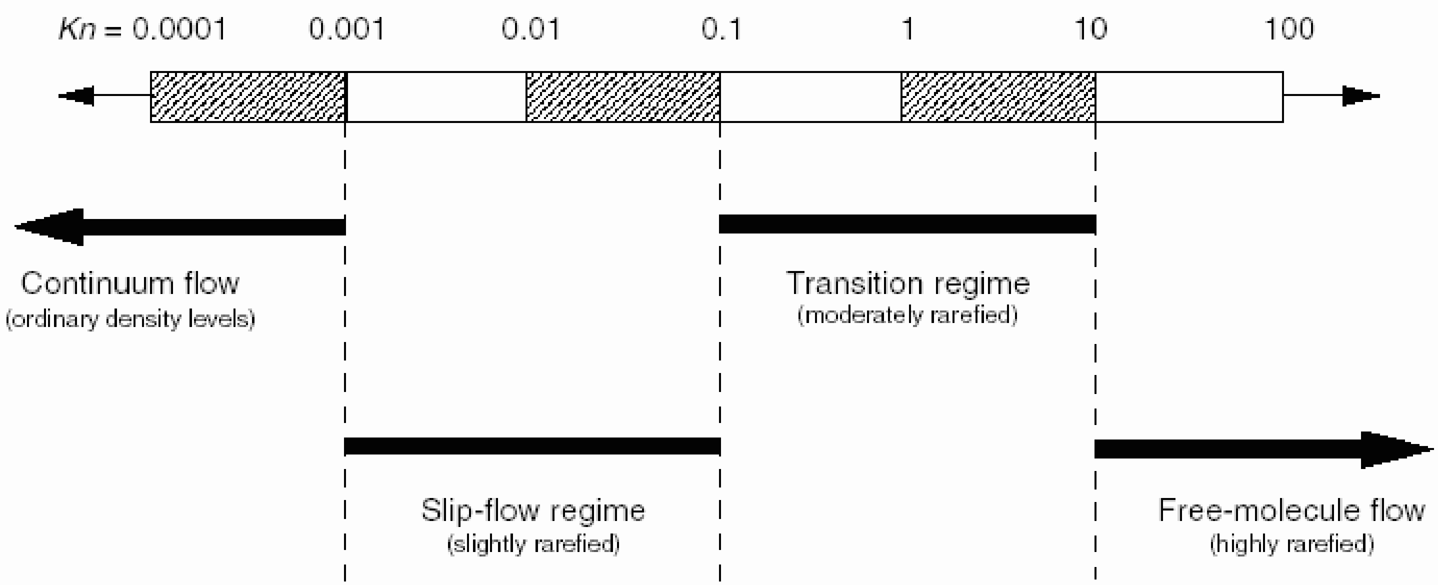

FIGURE 4.2 Knudsen number regimes. (From Gad-el-Hak, M. (1999) *J. Fluids Eng.* **121**, pp. 5–33, ASME, New York. With permission.)

Collisional Effects in the Atmosphere

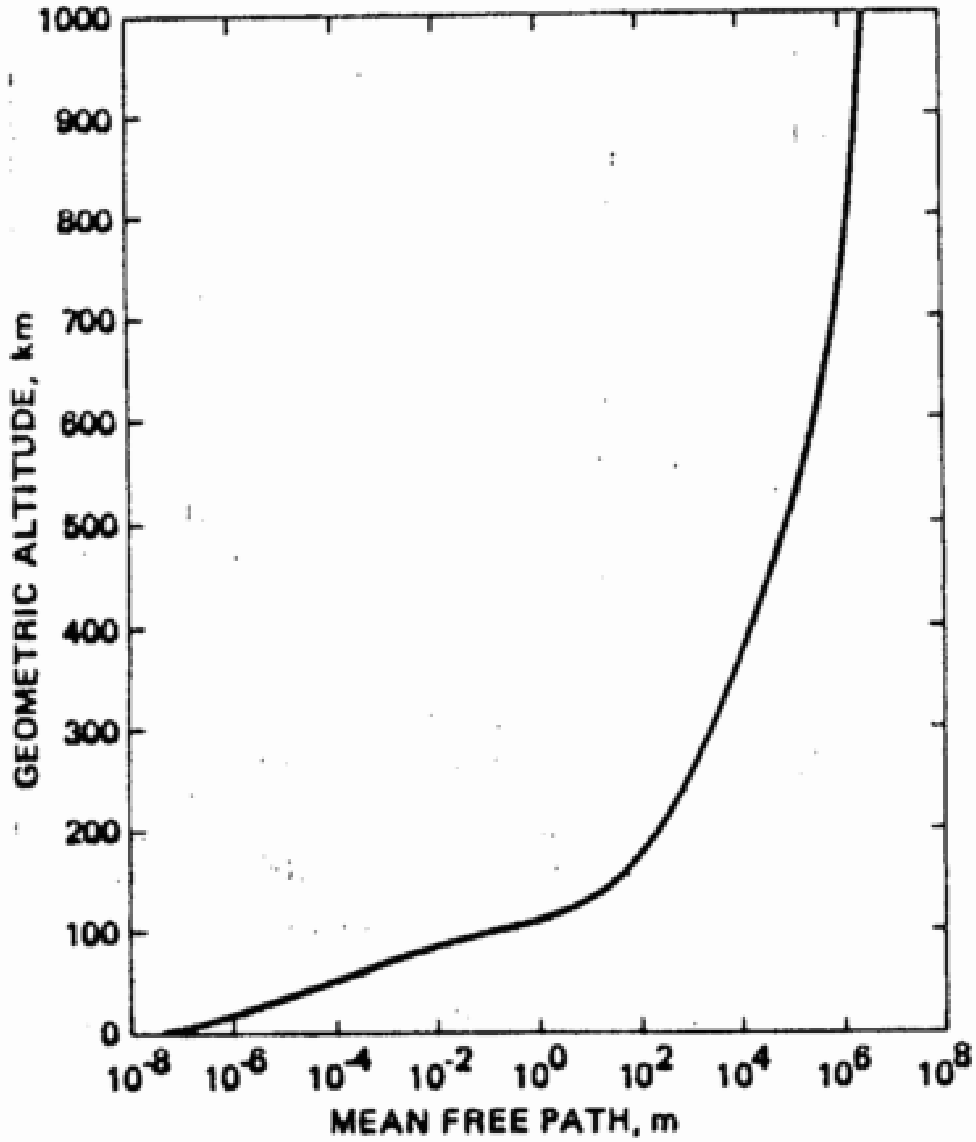

FIGURE 6. Mean free path as a function of geometric altitude.

