LA-UR-15-25378
Approved for public release; distribution is unlimited.

Title: On the numerical dispersion of electromagnetic Particle-In-Cell code: finite grid instability

Author(s): Huang, Chengkun

Intended for: http://cnls.lanl.gov/External/workshops_2015.php,
2015-05-04/2015-05-06 (Los Alamos, New Mexico, United States)
Web

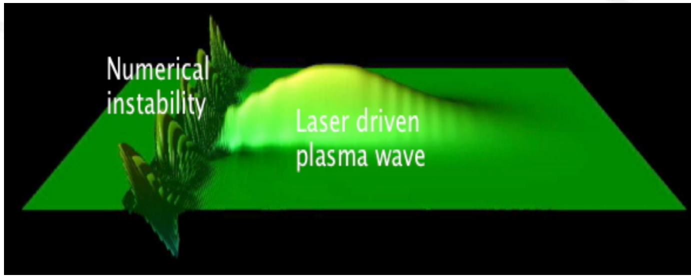
Issued: 2015-07-16

On the numerical dispersion of electromagnetic Particle-In-Cell code: finite grid instability

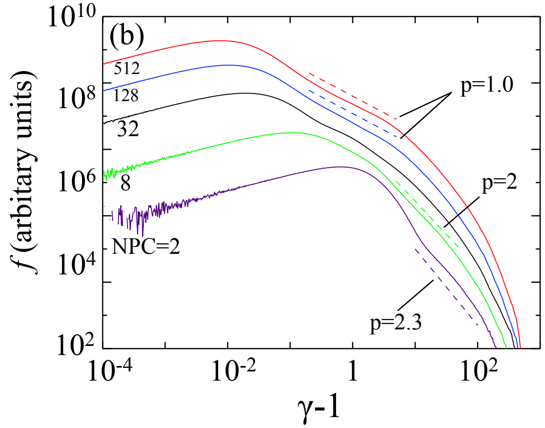
C.–K. Huang[1] , M. D. Meyers[1,2], Y. Zeng[1], S. A. Yi[1], B. J. Albright[1]
[1]Los Alamos National Laboratory. [2]University of California at Los Angeles

Outline

- The Particle-In-Cell algorithm.
  - Eulerian model for the fields and Larangian model for particles.
  - Source is only calculated at the grid points.



- The cause and effect of spatial and temporal aliasing in the PIC algorithm.
  - The PIC algorithm evinces only spatial aliasing.
- The finite difference dispersion relation.
- Numerical solutions of the dispersion relation.
  - Analysis of Finite Grid Instability
  - Analysis of ES grid instability for charge-conserving schemes
- Insight from dispersion analysis for the elimination of numerical instabilities



Guo et al. submitted to arxiv

Finite Difference Equations Advance the PIC Simulation

- PIC = grid-based field representation + Lagrangian particle model
- PIC operates on discrete time and both continuous and discrete spaces
- For a time centered scheme, the particle and field advancing equations are:

Continuous Expression **Finite Difference Expression**

$$\frac{d\vec{r}}{dt} = \vec{v} \longrightarrow \frac{\vec{r}_{n-1/2} - \vec{r}_{n-1}}{\Delta t/2} = \vec{v}_{n-1/2} \text{ and } \frac{\vec{r}_n - \vec{r}_{n-1/2}}{\Delta t/2} = \vec{v}_{n-1/2} \quad (1)$$

$$\frac{\partial \vec{E}}{\partial t} = \vec{\nabla} \times \vec{B} - 4\pi \vec{J} \longrightarrow \frac{\vec{E}_n - \vec{E}_{n-1}}{\Delta t} = \vec{\nabla} \times \vec{B}_{n-1/2} - 4\pi \vec{J}_{n-1/2} \quad (2)$$

$$\frac{\partial \vec{B}}{\partial t} = -\vec{\nabla} \times \vec{E} \longrightarrow \frac{\vec{B}_{n+1/2} - \vec{B}_{n-1/2}}{\Delta t} = -\vec{\nabla} \times \vec{E}_n \quad (3)$$

$$\frac{d(\gamma\vec{v})}{dt} = \frac{q}{m}\left(\vec{E} + \vec{v} \times \vec{B}\right) \longrightarrow \frac{(\gamma\vec{v})_{n+1/2} - (\gamma\vec{v})_{n-1/2}}{\Delta t} = \frac{q}{m}\left(\vec{E}_n + \vec{v}_n \times \vec{B}_n\right), \quad (4)$$

$$\frac{(\gamma\vec{v})^{+} - (\gamma\vec{v})^{-}}{\Delta t} = \frac{q}{2m\gamma_n}\left[(\gamma\vec{v})^{+} + (\gamma\vec{v})^{-}\right] \times \vec{B}_n \quad (5)$$

NNSA National Nuclear Security Administration

Spatial aliasing in PIC results from sampling

- In digital signal processing, sampling is the sole cause of aliasing.
  - Continuous signal ⇒ discrete signal (A/D, sampling) : aliasing
  - Discrete signal ⇒ continuous signal (D/A, interpolation) : convolution in spectrum, no aliasing
  - Discrete signal ⇒ discrete signal (interpolation, weighted averaging) : convolution, filtering in spectrum, no aliasing
- In PIC, the particle can move freely in continuous space, therefore particle distribution and quantities derived from particle distribution are also defined on continuous spatial variable, regardless of whether such quantities at arbitrary spatial location are calculated or used in the code.
  - Evaluating such a quantity (such as current) on the grid point only effectively involves a sampling operation.
  - This causes spatial aliasing in Fourier space.

