PRINCETON PLASMA PHYSICS LABORATORY

Eliminating Finite-Grid Instabilities in Gyrokinetic Particle-in-Cell Simulations

Ben Sturdevant[1] and Luis Chacón[2]

[1]Princeton Plasma Physics Laboratory
[2]Los Alamos National Laboratory

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EXASCALE COMPUTING PROJECT

HBPS
High-fidelity Boundary Plasma Simulation

Numerical Challenges with Kinetic Electrons

- Modern tokamak GK codes treat electrons kinetically (gyrokinetic or drift-kinetic), which introduces numerical challenges including:
  - Electrostatic models can generate the high-frequency ``omega-H" mode (ES limit of the shear Alfvén wave)

$$\omega_H = \pm \Omega_i \sqrt{\frac{m_i}{m_e}} \frac{k_{||}}{k_\perp}$$

  - Cancellation issues at long wavelengths; more problematic in particle codes
  - Electromagnetic models regularize ``omega-H" but have their own challenges at long λ:

Hamiltonian ($p_{||}$) formulation :

$$\dot{p}_{||} = -\frac{q_s}{m_s}\left(\nabla_{||}\phi - v_{||}\nabla_{||}A_{||}\right) + \ldots$$

$$-\nabla_\perp^2 A_{||} + \left(\sum_s \frac{q_s^2 \mu_0 n_s}{m_s}\right) A_{||} = \mu_0 \sum_s q_s \int p_{||} f_s dp_{||}$$

Large, non-physical current in Ampère must cancel in RHS

Symplectic ($v_{||}$) formulation :

$$\dot{v}_{||} = -\frac{q_s}{m_s}\left(\nabla_{||}\phi + \frac{\partial A_{||}}{\partial t}\right) + \ldots$$

$$-\nabla_\perp^2 A_{||} = \mu_0 \sum_s q_s \int v_{||} f_s dv_{||}$$

Partial time derivative in particle equations of motion

  - Several specialized numerical techniques have been developed over the years to mitigate these issues, but rigorous numerical analysis is often lacking
- **There are numerical problems that remain in the infinite particle, $\Delta t \longrightarrow 0$ limit: focus of this poster**

The Gyrokinetic Finite-Grid Instability for PIC

There is a severe issue which has not generated much discussion in the past :
The Gyrokinetic Finite-Grid Instability

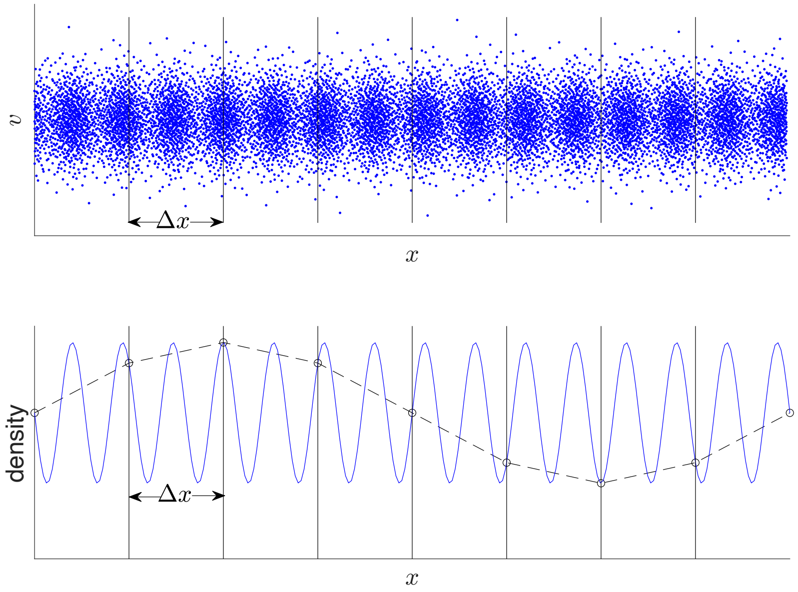
- Can be concealed by temporal instabilities due to ω_H , however, there are two key distinctions :
  1. The finite-grid instability is unique to PIC, i.e., it will not be present in continuum codes
  2. The finite-grid instability persists at arbitrary spatial and temporal resolutions
- Some history :
  - G. Wilkie and W. Dorland, PoP (2016): Converged instabilities shown to exist in minimal electrostatic GK δf PIC
  - B. McMillan, PoP (2020): This is just a manifestation of the well-known aliasing instability that requires us to ``resolve the Debye length" in Vlasov-Poisson PIC; Instability is present in gyrokinetic full-f PIC as well
  - The possibility of such an instability was alluded to in the early days of GK PIC : W. W. Lee, JCP (1987)

> and $\Delta x_\perp$ are coupled through ω_H. Following the previous derivation based on the NGP scheme, we can show that the largest growth occurs at $k_{||}\Delta x_{||} \cong \pi/1.4$ for $k_\perp \rho_s \cong 0.21$ regardless of the size of $\Delta x_{||}$—a rather unique feature. Numerical

  - Our own studies with implicit $v_{||}$ electromagnetic gyrokinetics see converged instabilities for certain parameters
- Recently, rigorous numerical analysis has shown that finite-grid instabilities in Vlasov-Poisson PIC can be tamed by using energy conserving interpolations : D. Barnes and L. Chacón, CPC (2021)

Aliasing in the Particle-in-Cell Method

- Both grid and particle quantities are present in PIC
- Particles can support many modes that cannot be represented on the grid → alias to grid modes
- Aliasing problem can exist in infinite particle limit



