

# Multi-Particle Simulation Techniques II

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U.S. DEPARTMENT OF  
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Science

ACCELERATOR TECHNOLOGY &  
APPLIED PHYSICS DIVISION



# Contrast of Non-Symplectic and Symplectic Integrator

## Example: Contrast of Non-Symplectic and Symplectic Advances

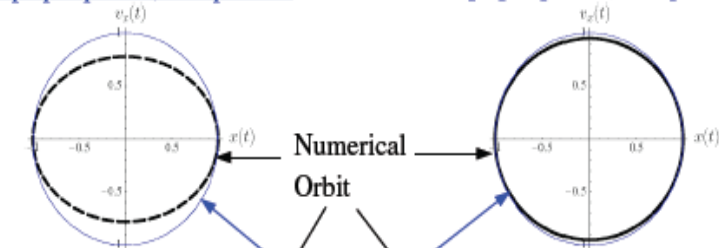
Contrast: Numerical and Actual Orbit for a Simple Harmonic Oscillator  
use scaled coordinates (max extents unity for analytical solution)

**Symplectic Leapfrog Advance:**

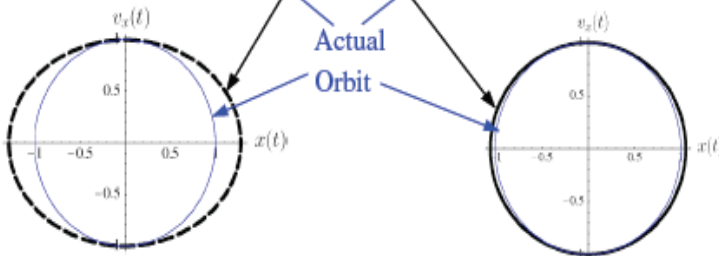
5 steps per period, 100 periods

10 steps per period, 100 periods

Cosine-type  
initial  
conditions



Sine-type  
initial  
conditions



SM Lund, USPAS, June 2008

Simulation Techniques 75

## Example: Contrast of Non-Symplectic and Symplectic Advances (3)

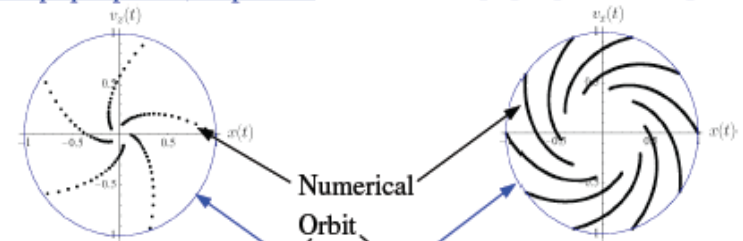
Contrast: Numerical and Actual Orbit for a Simple Harmonic Oscillator

**Non-Symplectic 4<sup>th</sup> Order Runge-Kutta Advance:** (analog to notes on 2<sup>nd</sup> order RK adv)

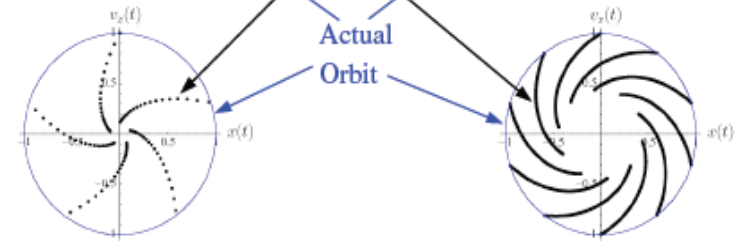
5 steps per period, 20 periods

10 steps per period, 200 periods

Cosine-type  
initial  
conditions



Sine-type  
initial  
conditions



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Simulation Techniques 77

Courtesy of S. Lund

# A Symplectic Multi-Particle Tracking Model (1)

multi-particle Hamiltonian  $H(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{p}_1, \mathbf{p}_2, \dots, s)$

$$H = \sum_i \mathbf{p}_i^2/2 + \frac{1}{2} \sum_i \sum_j q\phi(\mathbf{r}_i, \mathbf{r}_j) + \sum_i q\psi(\mathbf{r}_i)$$

↑
↑  
 space-charge      external focusing/acceleration  
 Coulomb potential

$$\frac{d\mathbf{r}_i}{ds} = \frac{\partial H}{\partial \mathbf{p}_i}$$

$$\frac{d\mathbf{p}_i}{ds} = -\frac{\partial H}{\partial \mathbf{r}_i} \quad \frac{d\zeta}{ds} = -[H, \zeta]$$

## A formal single step solution

$$\zeta(\tau) = \exp(-\tau(: H :))\zeta(0)$$

$$H = H_1 + H_2$$

$$\zeta(\tau) = \exp(-\tau(: H_1 : + : H_2 :))\zeta(0)$$

$$= \exp(-\frac{1}{2}\tau : H_1 :) \exp(-\tau : H_2 :) \exp(-\frac{1}{2}\tau : H_1 :) \zeta(0) + O(\tau^3)$$

$$\zeta(\tau) = \mathcal{M}(\tau)\zeta(0)$$

$$= \mathcal{M}_1(\tau/2)\mathcal{M}_2(\tau)\mathcal{M}_1(\tau/2)\zeta(0)$$

**$\mathcal{M}$**  would be symplectic if both  **$\mathcal{M}_1$**  and  **$\mathcal{M}_2$**  are symplectic

# A Symplectic Multi-Particle Tracking Model (2)

**2<sup>nd</sup> order:** 
$$\begin{aligned}\zeta(\tau) &= \mathcal{M}(\tau)\zeta(0) \\ &= \mathcal{M}_1(\tau/2)\mathcal{M}_2(\tau)\mathcal{M}_1(\tau/2)\zeta(0)\end{aligned}$$

**4<sup>th</sup> order:** 
$$\mathcal{M}(\tau) = \mathcal{M}_1\left(\frac{s}{2}\right)\mathcal{M}_2(s)\mathcal{M}_1\left(\frac{\alpha s}{2}\right)\mathcal{M}_2((\alpha - 1)s)\mathcal{M}_1\left(\frac{\alpha s}{2}\right)\mathcal{M}_2(s)\mathcal{M}_1\left(\frac{s}{2}\right)$$
  
where  $\alpha = 1 - 2^{1/3}$ , and  $s = \tau/(1 + \alpha)$

**higher order:** 
$$\mathcal{M}_{2n+2}(\tau) = \mathcal{M}_{2n}(z_0\tau)\mathcal{M}_{2n}(z_1\tau)\mathcal{M}_{2n}(z_0\tau)$$
  
where  $z_0 = 1/(2 - 2^{1/(2n+1)})$  and  $z_1 = -2^{1/(2n+1)}/(2 - 2^{1/(2n+1)})$

**Symplectic condition:** 
$$M_i^T J M_i = J$$
      **M is the Jacobi Matrix of  $\mathcal{M}$**

where  $J$  denotes the  $6N \times 6N$  matrix given by

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \quad \text{and } I \text{ is the } 3N \times 3N \text{ identity matrix}$$

Refs: E. Forest and R. D. Ruth, Physica D **43**, p. 105, 1990. H. Yoshida, Phys. Lett. A **150**, p. 262, 1990.

# A Symplectic Multi-Particle Tracking Model (3)

$$H_1 = \sum_i \mathbf{p}_i^2/2 + \sum_i q\psi(\mathbf{r}_i) \longrightarrow \mathcal{M}_1$$

- symplectic map for  $H_1$  can be found from charged particle optics method

$$H_2 = \frac{1}{2} \sum_i \sum_j q\phi(\mathbf{r}_i, \mathbf{r}_j) \longrightarrow \mathcal{M}_2$$

$$\mathbf{r}_i(\tau) = \mathbf{r}_i(0)$$

$$\mathbf{p}_i(\tau) = \mathbf{p}_i(0) - \frac{\partial H_2(\mathbf{r})}{\partial \mathbf{r}_i} \tau$$

$$M_2 = \begin{pmatrix} I & 0 \\ L & I \end{pmatrix} \quad \text{To satisfy the symplectic condition: } L = L^T$$

$$L_{ij} = \partial \mathbf{p}_i(\tau) / \partial \mathbf{r}_j = - \frac{\partial^2 H_2(\mathbf{r})}{\partial \mathbf{r}_i \partial \mathbf{r}_j} \tau$$

**$\mathcal{M}_2$  will be symplectic if  $p_i$  is updated from  $H_2$  analytically**

# Self-Consistent Space-Charge Transfer Map (1)

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = -\frac{\rho}{\epsilon_0}$$
$$\begin{aligned}\phi(x=0, y) &= 0 \\ \phi(x=a, y) &= 0 \\ \phi(x, y=0) &= 0 \\ \phi(x, y=b) &= 0\end{aligned}$$

$$\rho(x, y) = \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \rho^{lm} \sin(\alpha_l x) \sin(\beta_m y)$$

$$\phi(x, y) = \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \phi^{lm} \sin(\alpha_l x) \sin(\beta_m y)$$

$$\rho^{lm} = \frac{4}{ab} \int_0^a \int_0^b \rho(x, y) \sin(\alpha_l x) \sin(\beta_m y) dx dy$$

$$\phi^{lm} = \frac{4}{ab} \int_0^a \int_0^b \phi(x, y) \sin(\alpha_l x) \sin(\beta_m y) dx dy$$

where  $\alpha_l = l\pi/a$  and  $\beta_m = m\pi/b$

$$\phi^{lm} = \frac{\rho^{lm}}{\epsilon_0 \gamma_{lm}^2} \quad \text{where } \gamma_{lm}^2 = \alpha_l^2 + \beta_m^2$$

# Self-Consistent Space-Charge Transfer Map (2)

The charge density from macroparticles:

$$\rho(x, y) = \frac{1}{\Delta x \Delta y N_p} \sum_{j=1}^{N_p} S(x - x_j) S(y - y_j)$$

The solution of space-charge potential modes:

$$\begin{aligned} \phi^{lm} = & \frac{4\pi}{\gamma_{lm}^2} \frac{4}{ab} \frac{1}{N_p} \sum_{j=1}^{N_p} \frac{1}{\Delta x \Delta y} \int_0^a \int_0^b S(x - x_j) S(y - y_j) \\ & \times \sin(\alpha_l x) \sin(\beta_m y) dx dy \end{aligned} \quad ($$

The solution of space-charge potential:

$$\phi(x, y) = 4\pi \frac{4}{ab} \frac{1}{N_p} \sum_{j=1}^{N_p} \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \frac{1}{\gamma_{lm}^2} \sin(\alpha_l x) \sin(\beta_m y) \frac{1}{\Delta x \Delta y} \int_0^a \int_0^b S(\bar{x} - x_j) S(\bar{y} - y_j) \sin(\alpha_l \bar{x}) \sin(\beta_m \bar{y}) d\bar{x} d\bar{y}.$$

The space-charge potential on macroparticles:

$$\phi(x_i, y_i) = \frac{1}{\Delta x \Delta y} \int_0^a \int_0^b \phi(x, y) S(x - x_i) S(y - y_i) dx dy$$

# Self-Consistent Space-Charge Transfer Map (3)

The interaction potential:

$$\begin{aligned} \varphi(x_i, y_i, x_j, y_j) = & 4\pi \frac{4}{ab} \frac{1}{N_p} \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \frac{1}{\gamma_{lm}^2} \frac{1}{\Delta x \Delta y} \int_0^a \int_0^b S(x - x_j) S(y - y_j) \sin(\alpha_l x) \sin(\beta_m y) dx dy \\ & \times \frac{1}{\Delta x \Delta y} \int_0^a \int_0^b S(x - x_i) S(y - y_i) \sin(\alpha_l x) \sin(\beta_m y) dx dy. \end{aligned}$$

The space-charge Hamiltonian:

$$\begin{aligned} H_2 = & 4\pi \frac{K}{2} \frac{4}{ab} \frac{1}{N_p} \sum_{i=1}^{N_p} \sum_{j=1}^{N_p} \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \frac{1}{\gamma_{lm}^2} \frac{1}{\Delta x \Delta y} \int_0^a \int_0^b S(x - x_j) S(y - y_j) \sin(\alpha_l x) \sin(\beta_m y) dx dy \\ & \times \frac{1}{\Delta x \Delta y} \int_0^a \int_0^b S(x - x_i) S(y - y_i) \sin(\alpha_l x) \sin(\beta_m y) dx dy. \end{aligned}$$



# Symplectic Gridless Symplectic Space-Charge Model

$$\rho(x, y) = \sum_{j=1}^{N_p} w \delta(x - x_j) \delta(y - y_j)$$

$w$  is the particle charge weight

$$H_2 = \frac{1}{2\epsilon_0} \frac{4}{ab} w \sum_i \sum_j \sum_l \sum_m \frac{1}{\gamma_{lm}^2} \sin(\alpha_l x_j) \sin(\beta_m y_j) \sin(\alpha_l x_i) \sin(\beta_m y_i)$$

