Gyrokinetic Particle Simulation for Magnetic Fusion Plasmas*

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OUTLINE

- Progress in Particle Simulation
- Progress in Gyrokinetic Particle Simulation
- Integrated Gyrokinetic Particle Simulation
- Summary and Conclusions

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Why Particle Simulation?

Particle Simulation + Massively Parallel Computers:

- *a dynamite combination: local, explicit, scalable*

Particle Simulation is a Powerful Tool for:

- Tokamaks and Stellarators –
  microturbulence, neoclassical and MHD

- Minimal deviation from the original kinetic equations –
  linear and nonlinear kinetic effects

- Minimal numerical restrictions due to recent advances –
  large time step, large grid spacing, low numerical noise

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Particle Simulation of the Vlasov-Maxwell System

- The Vlasov equation,

$$\frac{dF}{dt} \equiv \frac{\partial F}{\partial t} + \mathbf{v} \cdot \frac{\partial F}{\partial \mathbf{x}} + \frac{q}{m}\left(\mathbf{E} + \frac{1}{c}\mathbf{v} \times \mathbf{B}\right) \cdot \frac{\partial F}{\partial \mathbf{v}} = C(F).$$

- Particle Pushing,

$$\frac{d\mathbf{x}_j}{dt} = \mathbf{v_j}, \qquad \frac{d\mathbf{v}_j}{dt} = \frac{q}{m}\left(\mathbf{E} + \frac{1}{c}\mathbf{v}_j \times \mathbf{B}\right)_{\mathbf{x}_j}.$$

- Klimontovich-Dupree representations,

$$F = \sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{x}_j)\delta(\mathbf{v} - \mathbf{v}_j),$$

Particle Simulation of the Vlasov-Maxwell System (cont.)

- Poisson's equation : $\mathbf{E} = -\nabla\phi$

$$\nabla^2\phi = -4\pi \sum_\alpha q_\alpha \sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{x}_{\alpha j})$$

- Ampere's Law

$$\nabla^2\mathbf{A} = -4\pi \sum_\alpha q_\alpha \sum_{j=1}^{N} \mathbf{v}_{\alpha j}\delta(\mathbf{x} - \mathbf{x}_{\alpha j})$$

- Field Quantities

$$\mathbf{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}$$

$$\mathbf{B} = \nabla \times \mathbf{A}$$

Particle Simulation of the Vlasov-Maxwell System (cont.)

- Vlasov equation is solved in Lagrangian coordinates
  - *Nonlinear PDE* $\Rightarrow$ *Linear ODE : Particle Pushing*
- Maxwell equations are solved in Eulerian coordinates
  - *Linear PDE*
- Collisions are treated as sub-grid phenomena
  - *Monte-Carlo processes*

Particle Simulation of the Vlasov-Maxwell System (cont.)

- Suitable for high frequency short wavelength physics, e.g.,

$$\omega \approx \omega_{pe} \quad k\lambda_D \approx 1$$

- Disparate spatial and temporal scales for physics of

$$\omega \approx \omega_*, \quad k\rho_s \approx 1$$

- Enhanced numerical noise (N: no. of particles)

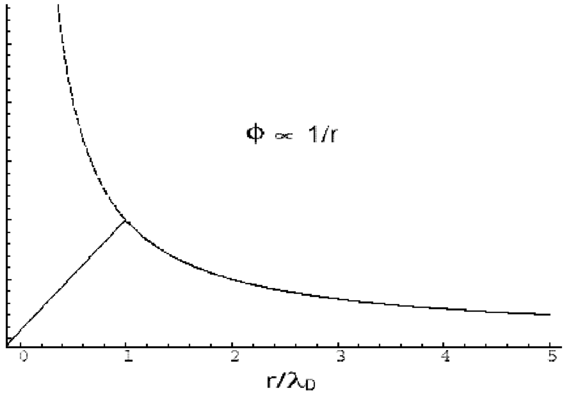
$$\delta n/n \gg 1/\sqrt{N}$$

Progress in Particle Simulation

- Early attempts [*Buneman (1959); Dawson (1962)*]

- Finite-Size Particles and Particle-in-Cell Simulation [*Dawson et al. BAPS (1968) and Birdsall et al. BAPS (1968)*]

  – Coulomb potential is modified for a finite size particle due to Debye shielding – no need to satisfy $1/(n\lambda_D^3) \ll 1$.



- Number of calculations for N particles

  – N^2 for direct interactions

  – $NlogN$ for PIC

- Collisionless Simulations [*Langdon et al. (1971)*]

- Collisions are re-introduced via Monte-Carlo methods [*Shanny, Dawson & Greene (1976)*]

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Progress in Particle Simulation (cont.)