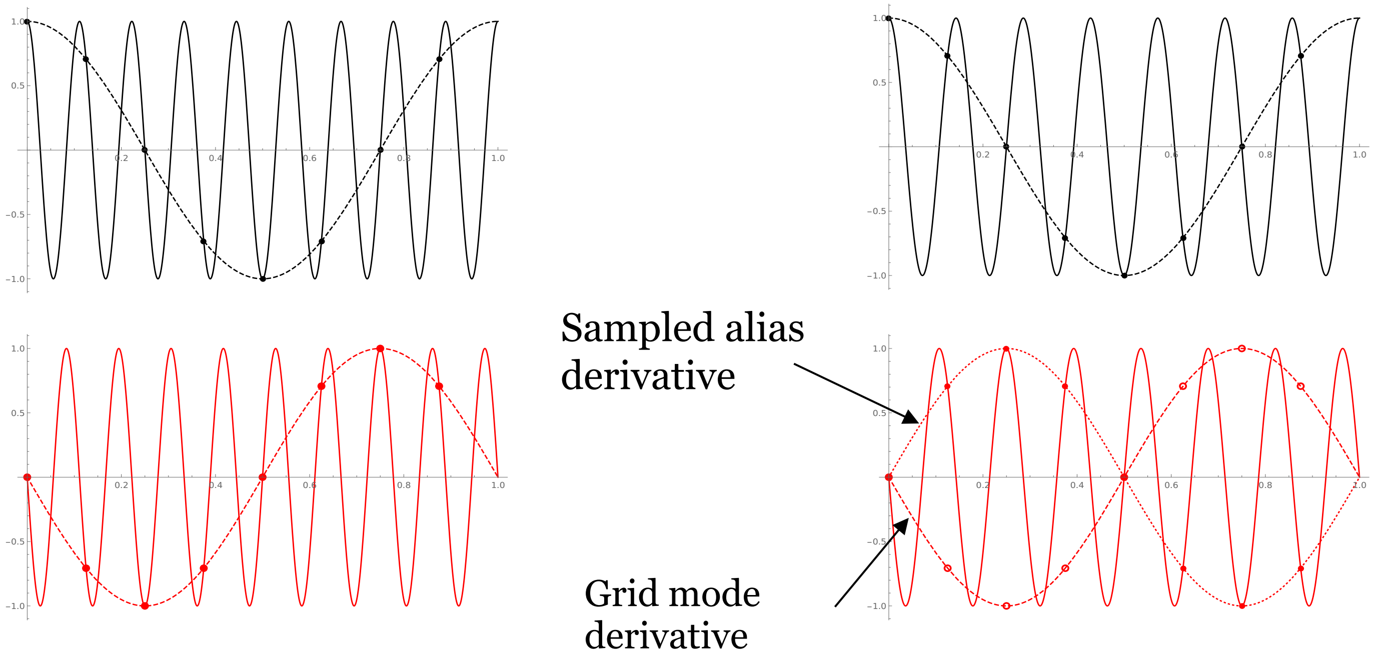
Aliasing in the Particle-in-Cell Method

- Derivatives of aliases can look like they have the wrong sign when restricted to the grid

$q < 0$ $$k_q = k - \frac{2\pi q}{\Delta x}$$ $q > 0$

Alias and grid modes :

Derivatives :



Momentum vs. Energy Conserving PIC

Naming conventions due to shape function symmetries that help ensure conservation of momentum or energy in ideal PIC models

Momentum Conserving :

$$\frac{d}{dt}P = \sum_j \rho_j E_j$$

- Deposit charge density with same shape function as used to interpolate electric field to particles

Energy Conserving :

- Shape function symmetry between charge density and potential

$$W_E = \frac{\Delta x}{2} \sum_j \rho_j \phi_j$$

- **Equivalently, between current density and electric field**

$$\frac{d}{dt}W_E = -\Delta x \sum_j J_j E_j$$

A. B. Langdon, JCP (1970)

$E-\rho$ symmetry :

$$\rho_j = \frac{1}{\Delta x}\sum_p q_p S(x_j - x_p)$$

$$E_p = \sum_j E_j S(x_j - x_p)$$

$$\epsilon_0 \frac{\phi_{j+1} - 2\phi_j + \phi_{j+1}}{\Delta x^2} = -\rho_j$$

$$E_j = -\frac{\phi_{j+1} - \phi_{j-1}}{2\Delta x}$$

$$\dot{x}_p = v_p$$

$$\dot{v}_p = -\frac{e}{m_e} E_p$$

Plane wave ansatz for grid quantities :

$$\psi_j(t) \sim e^{i(k\Delta x j - \omega t)}$$

$$\epsilon(\mathbf{k},\omega) = 1 - \frac{1}{2K^2\lambda_D^2}\sum_q \boxed{\kappa\, k_q} |S(k_q)|^2 k_q^{-2} Z'\left(\frac{\omega}{\sqrt{2}|k_q|\, v_e}\right) = 0$$