$\mathcal{M}_2$

$$p_{xi}(\tau) = p_{xi}(0) - \tau \frac{1}{\epsilon_0} \frac{4}{ab} w \sum_j \sum_l \sum_m \frac{\alpha_l}{\gamma_{lm}^2} \sin(\alpha_l x_j) \sin(\beta_m y_j) \cos(\alpha_l x_i) \sin(\beta_m y_i)$$

$$p_{yi}(\tau) = p_{yi}(0) - \tau \frac{1}{\epsilon_0} \frac{4}{ab} w \sum_j \sum_l \sum_m \frac{\beta_m}{\gamma_{lm}^2} \sin(\alpha_l x_j) \sin(\beta_m y_j) \sin(\alpha_l x_i) \cos(\beta_m y_i)$$

# Symplectic Particle-In-Cell Model (1)

$$p_{xi}(\tau) = p_{xi}(0) - \tau 4\pi K \frac{4}{ab} \frac{1}{N_p} \sum_{j=1}^{N_p} \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \frac{1}{\gamma_{lm}^2} \frac{1}{\Delta x \Delta y} \int_0^a \int_0^b S(x - x_j) S(y - y_j) \sin(\alpha_l x) \sin(\beta_m y) dx dy$$

$$\times \frac{1}{\Delta x \Delta y} \int_0^a \int_0^b \frac{\partial S(x - x_i)}{\partial x_i} S(y - y_i) \sin(\alpha_l x) \sin(\beta_m y) dx dy,$$

$$p_{yi}(\tau) = p_{yi}(0) - \tau 4\pi K \frac{4}{ab} \frac{1}{N_p} \sum_{j=1}^{N_p} \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \frac{1}{\gamma_{lm}^2} \frac{1}{\Delta x \Delta y} \int_0^a \int_0^b S(x - x_j) S(y - y_j) \sin(\alpha_l x) \sin(\beta_m y) dx dy$$

$$\times \frac{1}{\Delta x \Delta y} \int_0^a \int_0^b S(x - x_i) \frac{\partial S(y - y_i)}{\partial y_i} \sin(\alpha_l x) \sin(\beta_m y) dx dy,$$

$$p_{xi}(\tau) = p_{xi}(0) - \tau 4\pi K \frac{4}{ab} \frac{1}{N_p} \sum_{j=1}^{N_p} \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \frac{1}{\gamma_{lm}^2} \sum_{I'} \sum_{J'} S(x_{I'} - x_j) S(y_{J'} - y_j) \sin(\alpha_l x_{I'}) \sin(\beta_m y_{J'})$$

$$\times \sum_{I'} \sum_{J'} \frac{\partial S(x_{I'} - x_i)}{\partial x_i} S(y_{J'} - y_i) \sin(\alpha_l x_{I'}) \sin(\beta_m y_{J'}),$$

$$p_{yi}(\tau) = p_{yi}(0) - \tau 4\pi K \frac{4}{ab} \frac{1}{N_p} \sum_{j=1}^{N_p} \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \frac{1}{\gamma_{lm}^2} \sum_{I'} \sum_{J'} S(x_{I'} - x_j) S(y_{J'} - y_j) \sin(\alpha_l x_{I'}) \sin(\beta_m y_{J'})$$

$$\times \sum_{I'} \sum_{J'} S(x_{I'} - x_i) \frac{\partial S(y_{J'} - y_i)}{\partial y_i} \sin(\alpha_l x_{I'}) \sin(\beta_m y_{J'}),$$

# Symplectic PIC Model (2)

Define charge density on grid as:

$$\bar{\rho}(x_{I'}, y_{J'}) = \frac{1}{N_p} \sum_{j=1}^{N_p} S(x_{I'} - x_j) S(y_{J'} - y_j),$$

Space-charge  $\mathcal{M}_2$

$$p_{xi}(\tau) = p_{xi}(0) - \tau 4\pi K \sum_I \sum_J \frac{\partial S(x_I - x_i)}{\partial x_i} S(y_J - y_i) \\ \times \left[ \frac{4}{ab} \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \frac{1}{\gamma_{lm}^2} \sum_{I'} \sum_{J'} \bar{\rho}(x_{I'}, y_{J'}) \sin(\alpha_l x_{I'}) \sin(\beta_m y_{J'}) \sin(\alpha_l x_I) \sin(\beta_m y_J) \right],$$

$$p_{yi}(\tau) = p_{yi}(0) - \tau 4\pi K \sum_I \sum_J S(x_I - x_i) \frac{\partial S(y_I - y_i)}{\partial y_i} \\ \times \left[ \frac{4}{ab} \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \frac{1}{\gamma_{lm}^2} \sum_{I'} \sum_{J'} \bar{\rho}(x_{I'}, y_{J'}) \sin(\alpha_l x_{I'}) \sin(\beta_m y_{J'}) \sin(\alpha_l x_I) \sin(\beta_m y_J) \right].$$

# Symplectic PIC Model (3)

Define potential on grid as:

$$\phi(x_I, y_J) = \frac{4}{ab} \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \frac{1}{\gamma_{lm}^2} \sum_{I'} \sum_{J'} \bar{\rho}(x_{I'}, y_{J'}) \sin(\alpha_l x_{I'}) \sin(\beta_m y_{J'}) \sin(\alpha_l x_I) \sin(\beta_m y_J).$$

$\mathcal{M}_2$



$$p_{xi}(\tau) = p_{xi}(0) - \tau 4\pi K \sum_I \sum_J \frac{\partial S(x_I - x_i)}{\partial x_i} S(y_J - y_i) \phi(x_I, y_J)$$

$$p_{yi}(\tau) = p_{yi}(0) - \tau 4\pi K \sum_I \sum_J S(x_I - x_i) \frac{\partial S(y_J - y_i)}{\partial y_i} \phi(x_I, y_J)$$

$$S(x_I - x_i) = \begin{cases} \frac{3}{4} - \frac{(x_i - x_I)^2}{\Delta x^2}, & |x_i - x_I| \leq \Delta x/2, \\ \frac{1}{2} \left( \frac{3}{2} - \frac{|x_i - x_I|}{\Delta x} \right)^2, & \Delta x/2 < |x_i - x_I| \leq 3/2\Delta x, \\ 0 & \text{otherwise,} \end{cases}$$

$$\frac{\partial S(x_I - x_i)}{\partial x_i} = \begin{cases} -2\frac{(x_i - x_I)}{\Delta x}, & |x_i - x_I| \leq \Delta x/2, \\ \left(-\frac{3}{2} + \frac{(x_i - x_I)}{\Delta x}\right)/\Delta x, & \Delta x/2 < |x_i - x_I| \leq 3/2\Delta x, x_i > x_I, \\ \left(\frac{3}{2} + \frac{(x_i - x_I)}{\Delta x}\right)/\Delta x, & \Delta x/2 < |x_i - x_I| \leq 3/2\Delta x, x_i \leq x_I, \\ 0 & \text{otherwise.} \end{cases}$$

# Non-Symplectic PIC Model

$$\frac{d\mathbf{r}_i}{ds} = \mathbf{p}_i$$

$$\frac{d\mathbf{p}_i}{ds} = q(\mathbf{E}_i/v_0 - a_z \times \mathbf{B}_i)$$

$$\mathbf{r}(\tau/2)_i = \mathbf{r}(0)_i + \frac{1}{2}\tau\mathbf{p}_i(0)$$

$$E_x(x_I, y_J) = - \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \alpha_l \phi^{lm} \cos(\alpha_l x) \sin(\beta_m y)$$

$$E_y(x_I, y_J) = - \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \beta_m \phi^{lm} \sin(\alpha_l x) \cos(\beta_m y)$$

$$p_{xi}(\tau) = p_{xi}(0) + \tau \left( \frac{qE_x^{ext}}{v_0} - qB_y^{ext} \right) + \tau 4\pi K \sum_I \sum_J S(x_I - x_i) S(y_J - y_i) E_x(x_I, y_J)$$

$$p_{yi}(\tau) = p_{yi}(0) + \tau \left( \frac{qE_y^{ext}}{v_0} + qB_x^{ext} \right) + \tau 4\pi K \sum_I \sum_J S(x_I - x_i) S(y_J - y_i) E_y(x_I, y_J)$$

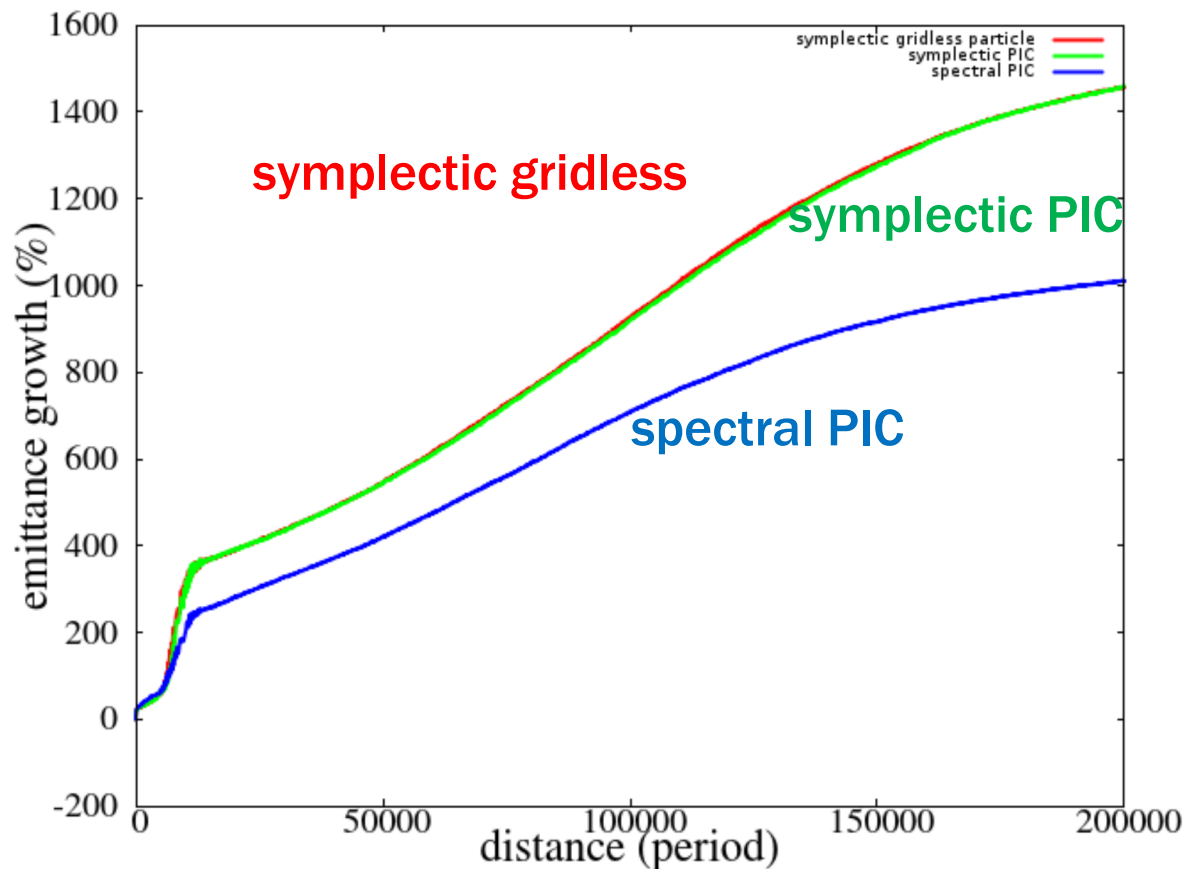
$$\mathbf{r}(\tau)_i = \mathbf{r}(\tau/2)_i + \frac{1}{2}\tau\mathbf{p}_i(\tau)$$

# Benchmark Case 1: FODO Lattice, Below 2<sup>nd</sup> Order Envelop Instability



- 1 GeV proton beam
- FODO lattice
- 0 current phase advance: 85 degrees
- Initial 4D Gaussian distribution

