Implicit δf Lorentz Ion Orbit Averaging and Sub-Cycling

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March 22, 2014

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PIC Simulation with Lorentz Ions: Introduction

- In regimes where gyrokinetic ordering may be in question, for example in the tokamak edge region with short gradient scales, a fully resolved Lorentz ion model can provide a useful validation tool or alternative to gyrokinetics.

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- Gyrokinetic simulations currently use time steps $\Omega_i \delta t \sim 1$ anyway. (Edge simulations of DIII-D $\Omega_i \delta t = 1$, NSTX $\Omega_i \delta t = 0.2$)
- Direct particle in cell (PIC) simulation results in unwanted cyclotron noise, and implicit stepping over the cyclotron motion does not resolve finite Larmor radius (FLR) effects well.

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Project Goal

To develop numerically stable algorithms to accurately reproduce FLR effects at low frequencies while filtering unwanted noise due to the high frequency ion cyclotron motion.

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- Equations for perturbed fields:

$$\frac{\partial \mathbf{B}_1}{\partial t} = -\nabla \times \mathbf{E}_1$$
$$\nabla \times \mathbf{B}_1 = \mu_0(\mathbf{J}_i + en_e\mathbf{V}_e)$$

where $\mathbf{J}_i$ is the perturbed ion current density and $\mathbf{V}_e$ is the electron flow velocity

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- The perturbed ion distribution function is calculated by:

$$\begin{aligned} f_1(\mathbf{x}, \mathbf{v}, t) &= \sum_{p=1}^{N_p} w_p(t)\delta(\mathbf{x} - \mathbf{x}_p(t))\delta(\mathbf{v} - \mathbf{v}_p(t)) \\ &\approx \sum_{p=1}^{N_p} w_p(t)\mathrm{S}(\mathbf{x} - \mathbf{x}_p(t))\delta(\mathbf{v} - \mathbf{v}_p(t)) \end{aligned}$$

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Implicit Time Discretization

- A second order accurate implicit scheme is used to push the ions.

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \frac{\Delta t}{2}(\mathbf{v}_{n+1} + \mathbf{v}_n)$$

$$\mathbf{v}_{n+1} = \frac{q\Delta t}{2m}\mathbf{E}_{n+1}(\mathbf{x}_{n+1}) + \underline{\underline{\mathbf{R}}} \cdot \left[\mathbf{v}_n + \frac{q\Delta t}{2m}\mathbf{E}_n(\mathbf{x}_n)\right]$$

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$$w_{n+1} = w_n - \frac{q_i \Delta t}{2T_i}\left[\mathbf{v}_n \cdot \mathbf{E}_n(\mathbf{x}_n) + \mathbf{v}_{n+1} \cdot \mathbf{E}_{n+1}(\mathbf{x}_{n+1})\right]$$

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- Picard iterations are used to solve the discrete equations at each time step.

Orbit Averaging and Sub-Cycling

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- Current densities are deposited only on macro time steps for sub-cycling. For orbit averaging, current densities are deposited on micro time steps and then time averaged.

$$\langle \mathbf{J}_i \rangle_{N+1/2} = \frac{1}{M+1} \sum_{n=0}^{M} \mathbf{J}_n \qquad \text{(Orbit Averaging)}$$

$$\langle \mathbf{J}_i \rangle_{N+1/2} = \frac{1}{2}(\mathbf{J}_{N+1} + \mathbf{J}_N) \qquad \text{(Subcycling)}$$

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- $\langle \mathbf{J}_i \rangle$ is used to solve for fields on the macro time step.

Orbit Averaging and Sub-Cycling

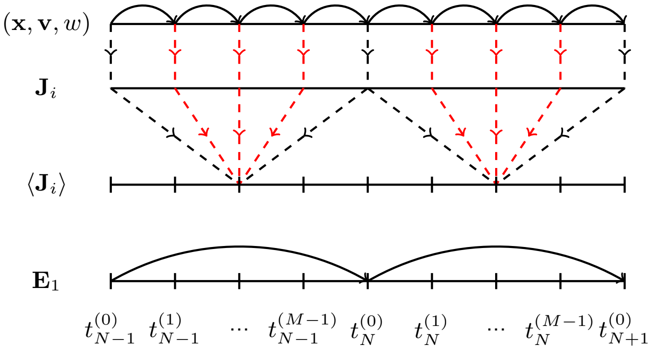

Figure: Orbit averaging and sub-cycling both advance particles over micro time steps and fields over macro time steps. Orbit averaging deposits current densities at each micro time step (represented by both the red and black lines), whereas sub-cycling only deposits current densites at the macro time steps (black lines only).

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- A test problem is used to study the numerical properties of the implicit time stepping algorithm and to compare with orbit averaging and sub-cycling algorithms.

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- Model assumptions:

  1. Electrostatic: $\mathbf{E}_1 = -\nabla\phi$
  2. Adiabatic electrons: $n_e = n_0 \frac{e\phi}{T_e}$
  3. Quasi-neutrality: $n_e = n_i = n$
  4. Uniform magnetic field: $\mathbf{B} = B_0 \hat{z}$

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- Assumptions along with the ion continuity equation yields:

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- Discretization with orbit averaged or sub-cycled current density:

$$\frac{\mathbf{E}_{N+1} - \mathbf{E}_N}{\Delta t} = \frac{T_e}{e^2 n_0} \nabla \left(\nabla \cdot \langle \mathbf{J}_i \rangle_{N+1/2} \right).$$

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- Discretization reduces to Crank-Nicholson method for orbit averaging and sub-cycling when $M = 1$.