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Collisional Effects in MEMS and NEMS

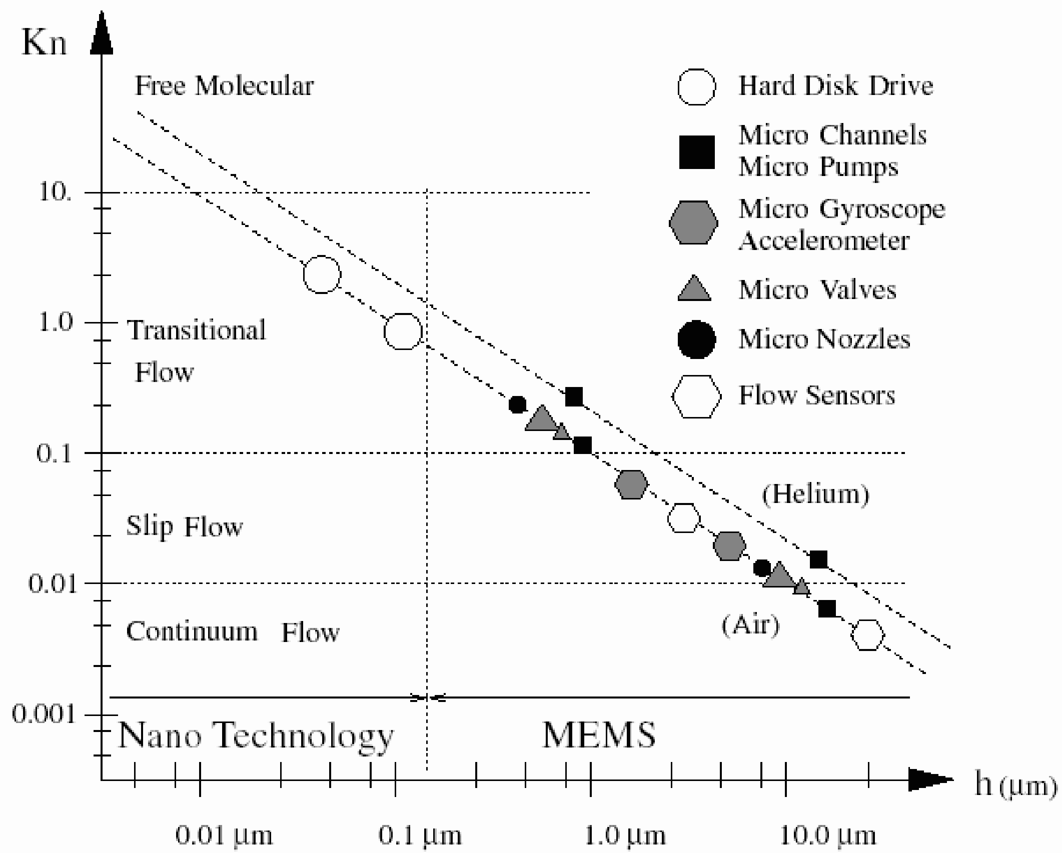

FIGURE 8.1 The Operation range for typical MEMS and nanotechnology applications under standard conditions spans the entire Knudsen regime (continuum, slip, transition and free molecular flow regimes).

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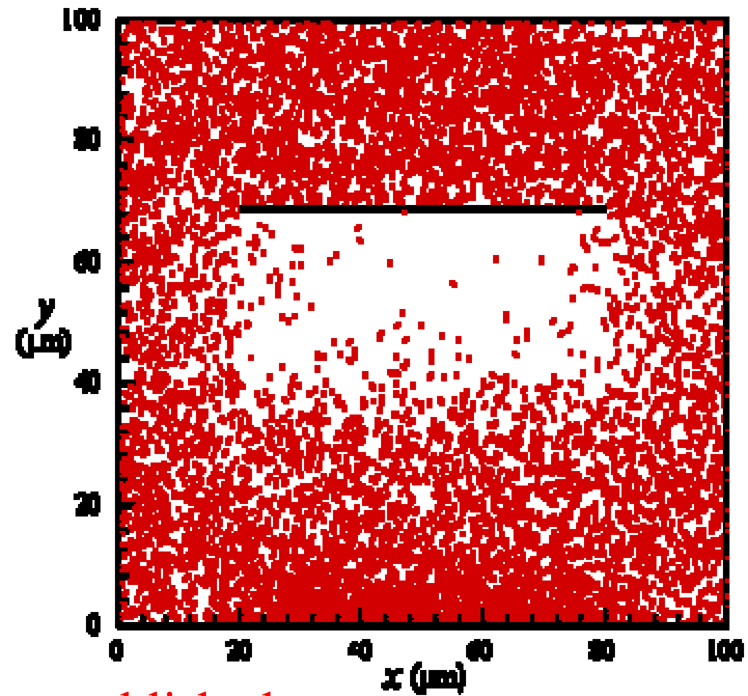
Boltzmann equation for rarefied gas dynamics (RGD)

- Statistical description replaces individual particles
  - density function f=f(x,v,t) in phase space (position x, velocity v) at time t
  - typical number of 10^{20} particles would be intractable
- Boltzmann equation for f

$$f_t + v \cdot \nabla_x f = \varepsilon^{-1} Q(f, f)$$



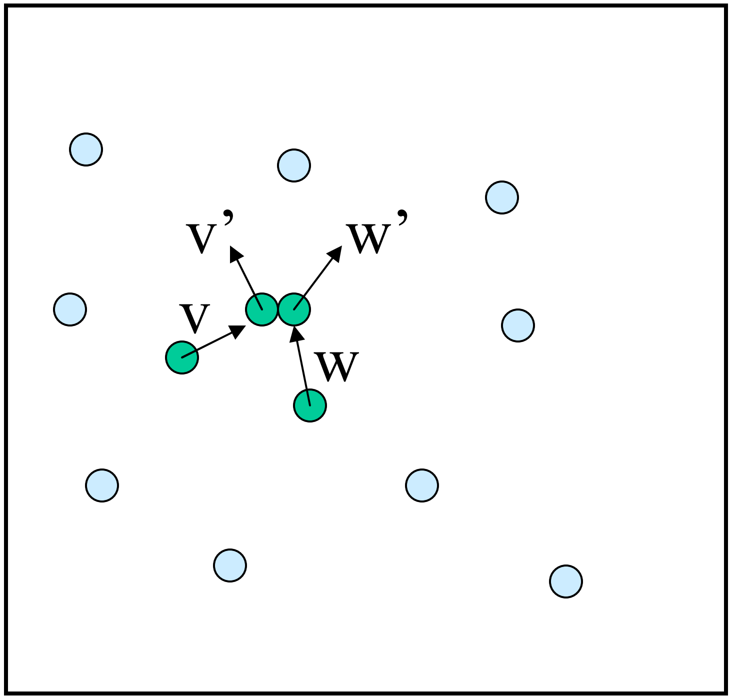
  - ε = Knudsen number
  - Q represents effect of binary collisions
- General existence theorem
  - Diperna & Lions 1989
  - “renormalized” solution
  - uniqueness, conservation of energy are not established

Collisions

- Velocities
  - -v,w before collision
  - -v', w' after collision
- Conservation of momentum and energy
  - $v + w = v' + w'$
  - $|v|^2 + |w|^2 = |v'|^2 + |w'|^2$

-Two free parameters

- $\Omega = (\varepsilon,\theta)$ on sphere
- θ = scattering angle
- ε = angle of plane of collision