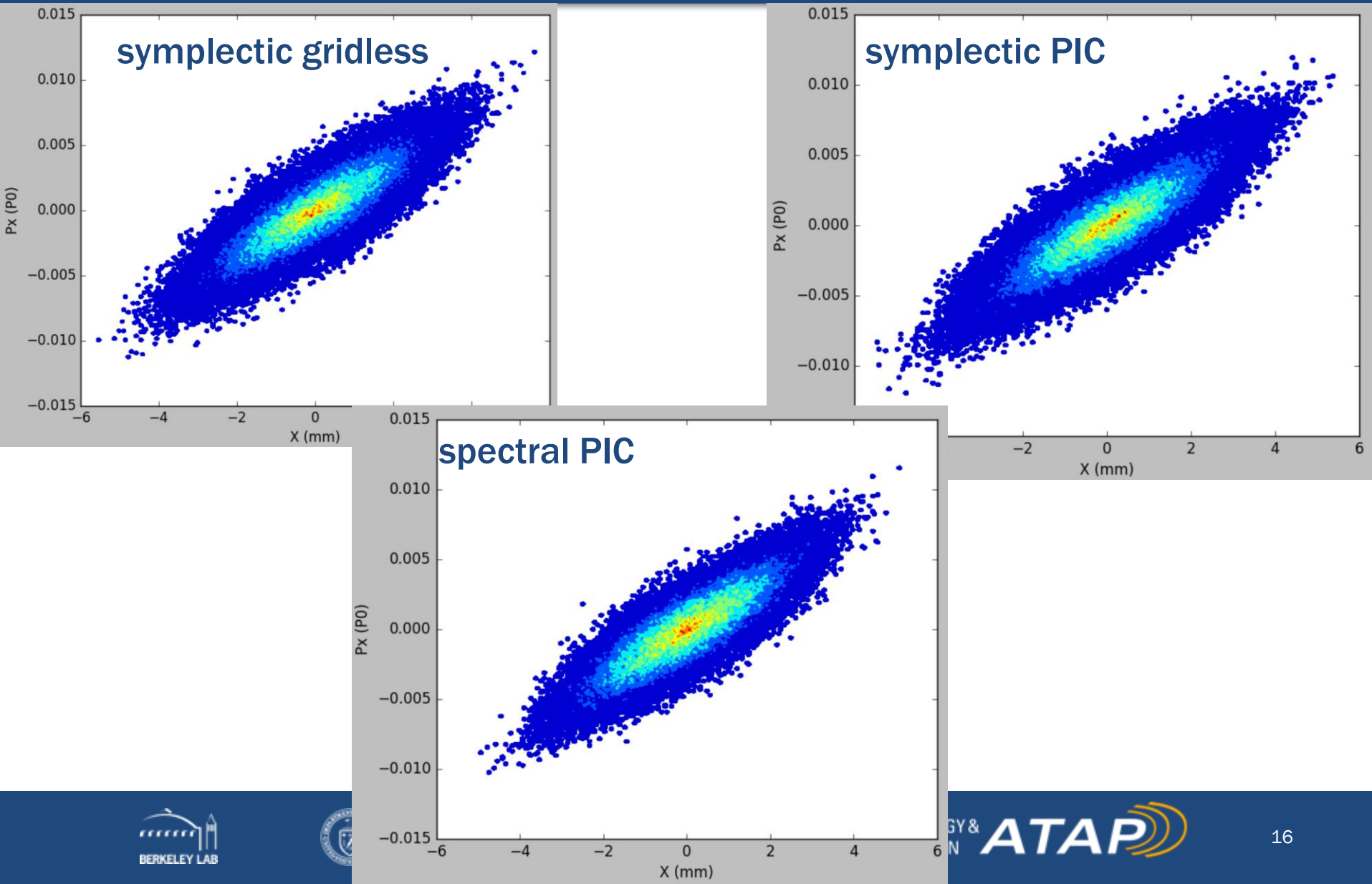
# Significant Difference in Final 4D Emittances Between the Symplectic and the Non-Symplectic Methods (Strong Space-Charge: Phase Advance Change 85 -> 42)



Two symplectic approaches show good agreement.

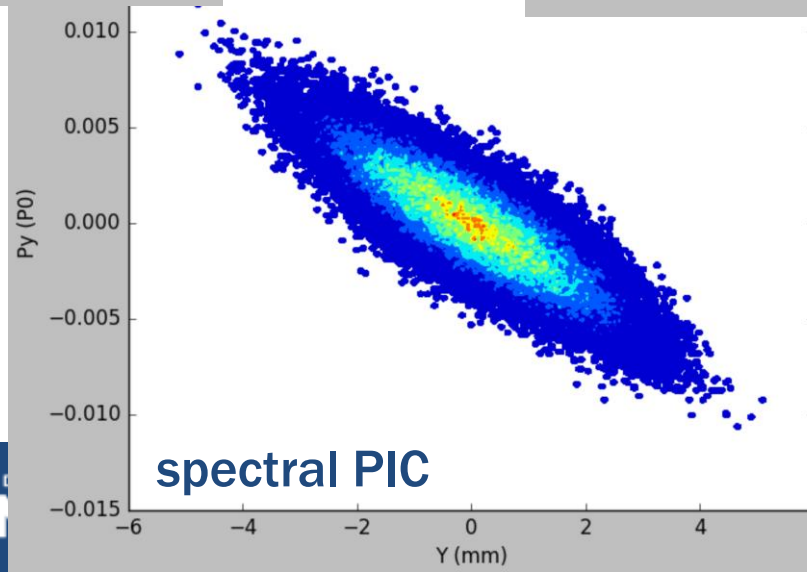
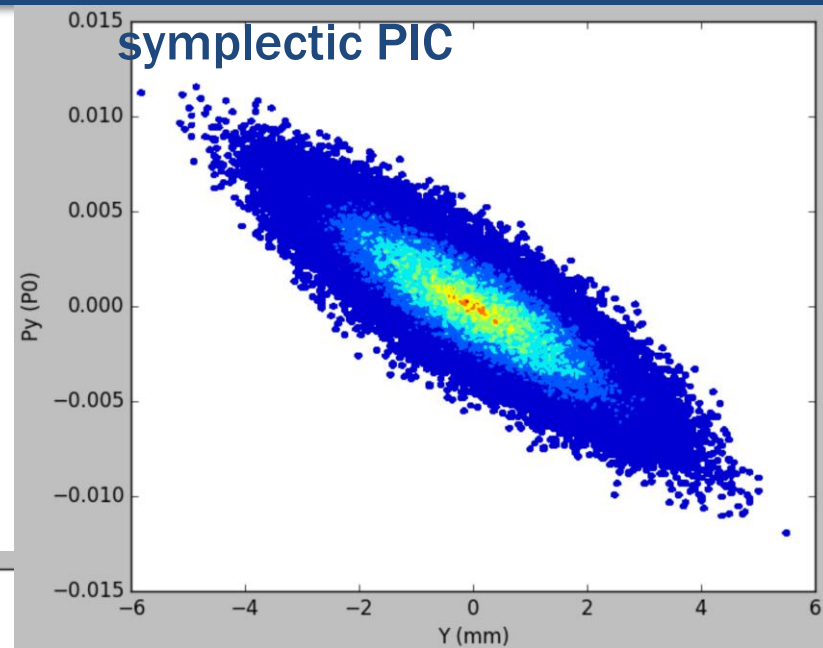
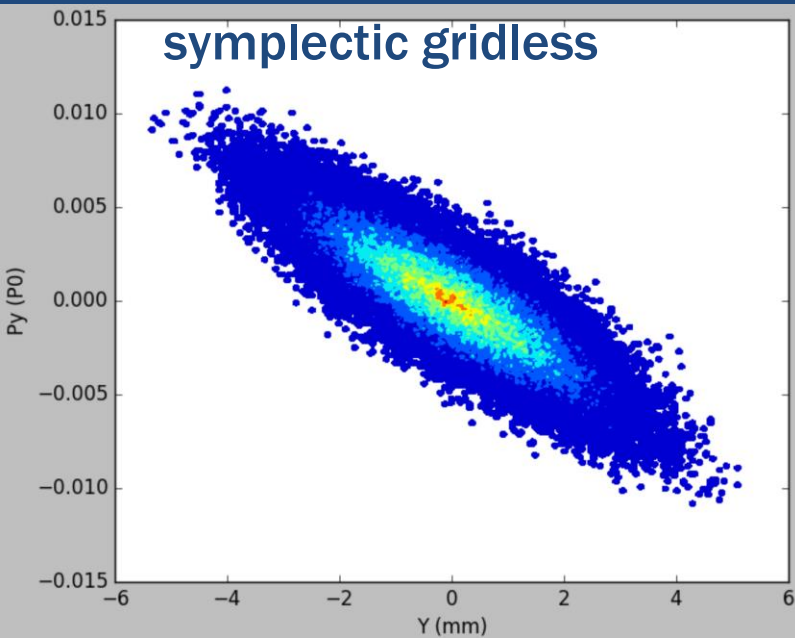
# Final Beam X-Px Phase Spaces Have Similar Shapes

## Non-Symplectic Model Has Smaller Area

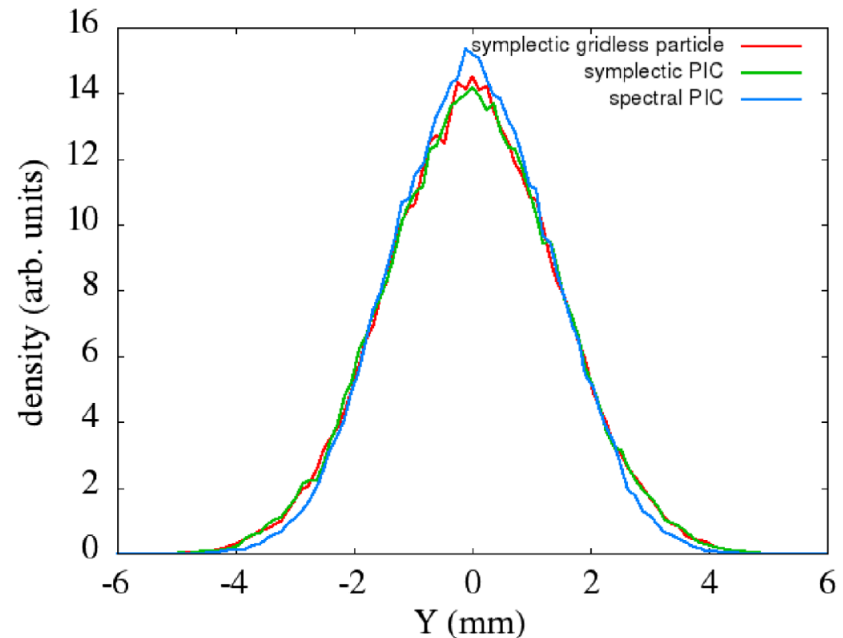
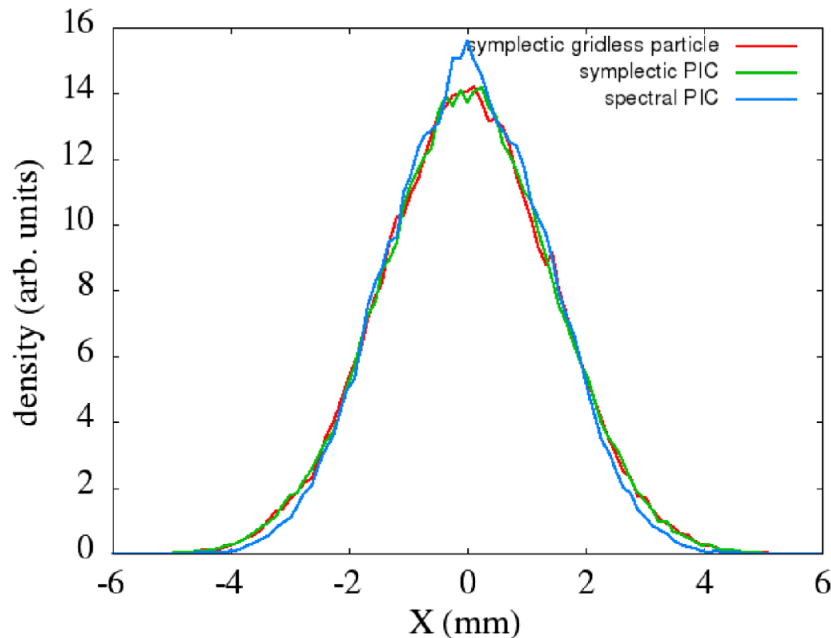