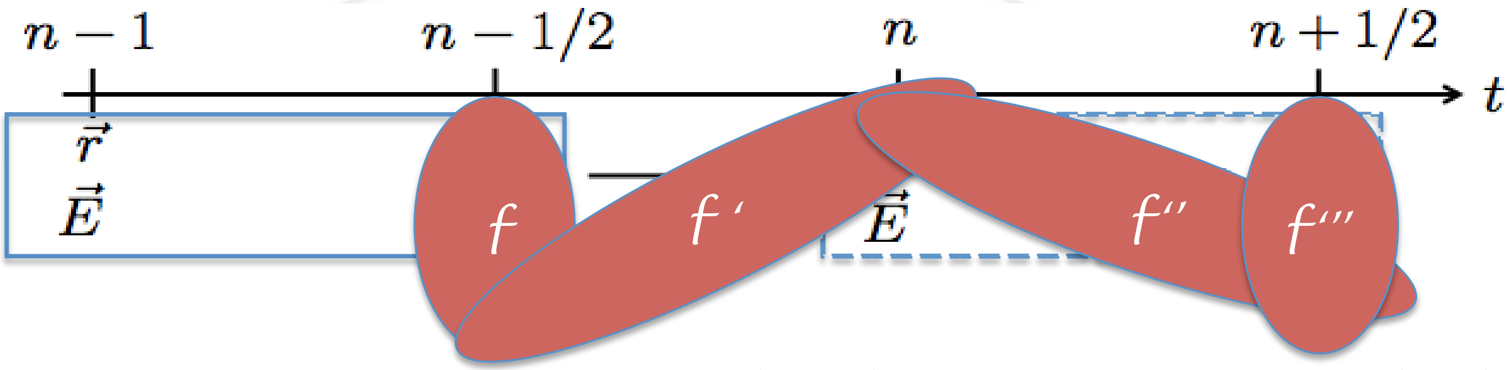
$$\rho(\mathbf{k}) = \sum_q S(\mathbf{k}_q) f(\mathbf{k}_q) \qquad \mathbf{k}_q = \mathbf{k} - 2\pi(q_x/\Delta x, q_y/\Delta y, q_z/\Delta z)$$

$$\mathbf{J}(\mathbf{k}) = \int \sum_q S(\mathbf{k}_q) f(\mathbf{k}_q, \mathbf{p}) d\mathbf{p}$$

However, there is no temporal aliasing

- The PIC algorithm operates entirely in a discrete time variable. In PIC, particles jump, they do not move smoothly.
  - no temporal sampling
  - operations like weighted averaging in time, or generation of particle information in between steps (e.g., for use in current deposition) do not constitutes sampling.
  - no temporal aliasing in Fourier space.
- Due to the use of discrete time variable, the corresponding Fourier space is periodic, thus correct to only consider the contribution from the fundamental Brillouin zone.
  - not equivalent to aliasing for which contribution from all Brillouin zones need to be summed.
  - The perturbation for the linear eigen modes analysis needs to be applied to the internal variables of the system.
  - Therefore, in PIC, time dependence of the perturbation should be in discrete form.

How is the system advanced?



- Leap frog advance $\vec{r}_{n-1}, \vec{v}_{n-1/2}, \vec{E}_{n-1}, \vec{B}_{n-1/2}$ ➡ $\vec{r}_{n}, \vec{v}_{n+1/2}, \vec{E}_{n}, \vec{B}_{n+1/2}$
- Assume number of particle per cell $N \to \infty$, the distribution function is smooth
- Current deposition using $f(\vec{r}_{n-1/2}, \vec{v}_{n-1/2})$ ➡ $J(\vec{r}, \vec{v})$, spatial sampling is implicit carried out.
- Half position update gives $\vec{r}_{n-1/2}, \vec{v}_{n-1/2}$ ➡ $f(\vec{r}_{n-1/2}, \vec{v}_{n-1/2}) = f_0 + f_1(\vec{r}_{n-1/2}, \vec{v}_{n-1/2})$
- Update fields to get $\vec{E}_{n}, \vec{B}_{n+1/2}$
- Full momentum update using $\vec{E}_{n}, \vec{B}_{n}$ gives $\vec{r}_{n-1/2}, \vec{v}_{n+1/2}$ ➡ $f''(\vec{r}_{n-1/2}, \vec{v}_{n+1/2})$
- Second half position update gives $\vec{r}_{n}, \vec{v}_{n+1/2}$ ➡ $f'''(\vec{r}_{n}, \vec{v}_{n+1/2})$

The PIC Algorithm is Analogous, Yet Different from the Klimontovich Equation

- PIC uses a Klimontovich (or Vlasov then $N \to \infty$) description of the distribution, but it evolves this distribution in a Newtonian way with operator splitting.

Klimontovich equation (linearized)	PIC
$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{\gamma} \nabla_x f = 0$	Two position half updates using method of characteristics $f'(\mathbf{p}, \mathbf{x}; t_{n+1/2}) = f(\mathbf{p}, \mathbf{x} - \mathbf{v} \cdot dt/2; t_n)$ $f'''(\mathbf{p}, \mathbf{x}; t_{n+1}) = f''(\mathbf{p}, \mathbf{x} - \mathbf{v} \cdot dt/2; t_{n+1/2})$
$\frac{\partial f}{\partial t} + \frac{q}{m} (\mathbf{E}_1 + \mathbf{v} \times \mathbf{B}_1) \nabla_p f_0 = 0$	Velocity update in phase space $f''(\mathbf{p}, \mathbf{x}; t_{n+1/2}) = \int [f_0(\mathbf{p}') + f'(\mathbf{p}', \mathbf{x}; t_{n+1/2})] \cdot \delta(\mathbf{p} - \mathbf{p}' - \Delta\mathbf{p}) d\mathbf{p}' - f_0(\mathbf{p}')$ $\Delta\mathbf{p}(\mathbf{p}', \mathbf{x}) = q\Delta t/m \, (\mathbf{E}_1 + \mathbf{p}' \times \mathbf{B}_1/\gamma)$

