Hybrid Monte Carlo Methods for Fluid and Plasma Dynamics

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Project Goals

- General goal
  - Hybrid numerical methods that combine particle simulations and continuum fluid solvers.
- Specific goals
  - Hybrid methods for Coulomb collisions in plasmas and applications to plasma kinetics, e.g., edge regions in fusion plasmas
  - Methods that combine particles and continuum throughout space (complementary to domain decomposition)

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Outline

- Particle collisions in rarefied gas dynamics (RGD)
  - Boltzmann equation vs. fluid eqtns
  - DSMC and its limitations
  - Hybrid method for RGD
- Coulomb collision in plasmas
  - Monte Carlo methods: Takizuka & Abe and Nanbu
  - ICEPIC
- Hybrid method for Coulomb collisions
  - Thermalization and dethermalization
  - Numerical Results
- Conclusions

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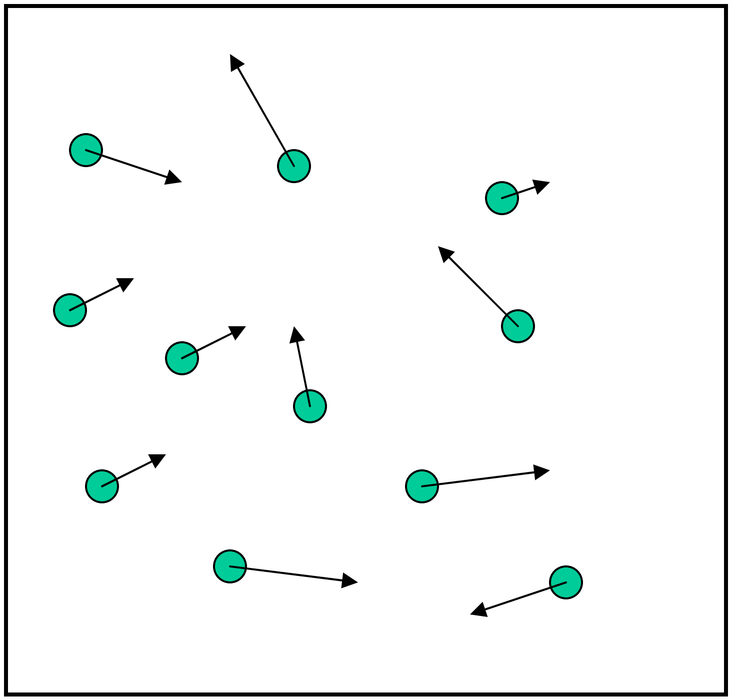
Particles vs. Continuum

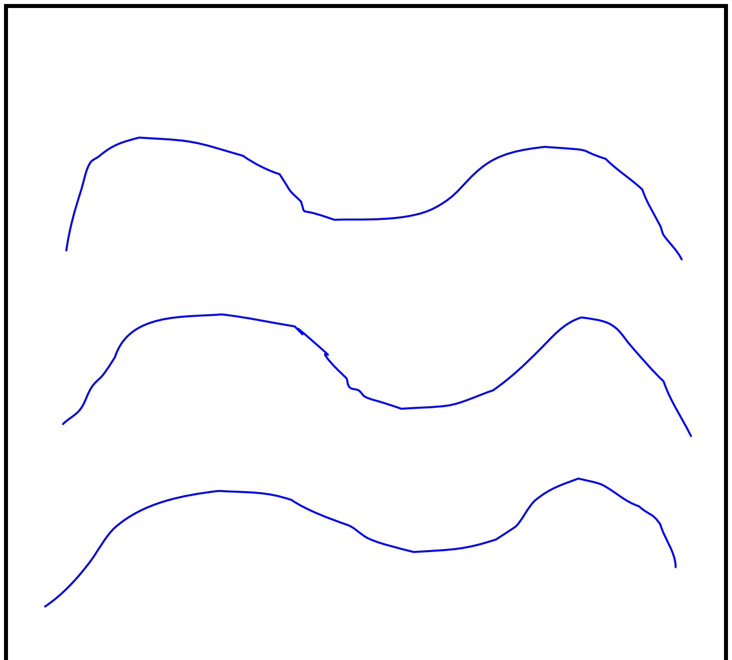
Particle description

- Discrete particles
- Motion by particle velocity
- Interact through collisions
- Statistical description through Boltzmann equation

Fluid (continuum) description

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





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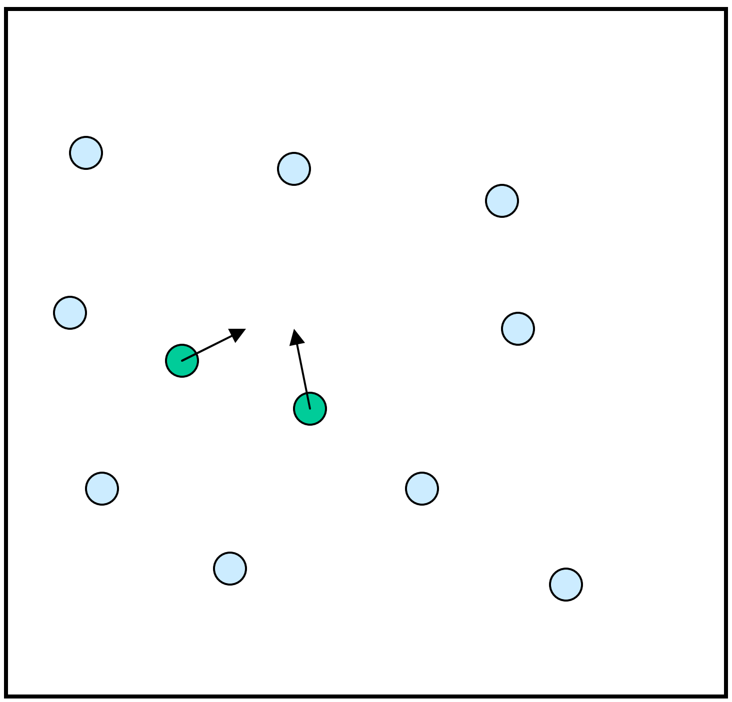

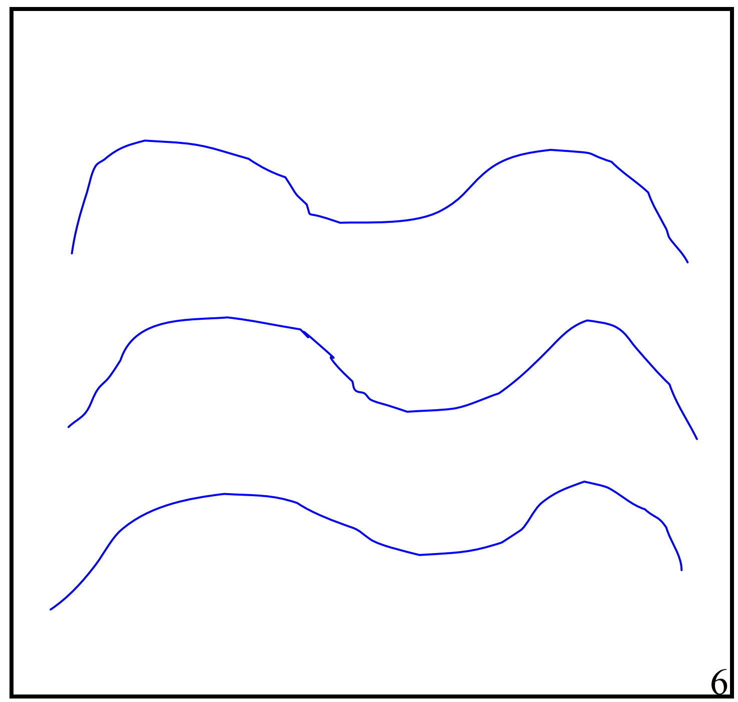

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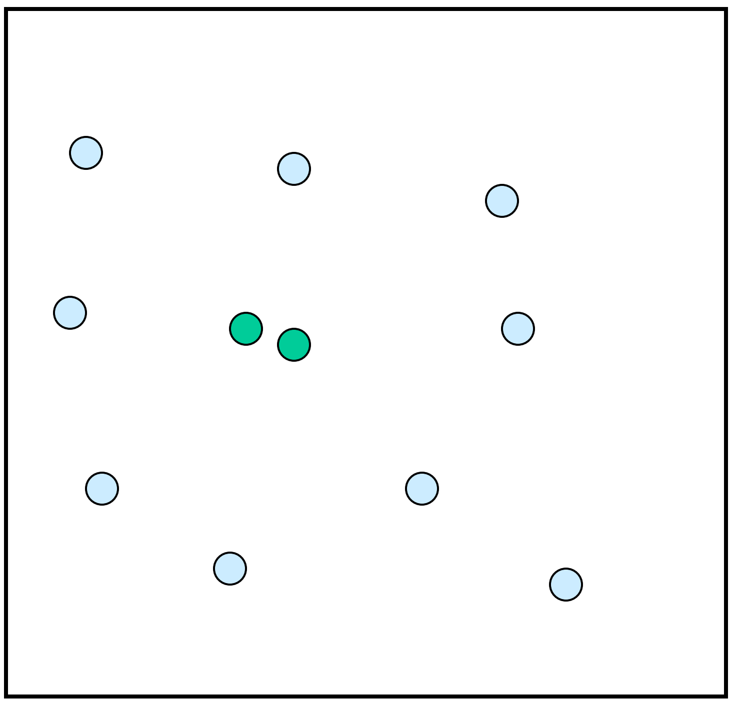

