#### **Particle Simulation of Magnetically Confined Plasmas**

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### **OUTLINE**

*PPPL*

- Progress in Particle Simulation
- Gyrokinetic Particle Simulation of Microinstabilities
- Future of Gyrokinetic Particle Simulation
- Particle Simulation of Relativistic Beams
- Summary and Conclusions
- Particle Simulation + Massively Parallel Computers **–***<sup>a</sup> dynamite combination: [Reynders, ..., Lin]* **–***local, explicit, scalar*
- Particle Simulation is a Powerful Tool:

**–**for Tokamaks and Stellarators *(microturbulence, neoclassical and MHD physics)* **–**for High Energy Particle Beams *(space charge effects)*

- Advantages of Particle Simulation
	- **–**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)*

• The Vlasov equation, on, $\frac{\partial P}{\partial F}$ 

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

 $dt$   $dt$ <br>• Particle Pushing,

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

at at the value of the set of the set of the set of the Klimontovich-Dupree representations,

\n- Klimontovich-Dupree representations,
\n- $$
F = \sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{x}_j) \delta(\mathbf{v} - \mathbf{v}_j),
$$
\n- Poisson's equation: 
$$
\mathbf{E} = -\nabla \phi
$$
\n

a<br>V

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

Ampere's Law and Faraday's Law

- **Particle Simulation of the Vlasov-Maxwell System (contability)**<br>• Vlasov equation is solved in Lagrangian coordinates<br>-*Nonlinear PDE*  $\Rightarrow$  *Linear ODE : Particle Pushing* • Vlasov equation is solved in Lagrangian coordinates  $\rightarrow$ *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*
- -*Monte-Carto processes*<br>• Suitable for high frequency short wavelength physics, e.g., Example 1988<br>
Equency short way<br>  $\omega \approx \omega_{ne} - k\lambda_D \approx$  $\frac{1}{2} \omega_{pe}$   $\frac{k}{\lambda_D}$ e<br>1
- $\omega \approx \omega_{pe} \kappa \lambda_D \approx 1$ <br>• Disparate spatial and temporal scales for physics of d temporal scales<br>  $\omega \approx \omega_*$ .  $k \rho_s \approx$

oral sca $_{*}, \;\; k\rho_{s}$ 1

 $\omega \approx \omega_*, \kappa \rho_s \approx 1$ <br>• Enhanced numerical noise (*N*: no. of particles)  $\omega$   $\approx$   $\omega$   $\approx$ ,  $k\rho_s \approx$ <br>
noise (N: no. of<br>  $\delta n/n \gg 1/\sqrt{N}$ .<br>1  $\frac{1}{2}$  $\begin{align} s^2 \ 0 \ \sqrt{2} \end{align}$ 

- 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 <sup>a</sup> finite size particle due to Debye shielding  $\mathcal{L}_{\mathcal{A}}$  , and the set of  $\mathcal{L}_{\mathcal{A}}$  no need to satisfy  $\frac{1}{1}$  $\frac{1}{\sqrt{2}}$ : a finite s<br>Debye sh<br>io need to<br> $(n \lambda_D^3) \ll$ )<br>)  $1/(n\lambda_D^3) \ll 1.$ <br>• Number of calculations for N particles



- Vumber of calculations for  $N$  particles<br>  $-N^2$  for direct interactions and  $N log N$  for PIC
- Collisionless Simulations [*Langdon et al. (1971)* ]
- Collisions are re-introduced via Monte-Carlo methods [*Shanny, Dawson & Greene* (1976)]

# **Progress in Particle Simulation (cont.)** *PPPL*

• Numerical Properties

**–Grid spacing imposed by Debye shielding [Langdon (71)]:**<br> $\Delta x < \lambda_D$ 

**–**Time step imposed by high freq. oscillat'ns [Langdon (79)]:  $\text{freq.}$  ( $\Delta t <$ 

 $\omega_{pe} \Delta t < 1$ ں<br>1

**–**Time step imposed by fast electrons [Langdon (79)]:  $\frac{letrc}{dt}$ 

 $kv_{te}\Delta t < 1$ u<br>1

-Noise enhanced by Debye shielding [Okuda et al. (71)]:<br> $\frac{\delta n}{\delta} \approx \frac{1}{\sqrt{1-\delta}}$ 

$$
\frac{\text{Debye shielding}}{n} \approx \frac{1}{\sqrt{N}(k\lambda_D)}
$$

• Implicit Schemes [Mason (1982); Denavit (1982); Langdon et. al (1982)] Implicit schemes [Maxtlength]  $\epsilon$ . al (1982)]<br>  $\epsilon$ **—Instability**:  $\omega_{pe} \Delta t >$ 