- The discrete velocity update in PIC can be linearized for dispersion analysis

$f'' \approx -\Delta\mathbf{p} \cdot \nabla_p f_0 + f'$ (This is a linearization to f needed for linear mode analysis)

Discrete update of the distribution in PIC

- Assume the distribution perturbation is in time- and spatial-harmonic form.

$$f(\mathbf{p},\mathbf{x};t_n) = \tilde{f}(\mathbf{p})e^{i\mathbf{k}\cdot\mathbf{x}-i\omega t_n}$$

- Note that the arguments $\mathbf{p}$ and $\mathbf{x}$ are continuous variables, but t is not, i.e., particles jump, they do NOT move in time, but they can have arbitrary position and momentum.
- With the exact operator for PIC position update and linearized operator for velocity update, the distribution evolution in one time step is,

$$\tilde{f}'''(\mathbf{p}) = \tilde{f}(\mathbf{p})e^{-i\mathbf{k}\cdot\mathbf{v}\Delta t} - q\Delta t/m\,(\mathbf{E}_1 + \mathbf{p}\times\mathbf{B}_1/\gamma)\cdot\nabla_p f_0 \cdot e^{-i\mathbf{k}\cdot\mathbf{v}\Delta t/2}$$

- Therefore, the distribution perturbation can be solved,

$$\tilde{f}'''(\mathbf{p}) = \tilde{f}(\mathbf{p})e^{-i\omega\Delta t} \longrightarrow \tilde{f}(\mathbf{p}) = \frac{q\Delta t/m\,(\mathbf{E}_1 + \mathbf{p}\times\mathbf{B}_1/\gamma)\cdot\nabla_p f_0 \cdot e^{-i\mathbf{k}\cdot\mathbf{v}\Delta t/2}}{e^{-i\mathbf{k}\cdot\mathbf{v}\Delta t} - e^{-i\omega\Delta t}}$$

- The pole determines the location of the alias modes
- The pole can also be written as $\csc((\omega-\mathbf{k}\cdot\mathbf{v})\Delta t/2) \to \sum_m (\omega' - \mathbf{k}\cdot\mathbf{v})^{-1}$

Force calculation by interpolating the fields from temporal and spatial grid with offsets

- The field interpolation, grid and time offset of E and B is incorporated as follows,

$$\tilde{\vec{F}}\left(\vec{k}_q,\vec{p},\omega\right)=q_e\left\{\tau_E\overleftrightarrow{\tilde{S}}_E\left(\vec{k}_q\right)\cdot\overleftrightarrow{O}_E\cdot\tilde{\vec{E}}\left(\vec{k},\omega\right)+\frac{\tau_B}{\gamma\omega_B}\vec{p}\times\overleftrightarrow{\tilde{S}}_B\left(\vec{k}_q\right)\cdot\left[\overleftrightarrow{O}_B\cdot\vec{k}_E\times\tilde{\vec{E}}\left(\vec{k},\omega\right)\right]\right\}$$

- Temporal and spatial phase factors are

$$\tau_E = e^{-i\omega\Delta t/2}$$

$$\tau_B = \left(e^{-i\omega\Delta t}+1\right)/2$$

$$O_{E,\alpha}^{\beta\beta}=\begin{cases}1, & \text{if } \alpha=\beta\\ (-1)^{q_\alpha+q_\beta}, & \text{if } \alpha\neq\beta\end{cases}$$

$$O_{B,\alpha}^{\beta\beta}=\begin{cases}(-1)^{q_\alpha+q_\beta+q_\gamma}, & \text{if } \alpha=\beta\\ (-1)^{q_\gamma}, & \text{if } \alpha\neq\beta\end{cases}.$$

The EM PIC numerical dispersion

- The numerical dispersion is derived from the wave equation

$$\vec{k}_B \times \vec{k}_E \times \tilde{\vec{E}} + \omega_B \omega_E \tilde{\vec{E}} = -i\omega_B \tilde{\vec{J}}(\tilde{k},\omega)$$

- The current source is given by for a simple, direct deposition scheme

$$\tilde{\vec{J}}(\vec{k},\omega) = \sum_{\vec{q}} \tilde{S}_j(\vec{k}_q) \left[\int \vec{p} \frac{\tilde{\vec{F}}\left(\vec{p},\vec{k}_q,\omega\right) \cdot \vec{\nabla}_p f_0 e^{-i\left(\vec{k}_q \cdot \vec{v} - \omega\right)\Delta t/2}}{\gamma(e^{-i\vec{k}_q \cdot \vec{v}\Delta t} - e^{-i\omega\Delta t})/\Delta t} d\vec{p} \right]$$

- The force term is

$$\tilde{\vec{F}}\left(\vec{k}_q,\vec{p},\omega\right) = q_e \left\{ \tau_E \overleftrightarrow{\tilde{S}}_E\left(\vec{k}_q\right) \cdot \overleftrightarrow{O}_E \cdot \tilde{\vec{E}}\left(\vec{k},\omega\right) + \frac{\tau_B}{\gamma\omega_B} \vec{p} \times \overleftrightarrow{\tilde{S}}_B\left(\vec{k}_q\right) \cdot \left[\overleftrightarrow{O}_B \cdot \vec{k}_E \times \tilde{\vec{E}}\left(\vec{k},\omega\right) \right] \right\}$$

- Finally, the dispersion tensor and dispersion relation are,

$$\overleftrightarrow{\epsilon} \cdot \tilde{\vec{E}} = 0. \qquad \mathrm{Det}\left|\overleftrightarrow{\epsilon}\right| = 0$$

The numerical dispersion for 1D cold drifting plasma

- For a cold drifting plasma, $f_0(\vec{p}) = \delta(p_x - p_0)\,\delta(p_y)\,\delta(p_z)$, the dispersion relation is

$$\omega_B \begin{vmatrix} \epsilon_a & 0 & 0 \\ 0 & \epsilon_b & 0 \\ 0 & 0 & \epsilon_b \end{vmatrix} = 0,$$