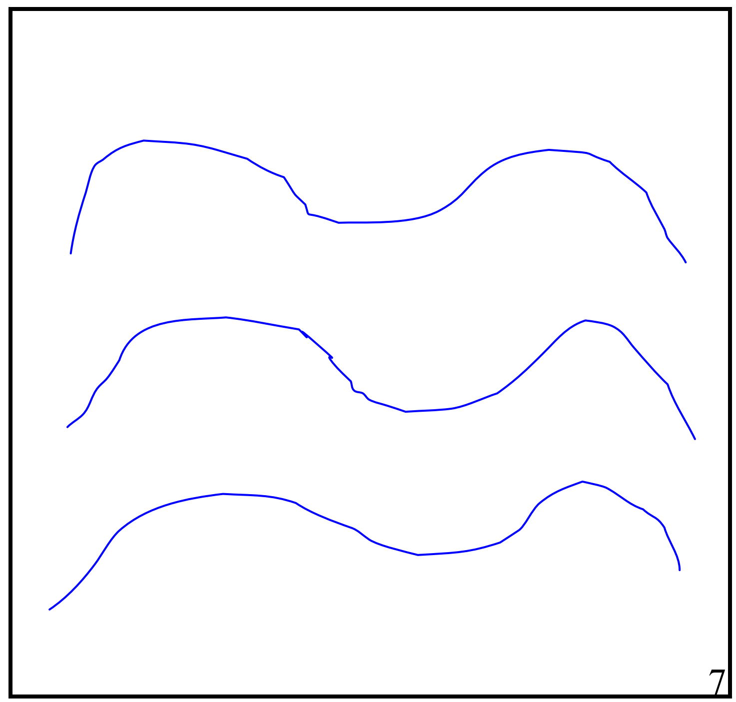

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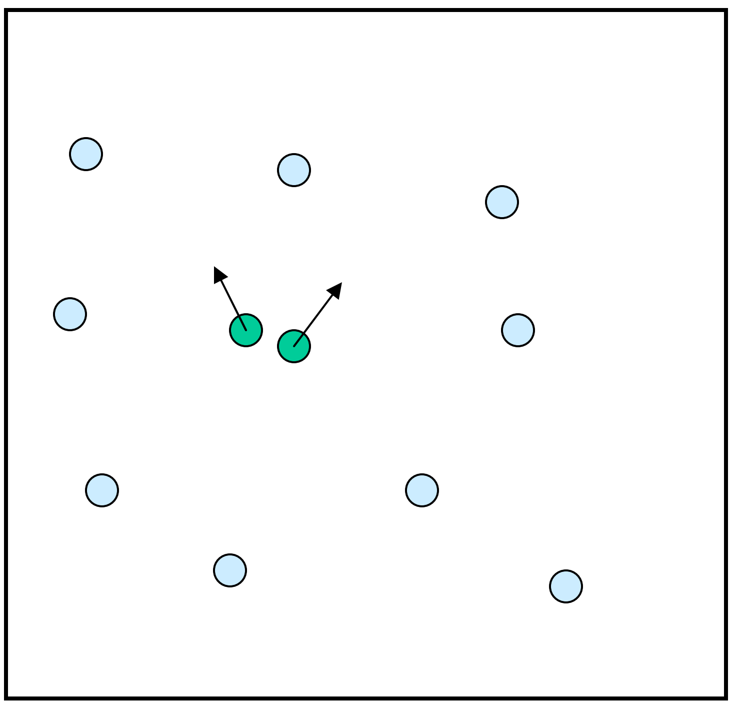

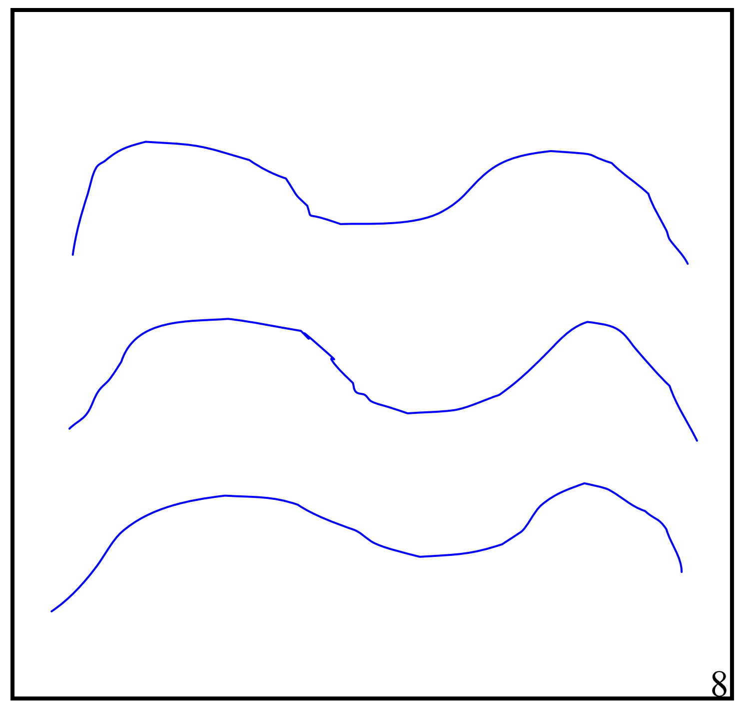

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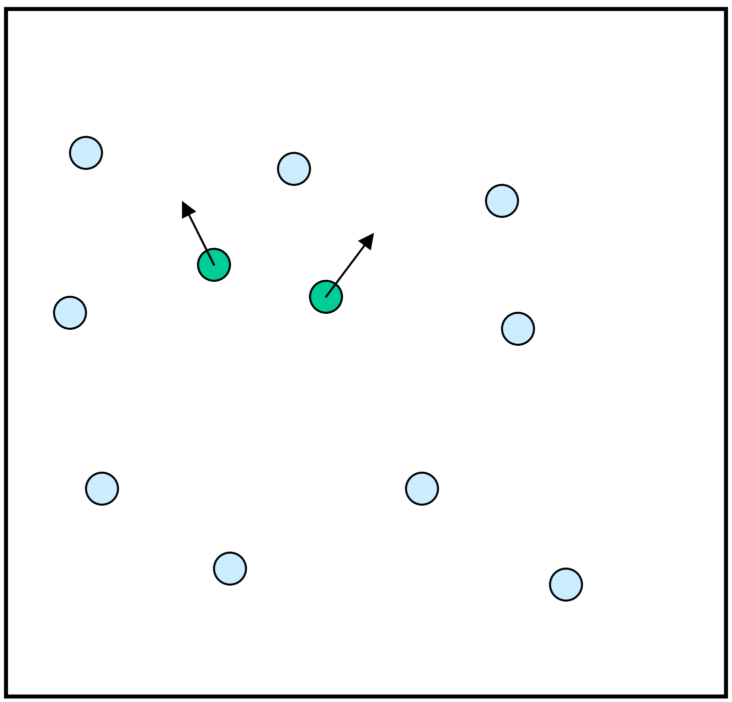