$\left(\frac{\Delta x}{\lambda_d}\right)^2$

Wrong sign for q > 0

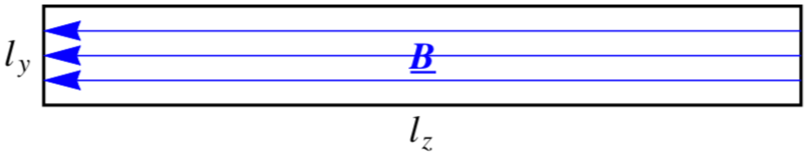
$$k_q = k - \frac{2\pi q}{\Delta x}$$

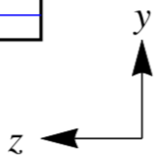
Strength of coupling

$$\kappa = \frac{\sin(k\Delta x)}{\Delta x} \qquad K^2 = \frac{4\sin^2\left(\frac{k\Delta x}{2}\right)}{\Delta x^2} \qquad S(k) = \left(\frac{2\sin\left(\frac{k\Delta x}{2}\right)}{(k\Delta x)}\right)^{m+1}$$

$\kappa\, k_q \approx -\frac{\partial^2}{\partial x^2}$ ... but positive semi-definite property is not preserved

A Minimal Drift/Gyrokinetic Electron Model





$$\frac{\partial}{\partial t}f_e + v_{||}\frac{\partial}{\partial z}f_e - \frac{e}{m_e}E_{||}\frac{\partial}{\partial v_{||}}f_e = 0$$

$$n_e = \int_{-\infty}^{\infty} f_e\, dv_{||} \qquad \Gamma_{||e} = \int_{-\infty}^{\infty} v_{||} f_e\, dv_{||}$$

GK Poisson :

$$-\frac{m_i n_{0i}}{B_0^2}\frac{\partial \phi}{\partial y^2} = q_i n_{0i} - e n_e$$

Ampère :

$$-\frac{1}{\mu_0}\frac{\partial A_{||}}{\partial y^2} = q_i \Gamma_{||0i} - e\Gamma_{||e}$$

Electric field with inductive component :

$$E_{||} = -\frac{\partial}{\partial z}\phi - \frac{\partial}{\partial t}A_{||}$$

Cold Dispersion analysis : Shear Alfvén Wave

$$\omega = \pm \frac{v_A k_{||}}{\sqrt{1 + d_e^2 k_\perp^2}}$$

Electrostatic limit ($\beta_e \rightarrow 0$) : Omega H mode

$$\beta_e = \frac{\mu_0 n_{0e} T_e}{B_0^2} \qquad \omega_H = \pm \Omega_i \sqrt{\frac{m_i}{m_e}}\frac{k_{||}}{k_\perp}$$

Modes are physically **stable**. With finite temperature they are Landau damped.

Analysis of a momentum-conserving scheme

$$\boxed{\delta n_j = \frac{1}{\Delta z}\sum_p w_p S(z_j - z_p)}$$

$$\delta \Gamma_j = \frac{1}{\Delta z}\sum_p w_p v_p S(z_j - z_p)$$

$$\boxed{E_p = \sum_j E_j S(z_j - z_p)}$$

Semi-discrete plane wave ansatz :

$$\psi_j(t) \sim e^{i(k\Delta z j + k_\perp y - \omega t)}$$

$$\epsilon(\omega, k) = 1 - \frac{1}{2k_\perp^2\rho_s^2}\sum_q \left(\boxed{\kappa k_q} - \frac{e m_i}{q_i m_e}\beta_e \frac{\omega^2}{v_e^2}\right)|S(k_q)|^2 k_q^{-2} Z'\left(\frac{\omega}{\sqrt{2}|k_q| v_e}\right) = 0$$

Sign issue from electrostatic potential

Analogy to Vlasov-Poisson PIC: McMillan PoP (2020)

$$\epsilon(\mathbf{k}, \omega) = 1 - \frac{1}{2K^2\lambda_D^2}\sum_q \kappa k_q |S(k_q)|^2 k_q^{-2} Z'\left(\frac{\omega}{\sqrt{2}|k_q| v_e}\right) = 0$$

$$k_q = k - \frac{2\pi q}{\Delta z}$$

$k_\perp \rho_s$ plays the role of $K\lambda_D = 2\sin\left(\frac{k\Delta x}{2}\right)\left(\frac{\lambda_D}{\Delta x}\right)$

Analysis of a Yee-lattice energy-conserving scheme

- D. Barnes and L. Chacón, CPC (2021) analyzes in detail the finite grid effects for Yee-lattice energy-conserving Vlasov-Poisson PIC
  - H.R. Lewis, JCP (1970), G. Chen et al., JCP (2011), L. Chacón et al., JCP (2013)
- Yee-lattice energy-conserving schemes can be implemented for idealized meshes, but not easily applicable for existing tokamak simulation codes

Momentum Conserving

$$\epsilon(\mathbf{k},\omega) = 1 - \frac{1}{2K^2\lambda_D^2}\sum_q \kappa\, k_q\, |S(k_q)|^2 k_q^{-2} Z'\left(\frac{\omega}{\sqrt{2}|k_q|\, v_e}\right) = 0$$

Yee-lattice energy-conserving

$$\epsilon(\mathbf{k},\omega) = 1 - \frac{1}{2K^2\lambda_D^2}\sum_q |S(k_q)|^2 Z'\left(\frac{\omega}{\sqrt{2}|k_q|\, v_e}\right) = 0$$

No sign issue here!