# Final Y-Py Phase Space Show Similar Shapes

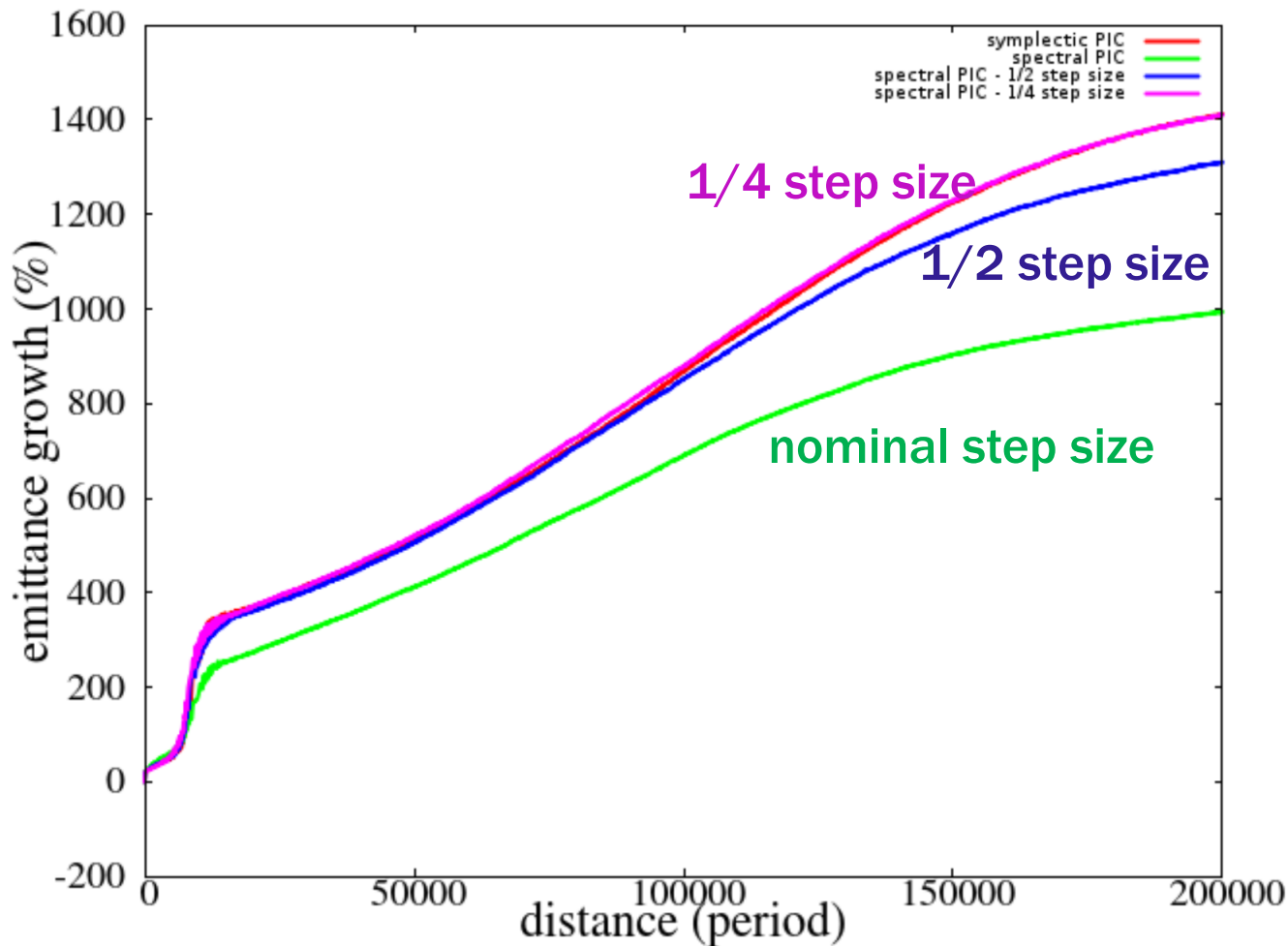


# Horizontal and Vertical Density Profiles from the Symplectic Gridless Model, the Symplectic PIC Model, and the Non-Symplectic Spectral PIC



- Two symplectic solvers produce similar density profiles
- Non-symplectic solver produces larger core density

# Finer Step Size Needed for Non-Symplectic PIC (Symplectic PIC vs. Non-Symplectic PIC)

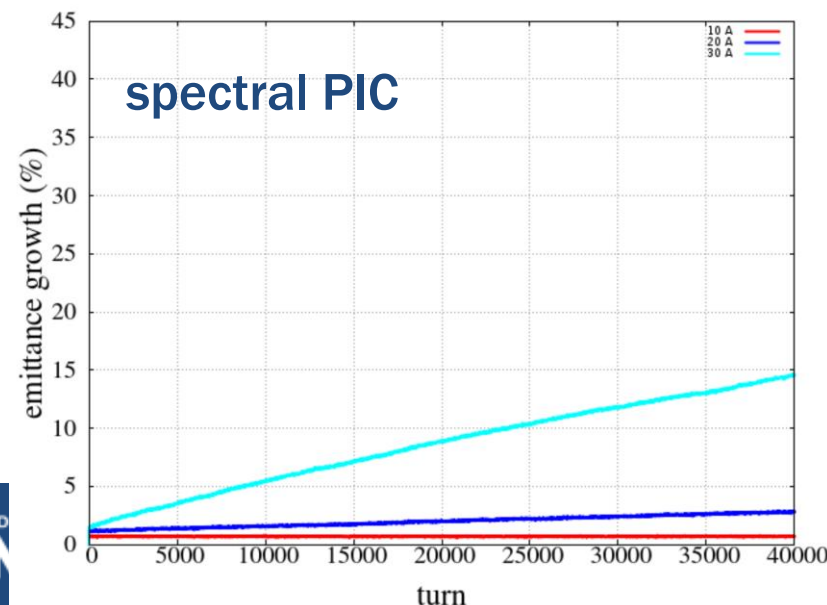
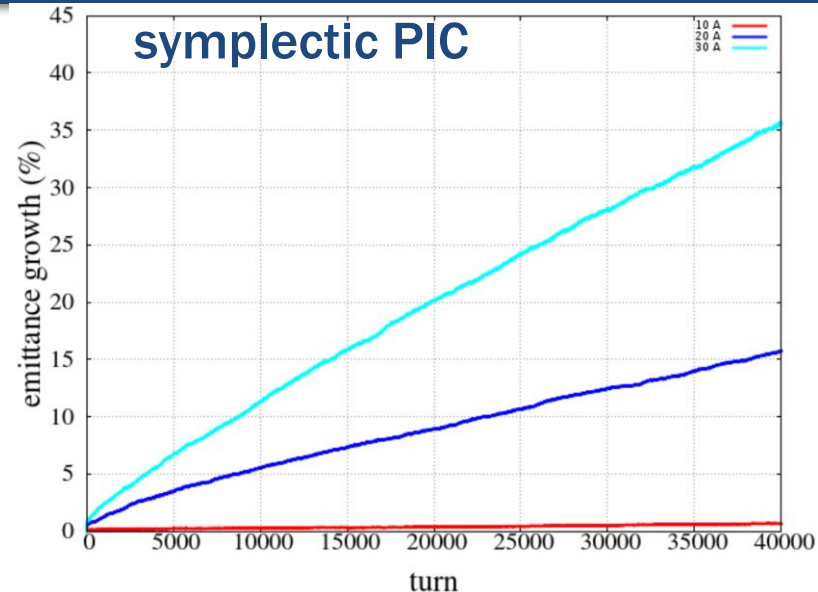
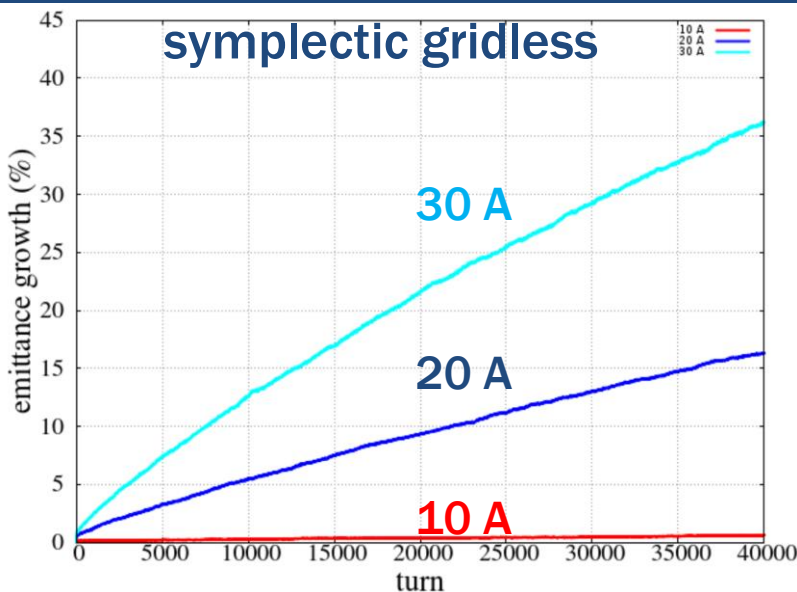


# Benchmark Case 2: 1 Turn = 10 FODOs + 1 Sextupole

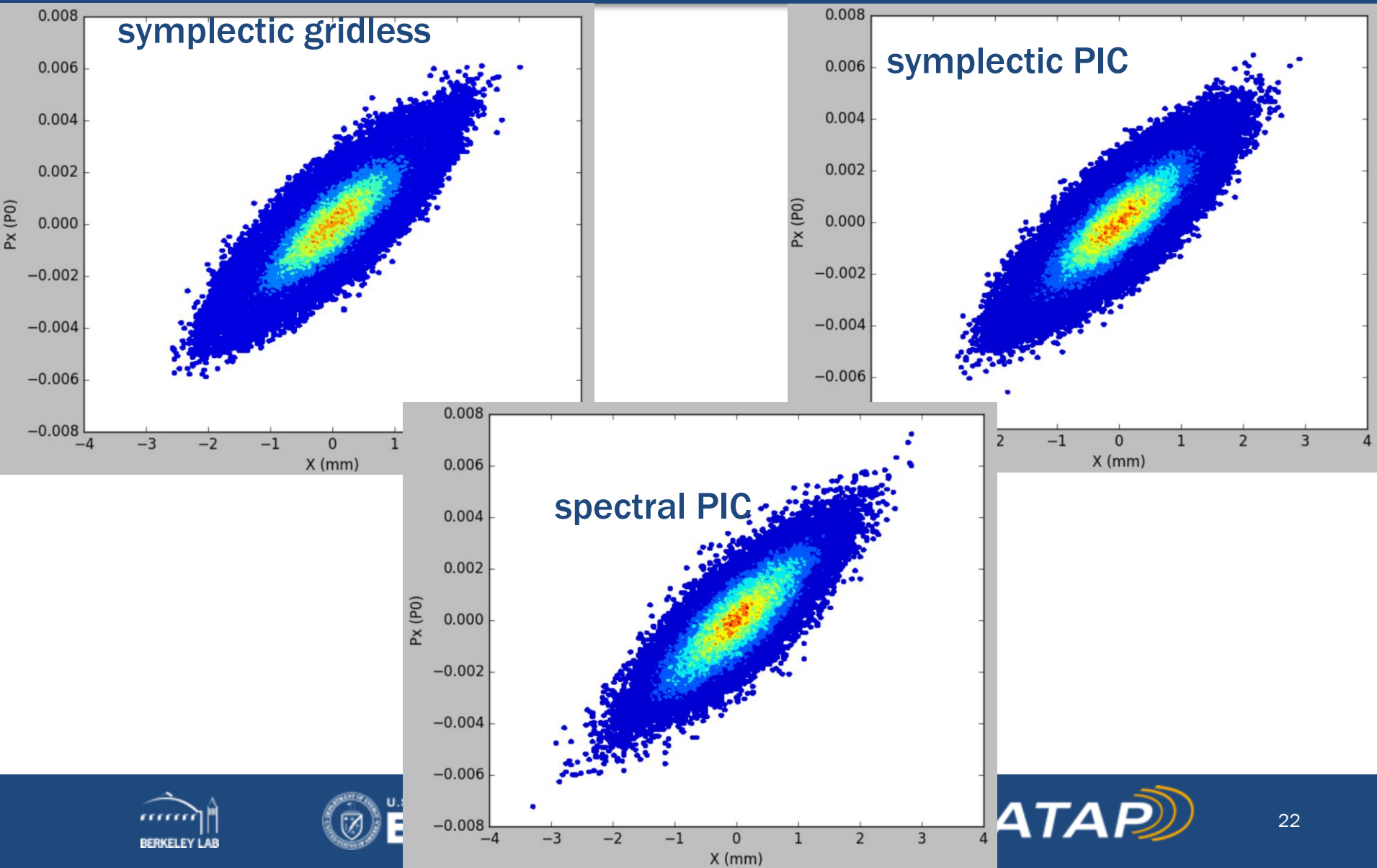


- 0 current tune 2.417, 30 A current, tune shift 0.113
- sextupole  $KL = 10 \text{ T/m/m}$