Equilibrium and Fluid Limit of Boltzmann

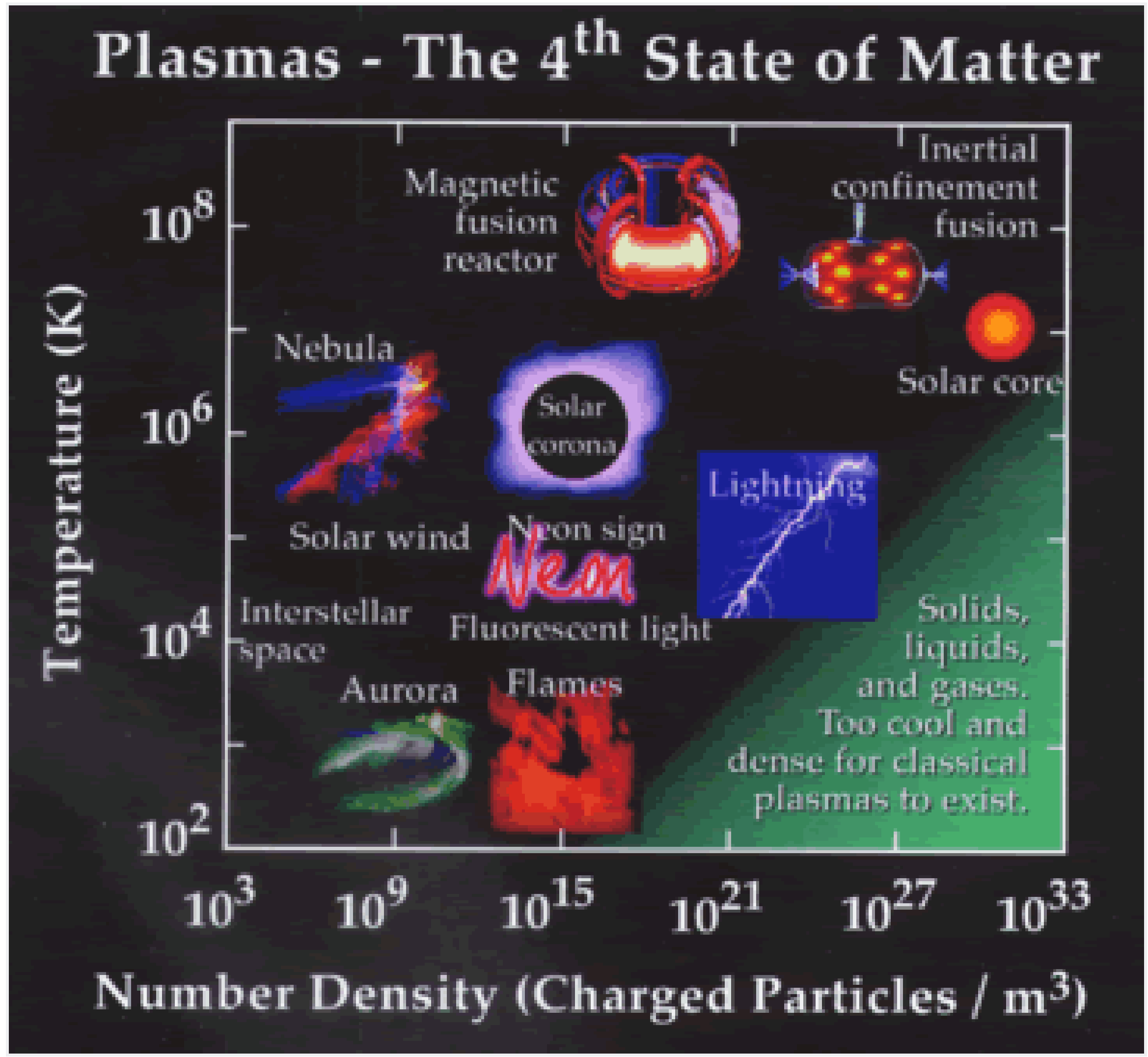
- Maxwellian equilibrium
  - Q(f,f) = 0 implies f = M(v;ρ,u,T)

$$M(\mathbf{v}) = \rho(2\pi T)^{-3/2}\exp(-(\mathbf{v}-\mathbf{u})^2/2T)$$

- Equilibration
  - f=f(v,t) spatially homogeneous
  - H= - Entropy $H(f) = \int f \log(f)dv$
  - Boltzmann's H-theorem $dH/dt \le 0$
  - H-theorem implies f →M as t →∞
- Fluid Limit (Hilbert, Grad, Nishida, REC)
  - ε→0
  - f(v,x,t)→ M(v;ρ,u,T), with ρ= ρ(x,t), etc.
  - ρ,u,T satisfy Euler (or Navier-Stokes)