|
|
| **-**Instability:  $\omega_{pe}\Delta t > 1$ <br>
-Inaccuracy:  $kv_{te}\Delta t = (\omega_{pe}\Delta t)(k\lambda_D) >$  $\frac{1}{\Delta}$ ) |
|
| -Instability:  $\omega_{pe}\Delta t > 1$ <br>-Inaccuracy:  $kv_{te}\Delta t = (\omega_p)$ <br>-for  $k\lambda_p \ll 1 \Rightarrow \omega_{pe}\Delta t > 1$  $\frac{1}{1}$  $t > 1$ <br>  $\Delta t = (\omega_{pe} \Delta t)(k \lambda_D) > 1$ <br>  $\omega_{pe} \Delta t > 1$  but keeping  $kv_{te} \Delta t <$ .<br>1

- Culprits: plasma waves originated from space charge effects
- Quasineutral waves are the waves of interest in tokamaks
- Reduced Vlasov-Maxwell equations:

**–**Gyrokinetic ordering:

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

**–**Gyrophase average

- Linear theory : Rutherford and Frieman (1968); Taylor and Hastie (1968); Catto (1978)
- Nonlinear Theory:

**–**Frieman and Chen (1982) – in Fourier k-space **–**Lee (1983) - in real space

- Nonlinear Theory Lie perturbation methods:
	- **–**Dubin et al. (1983) electrostatic slab
	- **–**Hahm (1988) electrostatic toroidal
	- **–**Hahm et al. (1988) electromagnetic slab
	- **–**Brizard (1989) electromagnetic toroidal and reduced MHD
	- **–**Qin et al.(1999) compressional-Alfven and Bernstein waves
	- **–**Qin et al. (2000) pressure balance
	- **–**Qin et. ql. (Sherwood 2000) Gyro-gauge theory

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**Gyrokinetic Particle Simulation** *PPPL*

[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.



**Gyrokinetic Particle Simulation (cont.)** *PPPL*

<sup>A</sup> charged ring is further approximated by 4-point average,

valid for  $k_{\perp} \rho_i \leq 2$ . i

 $\mathbb{L}^{n}$  =  $\mathbb{L}^{n}$ gyrokinetic model giving rise to quasineutral simulation, by<br>kii<br>V = re<sub>]</sub><br>vir<br>⇒ pola<br>quas:<br> $\nabla^2_\perp \phi$ Tration shieldin<br>
neutral simulation<br>  $= -4\pi e(\overline{n}_i - n_i)$ 

$$
\begin{aligned}\n\text{S} & \text{inetic model giving rise to quasineutral simulation,} \\
\nabla^2 \phi &= -4\pi \rho \quad \Rightarrow \quad (\frac{\rho_s}{\lambda_D})^2 \nabla^2 \phi = -4\pi e (\overline{n}_i - n_e), \\
\text{rations of Motion} & \text{or} \quad \cos \theta = \sqrt{\frac{\rho_s}{\lambda_D}} \quad \Rightarrow \quad \mu = v_\perp^2\n\end{aligned}
$$

 $\bullet$  Equations of Motion

$$
\begin{aligned}\n\text{equations of Motion} \\
\frac{d\mathbf{R}}{dt} &= U\hat{\mathbf{b}} + \mathbf{v}_d - \frac{c}{B}\frac{\partial \overline{\phi}}{\partial \mathbf{R}} \times \hat{\mathbf{b}}, \quad \frac{\mu}{B} \equiv \frac{v_\perp^2}{2B} = const., \\
\frac{dU}{dt} &= -[\hat{\mathbf{b}} + \frac{U}{\Omega}\hat{\mathbf{b}} \times (\hat{\mathbf{b}} \cdot \frac{\partial}{\partial \mathbf{R}})\hat{\mathbf{b}}] \cdot (\mu \frac{\partial}{\partial \mathbf{R}} lnB + \frac{q}{m} \frac{\partial \overline{\phi}}{\partial \mathbf{R}}),\n\end{aligned}
$$

• Numerical Properties of a Gyrokinetic Plasma **–**Grid spacing imposed by cold electron response posed by cold electron resp $\Delta x < \rho_s$ ;  $(\rho_s/\lambda_D \approx 100)$  $\Delta x < \rho_s$ ;  $(\rho_s/\lambda_D \approx 100)$ <br> **–Time step imposed by cold electron response**  $(\omega_H \equiv$  $\overline{\left( \right. }$ k  $\overline{\mathbb{R}}$  $\frac{k_{\parallel}}{k_{\perp}}$  $\lambda_D$  $\frac{\lambda_D}{\rho_s} \omega_{pe}$ )  $\Delta x < p_s,~~$   $(p_s / \Delta D \approx 100)$ <br>bosed by cold electron response (<br> $\omega_H \Delta t \ll 1;~~$   $(\omega_{pe}/\omega_H \approx 1000)$  $\omega_H \Delta t \ll 1$ ;  $(\omega_{pe}/\omega_H \approx 1000)$  $\overline{\left( \right. }$ **–**Time step restricted by streaming of thermal electrons: strear $k_{\parallel}v_{te}$ k  $\frac{1}{\text{ming}}$ ں<br>1  $\overline{\text{-Noise enhanced by }\omega_H}$  $\omega_H$ :<br>  $\delta n/n \approx 1/\sqrt{N} (k \rho_s)$ .  $\begin{array}{c} \n\searrow \n\end{array}$ 