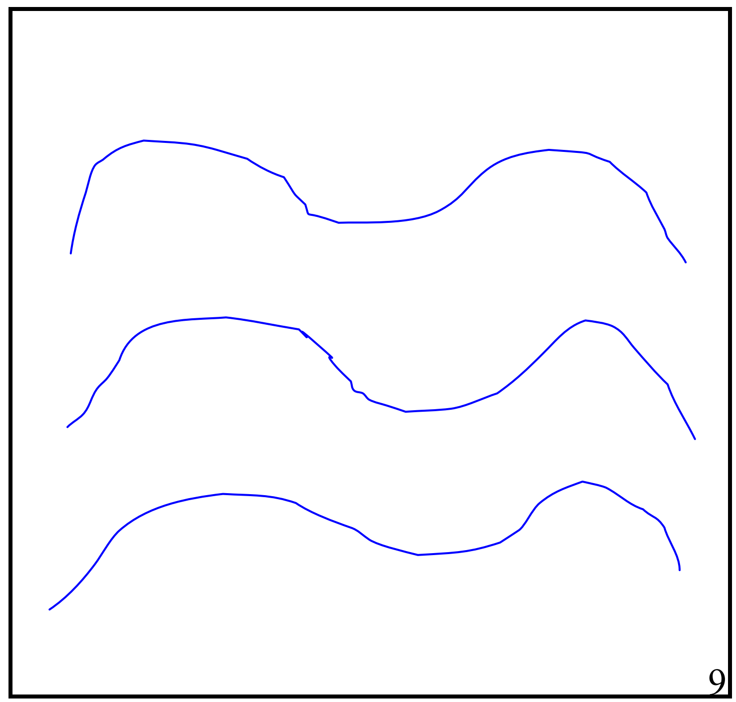

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Boltzmann equation for RGD

- Rarefied gas dynamics (RGD)
  - RGD required when effects of individual collisions are significant
  - Computational bottleneck in many simulations
- Boltzmann equation for density function f in phase space (position x, velocity v) at time t

$$f = f(v, x, t)$$

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

  - ε = Knudsen number = mean free path / characteristic length scale
  - Q represents effect of binary collisions
- Fluid Limit
  - $\varepsilon \to 0$, $f \to M(v;\rho,u,T)$

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

  - ρ,u,T satisfy Euler (or Navier-Stokes)

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Collisional Effects in the Atmosphere

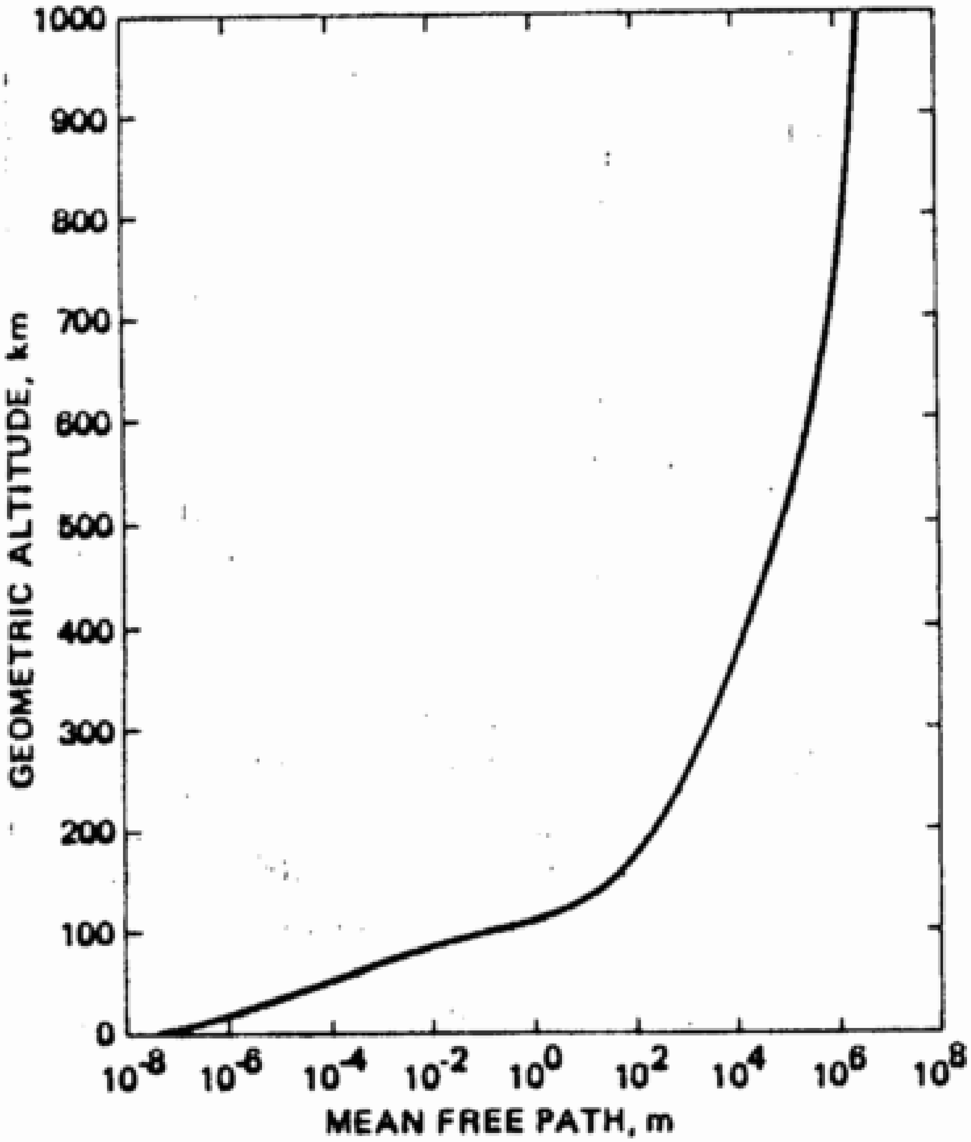

FIGURE 6. Mean free path as a function of geometric altitude.

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DSMC

- DSMC = Direct Simulation Monte Carlo
  - Invented by Graeme Bird, early 1970's
  - Represents density function 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 $dx_k / dt = v_k$
- Limitation of DSMC
  - DSMC becomes computationally intractable near fluid regime, since collision time-scale becomes small

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Hybrid method

- IFMC=Interpolated Fluid Monte Carlo
  - Combines DSMC and fluid methods
  - 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
    - $\alpha = 0 \leftrightarrow$ DSMC
    - $\alpha = 1 \leftrightarrow$ CFD
  - Remains robust near fluid limit
- Comparison to domain decomposition
  - Fluid description in some regions, RGD in others
  - Hybrid method uses mixture of fluid/RGD throughout

Thermalization Approximation

- Wild expansion

$$f(\Delta t) = \sum_{k=0}^{\infty} \tau_k f_k$$

  - f_k includes particles having k collisions
- Themalization approximation
  - Replace particles having 2 or more collisions in time step dt by Maxwellian M
  - Resulting evolution over dt