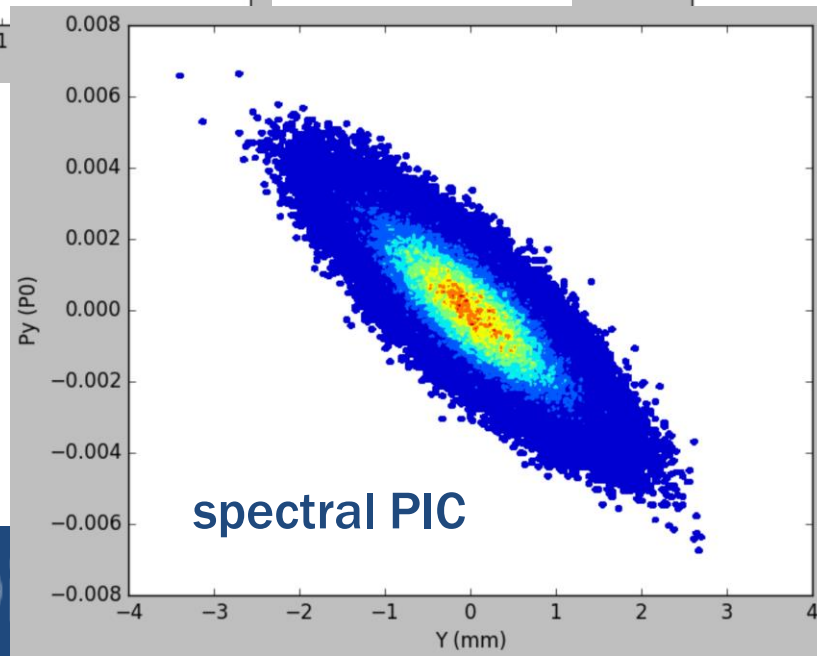
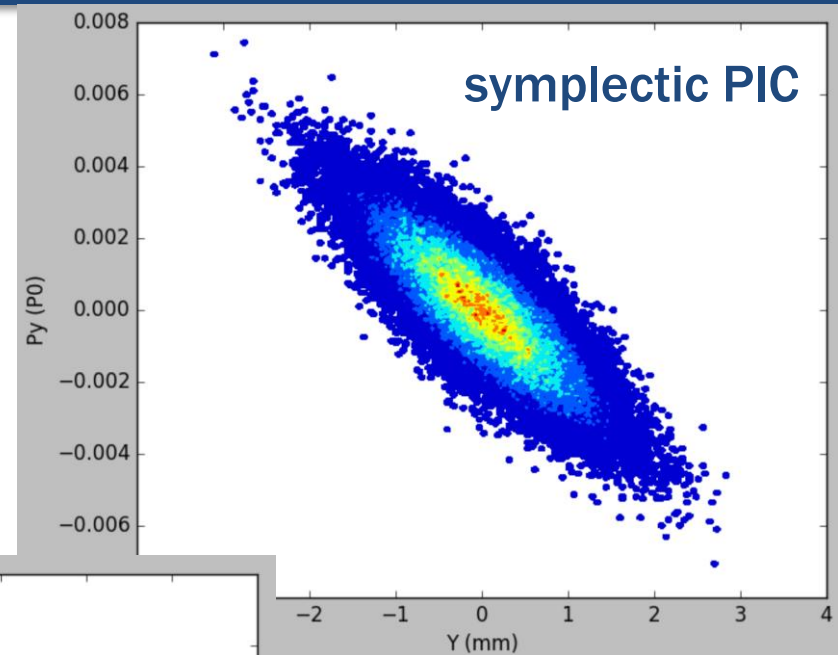
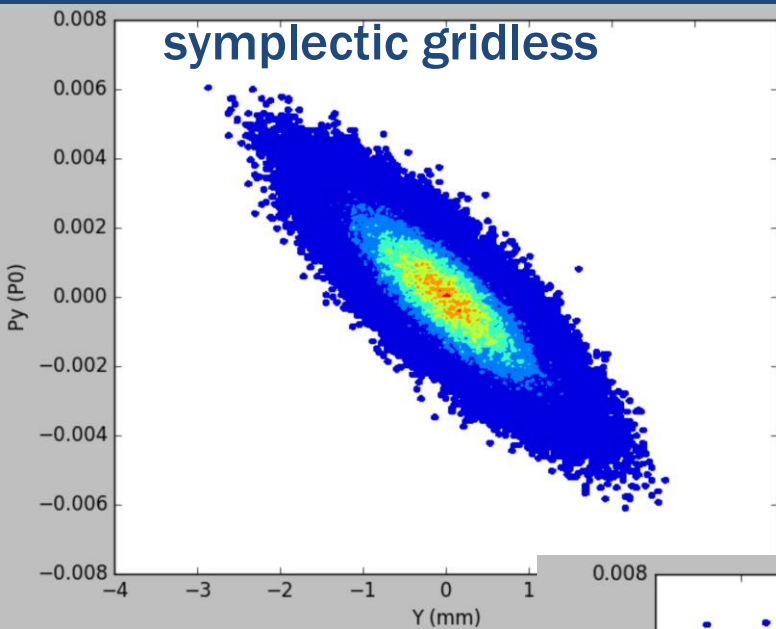
# Non-Symplectic PIC Shows Much Less Emittance Growth Compared with Two Symplectic Models (4D Emittance Evolution with Different Currents)



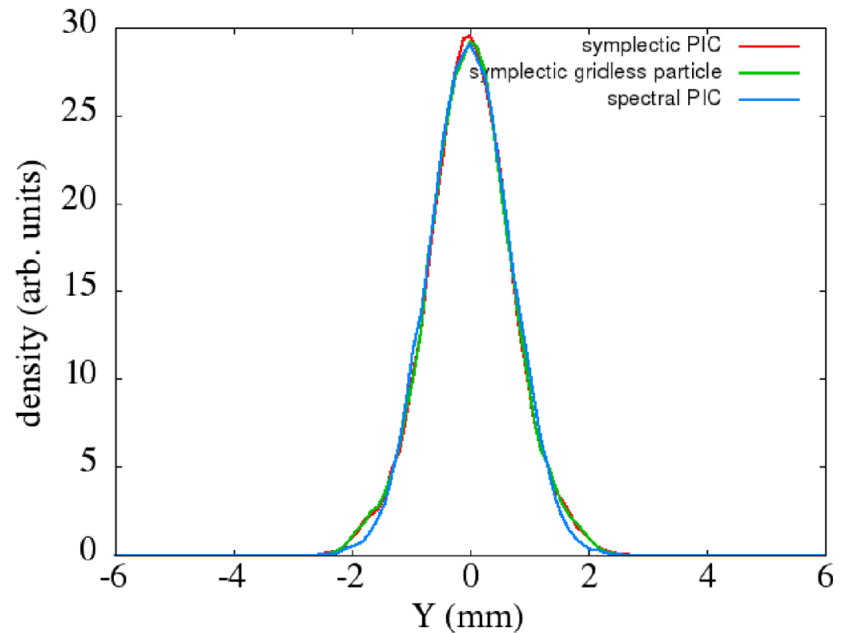
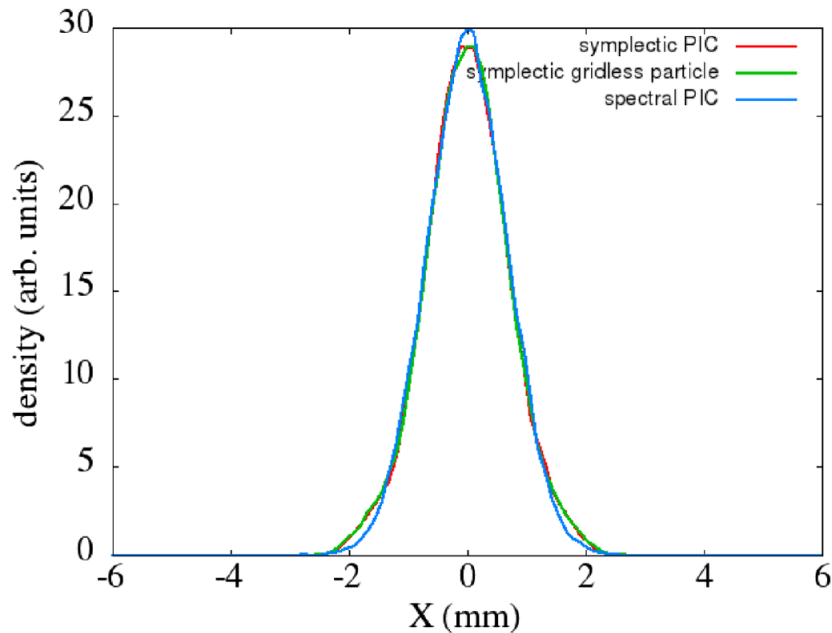
# Final Beam X-Px Phase Spaces Have Similar Shapes



# Final Beam Y-Py Phase Spaces Have Similar Shapes



# Comparison of Density Profiles

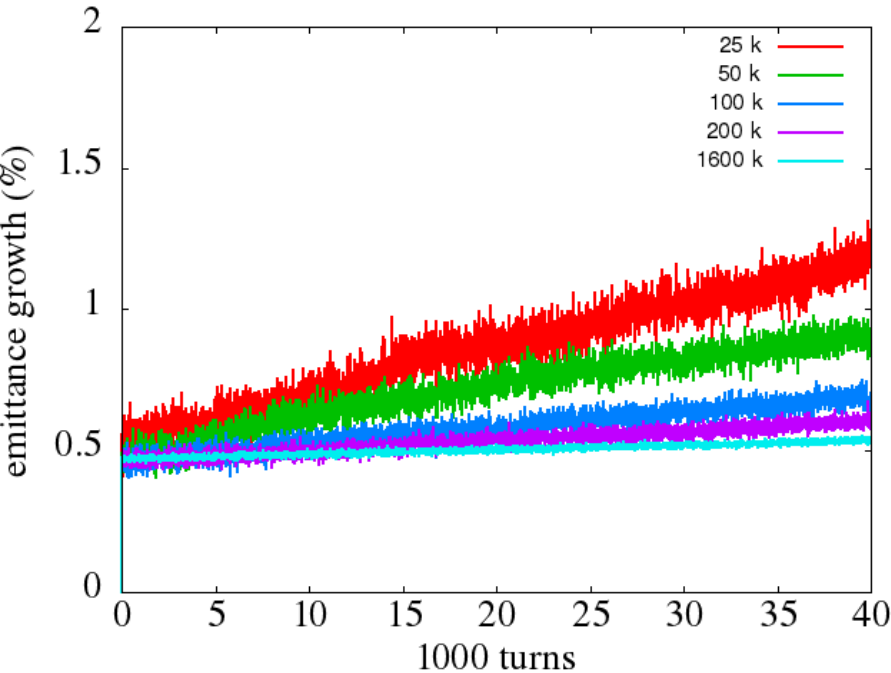


- Two symplectic solvers produce similar density profiles
- Non-symplectic solver produces larger less shoulder