|
|
| |

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

## Methods to further improve the numerical properties

- Methods to further improve the numerical properties<br>
 Adiabatic electron response  $(\delta n_e/n_0 \approx e\phi/T_e)$  can achieve all of the above, but by completely forfeiting non-adiabatic electron dynamics from simulation, e.g., wave-particle interactions.
- actions.<br>• Split weight  $\delta f$  simulation scheme can relax all the numerical restrictions: Split weight *o J* simulations:<br>al restrictions:<br>-Grid Spacing:  $\Delta x \gg \rho_s$ ula<br>>>
	-
	- al restrictions:<br> **–Grid Spacing:**  $\Delta x \gg \rho_s$ <br> **–Time Step:**  $\omega_* \Delta t < 1$  (or  $\omega_A \Delta t < 1$ ),  $k_{\parallel} v_{te} \Delta t \gg 1$ ;<br> **–Noise:**  $\delta n/n \approx 0 \rightarrow 1/\sqrt{N}$ . k  $\alpha$   $\sim$  1 (01  $\omega$ <sub>A</sub>)<br>0  $\rightarrow$  1/ $\sqrt{N}$ . ر<br>1  $\frac{1}{\sqrt{2}}$  $\frac{s}{\sqrt{2}}$
- With this scheme, accuracy now dictates the number of particle used in the simulation.

#### **The Perturbative**  $(\delta f)$  **Particle Simulation Scheme** *PPPL*

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

• The Vlasov equation,  $\frac{d}{dF}$  $\frac{d\mathbf{t}}{dt}$ uation,<br>  $\equiv \frac{\partial F}{\partial t} + \mathbf{v} \cdot \frac{\partial F}{\partial \mathbf{x}} + \frac{q}{m} \mathbf{E} \cdot \frac{\partial F}{\partial \mathbf{v}} = 0.$ • For  $F = F_o + \delta f$ ,  $d\delta f$  $\frac{d}{dt}$  $\frac{1}{2}$  =  $$  $dF_o$  $\frac{d}{dt}$ • Let  $W = \delta f / F$  to obtain

$$
dW = \delta f / F \text{ to obtain}
$$
  
\n
$$
\frac{d\mathbf{x}}{dt} = \mathbf{v}, \quad \frac{d\mathbf{v}}{dt} = \frac{q}{m} \mathbf{E}, \quad \frac{dW}{dt} = -(1 - W)\mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}} \left(\frac{q\phi}{T_e}\right),
$$
  
\n
$$
\delta f = \sum_{j=1}^{N} W_j \delta(\mathbf{x} - \mathbf{x}_j) \delta(\mathbf{v} - \mathbf{v}_j).
$$

- Easy access to both linear and nonlinear regimes
- Gyrokinetic Poisson's equation remains unchanged.

**Split Weight Perturbative**  $(\delta f)$  **Particle Simulation Scheme** 

*[Manuilskiy and Lee, PoP(2000)]*

*Let*  $\delta f_e = (e\phi/T_e)F_{0e} + \delta h_e$  to obtain )<br>)  $\frac{(e\phi/T_e)F_{0e} + \delta h_e \text{ to o}}{d\delta h_e}$ e  $\frac{dt}{dt}$  $T_e$ )  $I$ <br>= - $\frac{\partial}{\partial t}$  $\frac{1}{e\phi}$  $\frac{\text{d} \varphi}{T_e}$  $\frac{\delta h_e}{F_{0e}}$  + obtain<br> $\frac{\mathbf{v}}{2} \cdot \left[ \frac{\partial}{\partial \mathbf{x}} \right]$  $\ddot{\phantom{0}}$ a<br>|  $\overline{\phantom{a}}$  $\overline{\phantom{0}}$  $\overline{\phantom{0}}$  $\left(\frac{e\phi}{\pi}\right)$  $\frac{\text{d} \varphi}{T_e}$ )  $\frac{1}{2}$ |
|
| |
|
| **1** 7<br>7<br>1<br>7<br>2<br>7<br>2<br>2<br>2<br>2<br>2<br>2<br>2<br>  $\Bigl] \, F_{0e}$  $w^{NA}$  $\frac{dE}{dt} = -$ <br>=  $\delta h_e/F$ ,