$$f(\Delta t) = Af(0) + Bf_1 + CM$$

$$A = (1-\tau) \qquad B = \tau(1-\tau) \qquad C = \tau^2$$

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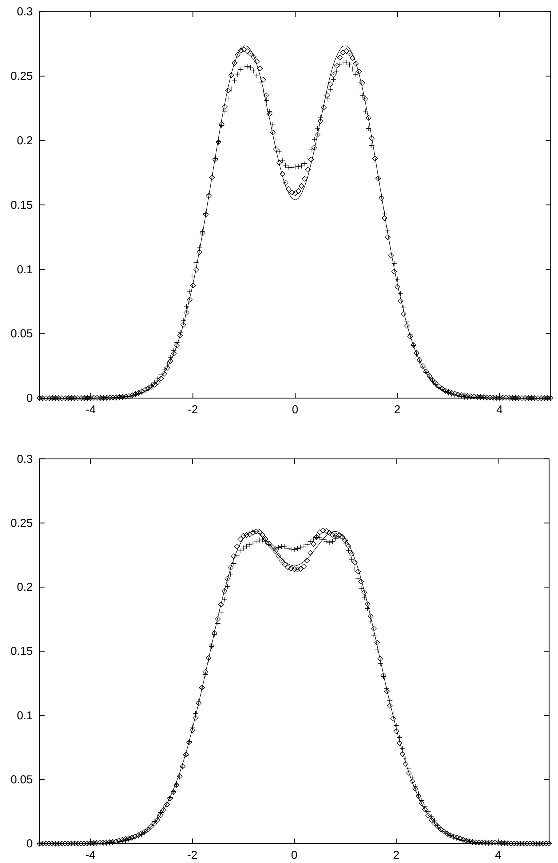
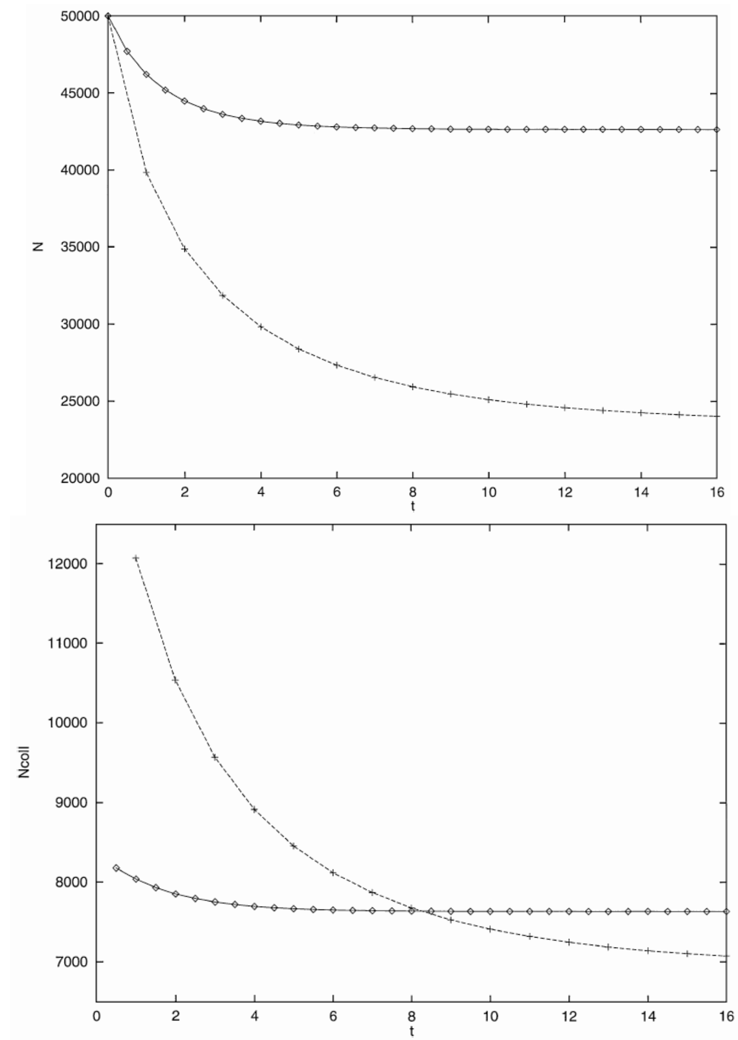
Relxation to Equilibrium

- Spatially homogeneous, Kac model
- Similarity solution (Krook & Wu, 1976)



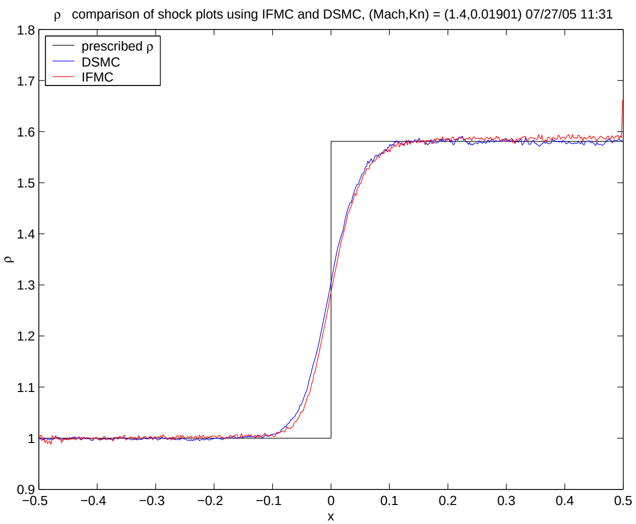
Comparison of DSMC(+) and IFMC(◊)
At time t=1.5 (top) and t=3.0 (bottom).



Number of particles (top) and number of collisions (bottom) for IFMC with dt=0.5(◊) and dt=1.0 (+).

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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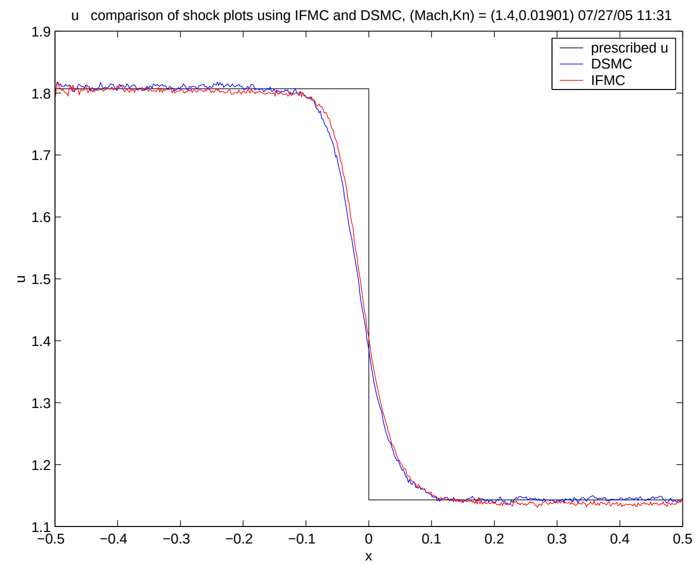

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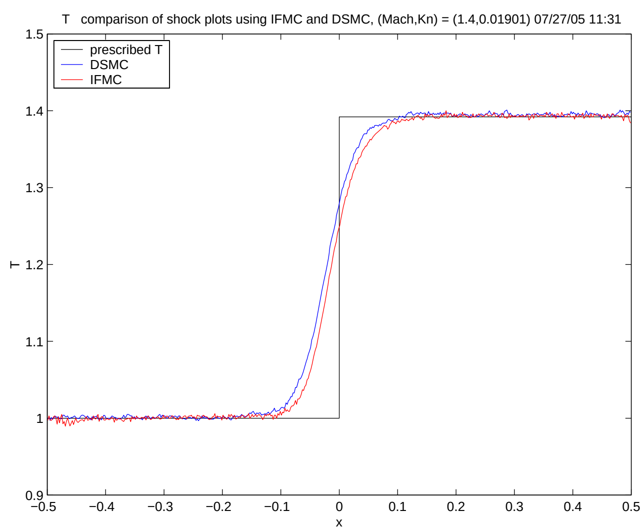
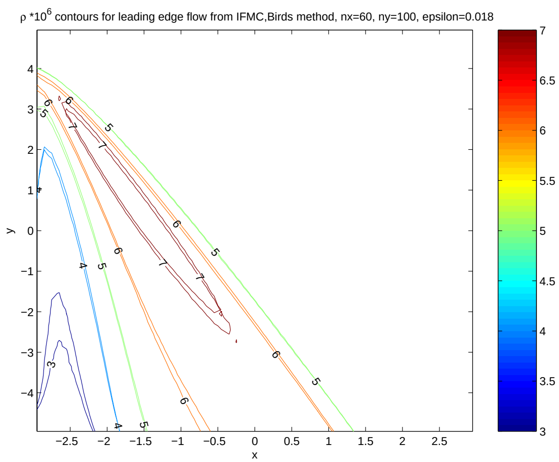


Comparison of DSMC (contours with num values) and IFMC (contours w/o num values) for the leading edge problem.

ρ



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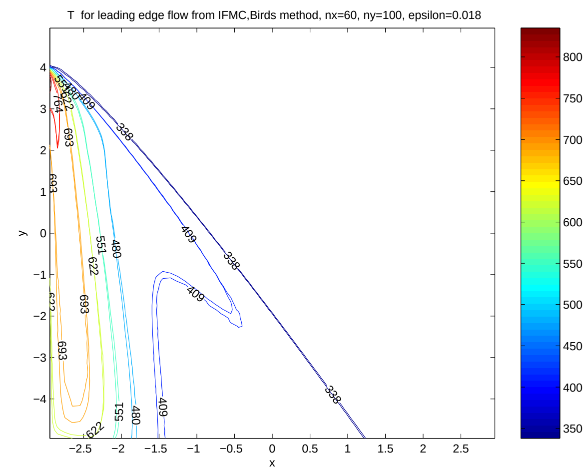