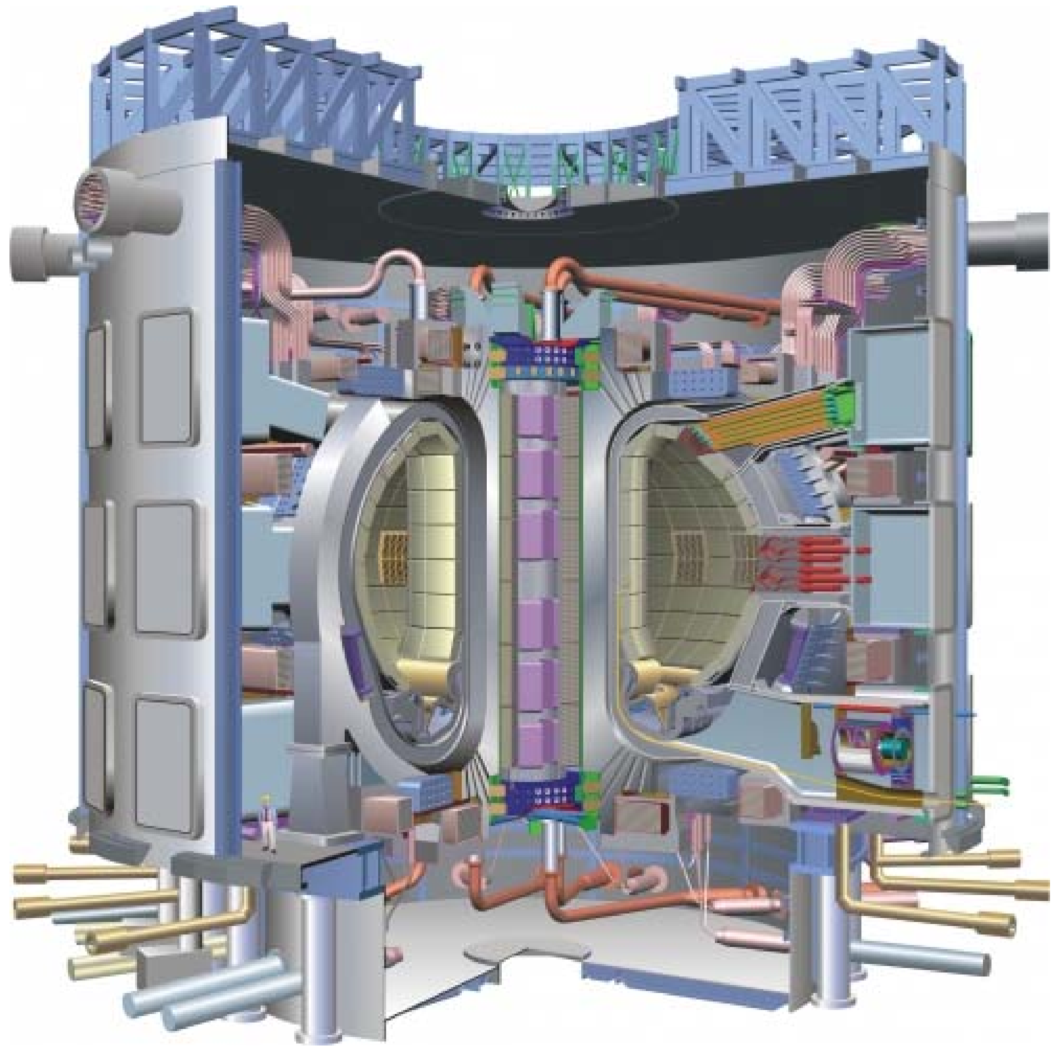
Plasmas

- Plasma
  - gas of ionized particles
  - 99% of visible matter
- Examples
  - fluorescent lights
  - sun
  - fusion energy plasmas



New experimental facilities are driving plasma physics

- ITER
  - tokamak (magnetic confinement fusion)
  - reactor chamber 840 m^3
  - originally the International Thermonuclear Experimental Reactor
  - international (China, EU, India, Japan, Korea, Russia, US)
  - located in southern France



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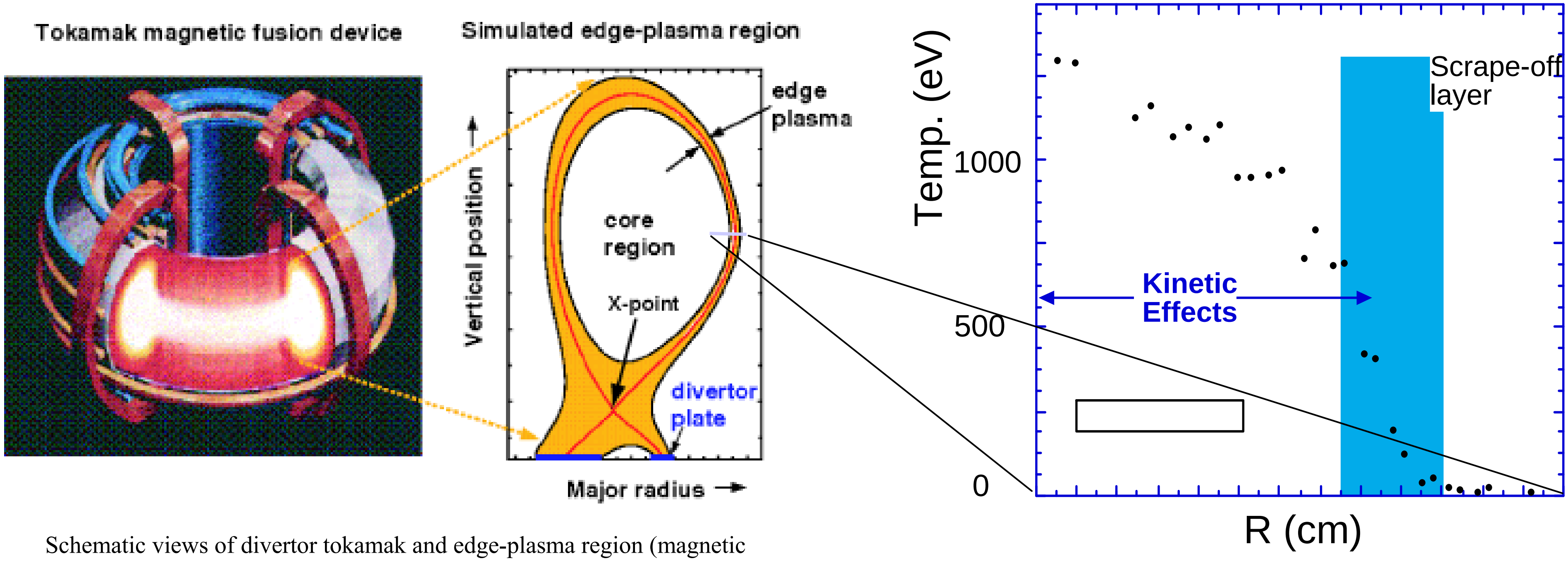
Where are collisions signifiant in plasmas?
Example: Tokamak edge boundary layer



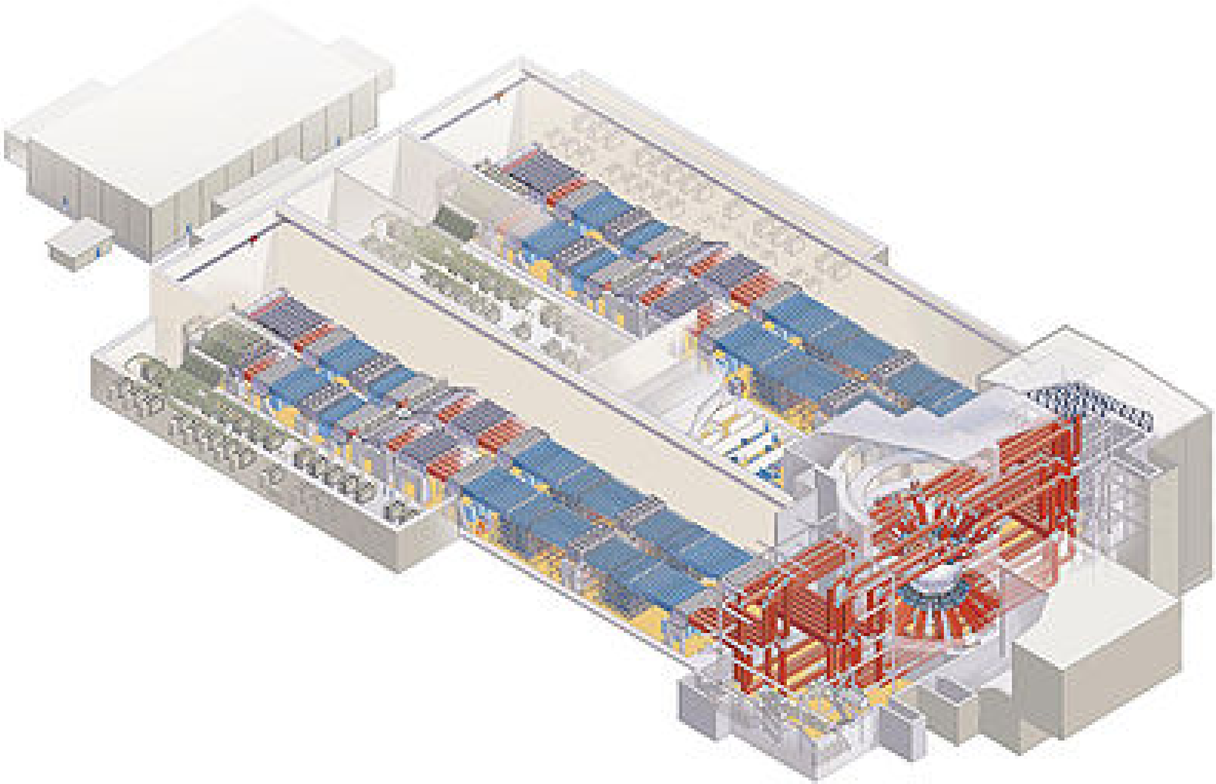
Schematic views of divertor tokamak and edge-plasma region (magnetic separatrix is the red line and the black boundaries indicate the shape of magnetic flux surfaces)

Edge pedestal temperature profile near the edge of an H-mode discharge in the DIII-D tokamak. [Porter*2000*]. Pedestal is shaded region.