- A discrete derivative on the grid is replaced by a derivative in the Lagrangian frame –> consistent signs
- Yee-lattice energy-conserving is absolutely stable for stationary Maxwellian
- Stable for drifting Maxwellian for Mach number below order 1
- But… relies on analytical properties of shape functions -> not easy to implement for complicated meshes

A new co-located energy-conserving scheme

- We have developed a new scheme that obtains density from the continuity equation[1]
- Allows all quantities to be co-located on a mesh
- Preserves sign in dispersion relation and is practical for fusion PIC codes

$$\delta\Gamma_j = \frac{1}{\Delta z}\sum_p w_p v_p S(z_j - z_p)$$

$$\frac{\partial}{\partial t}\delta n_j = -\sum_l D_{j,l}\delta\Gamma_l,$$

Instead of depositing density from marker particles :

1. Deposit flux density from marker particles
2. Advance density forward in time on the grid using the continuity equation
3. Use density from continuity equation in Poisson's equation

- Similarities to the vorticity equation formulation
- Applied to our drift/gyrokinetic electron model :

$$\epsilon(\omega,k) = 1 - \frac{1}{2k_\perp^2\rho_s^2}\sum_q\left(\boxed{\kappa^2} - \frac{e m_i}{q_i m_e}\beta_e\frac{\omega^2}{v_e^2}\right)|S(k_q)|^2 k_q^{-2} Z'\left(\frac{\omega}{\sqrt{2}|k_q|v_e}\right) = 0$$

No sign issue here!

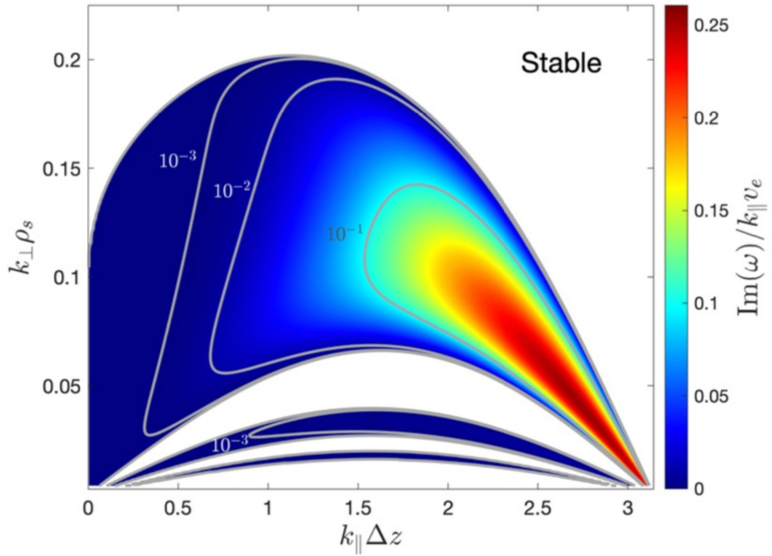
$$k_q = k - \frac{2\pi q}{\Delta z}$$

- A derivative in the Lagrangian frame is replaced by a discrete derivative on the grid –> consistent signs

[1]B. Sturdevant and L. Chacón, "Eliminating Finite-Grid Instabilities in Gyrokinetic Particle-in-Cell Simulations", submitted to J. Comput. Phys.

Investigation of the Numerical Dispersion Relations

Dispersion analysis for electrostatic ($\beta_e = 0$), stationary plasmas



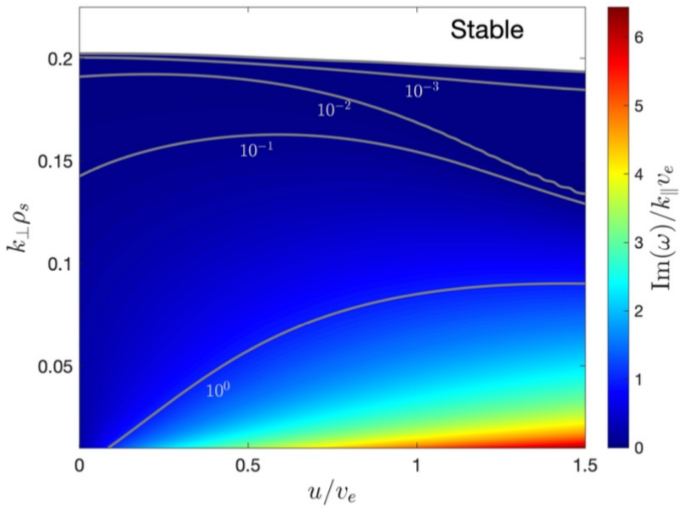
Predicted stability region for the momentum-conserving scheme

$$f_{0e} = \frac{n_{0e}}{\sqrt{2\pi}v_e} e^{-\frac{v_\parallel^2}{2v_e^2}}$$

- The momentum-conserving scheme has unstable regions in the parameter space shown to the left.
- **Note: the unstable regions are independent of numerical resolution**
- The same analysis shows the co-located energy-conserving scheme to be absolutely stable over the same parameter space.

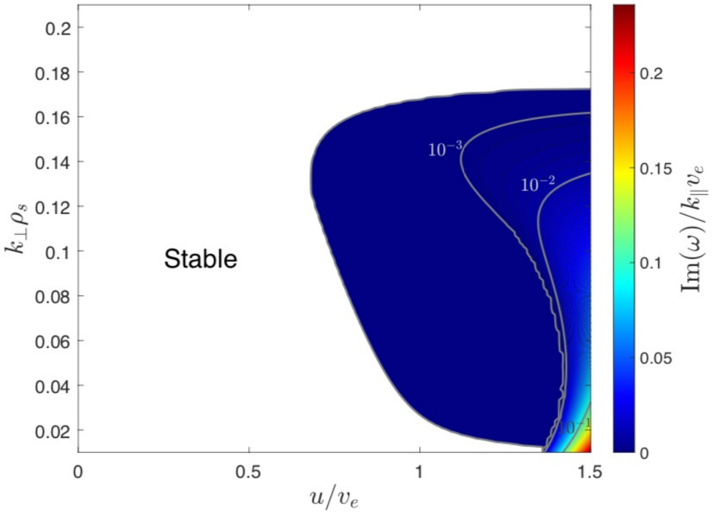
Dispersion analysis for electrostatic ($\beta_e = 0$), drifting plasmas