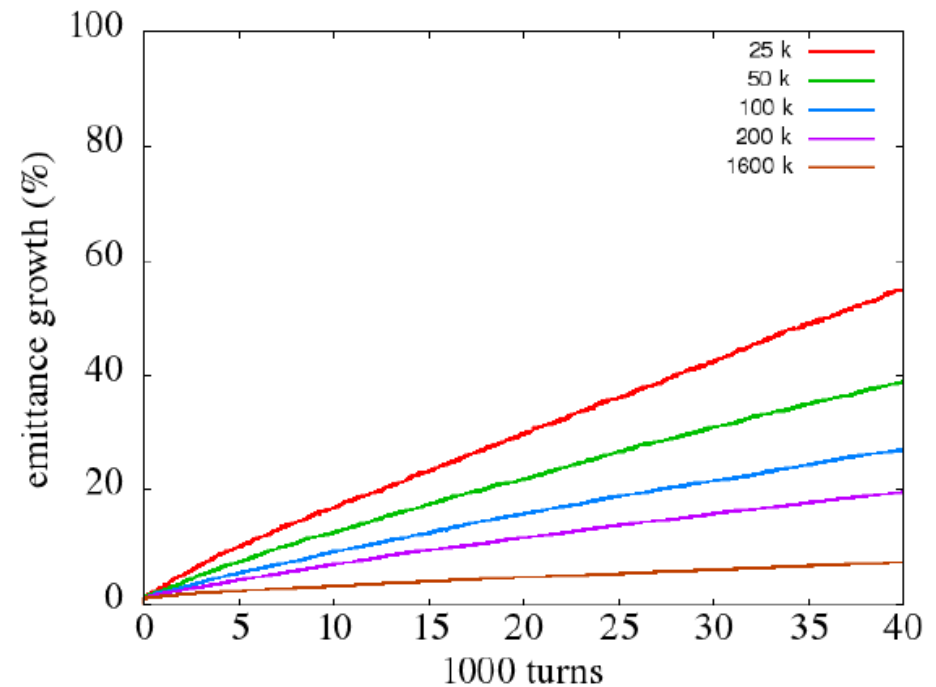


# Extra Numerical Emittance Growth with Small Number of Macroparticles

sextupole KL = 0, 64x64 modes



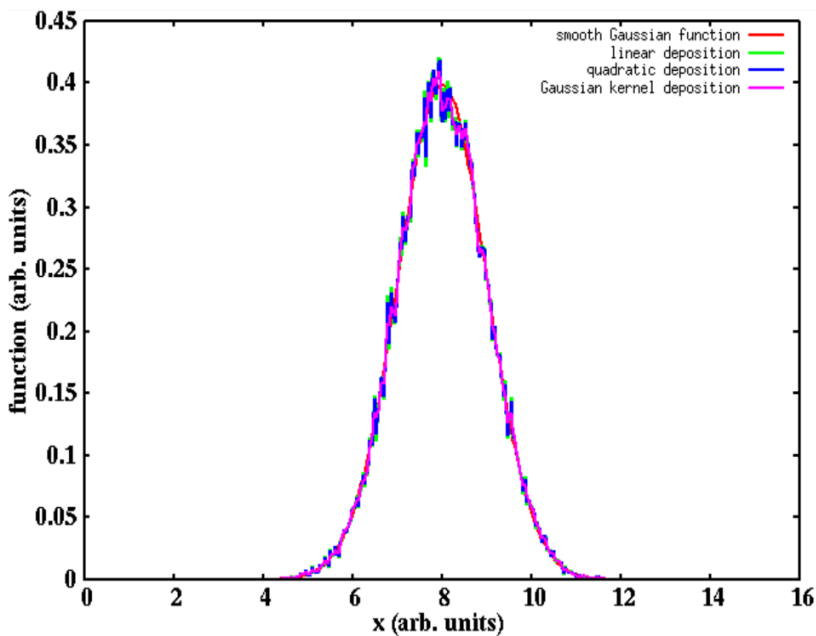
sextupole KL = 10, 64x64 modes



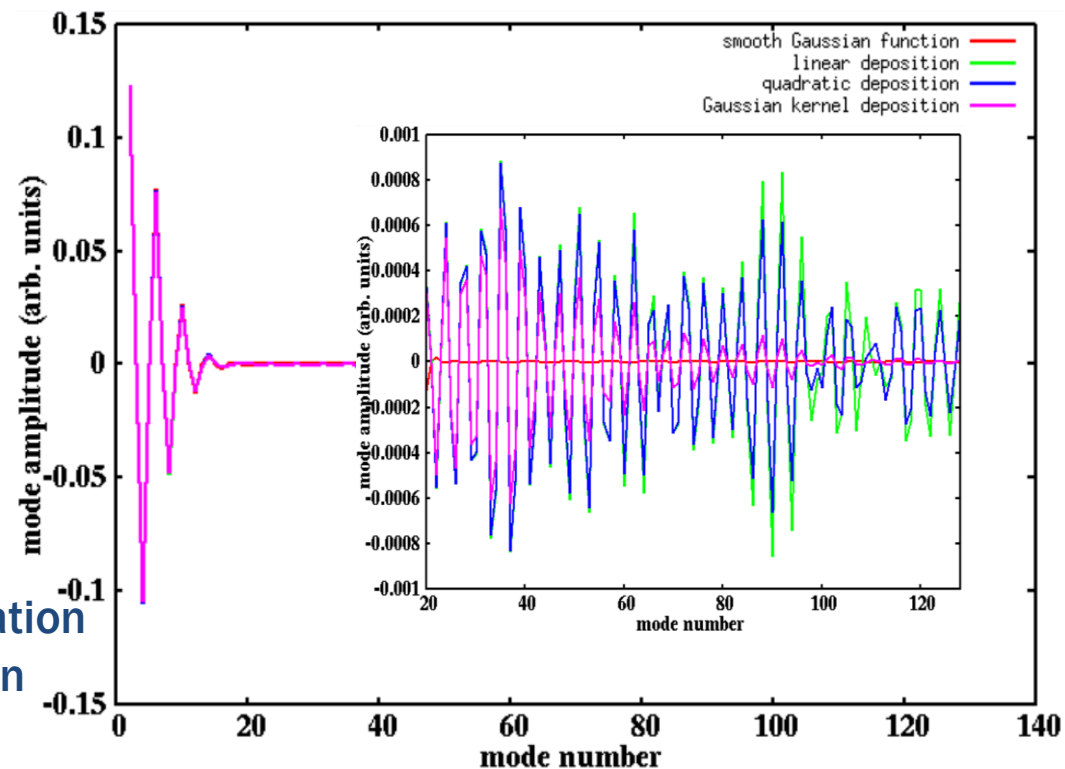
- Little emittance growth in the linear lattice
- Small emittance growth driven by the 3<sup>rd</sup> order resonance
- Sufficient number of macroparticles needed to suppress numerical emittance growth

# Understand the Numerical Emittance Growth from a 1D Model

The *smooth* and the reconstructed Gaussian distributions from macroparticle sampling with *linear*, *quadratic*, and *Gaussian kernel* deposition



The mode amplitude of the *smooth* and the reconstructed Gaussian distributions from macroparticle sampling with *linear*, *quadratic*, and *Gaussian kernel* deposition



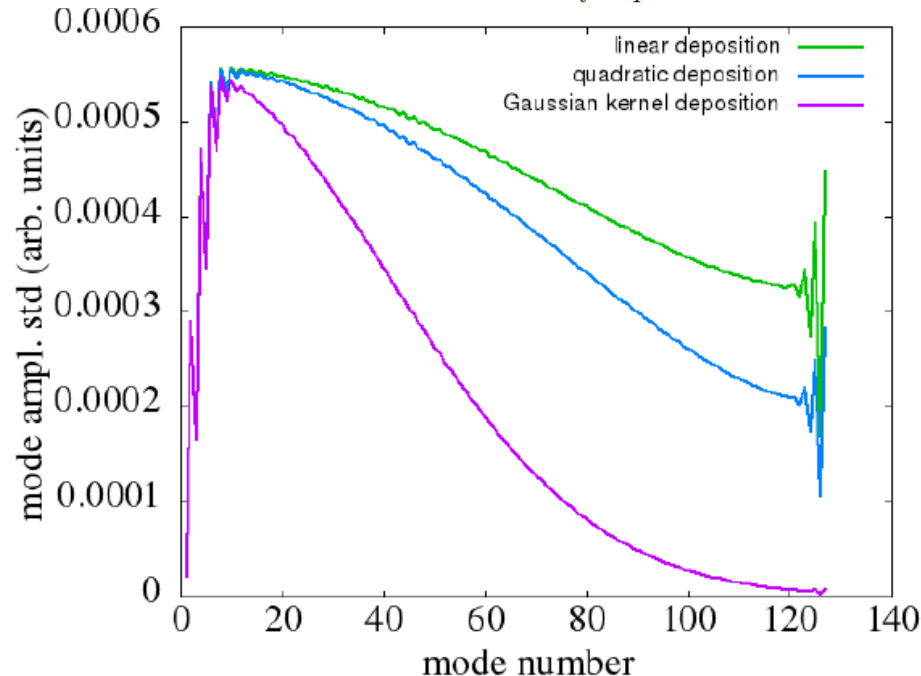
➤ Much larger mode amplitude fluctuation from the macroparticle depositions than that from the smooth distribution

# Quantify the Mode Amplitude Fluctuation with Standard Deviation

$$\rho^l = \frac{1}{N_p} \frac{2}{N_g \Delta x} \sum_i \sum_I S(x_I - x_i) \sin(\alpha_l x_i)$$

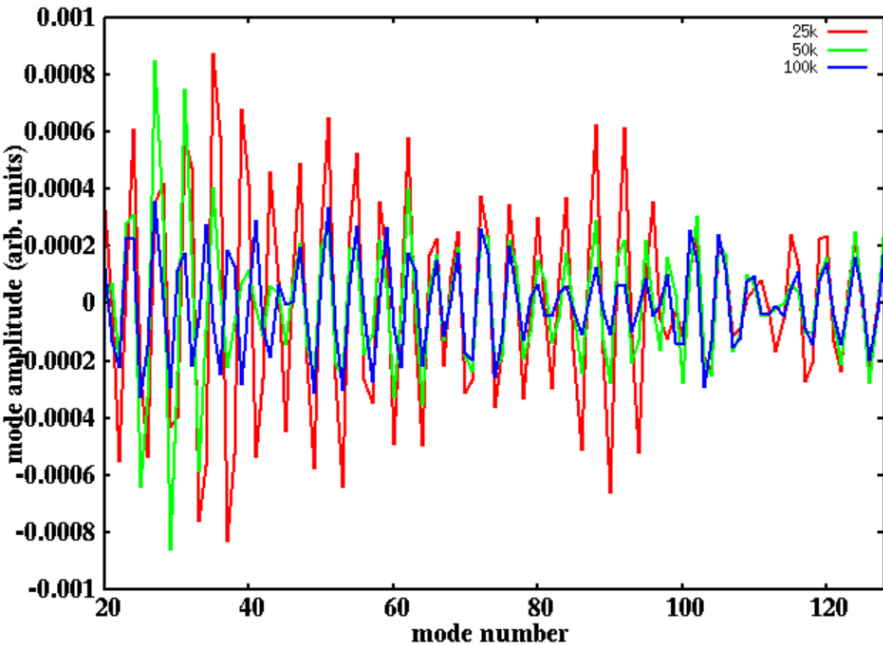
$$\text{var}(\rho^l) = \frac{1}{N_p} \text{var}\left(\frac{2}{N_g \Delta x} \sum_I S(x_I - x_i) \sin(\alpha_l x_i)\right)$$

$$\text{var}\left(\frac{2}{N_g \Delta x} \sum_I S(x_I - x_i) \sin(\alpha_l x_i)\right) \approx \frac{1}{N_p} \left(\frac{2}{N_g \Delta x}\right)^2 \sum_i \left[\sum_I S(x_I - x_i) \sin(\alpha_l x_i)\right]^2 - (\rho^l)^2$$