From G. W. Hammett, review talk 2007
APS Div Plasmas Physics
Annual Meeting, Orlando, Nov. 12-16.

New experimental facilities are driving plasma physics

- NIF
  - National Ignition Facility
  - 192 lasers
  - laser-based inertial confinement fusion (ICF) device
  - Lawrence Livermore National Laboratory



Interactions of Charged Particles in a Plasma

- Boltzmann equation for plasma with collisions

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + m^{-1} F_{EM} \cdot \nabla_v f = (\frac{\partial f}{\partial t})_{col}$$

$$F_{EM} = q\left(E + \frac{v \times B}{c} \right)$$

m=mass, q=charge

- Long range interactions
  - $r > \lambda_D$ ($\lambda_D =$ Debye length)
  - Electric and magnetic fields E, B
- Short range interactions
  - $r < \lambda_D$
  - Coulomb “collisions”

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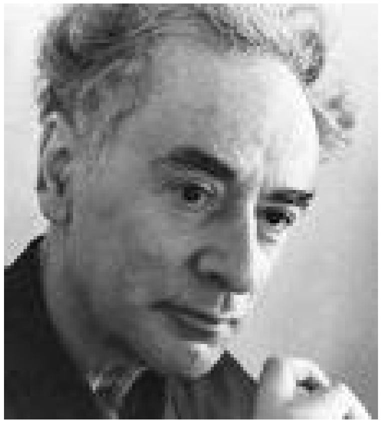
Landau-Fokker-Planck equation for collisions



- Coulomb interactions
  - collision rate ≈ u^{-3} for two particles with relative velocity u
- Fokker-Planck equation

$$\left(\frac{\partial f}{\partial t}\right)_{col} = -\frac{\partial}{\partial \mathbf{v}} g \mathbf{F}_d(\mathbf{v}) f(\mathbf{v}) + \frac{1}{2}\frac{\partial^2}{\partial \mathbf{v}\partial \mathbf{v}} : \mathbf{D}(\mathbf{v}) f(\mathbf{v})$$

$$\mathbf{F}_d(\mathbf{v}) = c_1 \frac{\partial H}{\partial \mathbf{v}} = c_1 \frac{\partial}{\partial \mathbf{v}} 2\int \frac{f(\mathbf{v}')}{|\mathbf{v}-\mathbf{v}'|} d\mathbf{v}'$$

$$\mathbf{D}(\mathbf{v}) = c_2 \frac{\partial^2 G}{\partial \mathbf{v}\partial \mathbf{v}} = c_2 \frac{\partial^2}{\partial \mathbf{v}\partial \mathbf{v}} \int f(\mathbf{v}') |\mathbf{v}-\mathbf{v}'| d\mathbf{v}'$$

Derivation of Landau Equation

- Linear Boltzmann equation (idealized)
  - collision integral

$$Lf(v) = \int k(v,v')f(v')dv' - \alpha(v)f(v)$$

  - conservation of mass

$$\int k(v,v')d\omega = \alpha(v)$$

- grazing collisions

$$k(v,v') \approx \alpha\delta(v' - (v+\Delta v))$$

$$\approx \alpha\delta(v'-v) + \beta\partial_v\delta(v'-v) + \gamma\partial_v^2\delta(v'-v)$$

  - derivation of Landau collision operator

$$Lf(v) \approx \int \left(\alpha - \beta\partial_{v'} + \gamma\partial_{v'}^2\right)\delta(v'-v)f(v')dv' - \alpha f(v)$$

$$= \left(\alpha + \partial_v\beta + \partial_v^2\gamma\right) f(v) - \alpha f(v)$$

$$= \left(\partial_v\beta + \partial_v^2\gamma\right) f(v)$$

Collisions in Gases vs. Plasmas

- Collisions between velocities v and v_*
  - $q = | v - v_* |$ relative velocity
- Gas collisions
  - hard spheres, σ = cross section area of sphere
  - collision rate is σq
  - any two velocities can collide → smoothing in v
- Plasma (Coulomb) collisions
  - very long range, potential $O(1/r)$
  - collisions are grazing, localized as in Landau eqtn
  - differential eqtn in v, as well as x,t
  - waves in phase space
  - Landau damping (interaction between waves and particles)

Boltzmann → Continuum: The original multiscale problem

- Maxwell calculated fluid transport coefficients
  - viscosity coefficient independent of density
- Hilbert performed perturbation expansion to derive Euler eqtns from Boltzmann eqtn

$$f = f_0 + \varepsilon f_1 + O(\varepsilon^2)$$

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Derivation of Euler equations

- Insert expansion into Boltzmann eqtn

$$f = f_0 + \varepsilon f_1 + O(\varepsilon^2)$$

$$f_t + v \cdot \nabla_x f = \varepsilon^{-1} Q(f, f)$$

- Expansion of eqtn

$$O(\varepsilon^{-1}): \quad Q(f_0, f_0) = 0$$

$$\Rightarrow f_0 = M = \rho (2\pi T)^{-3/2} \exp(-|v-u|^2 / 2T)$$

$$O(\varepsilon^0): \quad (\partial_t + v \cdot \nabla_x) f_0 = 2Q(f_0, f_1)$$

$$\int (1, v, v^2) Q dv = 0 \quad \Rightarrow \int (1, v, v^2)(\partial_t + v \cdot \nabla_x) M dv = 0$$

conservation of mass, momentum, energy

- Solveability condition (conservation)

$$\int \left(1, v, v^2\right)\left(\partial_t + v g\nabla_x\right) M dv = 0$$

- Equivalent to Euler eqtns

$$\partial_t \rho + \nabla \cdot (\rho u) = 0$$

$$\rho(\partial_t u + u \cdot \nabla u) + \nabla p = 0$$

$$\partial_t E + \nabla \cdot (u(E + p)) = 0$$

- Using integrals

$$\int \left(1, v, v^2\right) M dv = (\rho, \rho u, 2E)$$

$$\int \left(1, v, v^2\right) v M dv = (\rho u, \rho u u + pI, 2u(E + p))$$

$$E = \rho(|u|^2 + 3T)/2 \qquad p = \rho T$$

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Dominant numerical method for dilute flows

- DSMC = Direct Simulation Monte Carlo
  - Invented by Graeme Bird, early 1970's
  - Represents density f as collection of particles

$$F(v) = \sum_{k=1}^{N} \delta(v - v_k(t))\delta(x - x_k(t))$$

  - Directly simulates RGD by randomizing collisions
    - Collision v,w →v',w' conserving momentum, energy
    - Random choice of collision angles (ε,θ)
  - Particle advection $dx_k / dt = v_k$
  - Convergence (Wagner 1992)
- Limitation of DSMC
  - DSMC becomes computationally intractable near fluid regime, since collision time-scale becomes small

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What can mathematics contribute to DSMC?