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Direct Simulation Results ($M = 1$)

Direct simulation works well for zero or small values of $k_\perp \rho_i$.

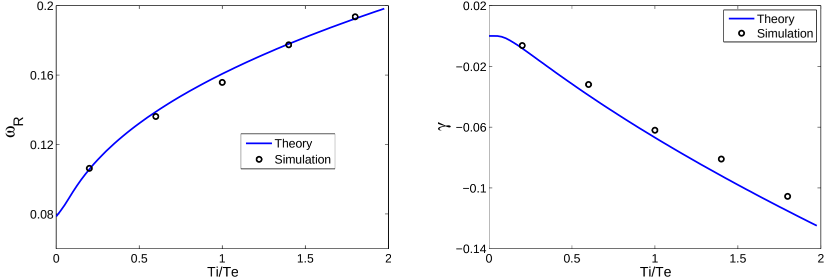

Figure: Real frequencies and damping rates for the ion acoustic wave as a function of ion temperature. Propagation is parallel to $\mathbf{B}$ ($k_\perp \rho_i = 0$) and results agree well with theory using direct simulation.

Direct Simulation Results ($M = 1$)

As $k_\perp \rho_i$ increases, simulations become dominated by cyclotron noise.

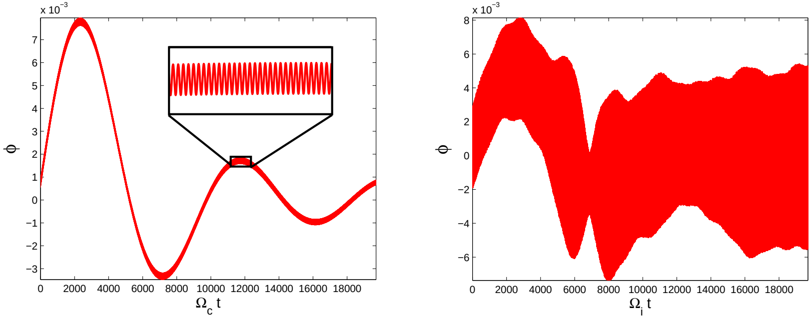

Figure: Time histories of Fourier mode amplitudes. On the left, $k_\perp \rho_i = 0.042$ and a small amount of cyclotron noise is present. On the right, $k_\perp \rho_i = 0.471$ and the cyclotron noise dominates.

Orbit Averaging/Sub-Cycling Results

- Orbit averaging successfully filters out cyclotron noise when $\Omega_i \Delta T$ is sufficiently large and produces accurate FLR effects.
- Sub-cycling increases the accuracy of the implicit integration scheme but suffers from noise when $k_\perp \rho_i = O(1)$.

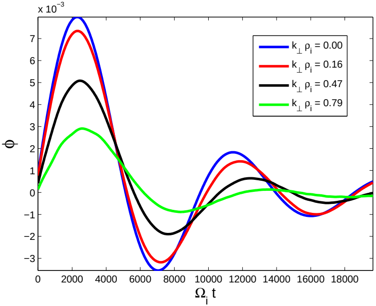

Figure: Time histories of Fourier mode amplitudes. Orbit averaging produces clean and accurate results even for $k_\perp \rho_i = O(1)$.

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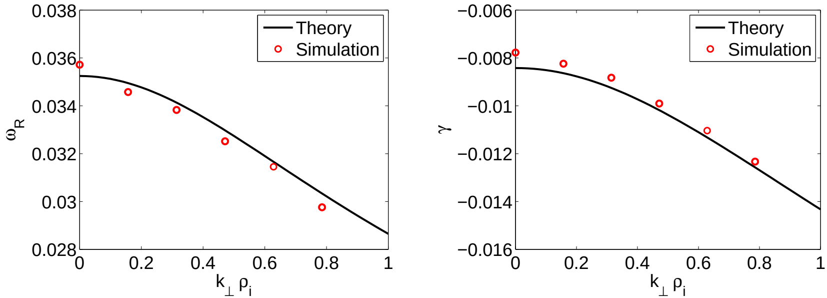

Figure: Real frequencies and damping rates for the ion acoustic wave as a function of $k_\perp \rho_i$. Orbit averaging accurately reproduces FLR effects.

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GPU Acceleration

- Implementation of particle pushes in a slab geometry code using one CPU and one GPU saw 4-8x speedup factors compared to using only one CPU.

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- A similar implementation with the test problem code is in process.
- We expect to improve on the slab code results by designing our implementation to eliminate the transfer of particle data between the host and the GPU.
- An efficient GPU deposit algorithm is being explored for the test code based on dividing the computational domain into tiles to utilize shared memory.

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- Further work to make optimal use of GPUs in PIC codes will be done.

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References and Acknowledgements

References:

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Acknowledgements:

Work supported by the DOE, SciDAC, Center for Extended Magnetohydrodynamics (CEEM), and Edge Physics Simulation Center (EPSI).

Questions?