• For 
$$
w^{NA} = \delta h_e/F
$$
,  
\n
$$
\frac{dw^{NA}}{dt} = \frac{1 - w^{NA}}{1 + e\phi/T_e} \left[ -\frac{\partial e\phi}{\partial t} + \frac{v}{2} \cdot \frac{\partial}{\partial x} \left( \frac{e\phi}{T_e} \right)^2 \right].
$$

 $dt = 1 + e\phi/T_e$   $dt/dtT_e = 2 \partial \mathbf{x} (T_e)$ <br>• Modified Poisson's equation and Charge Conservation

disson's equation and Charge Conse

\n
$$
\left(\lambda_D^2 \nabla^2 - 1\right) \frac{e\phi}{T_e} = \int \delta h_e d\mathbf{v} - \delta n_i,
$$
\n
$$
\lambda_D^2 \nabla^2 \left(\frac{\partial e\phi}{\partial t}\right) = -\frac{\partial}{\partial \mathbf{x}} \cdot \int \mathbf{v} \delta h_e d\mathbf{v},
$$
\n
$$
\delta h_e = \sum_{j=1}^N w_j^{NA} \delta(\mathbf{x} - \mathbf{x}_j) \delta(\mathbf{v} - \mathbf{v}),
$$

# **Split-weight scheme for finite- <sup>p</sup>lasmas** *PPPL*

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

*IW. W. Lee, J. L. V. Lewandowski and T. S. Hahm, Sherwood(2000)*<br>• The governing gyrokinetic Vlasov equation, E<br>E  $\frac{L}{L}$ 

The governing gyrokinetic Vlasov equation,  
\n
$$
\frac{dF_{\alpha}}{dt} \equiv \frac{\partial F_{\alpha}}{\partial t} + v_{\parallel} \hat{\mathbf{b}} \cdot \frac{\partial F_{\alpha}}{\partial \mathbf{x}} + c \frac{\mathbf{E}^{L} \times \hat{\mathbf{b}}_{0}}{B_{0}} \cdot \frac{\partial F_{\alpha}}{\partial \mathbf{x}} + \frac{q}{m} \mathbf{E} \cdot \hat{\mathbf{b}} \frac{\partial F_{\alpha}}{\partial v_{\parallel}} = 0,
$$
\n
$$
\hat{\mathbf{b}} = \hat{\mathbf{b}}_{0} + \frac{\delta \mathbf{B}}{B_{0}}, \quad \hat{\mathbf{b}}_{0} = \frac{\mathbf{B}_{0}}{B_{0}}
$$
\n
$$
\delta \mathbf{B} = \nabla A_{\parallel} \times \hat{\mathbf{b}}_{0},
$$
\n
$$
\mathbf{E} = E_{\parallel}^{T} \hat{\mathbf{b}}_{0} + \mathbf{E}^{L},
$$
\n
$$
\mathbf{E}^{L} = -\nabla \phi, \quad E_{\parallel}^{T} = -\frac{1}{c} \frac{\partial A_{\parallel}}{\partial t}.
$$

Gyrokinetic Poisson's equation & Ampere's law,

$$
(\frac{\rho_s}{\lambda_D})^2 \nabla_{\perp}^2 \phi = -4\pi e (n_i - n_e),
$$
  

$$
\nabla_{\perp}^2 A_{\parallel} = -\frac{4\pi}{c} J_{\parallel},
$$
  

$$
n_{\alpha} = \int F_{\alpha} dv_{\parallel}, \quad J_{\parallel} = \sum_{\alpha} q_{\alpha} \int v_{\parallel} F_{\alpha} dv_{\parallel}.
$$

• The generalized Ohm's law

lized Ohm's law  
\n
$$
[\frac{n_e}{n_i}\omega_{pe}^2 + \frac{n_i}{n_0}\omega_{pi}^2 - c^2 \nabla_{\perp}^2]E_{\parallel}/4\pi e
$$

$$
\left|\frac{1}{n_i}\omega_{pe} - \frac{1}{n_0}\omega_{pi} - c\right| \leq \left|\frac{1}{n_0}\right|^{4\pi e}
$$
\n
$$
= \hat{\mathbf{b}} \cdot \nabla \int v_{\parallel}^{2} (F_i - F_e) dv_{\parallel} - v_A^2 \hat{\mathbf{b}} \cdot \nabla \int (F_i - F_e) dv_{\parallel}
$$

#### $\textbf{Finite-}\beta$  **Simulation, (cont.)** *PPPL*

•  $F_{\alpha} = F_{0\alpha} + \delta f_{\alpha}$ ,  $\delta f_{e} = \psi F_{0e} + \delta h_{e}$ .