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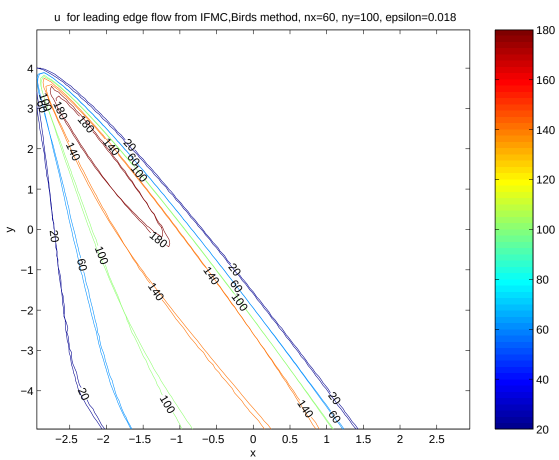
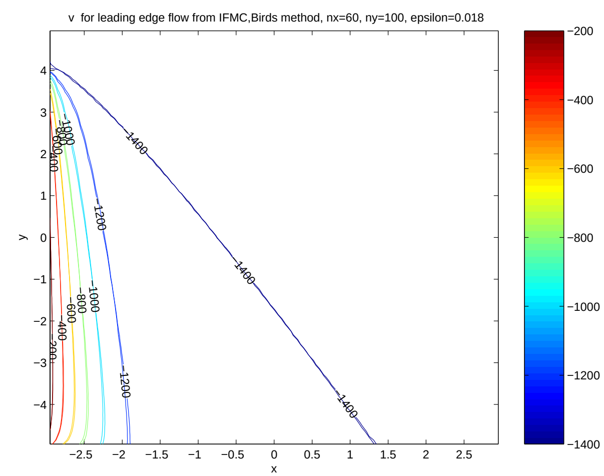


v



Interactions of Charged Particles in a Plasma

- Long range interactions
  - $r > \lambda_D$ ($\lambda_D =$ Debye length)
  - Electric and magnetic fields (e.g. using PIC)
- Short range interactions
  - $r < \lambda_D$
  - Coulomb interactions
  - Fokker-Planck equation

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

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

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

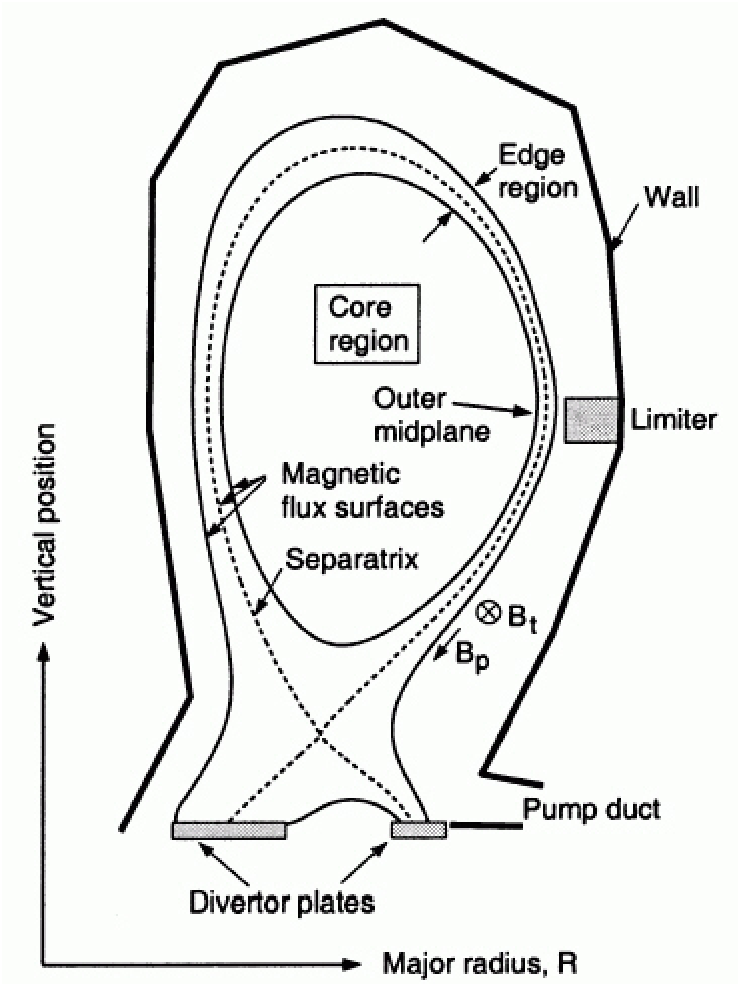
Monte Carlo Particle Methods for Coulomb Interactions

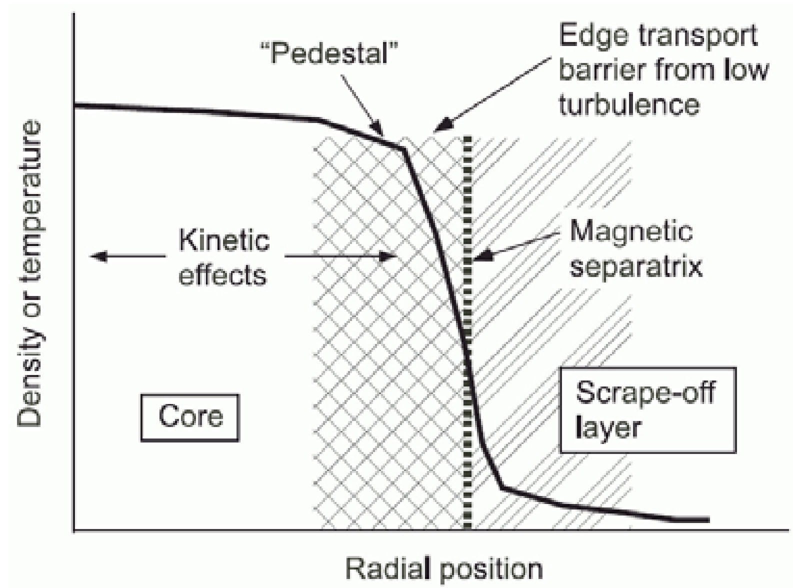
- Test particle - nonlinear field representation
  - Mannheimer, Lampe & Joyce, JCP 138 (1997)
  - Particles feel drag and diffusion

$$d\mathbf{v} = \mathbf{F}_d dt + \mathbf{D} d\mathbf{b}$$

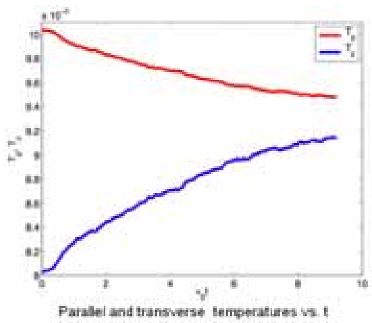
- Particle-particle representation
  - Takizuka & Abe, JCP 25 (1977), Nanbu, PRE 55 (1997)
    - T&A implemented in ICEPIC by Birdsall, Cohen and Procassini 1980's
    - Nanbu implemented in ICEPIC
  - Binary particle "collisions", from collision integral interpretation of FP equation
  - Comparison of Nanbu and T&A in poster of CM Wang.

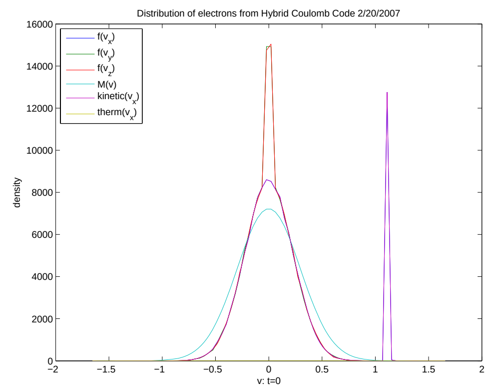
Kinetic Effects in Fusion Plasma Devices



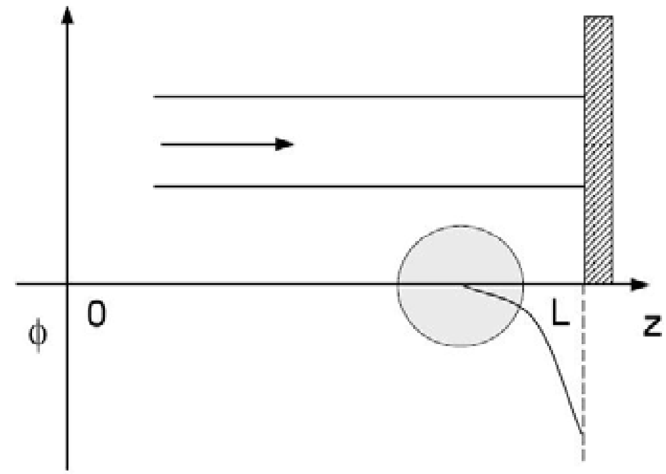


Test Problems for This Project

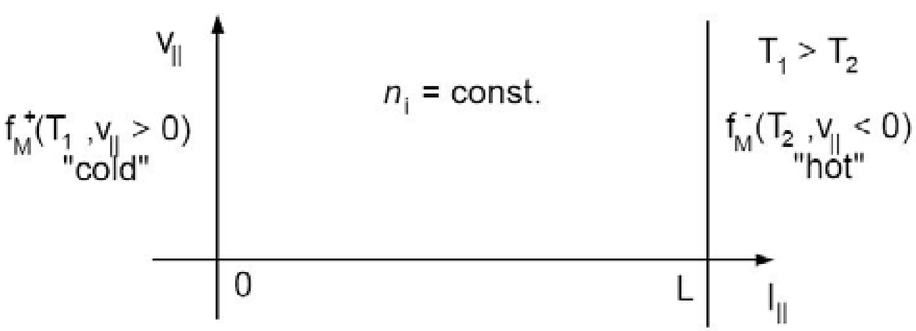




Relaxation of anistropic Maxwellian and bump on tail



Normal-incidence collisional sheath



Collisional oblique-incidence gyrosheath

Edge electron transport

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Takizuka & Abe Method

- T. Takizuka & H. Abe, *J. Comp. Phys.* 25 (1977).
- T & A binary collision model is equivalent to the collision term in Landau-Fokker-Planck equation
  - The scattering angle θ is chosen randomly from a Gaussian random variable δ

$$\delta \equiv \tan(\theta/2)$$

  - δ has mean 0 and variance

$$\left\langle \delta^2 \right\rangle = (e_\alpha^2 e_\beta^2 n_L \log \Lambda / 8\pi\varepsilon_0^2 m_{\alpha\beta}^2 u^3)\Delta t$$