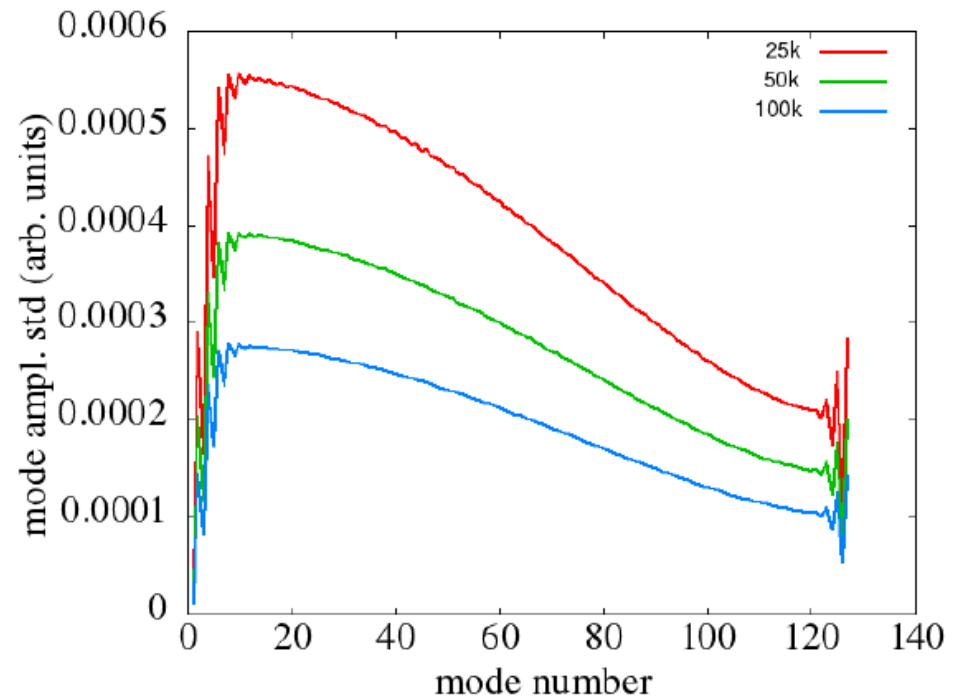


- Higher order macroparticle deposition scheme leads to smaller fluctuation

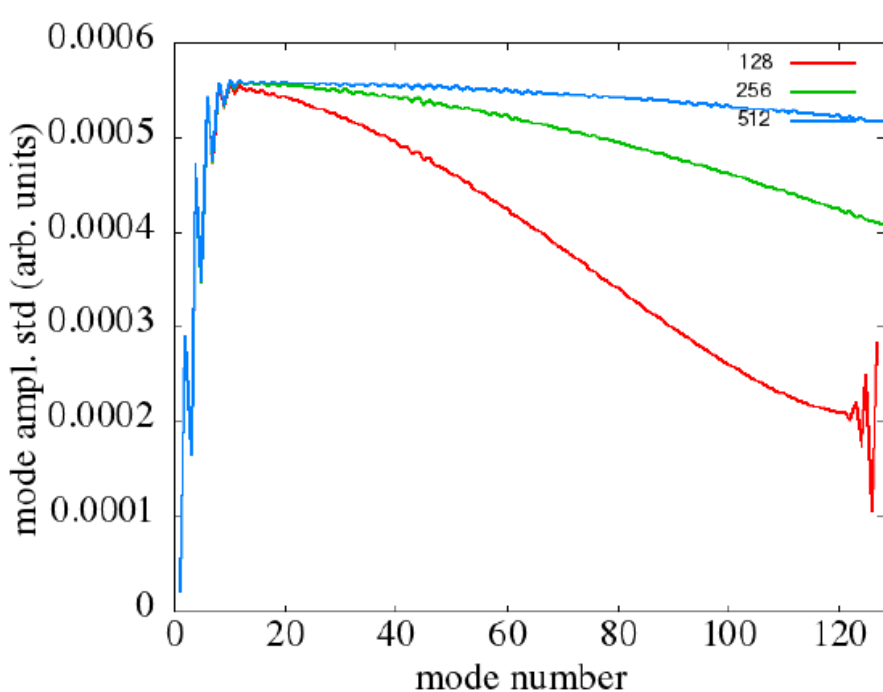
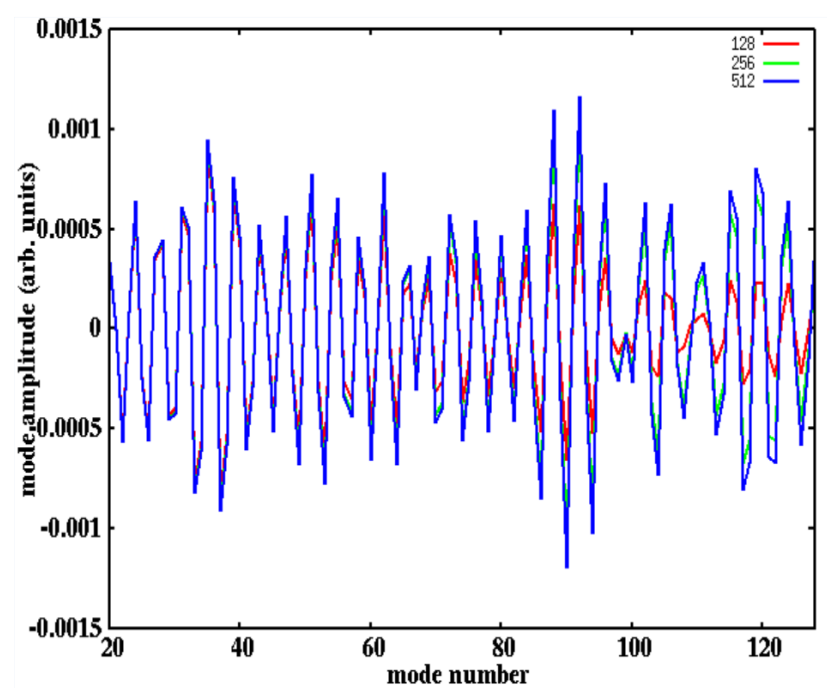
# Mode Amplitude Fluctuation Decreases with the Increase of Macroparticle Number



- Fluctuation standard deviation  $\sim 1/\sqrt{N_p}$



# Mode Amplitude Fluctuation Increases with the Increase of Grid Number



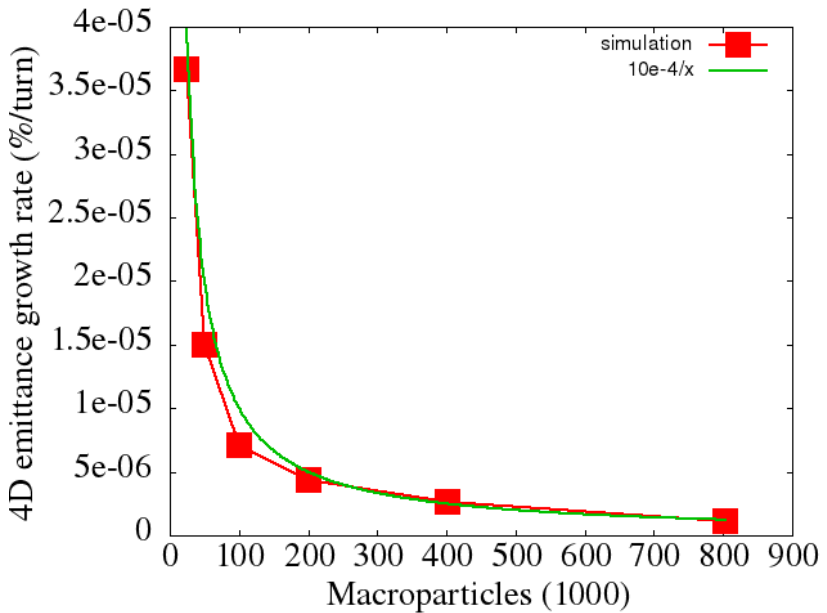
- Grid number mainly affects mode number > 10
- Larger grid number results in larger fluctuation

# Numerical Errors of in the Charge Density Distribution from Macroparticles Results in Numerical Emittance Growth

$$\Delta\epsilon \approx (\langle x^2 \rangle \langle x' \delta F \rangle - \langle x x' \rangle \langle x \delta F \rangle) \tau / \epsilon + \frac{1}{2} (\langle x^2 \rangle \langle (\delta F)^2 \rangle - \langle x \delta F \rangle^2) \tau^2 / \epsilon$$

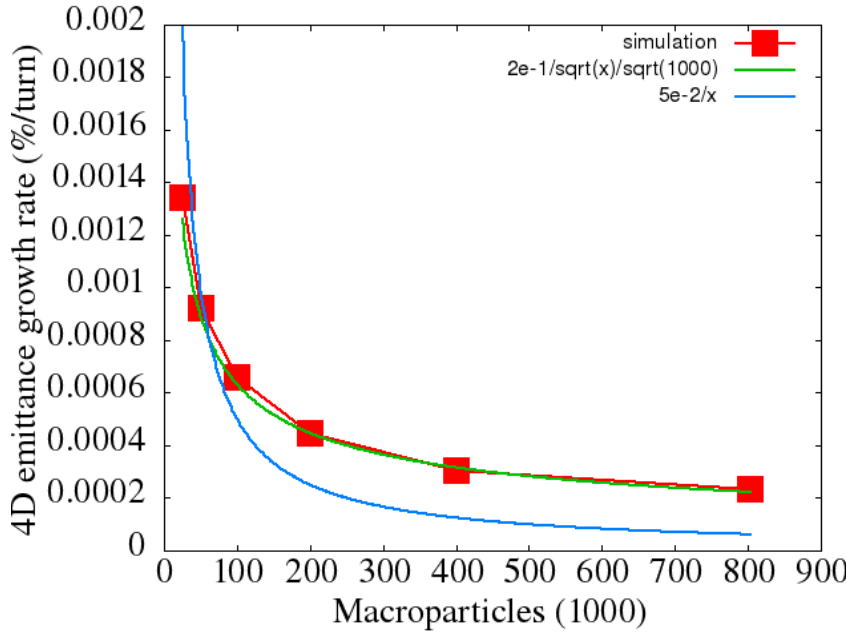
$$\frac{\Delta\epsilon}{\tau} \approx \frac{1}{2} \langle x^2 \rangle \langle (\delta F)^2 \rangle \tau / \epsilon$$

sextupole KL = 0, 64x64 modes



- Numerical emittance growth scales close to 1/Np as expected

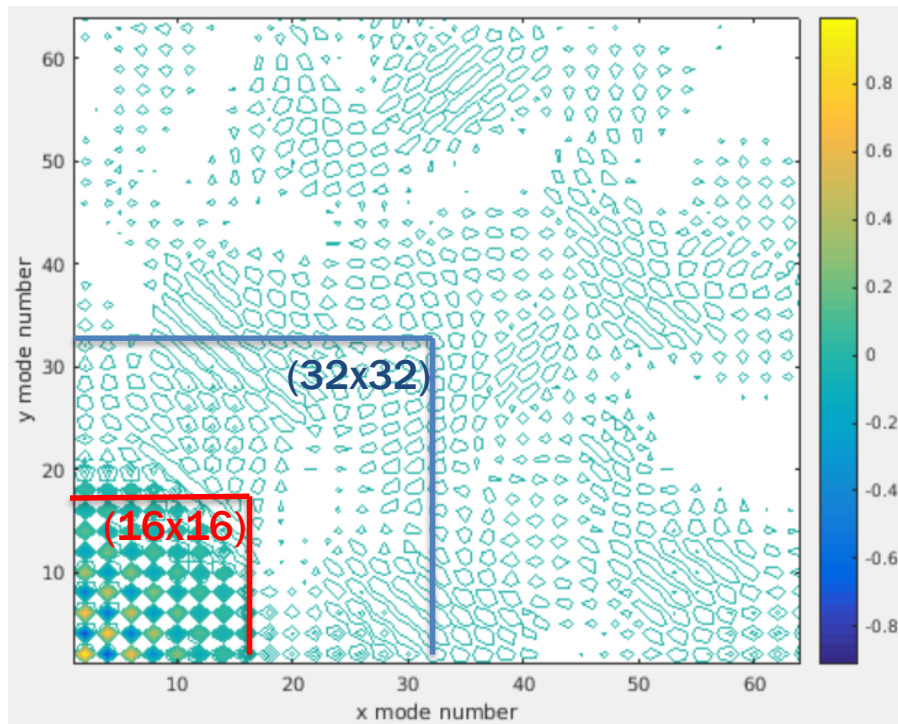
sextupole KL = 10, 64x64 modes



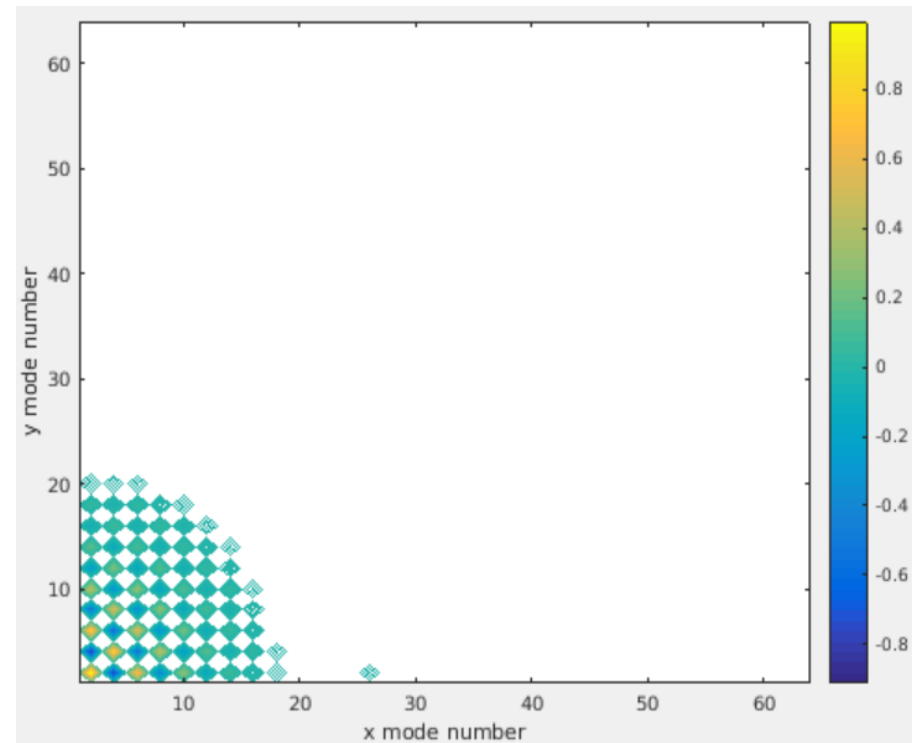
- Numerical emittance growth scales close to 1/sqrt(Np)
- The growth mechanism is more complicated

# Removing Small Amplitude Fluctuation Modes Using Relative Amplitude Threshold (1)

Spectral amplitude of a 2D Gaussian density  
(64x64 mode)