- $F_{\alpha} = F_{0\alpha} + \delta f_{\alpha}, \delta f_e = \psi F_{0e} + \delta h_e.$ <br>•  $E_{\parallel} = -\hat{\mathbf{b}} \cdot \nabla \psi = -\hat{\mathbf{b}} \cdot \nabla \phi (1/c)\partial A_{\parallel}/\partial t$ •  $E_{\parallel} = -b \cdot \nabla \psi = -b \cdot$ <br>• Generalized Ohm's law
- 

Generalized Ohm's law<br>  $[1 - \nabla_{\perp}^2] \psi = -\beta \int v_{\parallel}^2 (\delta f_i - \delta h_e) dv_{\parallel} + \int (\delta f_i - \delta h_e) dv_{\parallel}.$ 

 $\begin{aligned} \mathbf{L} - \mathbf{v} \mathbf{v} &= -\rho \mathbf{v} \end{aligned}$ <br>• Equations for  $\partial \psi / \partial t$ 

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

 $-\frac{\partial}{\partial x_{\parallel}}$  /  $v_{\parallel}(0)$ <br>• Split Weight:  $w^{NA} = \delta h_e/F_e$ ht:  $w^{\Lambda}$ <br>d $w^{NA}$ =  $\delta h_e/F_e$ <br>1 —  $w^{NA}$ 

$$
\mathcal{L}^{\mathbf{h}} = \frac{\delta h_e}{F_e} = \frac{1 - w^{NA}}{1 + \psi} \left[ -\frac{\partial \psi}{\partial t} + \frac{v_{\parallel} \partial \psi^2}{2 \partial x_{\parallel}} \right].
$$

#### Shear-Alfven Waves

One-Dimensional Simulation:

 $k_{\perp} \rho_s = 0.8, \beta = 10\%, k_{\parallel}/k_{\perp} = 0.01, T_e/T_i = 1$ 

• Split weight scheme:  $\omega \Delta t \approx 0.033$ ,  $k_{\parallel} v_{te} \Delta t \approx 0.344$ 



Original  $\delta f$  scheme:



**Gyrokinetic Particle Simulation Codes** *PPPL*

 $\Rightarrow$ 1,2&3D electrostatic and electromagnetic (Darwin) slab codes  $\Rightarrow$  3D electrostatic global toroidal code in magnetic coordinates

GTC [Lin et al. *Science* (1998)]

Basic formalism for GTC



asic formatism for GTC<br>  $-$ magnetic coordinates  $(\psi, \theta, \zeta)$  [Boozer, 1981]

- **–**guiding center Hamiltonian [White and Chance, 1984]
- **–**non-spectral Poisson solver [Lin and Lee, 1995]

Advanced features for GTC

- **–**general geometry (e.g., stellarator)
- **–**profile effects (e.g., low-aspect ratio, steep gradient)
- **–**capable of simulating full poloidal cross section (*global*) or thin annulus box (*local* )

### **Global Field-line Coordinates**

*[Z. Lin, in preparation]*

[Z. Lin, in preparation]<br>• Microinstability wavelength:  $\lambda_{\perp} \propto \rho_i$ ,  $\lambda_{\parallel} \propto qR$ Lin, in preparation]<br>**Microinstability<br><del>–grid</del> # N**  $\propto a^2$ ,  $a:$  minor radius

- Most global codes: w/o field-line coordinates Most global cod<br>  $-\text{grid}$  #  $N \propto a^3$
- $-\text{grid} \# N \propto a^{\circ}$ <br>• GTC global code: use field-line coordinates bal code: use field-line coors<br>  $(\psi, \alpha, \zeta), \quad \alpha = \theta - \zeta/q$  $\frac{1}{2}$

 $(\psi, \alpha, \phi)$ <br>
–grid #  $N \propto a^2$ 

 $-\text{grid} \# N \propto a^2$ <br>—larger time step: no high *k*  $\parallel$  modes

- **–**order of magnitude saving of computing time for reactor size simulations
- Field-line coordinates in flux-tube codes [Dimits and Beer]



*PPPL*





# **Gyrokinetic Particle Simulation of Microinstabilities***PPPL*

Codes:

**–**1&2D slab codes

**–**3D global toroidal code in general geometry

Physics:

**–**wave-particle interactions: nonlinear saturation

**–**zonal flows: reduction of fluctuation and transport

**–**collisional effects: enhancement of transport due to weak  $\nu_{ei}, \nu_{ii}$ 

• Scaling trends:

caling trends:<br>–Mixing Length Rule:  $\gamma_L/k_\perp^2,$  $\frac{1}{\Delta}$ 