  - Parameters
    - Log Λ = Coulomb logarithm
    - u = relative velocity
- Simulation
  - Every particle collides once in each time interval
    - Scattering angle depends on dt
    - cf. DSMC for RGD: each particle has physical number of collisions
  - Implemented in ICEPIC by Birdsall, Cohen and Procassini.

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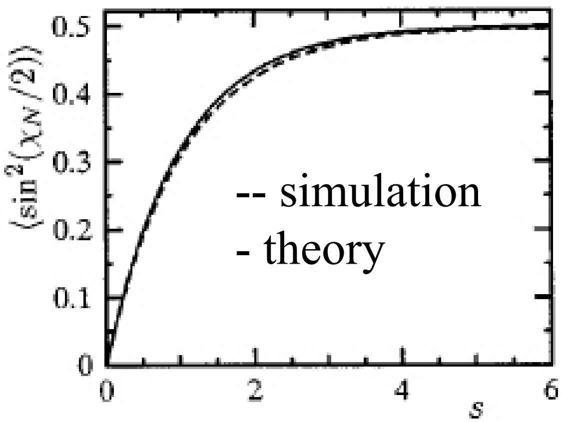
Nanbu's Method

- Combine many small-angle collisions into one aggregate collision
  - K. Nanbu. *Phys. Rev. E.* 55 (1997)
- Scattering in time step dt
  - χ_N = cumulative scattering angle after N collisions
  - N-independent scattering parameter s

$$\langle \sin^2(\chi_N/2) \rangle \cong (1-e^{-s})/2$$

$$s = N\langle \theta^2 \rangle /2$$



  - Aggregation is only for collisions between two given particle velocities
- Steps to compute cumulative scattering angle:
  - At the beginning of the time step, calculate s

$$s = c_3 u^{-3}(\ln \Lambda)\Delta t$$

  - Determine A from

$$\coth A - A^{-1} = e^{-s}$$

  - Probability that postcollison relative velocity is scattered into dΩ is

$$f(\chi)d\Omega = \frac{A}{4\pi \sin hA} e^{A\cos\chi} d\Omega$$

  - Implemented in ICEPIC by Wang & REC

Accelerated Simulation Methods for Coulomb collisions

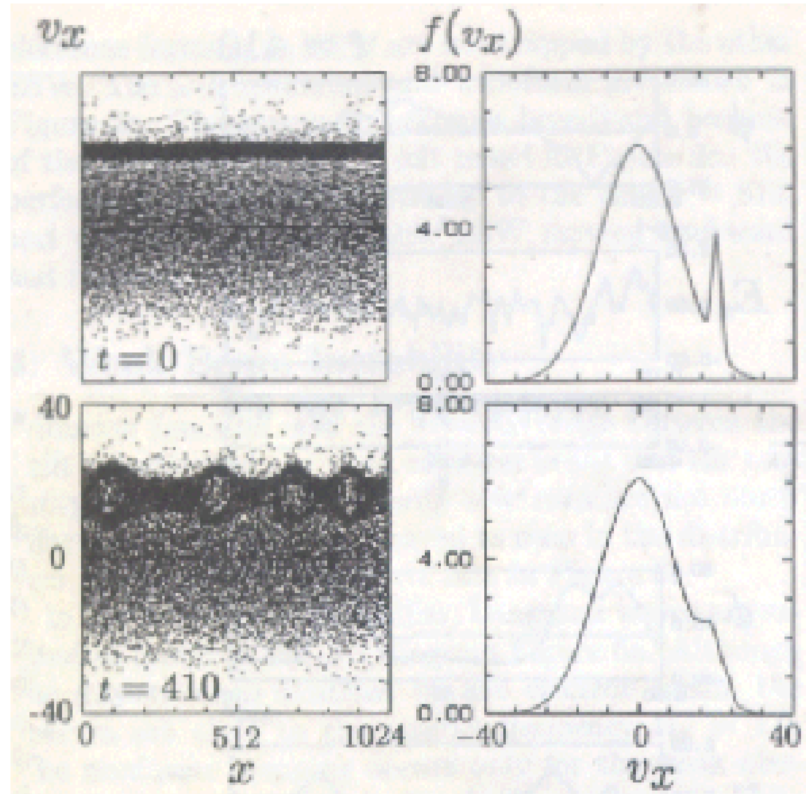
- Domain decomposition
- δf methods: $f = M + \delta f$
  - simulate (small) correction to approximate result (Kotschenruether 1988)
  - δf can be positive or negative
  - Particle weights: "quiet" & partially linearized methods (Dimits & Lee 1993)
  - Stability problems
- New hybrid method
  - Hybrid representation (as in RGD)

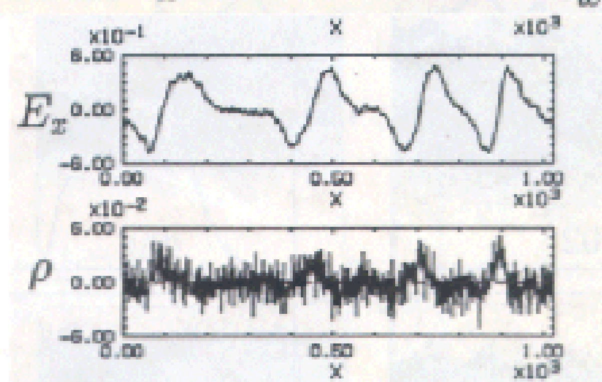
$$F(v) = m + g$$

    - m = equilibrium component (Maxwellian)
    - g = kinetic (nonequilibrium) component
  - Thermalization rate must vary in phase space
    - $\alpha = \alpha(x,v)$ = fraction of particles in m
    - $(u_m, T_m) \neq (u_F, T_F)$

Variable thermalization across phase space

- Bump-on-tail
  - Persistent because Coulomb cross section decreases as v increases





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

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T/D Hybrid Collision Algorithm

- Hybrid representation (as in RGD)

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

  - g represented by particles

$$g = \sum_{k=1}^{n} \delta(v - v_k(t))$$

- Collisions
  - m-m: leaves m unchanged
  - g-g: as in DSMC
  - m-g: select particle from g, sample particle from m, then perform collision
- T/D step
  - Particle from g is thermalized (moved to m) with probability p_t
  - Particle sampled from m is dethermalized (moved to g) with probability p_d
- Change (ρ_m, u_m, T_m) to conserve mass, momentum, energy
- Implemented in ICEPIC

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Choice of Probabilities p_d and p_t

- T/D step
  - $F_n = F(n\,dt) = m_n + g_n$
  - One step

$$m_1 = (1 - p_d)m_0 + p_t g_0$$

$$g_1 = p_d m_0 + (1 - p_t)g_0$$

- Detailed balance requirement

$$\boxed{F_0 = M = m + g \quad \rightarrow \quad F_1 = M = m + g}$$

$$\Rightarrow g = p_d m + (1 - p_t)g$$

$$\Rightarrow g = (p_d / p_t)m$$

$$\Rightarrow M = (1 + p_d / p_t)m$$

$$\Rightarrow (1 + p_d / p_t) = c\exp(|v|^2 / \tau)$$

  - Assuming $u_M = u_m = 0$
- Simple choice
  - $p_t = 1$ for $v < v_1$ (i.e., complete thermalization)
  - $p_d = 1$ for $v > v_2$ (i.e., complete dethermalization)