- Traditionally, math contributed little to DSMC
  - only difficulties are computational complexity
  - no stability, consistency issues
- Flows near fluid limit
  - DSMC becomes intractable
  - math needed to design methods that overcome this difficulty!

Current Multiscale Methods: What's New?

- Current multiscale methods
  - e.g. quasi-continuum, HMM, equations-free method
  - combine multiple scales and multiple physics into a single numerical method
- Multiscale methods for dilute fluids and plasmas (my title!)
  - applicable in near fluid regime
  - combine fluid and particle descriptions
  - provide considerable acceleration over traditional methods

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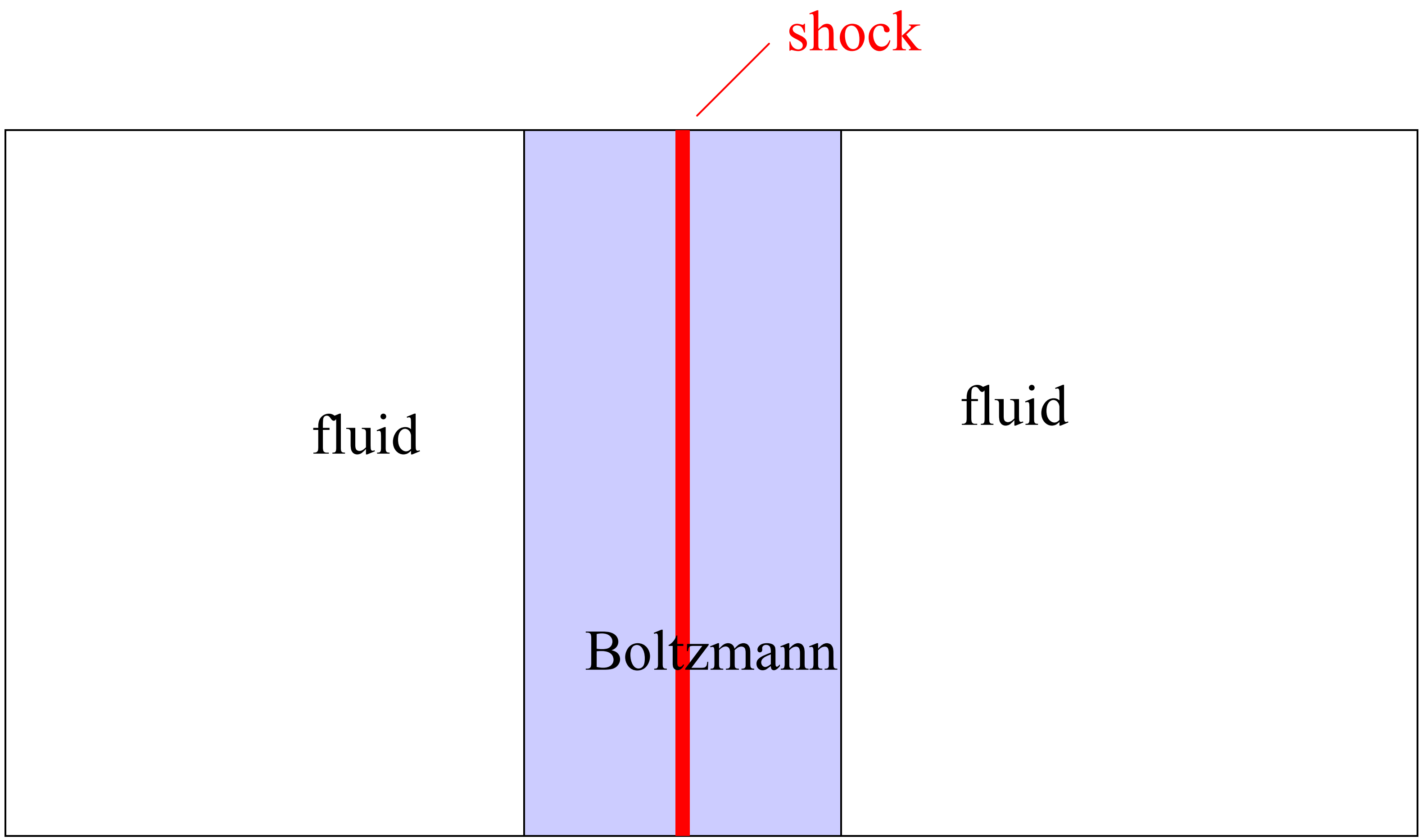
Accelerated Methods for RGD

- Domain decomposition
  - DSMC in one region, CFD in another region
  - Hash & Hassan (1996), Letallec & Mallinger (1997), Tiwari & Klar (1998), Garcia, Bell Crutchfield & Alder (1999), Boyd (2006),…
- Asymptotic-preserving methods
  - Fluid limit for numerical method consistent with limit for Boltzmann
  - Larsen (neutron transport), Levermore, Jin, Degond, …
- Hybrid methods
  - Combine fluids and Monte Carlo throughout space
  - Roveda, Goldstein & Varghese (1998), Pareschi & REC (1999), Pareschi & Russo (2000), Crouseilles, Degond & Lemou (2004), REC, Luo, Pareschi (2006)
- Complex particle methods
  - add additional degrees of freedom to particles, representing fluid state
  - not closely related to the other types of methods

Domain decomposition



- Method required for finding domain interfaces
- Fluid/particle BCs needed across interfaces
- On Boltzmann side of interface, computation is still stiff

Asymptotic Preserving Methods

Boltzmann solver (ε,N,dx) —— $\varepsilon \to 0$ ——→ limit of Boltzmann solver (N,dx)

Boltzmann solver (ε,N,dx) ↓ $N \to \infty$, $dx \to 0$ ↓ Boltzmann eqtn (ε)

limit of Boltzmann solver (N,dx) ↓ $N \to \infty$, $dx \to 0$ ↓ Fluid eqtns

Boltzmann eqtn (ε) —— $\varepsilon \to 0$ ——→ Fluid eqtns

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Hybrid method

- Combine fluid and particle methods
- Pareschi & REC
  - Representation of density function as combination of Maxwellian and particles