 $-$ Mixing Length Rule:  $\gamma_L/k_{\perp}^2$ ,<br>--Resonance Broadening:  $\Delta \omega_{NL}/k_{\perp}^2$ ,

**Gyrokinetic Particle Simulation of Microinstabilities (cont.)** 

**Nonlinear Saturation: Three Mode Coupling in Slab Geometry**<br>• 1D drift instability: (linear:  $\omega \Delta t \approx 0.72$ .  $k_{\parallel}v_{te}\Delta t \approx 2.7$ )

**Nonlinear Saturation: Three Mode Coupling in Slab Geom**<br>• 1D drift instability: (linear:  $\omega \Delta t \approx 0.72$ ,  $k_{\parallel} v_{te} \Delta t \approx 2.7$ )  $\overline{\mathbf{r}}$ 



*[Parker and Lee ('93); Manuilskiy and Lee ('00)]*

- The space  $P_{\text{a}_{i}}$ <br>
[Parker and Lee ('93); Manuilskiy and Lee ('00)]<br>
 2D drift instability:  $E \times B$  trapping of resonant particles
- 2D drift instability:  $E \times B$  trapping of resonant particles<br>• 2D drift instability with collisions: saturation level caused<br>by  $E \times B$  trapping is greatly enhanced by weak collisions. by  $E$   $\times$ by  $E \times B$  trapping is greatly enhanced by weak collisions.<br>
• 2D ITG drift instability:  $E \times B$  trapping of resonant particles  $\frac{1}{16}$
- *[Lee et al., ('84), Federici et al. ('87), Lee and Tang ('88)]*

**Gyrokinetic Particle Simulation of Microinstabilities (cont.)** 

Global Toroidal Simulation

Without zonal flow *[Lee and Santoro, PoP (1997)]*  $\frac{dS}{E}$ 

Vithout zonal flow *[Lee and Santoro, PoP (1997)]*<br>
-Nonlinear saturation :  $E \times B$  trapping of resonant particles **–**Energy cascade to low (m,n) modes

**–**Consistent with Resonance Broadening Scaling (Dupree):

It with Reso $\chi_i \propto (k_\perp \rho_s)$ i  $\overline{\left( \right. }$ ) ance Broadening Scaling<br>  $\frac{2}{e\phi/T_e}$   $\frac{2}{(1/k_{\parallel}\rho_s)(cT/eB)}$ k )

With zonal flow: Reduction of Turbulent Transport *[Z. Lin et al.,*



**Gyrokinetic Particle Simulation of Microinstabilities (cont.)** 

Collisional Effects on Toroidal ITG modes

Weak collisions have negligible effects on linear growth, but can enhance transport due to collisional damping of the zonal<br>flow, i.e.,<br> $\chi_i \propto \nu^*$ flow, i.e.,  $\frac{1}{\chi}$  $\overline{\nu}$  $\ast$ 

$$
\chi_i \propto \nu^*
$$



Bursting Behavior



**large bursts of fluctuation in TFTR RS plasmas observed period ~ collisional flow damping time** **collisional damping of zonal flows causes bursts of turbulent transport in gyrokinetic simulations**

**Gyrokinetic Particle Simulation of Neoclassical Transport**<br>
• Neoclassical  $\delta f$  scheme:  $f = f_0 + \delta f$ 

**Gyrokinetic Particle Simulation of No.<br>• Neoclassical**  $\delta f$  **scheme:**  $f = f_0 + \delta f$  $f_0$ : local Maxwellian;  $\delta f$ : deviations due to magnetic drift

*[Lin, Tang, and Lee, 1995; Sasinowski and Boozer, 1995]*

- Advantages: reduced noise; steady state; Forker-Planck collision operators conserving momentum and energy
- Formal derivation and validation of collisional  $\delta f$  method: source and sink; nonlinear collision operators

*[Chen and White, 1997]*

[Chen and White, 1997]<br>• Neoclassical  $\chi_i$  near magnetic Axis

*[Lin, Tang, and Lee, 1997]*

Widely used in stellarator neoclassical transport calculation

## **Neoclassical**  $\chi_i$  **Near Magnetic Axis** *PPPL*

- Ion thermal transport levels in ERS plasmas observed to fall below the neoclassical theory "irreducible minimum level"
- Simulations lead to improved calculation of neoclassical  $\chi_i$

*[Lin, Tang, and Lee, Phys. Rev. Lett. , 1997]*

- Physical picture:
	- $\alpha$ -orbit size reduced due to  $\rho_p \sim r$
	- **–**higher energy particle: larger reduction
	- **–**outward energy flux reduced
	- $-\chi_i$  decreases for smaller minor radius