- The 1D E.S.-like and E.M.-like numerical dispersion are,

E.S.-like

$$\epsilon_a = \frac{\sin(\omega\Delta t/2)}{\Delta t/2} - \frac{4\Delta t}{\gamma^3}\sin^4(k\Delta x/2) \times \sum_{q=-\infty}^{\infty} \frac{2\sin\{(\omega - k_q v_0)\Delta t/2\} + k_q v_0 \Delta t \cos\{(\omega - k_q v_0)\Delta t/2\}}{k_q^4 \Delta x^4} \csc^2\{(\omega - k_q v_0)\Delta t/2\}$$

E.M.-like

$$\epsilon_b = \frac{\sin^2(\omega\Delta t/2)}{(\Delta t/2)^2} - \frac{\sin^2(k\Delta x/2)}{(\Delta x/2)^2} + \frac{16}{\gamma\Delta x}\sin^4(k\Delta x/2) \times \sum_{q=-\infty}^{\infty} \csc\{(\omega - k_q v_0)\Delta t/2\} \times \frac{(-1)^q v_0 \Delta t \cos(\omega\Delta t/2)\sin(k\Delta x/2) - \Delta x \sin(\omega\Delta t/2)}{k_q^4 \Delta x^4}$$

PIC Numerical Dispersion with Aliases : 1D E.S. Example

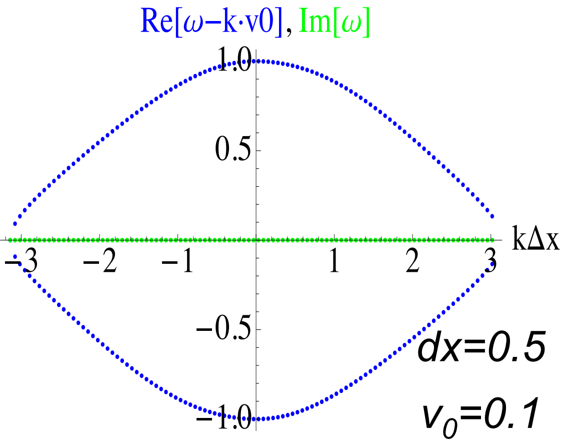
- The 1D dispersion for E.S. momentum-conserving PIC with continuous time variable is solved numerically with all aliases included

$$1-\frac{(k\cdot \mathrm{dx}/2)^2}{k^2\mathrm{Sin}^2(k\cdot \mathrm{dx}/2)}\sum_q \frac{16\mathrm{Sin}^4(\frac{\mathrm{dx}\cdot \mathrm{k}_q}{2})\mathrm{Sin}(\mathrm{dx}\cdot \mathrm{k}_q)}{\mathrm{dx}^5\mathrm{k}_q^5(-\mathrm{v}_0+\omega/\mathrm{k}_q)^2}=0$$

(Birdsall & Langdon)

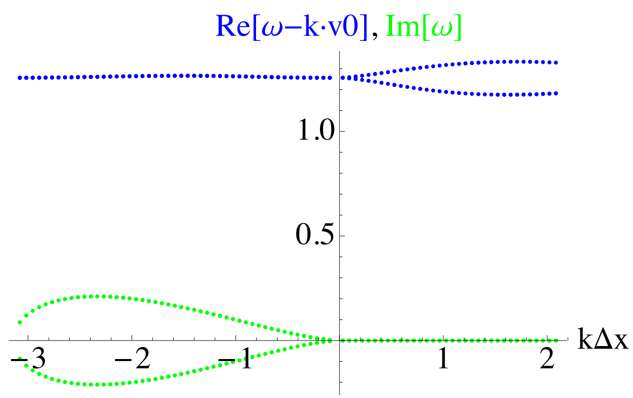
Each alias introduces one resonance

- Unstable modes (grid instability) from q ≠ 0 resonances.



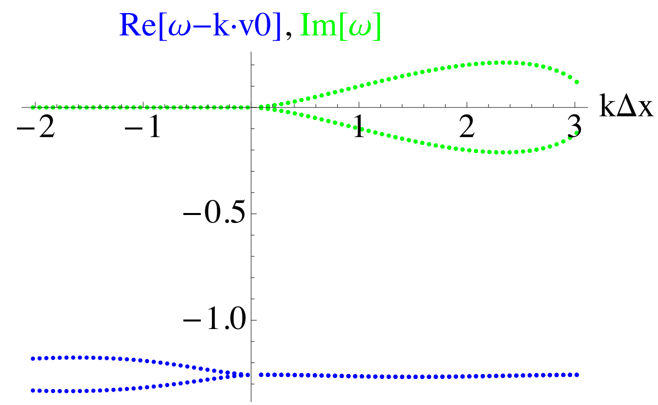
$\omega - \mathrm{k}\cdot \mathrm{v}_0 = 0$

Only real roots from q=0 resonance



$\omega - \mathrm{k}\cdot \mathrm{v}_0 = 2\pi \mathrm{v}_0/\mathrm{dx}$

Complex roots from q=-1 resonance when k<0



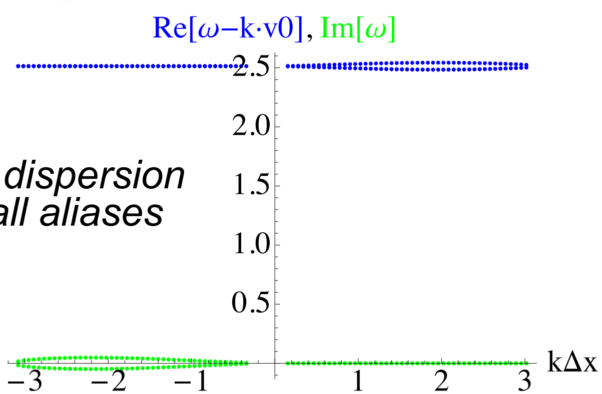
$\omega - \mathrm{k}\cdot \mathrm{v}_0 = -2\pi \mathrm{v}_0/\mathrm{dx}$