Momentum-conserving



$$f_{0e} = \frac{n_{0e}}{\sqrt{2\pi} v_e} e^{-\frac{(v_\parallel - u)^2}{2 v_e^2}}$$

Co-located energy-conserving

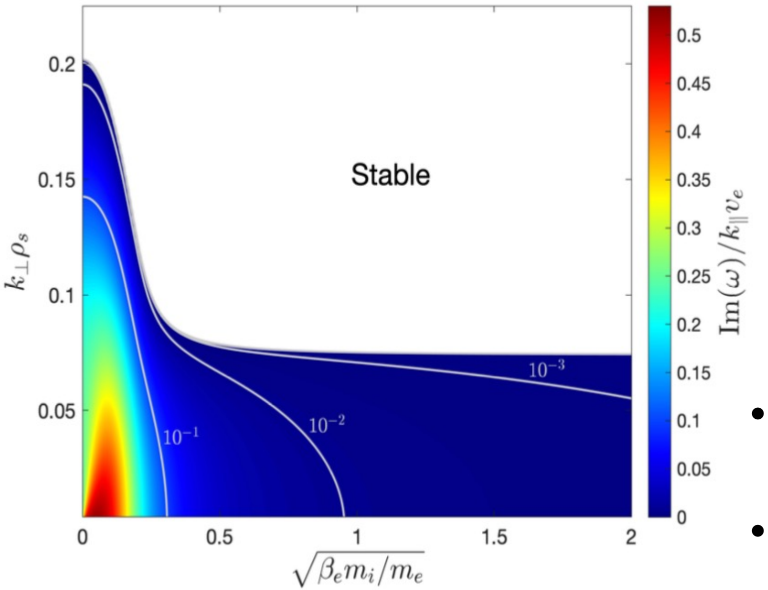


- Another type of finite-grid instability can be present in drifting plasmas
- With co-located energy-conserving scheme, this is generally harmless for plasmas of interest
- Stable for electron Mach numbers $\lesssim 1$
- Similar results were found in Barnes and Chacón, CPC (2021) for Yee-lattice energy conserving schemes in Vlasov-Poisson PIC

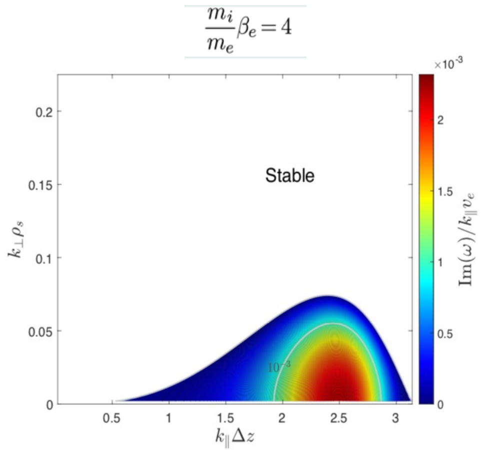
Investigation of the Numerical Dispersion Relations

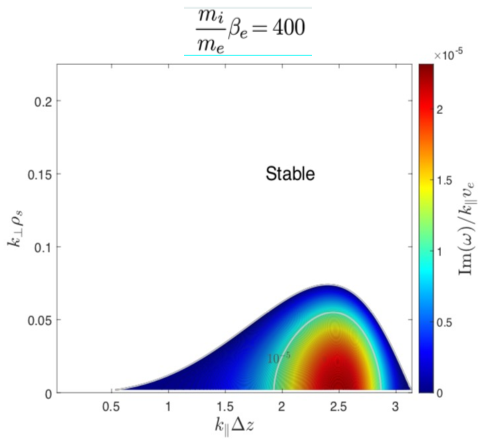
Dispersion analysis for finite - β_e , stationary plasmas

Maximized over $k\Delta z$



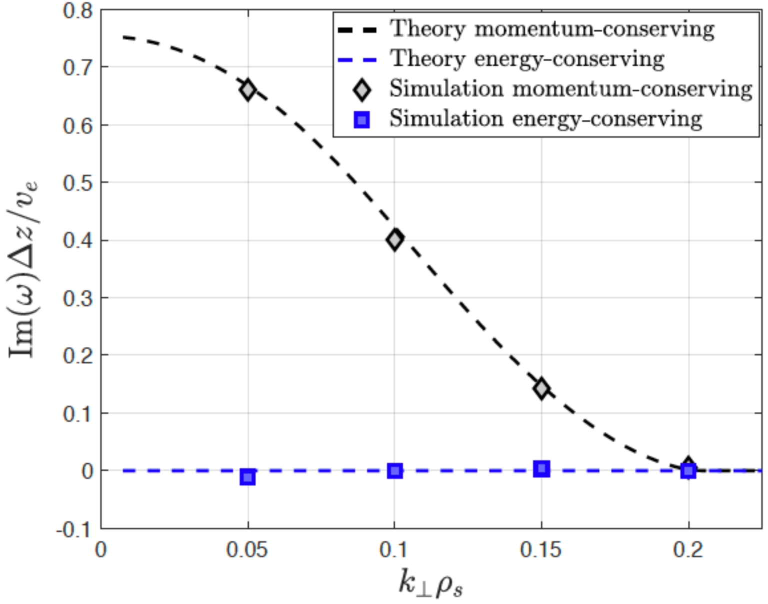
Predicted stability regions for the momentum-conserving scheme





- The co-located energy-conserving scheme is again found to be absolutely stable.
- Finite beta helps stabilize the momentum-conserving scheme but does not eliminate instabilities. At high beta, numerical growth rates are inversely proportional to beta.