- Numerical Properties

  – Grid spacing imposed by Debye shielding [Langdon ‘71]:

$$\Delta x < \lambda_D$$

  – Time step imposed by high frequency waves [Langdon ’79]:

$$\omega_{pe}\Delta t < 1$$

  – Time step imposed by fast electrons [Langdon ‘79]:

$$k v_{te}\Delta t < 1$$

  – Noise enhanced by Debye shielding [Okuda et al. ‘71]:

$$\frac{\delta n}{n} \approx \frac{1}{\sqrt{N}(k\lambda_D)}$$

Progress in Particle Simulation (cont.)

Culprits: plasma waves

- originated from space charge or charge separartion effects
- however, quasineutral waves are the waves of interest, such as those in tokamaks and space ...

Implicit Schemes: *[Mason (82); Denavit (82); Langdon et. al (82)]*

- Instability: $\omega_{pe}\Delta t > 1$
- Inaccuracy: $kv_{te}\Delta t = (\omega_{pe}\Delta t)(k\lambda_D) > 1$
- for $k\lambda_D \ll 1 \Rightarrow \omega_{pe}\Delta t > 1$ but keeping $kv_{te}\Delta t < 1$

Reduced Vlasov-Maxwell equations: gyrophase averaging

- Gyrokinetic ordering:

$$\frac{\omega}{\Omega_i} \sim \frac{k_\parallel}{k_\perp} \sim \frac{\rho}{L_{eq}} \sim \frac{\delta B}{B} \sim \frac{e\phi}{T} \sim O(\epsilon); k_\perp \rho \sim O(1)$$

- Gyrocenter Gauge Theory: $\rho/L_{eq} \sim O(\epsilon)$

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Gyrokinetic Theory

- Linear theory:
  - Rutherford and Frieman (1968);Taylor and Hastie (1968); Catto (1978)
- Nonlinear Theory:
  - Frieman and Chen (1982) – in Fourier k-space without velocity space nonlinearity
  - Lee (1983) - in real space
- Nonlinear Theory – Lie perturbation methods:
  - Dubin et al. (1983) - ES slab;
  - Hahm (1988) - ES toroidal; Hahm et al. (1988) - EM slab;
  - Brizard (1989) - EM toroidal and reduced MHD;
  - Qin et al.(1999) - compressional-Alfven and Bernstein waves;
  - Qin et al. (2000) - pressure balance;
  - Qin et. al. (2000) - gyrocenter gauge theory

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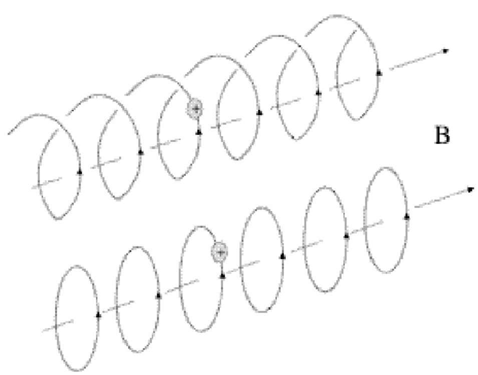
Gyrokinetic Particle Simulation

[Lee, PF ('83); Lee, JCP ('87)]

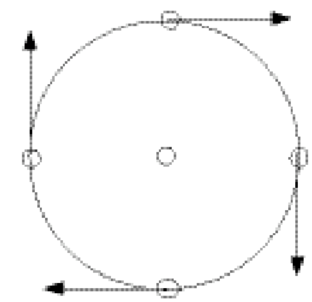
- Gyrophase-averaged Vlasov-Maxwell equations for low frequency microinstabilities.

- The spiral motion of a charged particle is modified as a rotating charged ring subject to guiding center electric and magnetic drift motion as well as parallel acceleration + polarization drifts.



Gyrokinetic Particle Simulation (cont.)

- A charged ring is approximated by 4 points for $k_\perp \rho_i \leq 2$.
- Polarization drifts now appear in the field equations:



  – ES polarization drift repalces Debye shielding in the gyrokinetic Poisson's giving rise to quasineutral simulation and ES shear-Alfven waves,

$$\nabla^2\phi = -4\pi\rho \quad \Rightarrow \quad \nabla^2\phi + (\frac{\rho_s}{\lambda_D})^2\nabla_\perp^2\phi = -4\pi e(\overline{n}_i - n_e)$$

  – EM polarization drift appears in Ampere's law giving rise to shear and compressional Alfven waves,

$$\nabla^2\mathbf{A} - \frac{1}{v_A^2}\frac{\partial^2\mathbf{A}_\perp}{\partial t^2} = -\frac{4\pi}{c}(\overline{\mathbf{J}}_{\perp i} + \overline{\mathbf{J}}_{\| i} + \overline{\mathbf{J}}_{\perp e} + J_{\| e})$$

Gyrokinetic Particle Simulation (cont.)