## **Plans for Gyrokinetic Particle Simulation** *PPPL*

- Trapped electron physics:
- Field-line coord. <sup>+</sup> Split-weight <sup>+</sup> Adiabatic field pusher d. + Split-weight + Adiaba<br>  $k_{\parallel}v_{te}\Delta t >> 1, \quad \omega \ll \omega_{be}$ cs:<br>
Split-weight + Ac<br>  $\Delta t >> 1$ ,  $\omega \ll$

k

- $\|v_{te}\|$   $\geq$  1, a
	- Shear-Alfven waves: split-weight for passing electrons
- Gyrokinetic MHD: neoclassical drive and turbulence drive
	- Compressional Alfven Waves *[Qin et al., 1999]*
	- **–** Pressure Balance *[Qin et al. to appear]*
- Wave Heating high frequency gyrokinetics *[Qin et al. 1999]* **–**IBW physics

## **Perturbative Particle Simulation of Space Charge Dominated Relativistic Beams** *PPPL*

- f simulation model *[Lee, Qian, and Davidson, 1997] s* sinuration moder *[Lee, Qian, and Dav*  $-$ based on KV equilbrium:  $F_0 \propto \delta$ **vistic E**<br>a Davidson<br> $\propto \delta$  (W  $\overline{\left( \right. }$ )
- Non KV equilibrium:
	- **–**simulation: *[Stoltz, Davidson, Lee, 1999]*
	- **–**theory: *[Davidson, Qin, Channell, 1999]*
- $\bullet$  3D multi-species NL  $\delta f$  code: *[Qin, Davidson, Lee, 1999]* Beam Equlibrium, Stability, Transport (BEST) Code
- e-p instability (two-stream)
	- **–**theory: *[Davidson et al, 1999]*
	- **–**simulation: *[Qin, Davidson and Lee, <sup>1999</sup> and 2000]*
- Darwin model: nonradiative simulation for chamber transport
	- *[Lee, Qin, and Davidson, 2000]*

 $\left\{ \right.$ 

**Darwin Model for Bean Physics**  
\n
$$
\mathbf{F}_{j}^{foc} = -\gamma_{j} m_{j} \omega_{\beta j}^{2} \mathbf{x}_{\perp},
$$
\n
$$
\{\frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}} - [\gamma_{j} m_{j} \omega_{\beta j}^{2} \mathbf{x}_{\perp} + e_{j} \nabla_{\perp} (\phi - \frac{v_{z}}{c} A_{z})] \cdot \frac{\partial}{\partial \mathbf{p}_{\perp}}
$$
\n
$$
-e_{j} \frac{\partial}{\partial z} (\phi - \frac{v_{z}}{c} A_{z}) \frac{\partial}{\partial P_{z}} \} f_{j}(\mathbf{x}, \mathbf{p}_{\perp}, P_{z}, t) = 0,
$$
\n
$$
\nabla^{2} \phi = -4\pi \sum_{j} e_{j} \int d^{2} p_{\perp} dP_{z} f_{j}(\mathbf{x}, \mathbf{p}_{\perp}, P_{z}, t),
$$
\n
$$
\nabla^{2} A_{z} = -\frac{4\pi}{c} \sum_{j} e_{j} \int d^{2} p_{\perp} dP_{z} v_{z} f_{j}(\mathbf{x}, \mathbf{p}_{\perp}, P_{z}, t).
$$
\n
$$
\mathbf{v}_{\perp} = \mathbf{p}_{\perp} / \gamma_{j} m_{j}
$$
\n
$$
v_{z} = (P_{z} - \frac{e_{j}}{c} \delta A_{z}) / \gamma_{j} m_{j}
$$

## **Darwin Model for Beam Physics (cont.)** *PPPL*

$$
\frac{d\mathbf{x}_{ji}}{dt} = \mathbf{v}_{ji},
$$

$$
\frac{d\mathbf{p}_{\perp ji}}{dt} = \mathbf{v}_{ji},
$$

$$
\frac{d\mathbf{p}_{\perp ji}}{dt} = -\gamma_j m_j \omega_{\beta j}^2 \mathbf{x}_{\perp ji} - e_j \nabla_\perp (\phi - \frac{v_{zji}}{c} A_z).
$$

$$
i j^{\mu} j^{\mu} \beta j^{\lambda} \perp j i \qquad c_j \vee \perp (\varphi)
$$

$$
\frac{dP_{zji}}{dt} = -e_j \frac{\partial}{\partial z} (\phi - \frac{v_{zji}}{c} A_z).
$$