Stationary Electrostatic Simulations



Comparisons of measured growth rates from simulations to growth rates predicted from the numerical dispersion relations.

- Timestep size is chosen to resolve ω_H frequencies for all values of $k_{||}\Delta z \in [-\pi, \pi]$. In particular, we choose:

$$\frac{v_e}{k_\perp \rho_s} \frac{\Delta t}{\Delta z} = 0.128$$

- A large number (1×10^4) of particles per cell is taken to isolate the effects of the finite-grid instability from particle noise

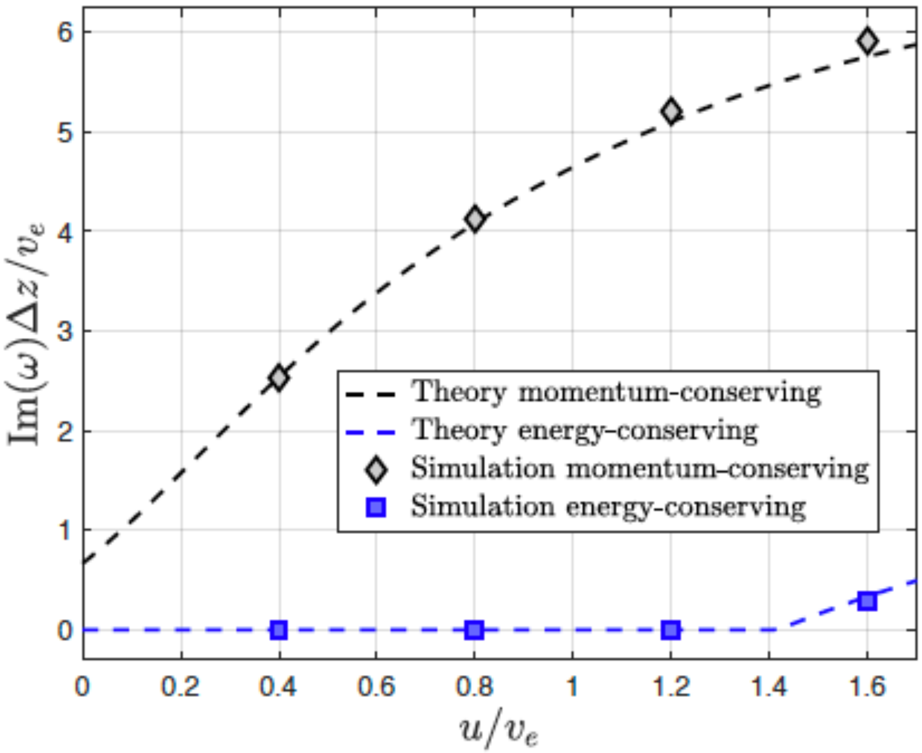
- Parallel resolution: $n_z = 64$

Electrostatic Simulations with Finite Mean Parallel Velocity

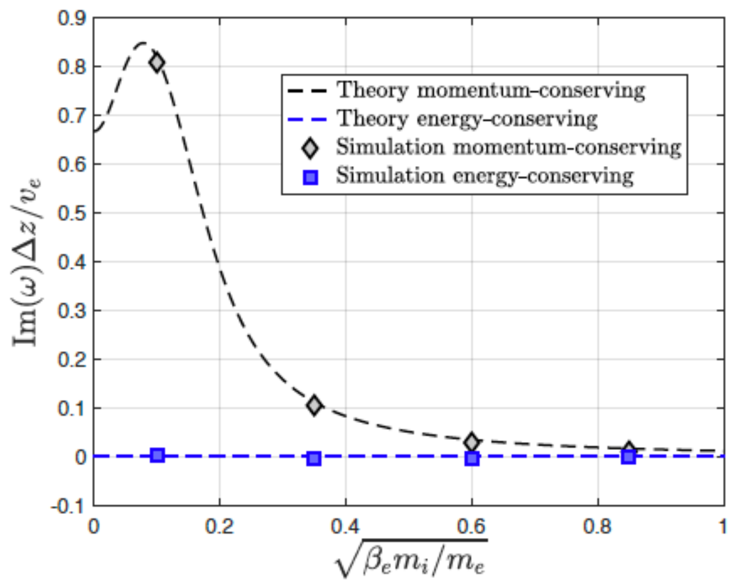
Right: Comparisons of measured growth rates from simulations to growth rates predicted from the numerical dispersion relations.

$$k_\perp \rho_s = 0.05$$

The same numerical parameters are used as in the stationary case



Electromagnetic Simulation Results



Comparisons of measured growth rates from simulations to growth rates predicted from the numerical dispersion relations.