- Equations of Motion:

$$\frac{d\mathbf{R}}{dt} = U\hat{\mathbf{b}} + \mathbf{v}_d - \frac{c}{B}\frac{\partial\overline{\phi}}{\partial\mathbf{R}} \times \hat{\mathbf{b}},$$

$$\mu \equiv \frac{v_\perp^2}{2B_0}\left(1 - \frac{mc}{e}\frac{v_\parallel}{B_0}\hat{\mathbf{b}}_0 \cdot \nabla \times \hat{\mathbf{b}}_0\right) \approx cons.,$$

$$\frac{dU}{dt} = -[\hat{\mathbf{b}} + \frac{U}{\Omega}\hat{\mathbf{b}} \times (\hat{\mathbf{b}} \cdot \frac{\partial}{\partial\mathbf{R}})\hat{\mathbf{b}}] \cdot (\mu\frac{\partial}{\partial\mathbf{R}} lnB - \frac{q}{m}E_\parallel),$$

- Field Quantities:

$$E_\parallel = E_\parallel^L + E_\parallel^T = -\hat{\mathbf{b}} \cdot \nabla\overline{\phi} - \frac{1}{c}\frac{\partial\overline{A_\parallel}}{\partial t},$$

$$\hat{\mathbf{b}} \equiv \frac{\mathbf{B}}{B} \approx \hat{\mathbf{b}}_o + \frac{\delta\mathbf{B}}{B_0} = \hat{\mathbf{b}}_o + \frac{\nabla \times \overline{\mathbf{A}}}{B_o}.$$

Improvement of Numerical Properties of a Gyrokinetic Plasma

- Grid spacing imposed by cold electron response

$$\Delta x < \rho_s \quad (\rho_s/\lambda_D \approx 100)$$

- Time step imposed by cold electron response $(\omega_H \equiv \frac{k_\parallel}{k_\perp}\frac{\lambda_D}{\rho_s}\omega_{pe})$

$$\omega_H \Delta t \ll 1 \quad (\omega_{pe}/\omega_H \approx 1000)$$

- Time step restricted by streaming of thermal electrons:

$$k_\parallel v_{te} \Delta < 1$$

- Noise enhanced by ω_H:

$$\delta n/n \approx 1/\sqrt{N}(k\rho_s).$$

- We need to get rid of cold electron response to lift these restrictions.

Methods to Further Improve Numerical Properties

- Adiabatic electron response ($\delta n_e/n_0 \approx e\phi/T_e$) is one way to lift the restrictions, but by completely forfeiting wave-particle interactions in the simulation.

- Split-weight δf simulation scheme can also relax most of the numerical restrictions:
  - Grid Spacing: $\Delta x \gg \rho_s$
  - Time Step: $\omega_* \Delta t < 1$ (or $\omega_A \Delta t < 1$), $k_\| v_{te} \Delta t \gg 1(?)$;
  - Noise: $\delta n/n \approx 0 \to 1/\sqrt{N}$.

- With split-weight δf scheme, accuracy in the simulation alone now dictates the number of particles N_p required for statistics and time step Δt required for zeroth-order trajectories.

The Perturbative (δf) Particle Simulation Scheme

[Dimits and Lee, JCP (1993); Parker and Lee, FPB (1993)]

- The Vlasov equation,

$$\frac{dF}{dt} \equiv \frac{\partial F}{\partial t} + \mathbf{v} \cdot \frac{\partial F}{\partial \mathbf{x}} + \frac{q}{m}\mathbf{E} \cdot \frac{\partial F}{\partial \mathbf{v}} = 0.$$

- For $F = F_o + \delta f$,

$$\frac{d\delta f}{dt} = -\frac{dF_o}{dt}$$

- Let $W = \delta f / F$ to obtain

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}, \quad \frac{d\mathbf{v}}{dt} = \frac{q}{m}\mathbf{E}, \quad \frac{dW}{dt} = -(1 - W)\mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}}(\frac{q\phi}{T_e}),$$

$$\delta f = \sum_{j=1}^{N} W_j \delta(\mathbf{x} - \mathbf{x}_j)\delta(\mathbf{v} - \mathbf{v}_j).$$