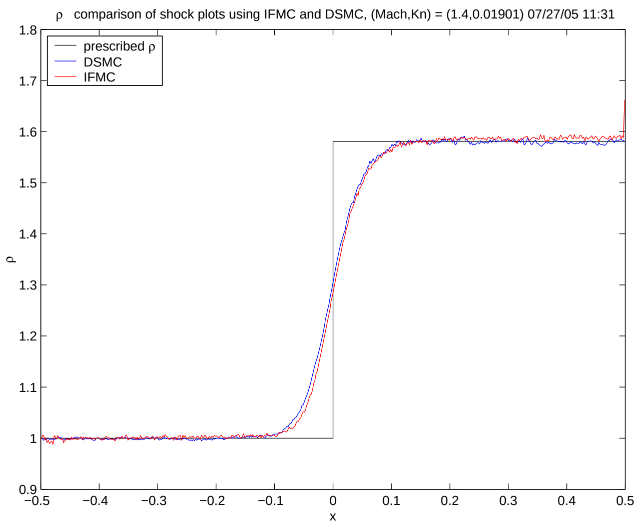
$$F(v) = \alpha M(v) + m \sum_{k=1}^{(1-\alpha)N} \delta(v - v_k(t))$$

$$M(v) = \rho (2\pi T)^{-3/2} \exp(-(v-u)^2 / 2T)$$

  - ρ, u, T solved from fluid eqtns, using Boltzmann scheme for CFD
  - DSMC used for particles
- Thermalization coefficient α
  - independent of v (cf. plasma)
  - $\alpha = 0 \leftrightarrow$ DSMC
  - $\alpha = 1 \leftrightarrow$ CFD
  - Remains robust near fluid limit

Comparison of DSMC (blue) and IFMC (red) for a shock with Mach=1.4 and Kn=0.019
Direct convection of Maxwellians

ρ



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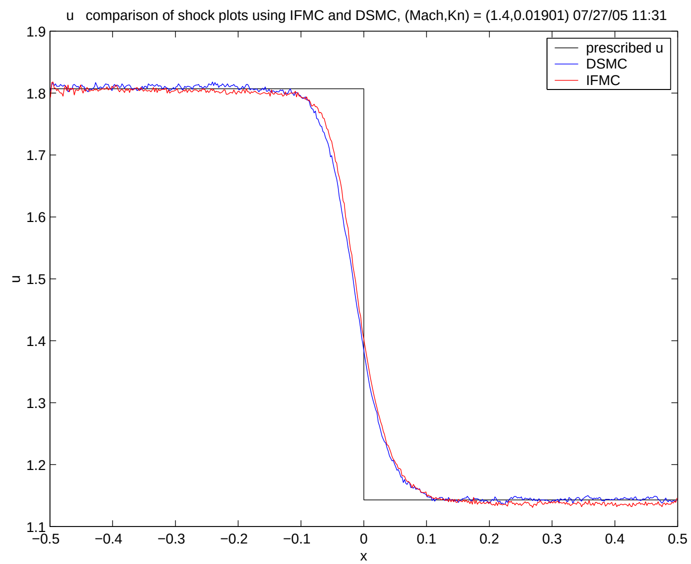

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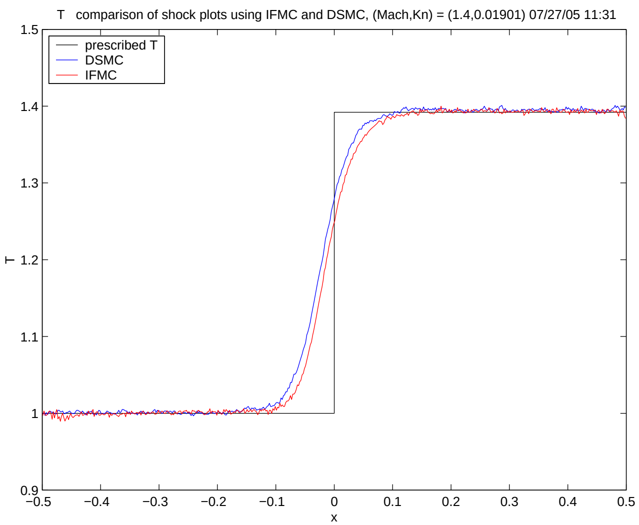

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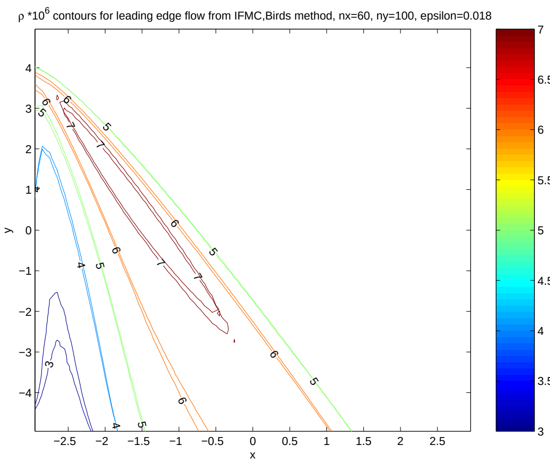
Comparison of DSMC (contours with num values) and IFMC (contours w/o num values) for the leading edge problem.

ρ



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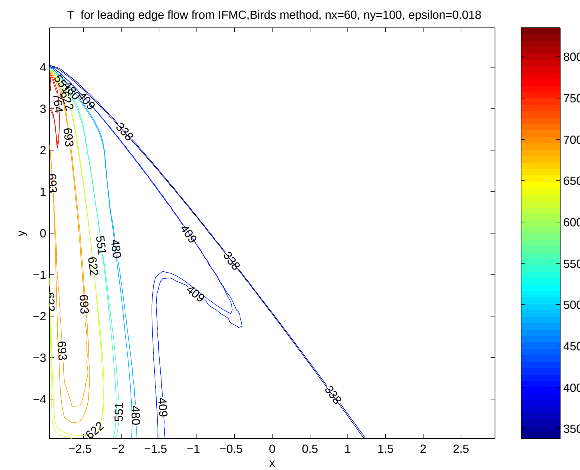

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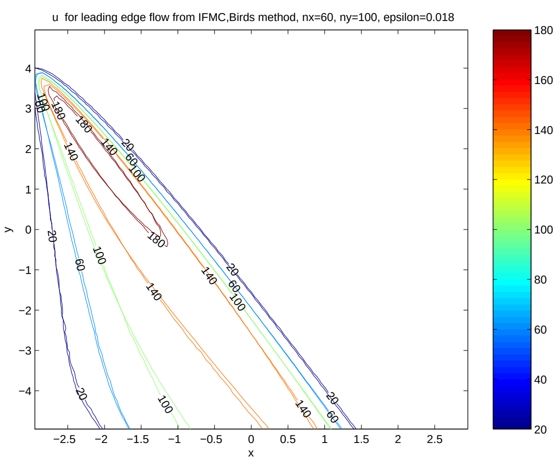
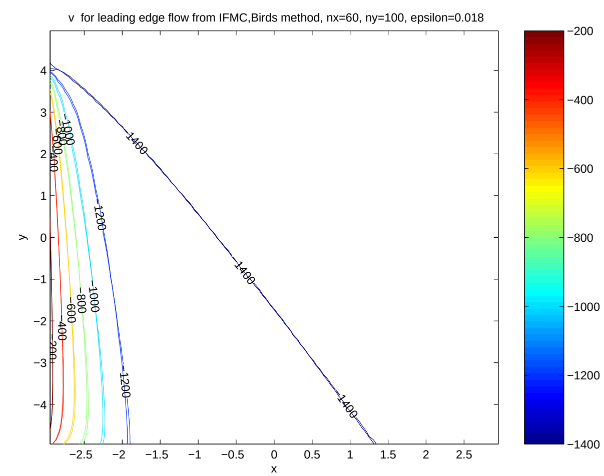