- Timestep size is chosen to resolve Alfvén frequencies for all values of $k_{||}\Delta z \in [-\pi,\pi]$. In particular, we choose:

$$v_A \frac{\Delta t}{\Delta z} = 0.128$$

- A large number (1×10^4) of particles per cell is taken to isolate the effects of the finite-grid instability from particle noise
- Parallel resolution: $n_z = 64$
- Fixed $k_\perp \rho_s = 0.05$

Demonstration in XGC

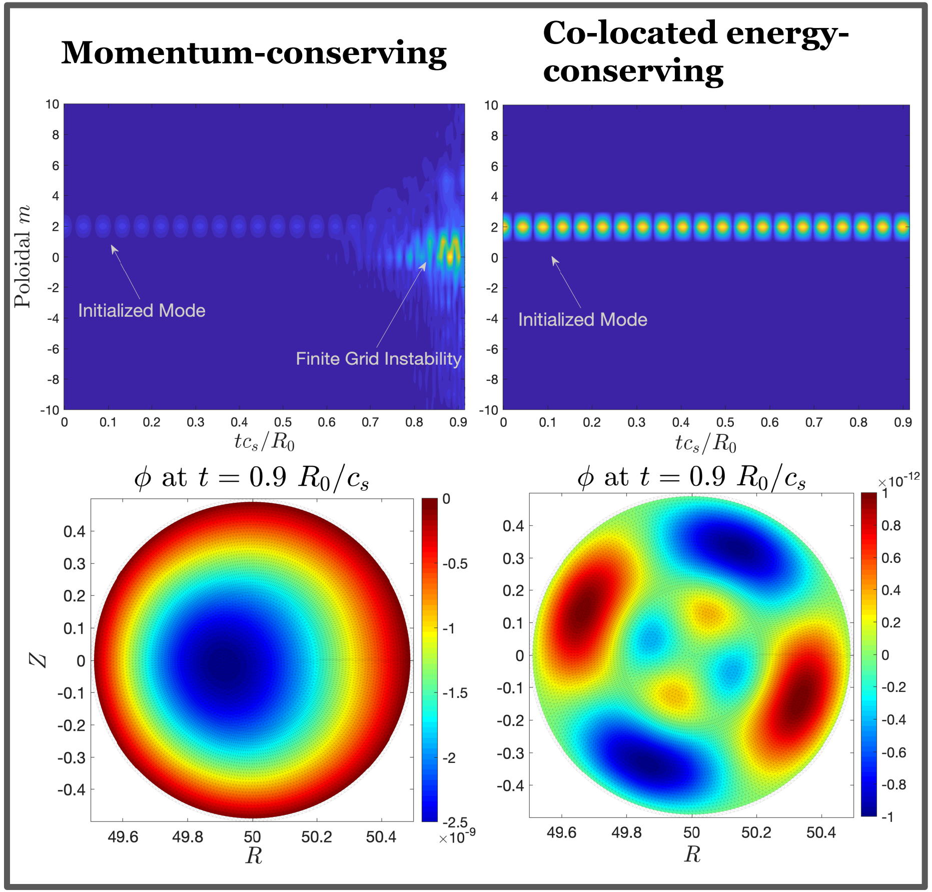


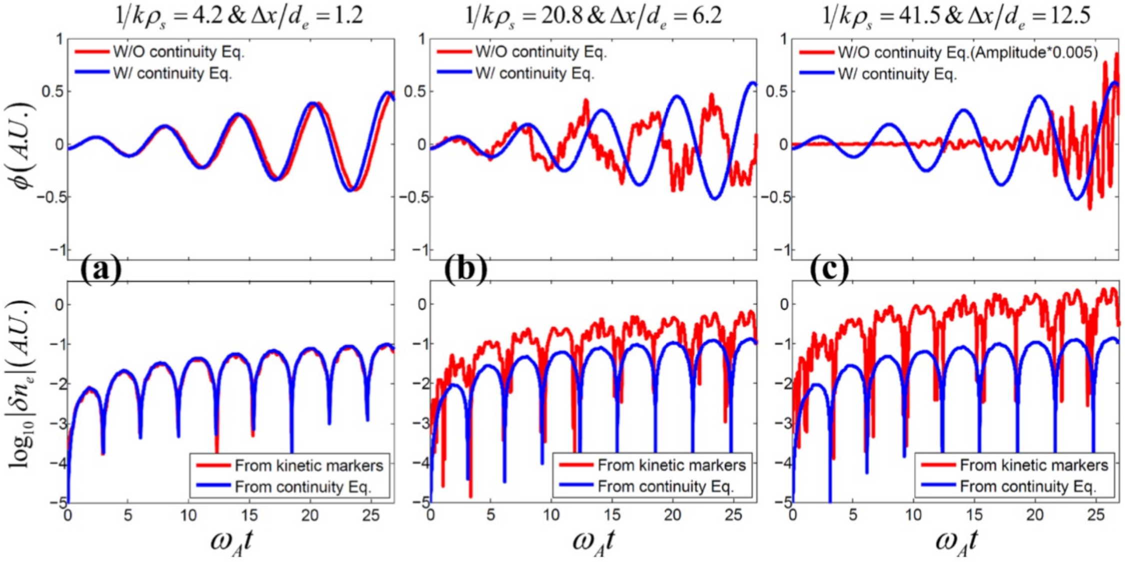
Figure: Shear Alfvén waves are excited from an initial perturbation in XGC. With the momentum-conserving scheme (left), the finite-grid instability, characterized by long wavelengths in the poloidal plane, quickly develops. The co-located energy-conserving scheme (right) allows for clean, numerically stable simulations.