Complex roots from q=1 resonance when k>0

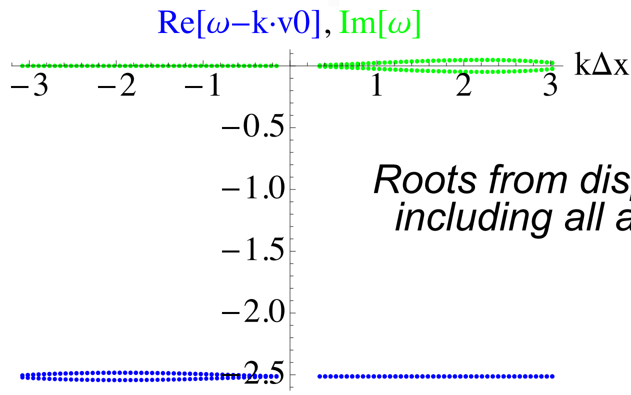
PIC Numerical Dispersion with Aliases : 1D E.S. Example

- Higher q resonances behave similarly but has smaller growth rate

Roots from dispersion including all aliases



$$\omega - k \cdot v_0 = 4\pi v_0/dx$$



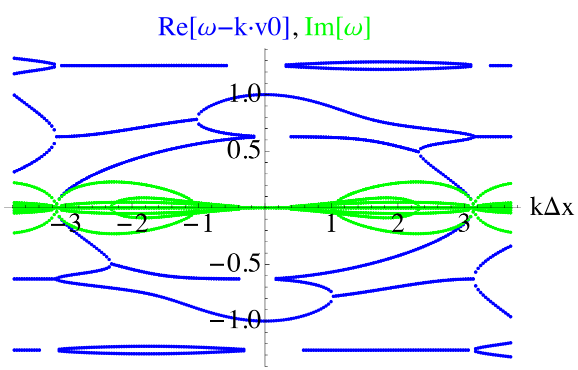
Roots from dispersion including all aliases

$$\omega - k \cdot v_0 = -4\pi v_0/dx$$

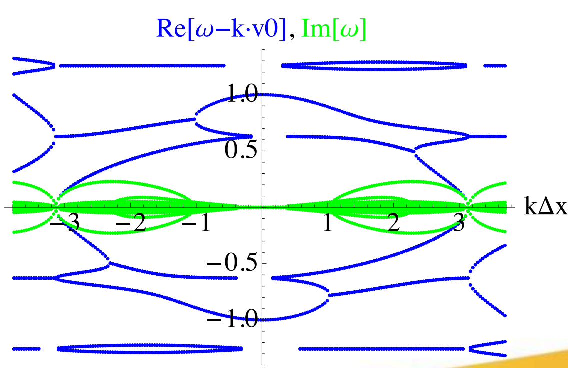
- When resonance separation $2\pi v_0/dx<1$, modes mix together. However, the dispersion can still be solved accurately with a few aliases.

dx=1

v_0=0.1



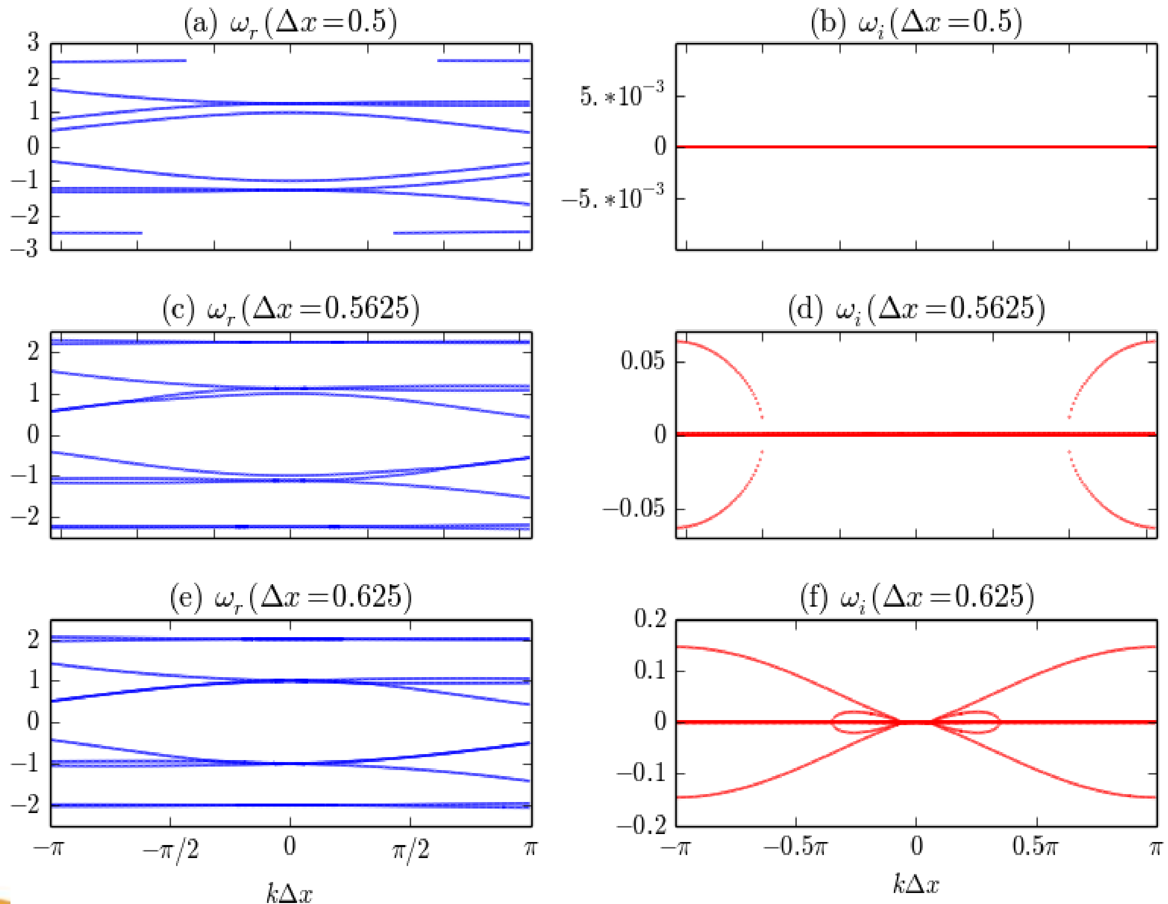
Roots from dispersion with 5 aliases (q=-2,-1,0,1,2)