v



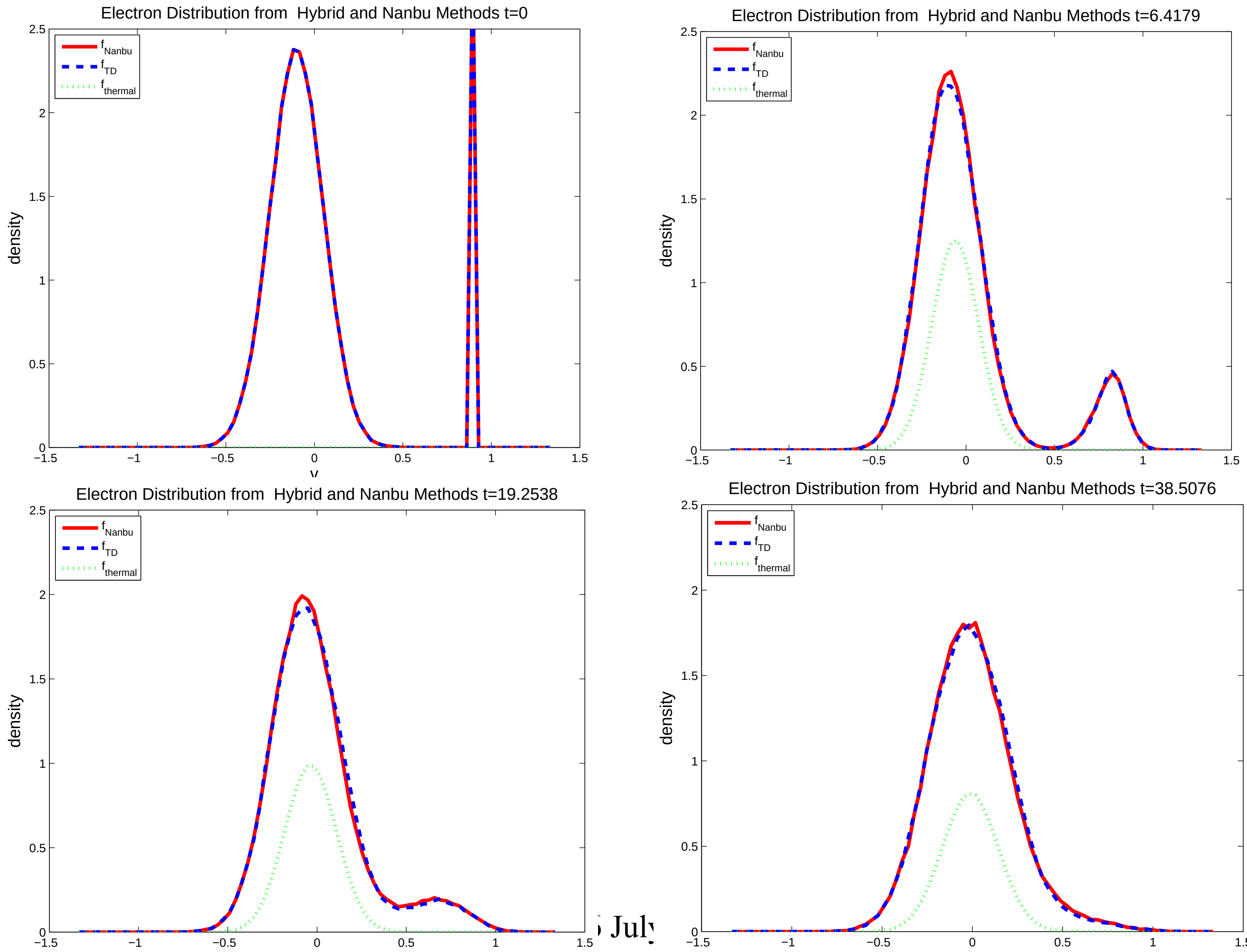
Hybrid method for plasmas
Thermalization/Dethermalization Method

- Hybrid representation (as in RGD)

$$F(v) = m + g$$

- Thermalization and dethermalization (T/D)
  - Thermalize particle (velocity v) with probability p_t
    - Move from g to m
  - Dethermalize particle (velocity v) with probability p_d
    - Move from m to g

Hybrid Method for Bump-on-Tail



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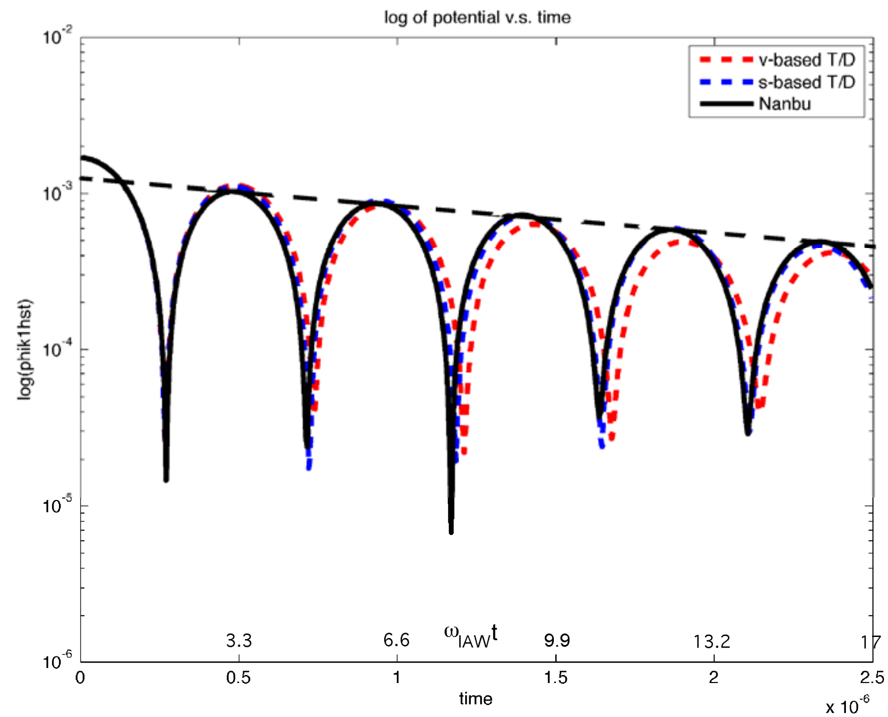
Ion Acoustic Waves

- kinetic description needed for ion Landau damping and ion-ion collisions
- wave oscillation and decay shown at right
- agreement with "exact" solution from Nanbu



Nanbu (–), hybrid (–), older hybrid method (–)

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Conclusions and Prospects

- Lots of opportunities for mathematics in plasma physics
- Current simulation methods for kinetics have trouble in the fluid and near-fluid regime
- Math leading to new methods that are robust in fluid limit