Alternative: S Hybrid Collision Algorithm

- Thermalization for particle pairs v, v_1 that are "strongly colliding"
  - Strength measured by Nanbu parameter s

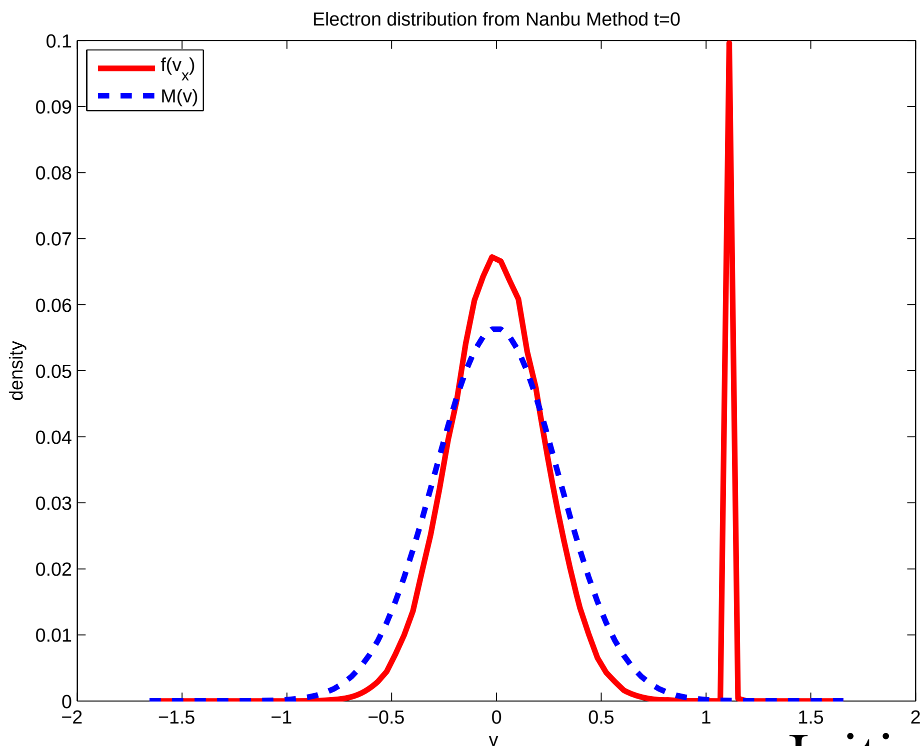
$$s = c_3 u^{-3} (\ln \Lambda) \Delta t \cong N \left\langle \theta^2 \right\rangle / 2$$

    - $u=|v-v_1|$, N = # aggregated collisions

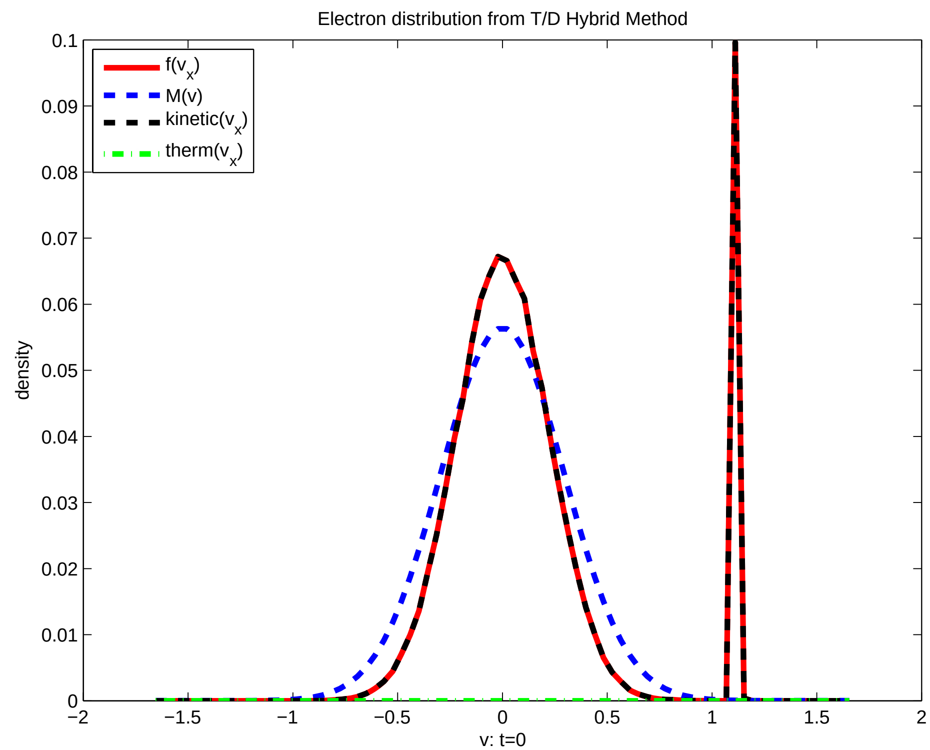
- Implementation in ICEPIC
  - Move particles v, v_1 into Maxwellian m, if s>6
  - Alternative to thermalization/dethermalization (T/D) probabilities
- Future work: formulate s-dependent T/d probabilities

Relaxation of Bump on Tail

- Bump disjoint from Maxwellian
  - v_{bump}=5*sqrt(temp)
  - m_{bump}=0.1 * m_{total}
  - Hybrid method is initially all particles
    - after brief transient 2/3 mass in equilibrium component