Roots from dispersion with all aliases

Finite Grid Instability (dt=0) in 1D EM PIC

$$(\omega_t + k v_0)\left[1 - \frac{16\Delta x^2}{\gamma^3}\sin^4(k\Delta x/2)\sum_{q=-\infty}^{\infty}\frac{1}{(k\Delta x - 2\pi q)^4(\omega_t \Delta x + 2\pi q v_0)^2}\right] = 0$$



- Alias mode is stable by itself when separated from other modes
- Alias vertical location is proportional to alias mode index q
- FGI for dt=0 case has a threshold which corresponds to q=0,±1 mode intersection at kΔx=±***π***

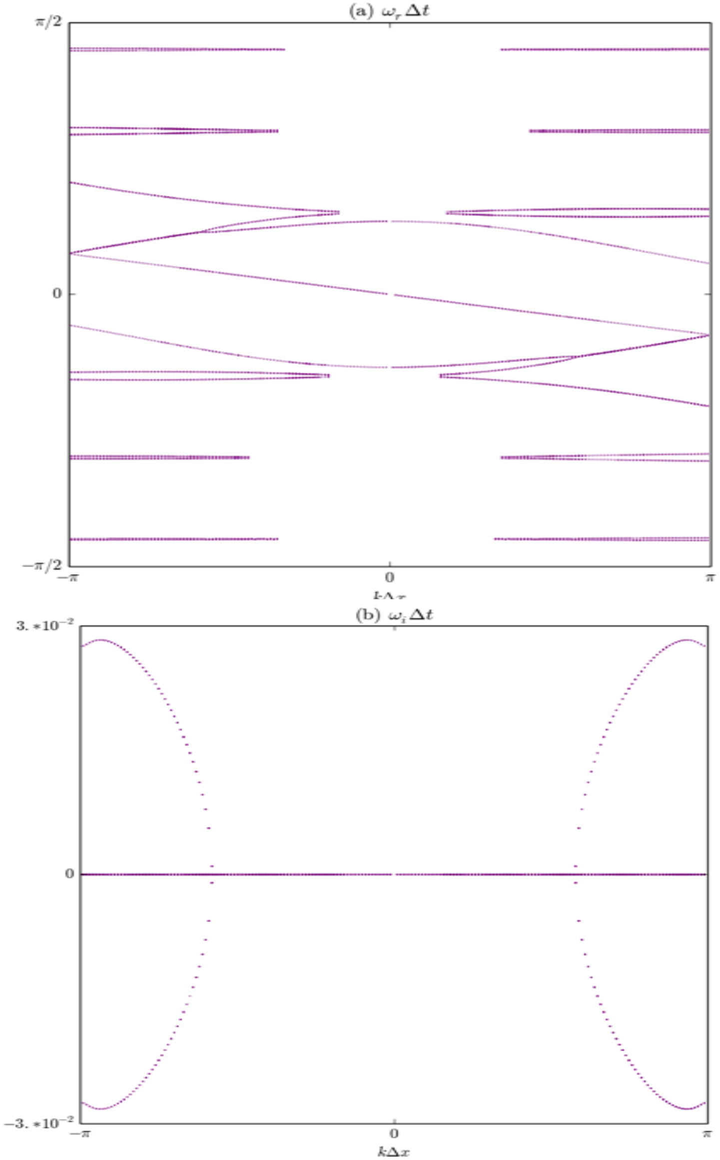
$$\Delta x_{\mathrm{th}} = \frac{\pi^3\gamma^{3/2}v_0}{4\sqrt{2}}.$$

- Peak growth rate :

$$|\omega_i(k\Delta x = \pm\pi)| = \sqrt{\left|16\pi^{-4}\gamma^{-3} + \left(\frac{\pi v_0}{\Delta x}\right)^2 - 8\pi^{-2}\gamma^{-3}\sqrt{4\pi^{-4} + \left(\frac{\pi v_0}{\Delta x}\right)^2\gamma^3}\right|}.$$

Finite Grid Instability (dt>0) in 1D EM PIC

$$\epsilon_a^N = \frac{\gamma^3 \csc^4(k\Delta x/2)}{2S^2\Delta x^2} \sin\left[(Sv_0 k\Delta x + \omega_t \Delta t)/2\right]$$
$$- \sum_{q=-N}^{N} \frac{2}{(k\Delta x - 2\pi q)^4} \csc(\pi q S v_0 + \omega_t \Delta t/2)$$
$$+ \frac{Sv_0}{(k\Delta x - 2\pi q)^3} \csc^2(\pi q S v_0 + \omega_t \Delta t/2) \cos(\pi q S v_0 + \omega_t \Delta t/2),$$