Preliminary results with a fully implicit electromagnetic version of XGC[1] show the existence of the finite-grid instability and the effectiveness of our new scheme to eliminate it.

[1] B. Sturdevant et al., *Phys. Plasmas,* Vol. 28, No. 7, 072505 (2021)

Connection to other schemes used in fusion PIC codes

- J. Bao, Z. Lin, and Z. X. Lu, ``A conservative scheme for electromagnetic simulation of magnetized plasmas with kinetic electrons”, PoP (2018)
- Reformulation in GTC using continuity equation gives much cleaner simulation results, although their motivation was different (cancellation issue)



Connection to other schemes used in fusion PIC codes : reformulation used in the split-weight scheme

- Original split-weight paper :

PHYSICS OF PLASMAS VOLUME 7, NUMBER 5 MAY 2000

The split-weight particle simulation scheme for plasmas

Igor Manuilskiy and W. W. Lee
Plasma Physics Laboratory, Princeton University, Princeton, New Jersey 08543

- Reformulation is to avoid using a time differenced potential in the weight equation
- However, this also has the effect of moving a derivative in the Lagrangian frame to the grid, which would be beneficial for avoiding finite grid instabilities
- Could partially explain why split-weight scheme is more robust in handling omega-H and is better for cancellation issue

$$\frac{dw^{NA}}{dt} = \frac{1}{F_e}\frac{d\delta h_e}{dt} = \frac{1-w^{NA}}{1+e\phi/T_e}\left[-\frac{\partial}{\partial t}\frac{e\phi}{T_e} - \left(1+\frac{e\phi}{T_e}\right)\frac{c}{B}\frac{\partial\phi}{\partial \mathbf{x}}\times\hat{\mathbf{b}}\cdot\boldsymbol{\kappa}_e + \frac{v_\parallel}{2}\frac{\partial}{\partial x_\parallel}\left(\frac{e\phi}{T_e}\right)^2\right]. \qquad (15)$$

However, serious numerical instabilities may arise from Eq. (15) because of the existence of time derivatives on both sides of the equation. Although for a different reason, this situation is similar to the problem of Darwin model for non-radiative simulation encountered by Nielson and Lewis.[8] To avoid the numerical difficulty, we first take the partial time derivative of Eq. (5) and substitute the $\partial\delta n_\alpha/\partial t$ term by using the continuity equation from Eq. (1) to obtain

$$\rho_s^2\nabla_\perp^2\left(\frac{\partial}{\partial t}\frac{e\phi}{T_e}\right) = -\frac{\partial\delta u_e}{\partial x_\parallel} + \frac{\partial \delta u_i}{\partial x_\parallel} + \frac{c}{B}\frac{\partial\phi}{\partial\mathbf{x}}\times\hat{\mathbf{b}}\cdot\frac{\partial}{\partial\mathbf{x}}\left(\rho_s^2\nabla_\perp^2\frac{e\phi}{T_e}\right), \qquad (17)$$

Connection to other schemes used in fusion PIC codes : reformulation used in the split-weight scheme

- Y. Chen and S. E. Parker, JCP (2007)

Split-weight and cancellation paper

been demonstrated numerically, and is not well understood. A prominent feature of the split-weight scheme is the extra field equation for the rate of change of the electric potential, $\dot{\phi}$. While in the continuum limit, i.e. with vanishing grid size and time step, and infinite number of particles, solving both the quasi-neutrality condition and the equation for $\dot{\phi}$ is redundant, the two equations are not consistent on the grid scale, due to the use of finite grid sizes. In this paper, we show that the key to the efficacy of the split-weight scheme is this inconsistency, which tends to suppress grid-scale numerical instabilities.

- To investigate numerical properties of the split-weight scheme, an equation for $\frac{\partial \phi}{\partial t}$ is derived directly from discretized GK Poisson

$$\dot{n}_{\mathrm{p}} = \frac{V}{N}\sum_j \frac{1}{\Delta V_j}\left(\left(\mathbf{v}_E + v_\parallel \frac{\delta \mathbf{B}_\perp}{B}\right)_j \cdot \boldsymbol{\kappa}_j + \dot{\varepsilon}_{pj}\right) S(\mathbf{x}-\mathbf{x}_j) + \frac{V}{N} \sum_j \frac{1}{\Delta V_j}(w_j + \varepsilon_g \tau \phi(\mathbf{x}_j,t))\mathbf{v}_{Gj} \cdot \nabla S(\mathbf{x}-\mathbf{x}_j) + \text{ion terms}, \tag{38}$$

- Grid scale instabilities were found with this formulation but not when continuity form is discretized directly. This is consistent with our findings.

Summary and Conclusions

We've gained new insights into an instability plaguing gyrokinetic PIC simulations and have found a simple solution by reformulating the discrete equations using the continuity equation. This work can provide direction for further GK PIC algorithm development.

- Finite-grid instabilities show up in unusual ways in drift/gyrokinetic electron PIC models
- Numerical analysis and aliasing theory can be powerful tools for understanding and designing GK PIC algorithms
- With certain shape function symmetries, finite-grid instabilities can be eliminated for parameter regimes of interest in both electrostatic (omega-H) and electromagnetic (Shear Alfvén wave)
- The present numerical analysis could help understand why some PIC schemes have been more successful in simulating tokamak plasmas.

It is interesting to look back on previously successful schemes with this new perspective. Future studies could be done to give a more complete understanding – what is the role of the finite timestep size, particle noise, how does this show up in $p_{\|}$ formalism, etc ?