- Easy access to both linear and nonlinear regimes

Electrostatic Split-Weight Particle Simulation Scheme

[Manuilskiy and Lee, PoP(2000)]

- Let $\delta f_e = (e\phi/T_e)F_{0e} + \delta h_e$ to obtain

$$\frac{d\delta h_e}{dt} = -\frac{\partial}{\partial t}\frac{e\phi}{T_e}F_{0e} + \frac{\mathbf{v}}{2}\cdot\left[\frac{\partial}{\partial \mathbf{x}}(\frac{e\phi}{T_e})^2\right]F_{0e}$$

- For $w^{NA} = \delta h_e/F$,

$$\frac{dw^{NA}}{dt} = \frac{1-w^{NA}}{1+e\phi/T_e}\left[-\frac{\partial}{\partial t}\frac{e\phi}{T_e} + \frac{\mathbf{v}}{2}\cdot\frac{\partial}{\partial \mathbf{x}}\left(\frac{e\phi}{T_e}\right)^2\right].$$

- Modified Poisson's equation and Charge Conservation

$$\left(\lambda_D^2\nabla^2 - 1\right)\frac{e\phi}{T_e} = \int \delta h_e d\mathbf{v} - \delta n_i, \quad \lambda_D^2\nabla^2\left(\frac{\partial}{\partial t}\frac{e\phi}{T_e}\right) = -\frac{\partial}{\partial \mathbf{x}}\cdot\int \mathbf{v}\delta h_e d\mathbf{v},$$

$$\delta h_e = \sum_{j=1}^{N} w_j^{NA}\delta(\mathbf{x}-\mathbf{x}_j)\delta(\mathbf{v}-\mathbf{v}_j),$$

Finite-β Split-Weight Particle Simulation Scheme

[W. Lee, J. L. V. Lewandowski, T. S. Hahm, and Z. Lin, PoP(2000)]

Non-adiabatic perturbed distribution:

$$F_\alpha = F_{0\alpha} + \delta f_\alpha, \delta f_e = \psi F_{0e} + \delta h_e,$$

$$E_\parallel = -\hat{\mathbf{b}} \cdot \nabla \psi = -\hat{\mathbf{b}} \cdot \nabla \phi - (1/c)\partial A_\parallel / \partial t$$

Generalized Ohm's laws:

$$[1 - \nabla_\perp^2]\psi = -\beta \int v_\parallel^2 (\delta f_i - \delta h_e) dv_\parallel + \int (\delta f_i - \delta h_e) dv_\parallel .$$

$$(\beta \frac{m_i}{m_e} - \nabla_\perp^2) \frac{\partial \psi}{\partial t} = \beta \frac{\partial}{\partial x_\parallel} \int v_\parallel^3 (\delta f_i - \delta h_e) dv_\parallel - \frac{\partial}{\partial x_\parallel} \int v_\parallel (\delta f_i - \delta h_e) dv_\parallel$$

Split Weight: $w^{NA} = \delta h_e / F_e$

$$\frac{dw^{NA}}{dt} = \frac{1 - w^{NA}}{1 + \psi} \left[-\frac{\partial \psi}{\partial t} + \frac{v_\parallel}{2} \frac{\partial \psi^2}{\partial x_\parallel} \right].$$

Integrated Gyrokinetic Particle Simulation

- Microturbulence simulation including trapped electrons and finte-β physics:
  - Zeroth-order orbit sets the maximum time step, e.g., $0.1\mu sec$.
  - FL-coord. + Split-weight + Adiabatic field pusher
  - Simulation time to reach steady-state turbulence: e.g. $1msec$.
- Gyrokinetic MHD: Equilbria
  - Compressional Alfven Waves
  - Pressure Balance
- Elliptic Multi-grid Solver
- Transport time scale: e.g. $1sec$.
  - Profile evolution based on entropy production
  - Brute force

Summary and Conclusions

- The combination gyrokinetic particle simulation and MultiGrid Elliptic Solver are the most powerful tool for solving the Darwin-Vlasov-Maxwell system on the massively parallel computers. *(Darwin model negelects the displacement current* $\partial \mathbf{E}^T / \partial t$*.)*

- The computing time is (*nearly*) linearly proportional to number of particles (N_p) and number of cells (N_c) (*Typically, 4 - 10 particles per cell.*), and the computing power is also (*nearly*) increases linearly with number of processors (N_s).

- Simulations of NSTX and NCSX plasmas in the near future.

- The availability of new class of MPPs in the future makes it possible to simulate reactor-size plasmas.