$$
dt = c_j \frac{\partial z}{\partial z} + c \frac{\partial z}{\partial z}.
$$

$$
\frac{dw_{ji}}{dt} = -(1 - w_{ji}) \frac{1}{f_{j0}} \left[ \frac{\partial f_{j0}}{\partial \mathbf{p}_{\perp}} \cdot \delta \left( \frac{d\mathbf{p}_{\perp ji}}{dt} \right) + \frac{\partial f_{j0}}{\partial P_z} \delta \left( \frac{dP_{zji}}{dt} \right) \right],
$$

$$
\delta \left( \frac{d\mathbf{p}_{\perp ji}}{dt} \right) = -\frac{\partial}{\partial \mathbf{p}_{\perp}} \left( \delta \mathbf{p}_{\perp} \right) \frac{\partial z_{ji}}{\partial \mathbf{p}_{\perp}} \frac{\partial z_{ji}}{\partial \mathbf{p}_{\per
$$

$$
\begin{aligned}\n\zeta \frac{d\mathbf{p}_{\perp ji}}{dt} f_{j0} \, \mathbf{p}_{\perp} &\quad \zeta \frac{d\mathbf{p}_{\perp ji}}{dt} \\
\delta \left( \frac{d\mathbf{p}_{\perp ji}}{dt} \right) &= -e_j \nabla_{\perp} (\delta \phi - \frac{v_{zji}}{c} \delta A_z), \\
\delta \left( \frac{dP_{zji}}{dt} \right) &= -e_j \frac{\partial}{\partial \phi} (\delta \phi - \frac{v_{zji}}{c} \delta A_z).\n\end{aligned}
$$

$$
\delta(\frac{dP_{zji}}{dt}) = -e_j \frac{\partial}{\partial z} (\delta \phi - \frac{v_{zji}}{c} \delta A_z),
$$

$$
\pmb{PPPL}
$$

$$
\delta f_j = \sum_{i=1}^{N_{sj}} w_{ji} \delta(\mathbf{x} - \mathbf{x}_{ji}) \delta(\mathbf{p}_{\perp} - \mathbf{p}_{\perp ji}) \delta(P_z - P_{zji}),
$$
  

$$
\nabla^2 \delta \phi = -4\pi \sum_j e_j \delta n_j,
$$
  

$$
\nabla^2 \delta A_z = -\frac{4\pi}{c} \sum_j \delta j_{zj},
$$
  

$$
\delta n_j = \int d^2 p_{\perp} dP_z \delta f_j(\mathbf{x}, \mathbf{p}_{\perp}, P_z, t) = \sum_{i=1}^{N_{sj}} w_{ji} S(\mathbf{x} - \mathbf{x}_{ji}),
$$

$$
\delta j_{zj} = e_j \int d^2 p_\perp dP_z v_{zj} \delta f_j(\mathbf{x}, \mathbf{p}_\perp, P_z, t) = e_j \sum_{i=1}^{N_{sj}} v_{zji} w_{ji} S(\mathbf{x} - \mathbf{x}_{ji}).
$$

Equilibrium Distribution  
\n
$$
f_{b0}(r, \mathbf{p}_{\perp}, P_z) = \frac{\hat{n}_b}{\gamma_b (2\pi \gamma_b m_b T_b)^{3/2}}
$$
\n
$$
\times \exp\{-\frac{p_{\perp}^2 / 2\gamma_b m_b + \gamma_b m_b \omega_{\beta b}^2 r^2 / 2 + e_b(\phi_0 - \beta_b A_{z0})}{T_b}\}\times \exp\{-\frac{(P_z - \gamma_b m_b \beta_b c)^2}{2\gamma_b^3 m_b T_b}\},
$$

# Adiabatic Pusher<br>in  $x - y$  plane lin

- Adiabatic Pusner<br>Fast electron motion in  $x y$  plane limits the time step.
- Treat electrons as charged strings.
- Push ions and solve field equations in the time scale of the frequency of interest, i.e., less often.

When <sup>a</sup> background electron componen<sup>t</sup> is introduced in <sup>a</sup> proton storage ring, the dipole surface mode can be destabilized.



Electrostatic/Magnetostatic Model [H. Qin, R. C. Davidson and W. W. Lee, Phys. Lett. A (in press)].

- Particle simulation finally emerges as one of the most promising tools for plasma physics research
- With thousand-processor parallel computers at NERSC and ACL/LANL, we can investigate:
- With thousand-processor parallel computers at NER<br>ACL/LANL, we can investigate:<br>MFE:  $(0.1 1) \times 10^9$  particles with 10,000 time steps<br> $\sim (30 300)$  hours on 256PE / T3E-900
	- **–**Transport scaling for large tokamaks
	- **–**NSTX simulation
	- **–**NCSX design
- $-$ NCSX design<br>IFE:  $(1 10) \times 10^6$  particles with 1,000,000 time steps
	- **–**two stream instability
	- **–**filamentation instability