- Similar threshold as the dt=0 case for q=0,±1 mode intersection

$$\Delta x_{th}^{\delta} = 2\pi v_0 \gamma^{3/2},$$

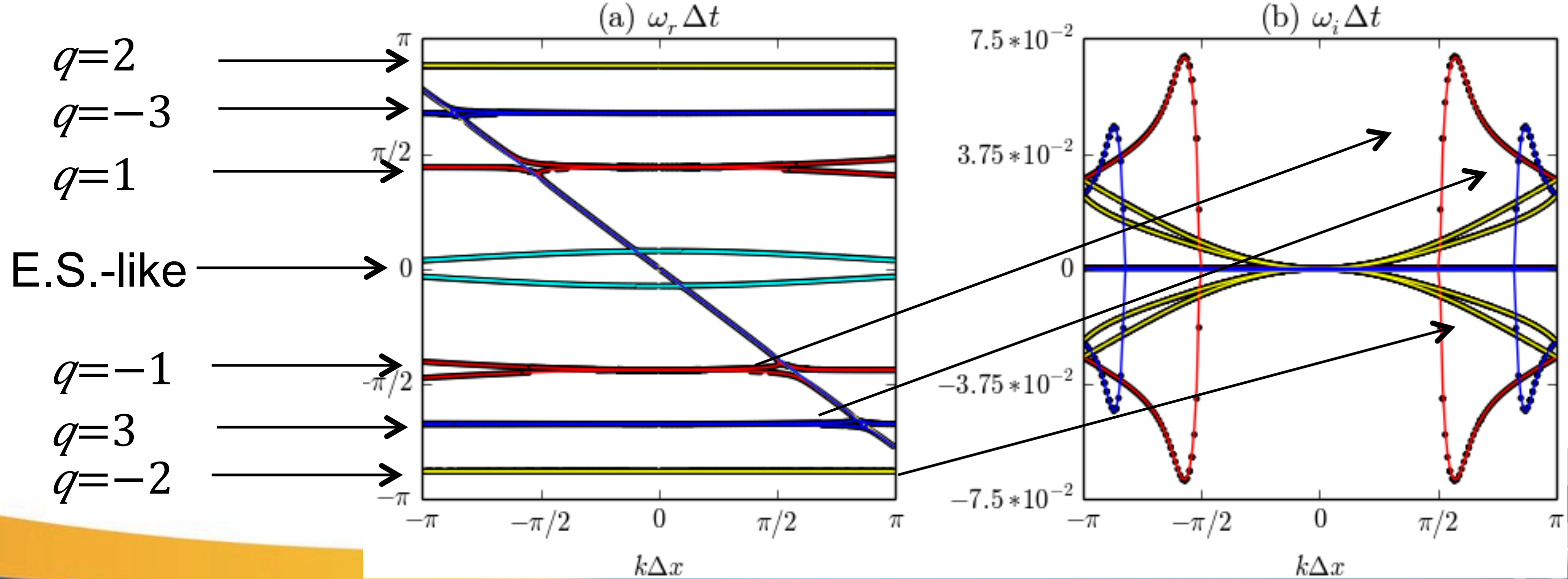
- This condition is easily satisfied in typical simulation with large drift velocity

Finite Grid Instability (dt>0) in 1D EM PIC

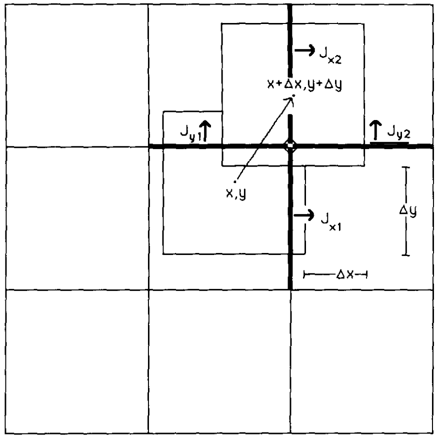
M. D. Meyers et al., submitted to JCP

- The location of the qth alias mode is at $\omega_t^q \Delta t = 2\pi(n - q\mathcal{S})$, $\mathcal{S} = S v_0$
- Alias modes fold into the zeroth Brillouin zone when $|qSv_0| > 1/2$
- Linear mode due to non-charge conserving current deposition
- The folded alias mode can intersect with ω=0 mode causing instability
- This is the dominate FGI for the case with large drift velocity

Peak growth rate : $\omega_i \Delta t \approx \frac{(-1)^{n+1} \sqrt{3} (n\pi)^{1/3}}{\gamma} \left[\mathrm{sinc}^2 (n\pi/\mathcal{S}) S \Delta x/2\right]^{2/3}$



Equivalent velocity for charge-conserving deposition



- Charge-conservation can be enforced in current deposition on microscopic (grid) scale and macroscopic (cell) scale.
- Esirkepov scheme and Villasenor-Buneman scheme are examples of these two views.
- These two schemes are equivalent in 1D, but not so in higher dimension
- Equivalent velocity in spectral domain can be defined:

Villasenor-Buneman:

$$\vec{v}_{\text{VB}} = \begin{pmatrix} \frac{\sin\left(k_q^x v_x \Delta t/2\right)}{k_{qB}^x \Delta t/2} \text{sinc}\left\{\left(k_q^y v_y + k_q^z v_z\right)\Delta t/2\right\} \\ \frac{\sin\left(k_q^y v_y \Delta t/2\right)}{k_{qB}^y \Delta t/2} \text{sinc}\left\{\left(k_q^z v_z + k_q^x v_x\right)\Delta t/2\right\} \\ \frac{\sin\left(k_q^z v_z \Delta t/2\right)}{k_{qB}^z \Delta t/2} \text{sinc}\left\{\left(k_q^x v_x + k_q^y v_y\right)\Delta t/2\right\} \end{pmatrix}.$$

Esirkepov:

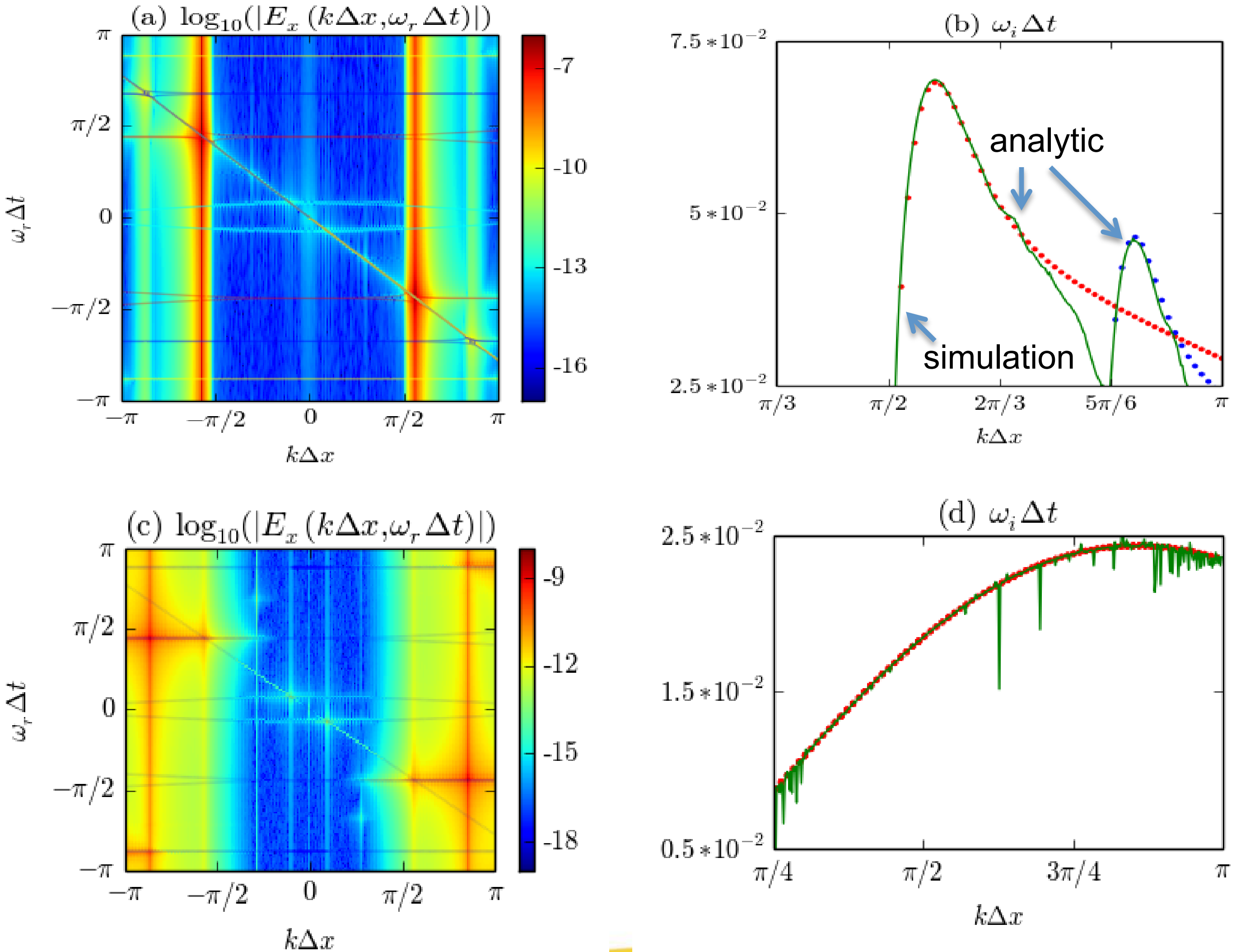
$$\vec{v}_{\text{E}} = \begin{pmatrix} \frac{\sin\left(k_q^x v_x \Delta t/2\right)}{k_{qB}^x \Delta t/2} \left[\cos\left(k_q^y v_y \Delta t/2\right)\cos\left(k_q^z v_z \Delta t/2\right) - \frac{1}{3}\sin\left(k_q^y v_y \Delta t/2\right)\sin\left(k_q^z v_z \Delta t/2\right)\right] \\ \frac{\sin\left(k_q^y v_y \Delta t/2\right)}{k_{qB}^y \Delta t/2} \left[\cos\left(k_q^z v_z \Delta t/2\right)\cos\left(k_q^x v_x \Delta t/2\right) - \frac{1}{3}\sin\left(k_q^z v_z \Delta t/2\right)\sin\left(k_q^x v_x \Delta t/2\right)\right] \\ \frac{\sin\left(k_q^z v_z \Delta t/2\right)}{k_{qB}^z \Delta t/2} \left[\cos\left(k_q^x v_x \Delta t/2\right)\cos\left(k_q^y v_y \Delta t/2\right) - \frac{1}{3}\sin\left(k_q^x v_x \Delta t/2\right)\sin\left(k_q^y v_y \Delta t/2\right)\right] \end{pmatrix}$$

- Alias mode is unstable by itself

Simulation verification

Direct deposition

Charge-conserving deposition



Summary

- The PIC algorithm operates in a discrete time variable and there is no temporal aliasing.
  - Only sampling causes aliasing, and there is no temporal sampling
  - There is spatial sampling and each Brillouin zone in Fourier space contributes to the zeroth zone.
- The correct forms of the finite difference operators in the current are critical to obtaining correct dispersion relations.
  - The numerical solutions will depend on these operators.
  - The location of the alias mode also depend on the form of the pole
- Finite Grid Instability is investigated for both E.S. and E.M. PIC in the 1D case
  - In the E.S. code and charge-conserving E.M. code, alias mode itself is unstable
  - Intersection of alias modes and ω=0 mode is a major source of FGI in non charge-conserving E.M. PIC for large drift velocity
- Preliminary work indicates that phase distortion in the charge/current deposition is the root cause of numerical instabilities
  - Phase distortion can corrected, spectral accuracy and discrete continuity can be preserved
  - Simulation is stable even with NGP shape