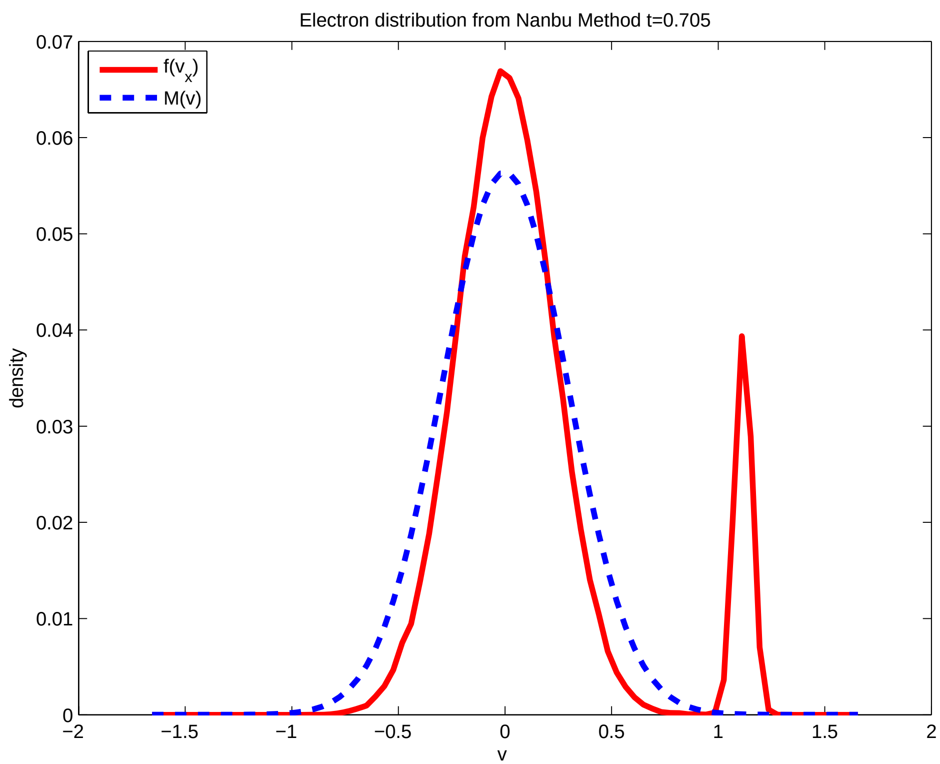
Nanbu

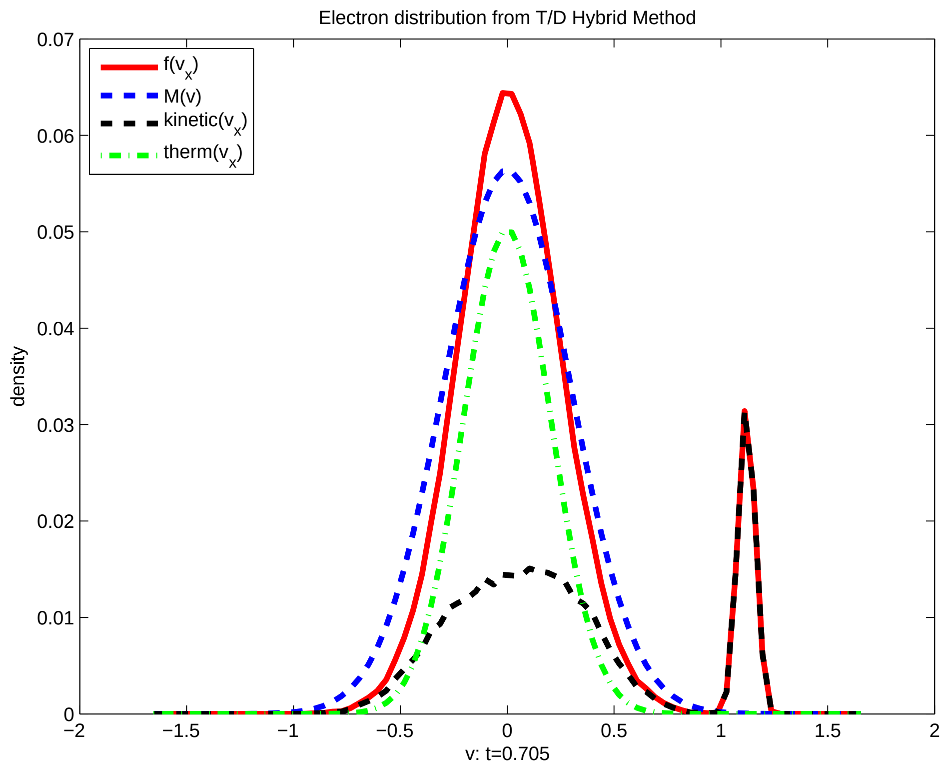


Hybrid

Initial data

Relaxation of Bump on Tail





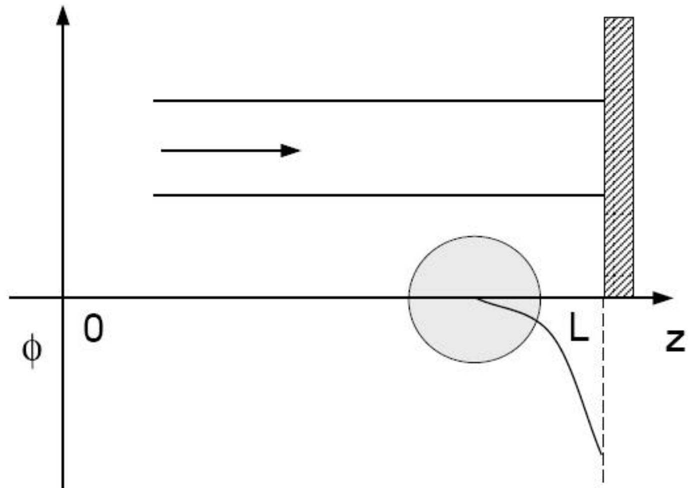
Nanbu

t =.705

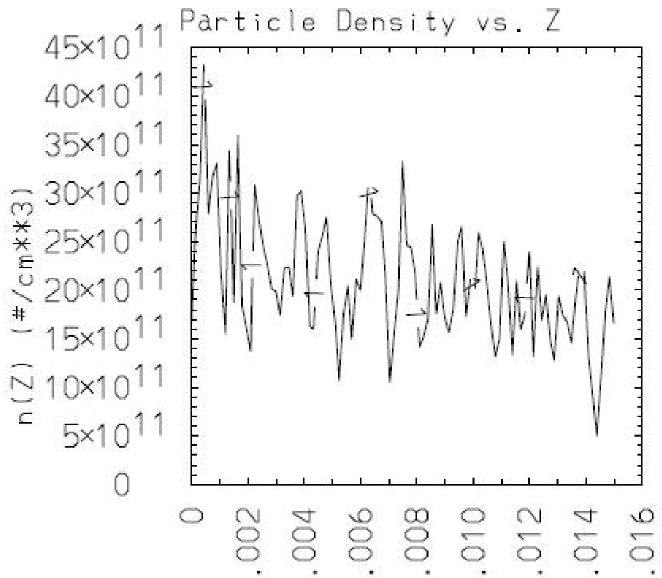
Hybrid

Sheath Calculation

- Steady boundary layer
  - Ions represented as particles
  - Electrons in a background Maxwellian
  - Maxwellian influx of ions at left
  - Absorbing bdry at right
  - E & M fields
- Parameters
  - Injection drift velocity=0 (subcritical)
  - Background drift velocity = 0
  - Flux of particles at left = 16.5 (large)
  - Coulomb collision parameter = 200 (small)



Sheath geometry

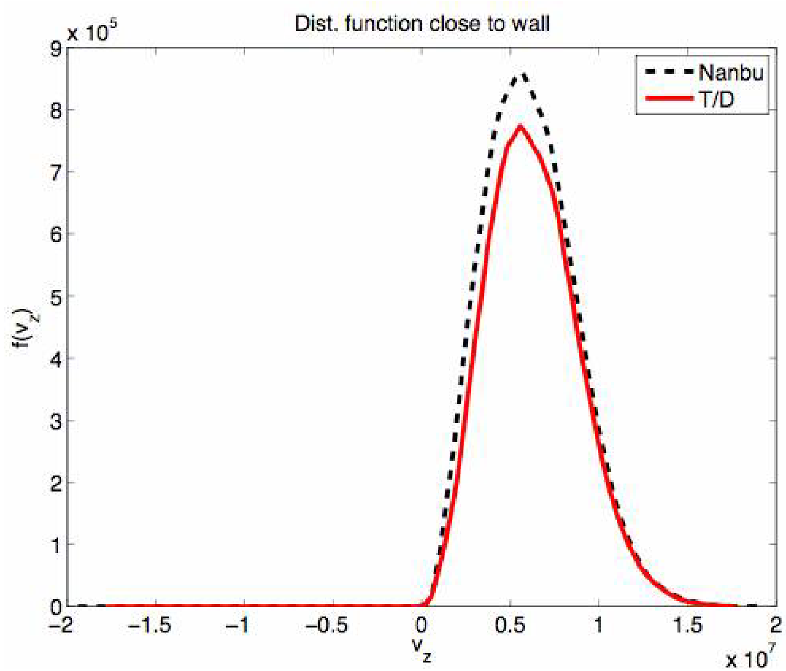


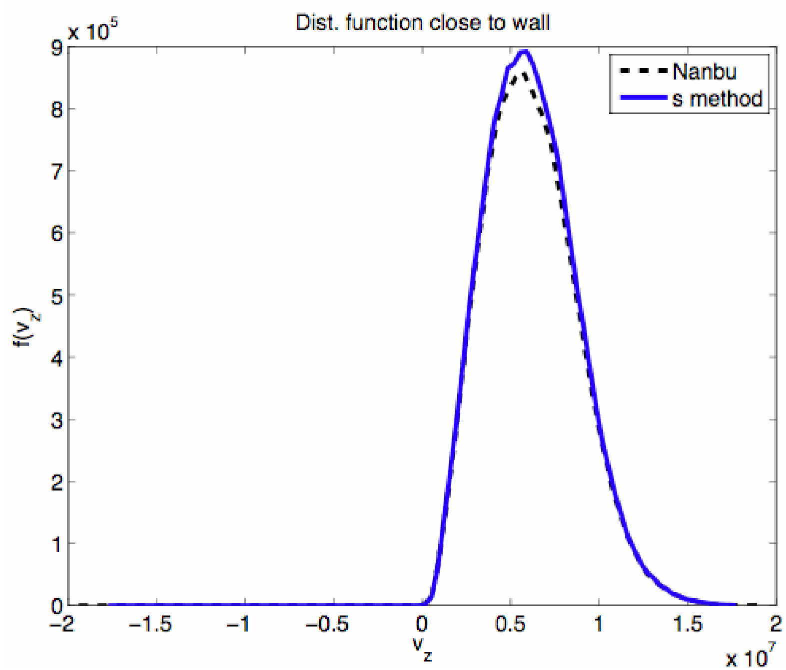
Particle density vs. z

Initial data

Sheath Calculation

- Application of hybrid method
  - Collisions as in relaxation problems
  - Advection of particle components
  - Advection of Maxwellian m by sampling and moving particles
    - Future: fluid solver for Maxwellian component





Parallel velocity distribution function from hybrid methods: T/D (left) and s (right) from poster of Wang.

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Conclusions and Prospects

- Hybrid method for RGD that performs uniformly in the fluid and near-fluid regime
  - Applications to aerospace, materials, MEMS
- Extension of hybrid method to Coulomb collisions
  - Thermalization/dethermalization probabilities
  - Probabilities vary in phase space (x,v)
- Application
  - Relaxation of anistropic Maxwellian
  - Relaxation of bump-on-tail
  - Ionic sheath