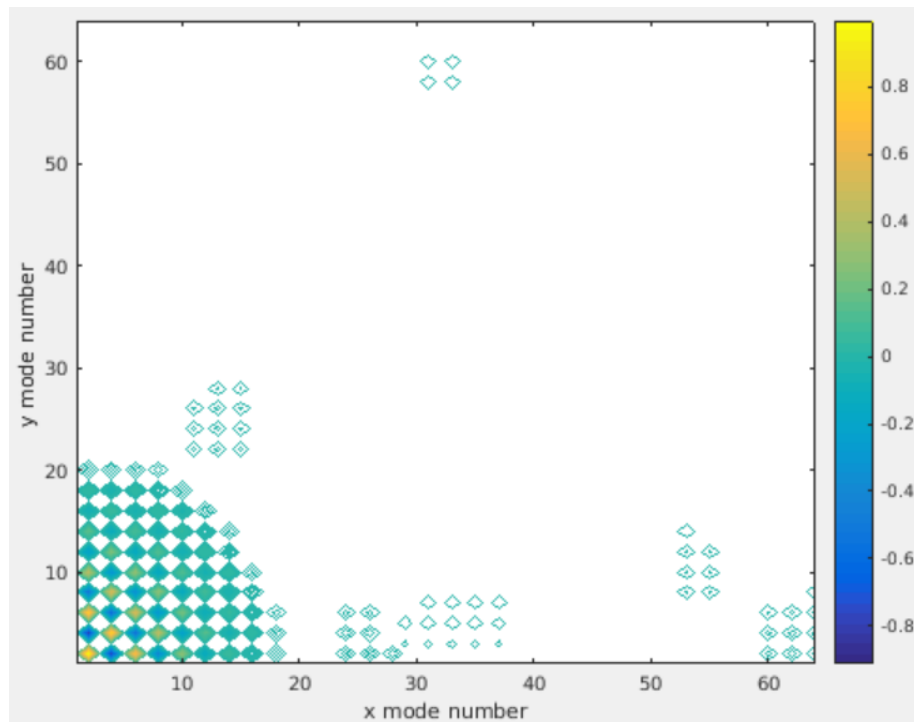


Spectral amplitude of a 2D Gaussian density  
with 1% threshold

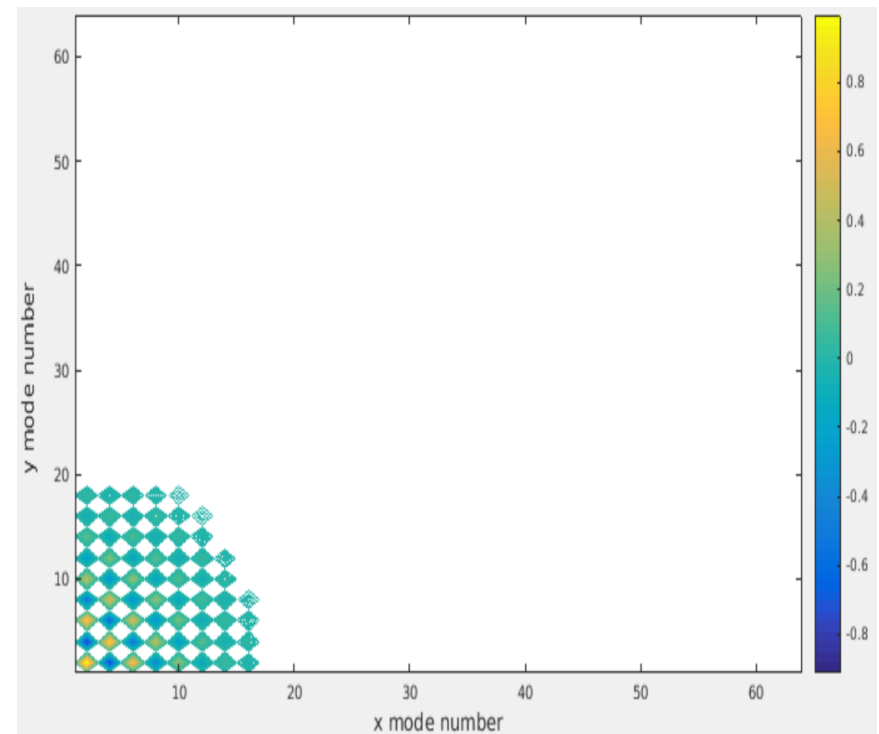


# Removing Small Amplitude Fluctuation Modes Using Relative Amplitude Threshold (2)

Spectral amplitude of a 2D Gaussian density with 2 sigma threshold



Spectral amplitude of a 2D Gaussian density with 4 sigma threshold

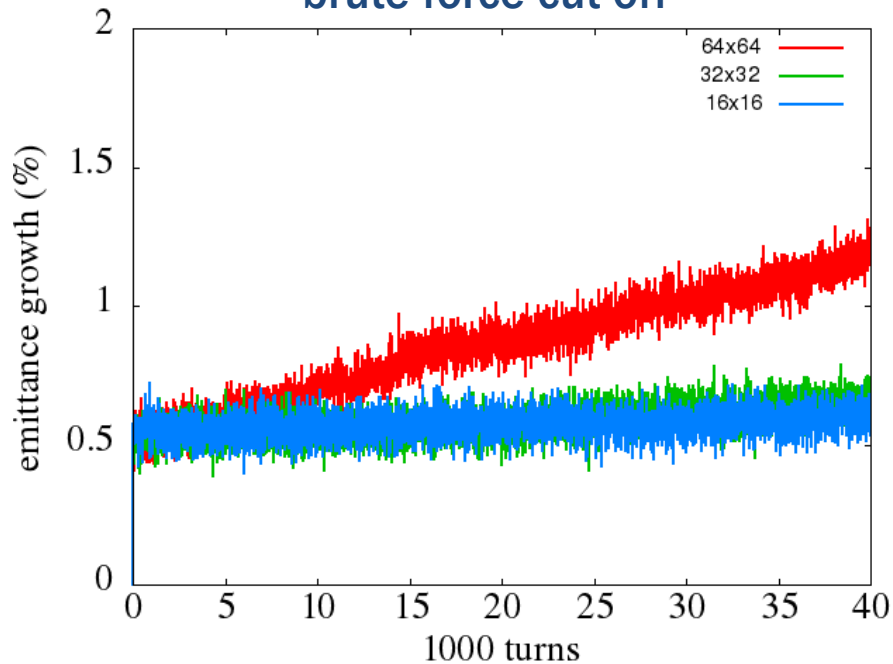




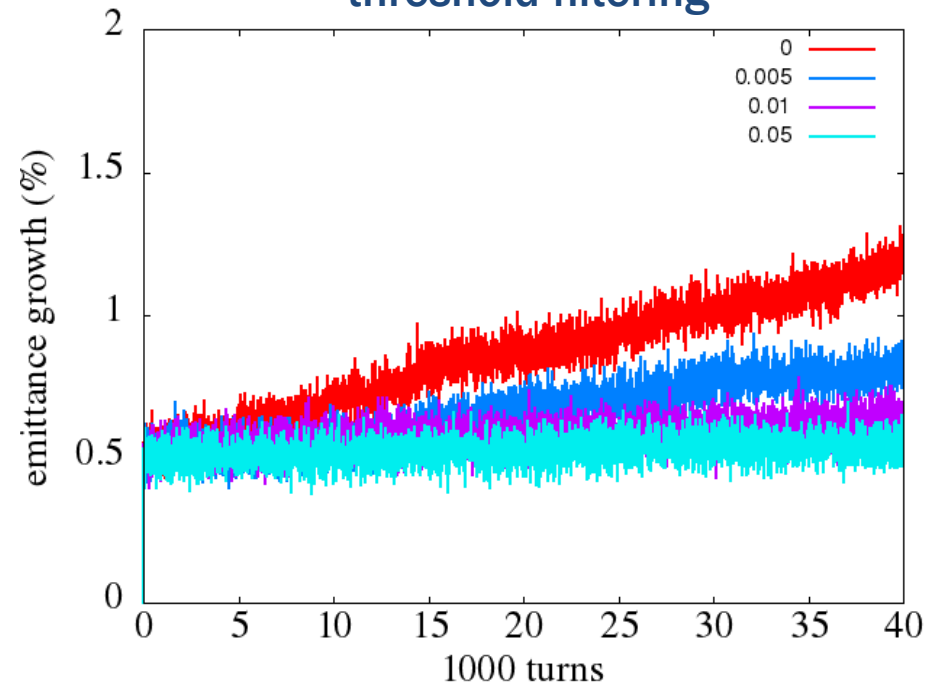
# Mitigate the Numerical Emittance Growth by Removing High Frequency Modes in Linear Lattice

sextupole KL = 0, current = 30 A, 25 k macroparticles

brute force cut-off



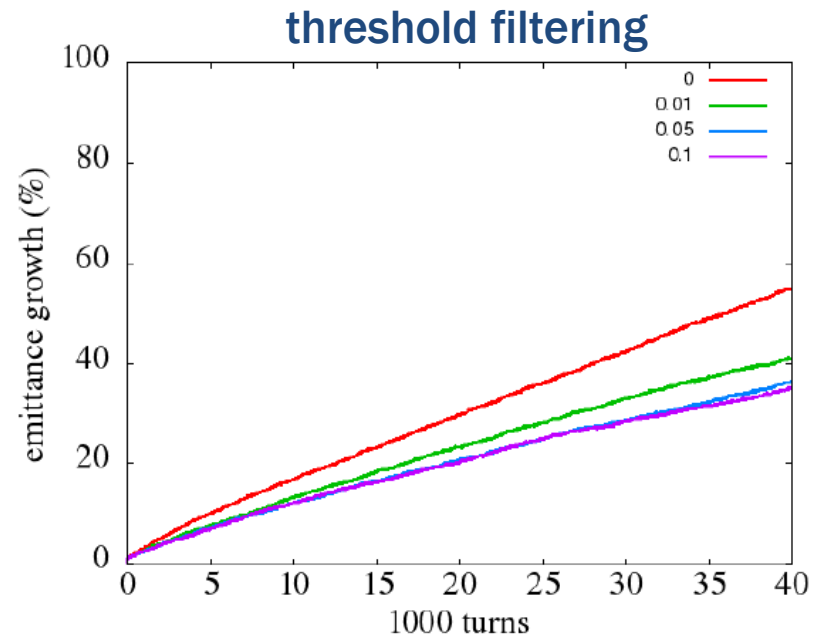
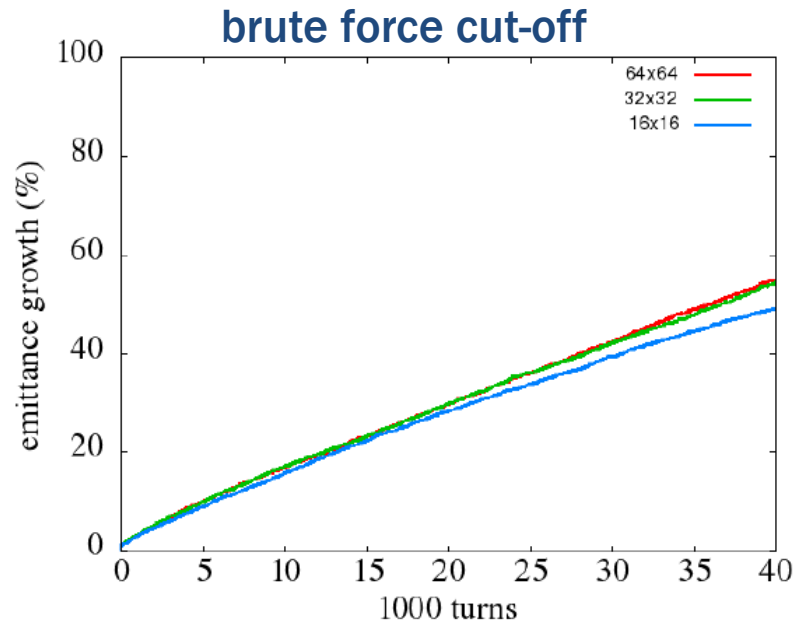
threshold filtering



- Both numerical filters work well
- Numerical emittance growth is mainly due high frequency errors

# Mitigate the Numerical Emittance Growth through Threshold Filtering in Nonlinear Lattice

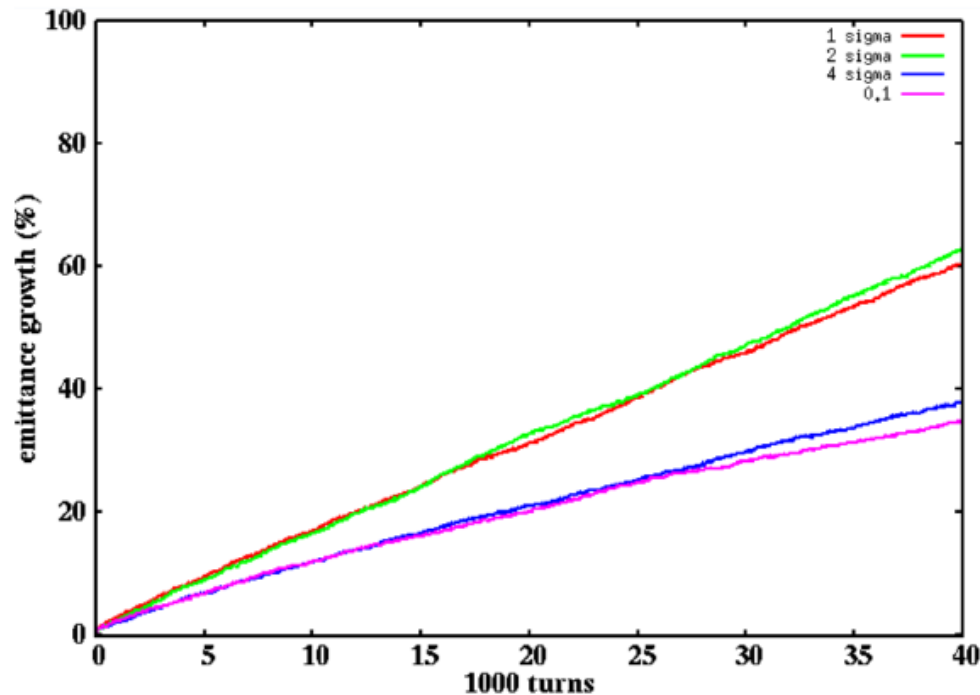
sextupole KL = 10, current = 30 A, 25 k macroparticles



- Direct brute force cut-off filtering is not efficient
- Numerical emittance growth can be mitigated with threshold filtering
- The numerical growth is mainly due low frequency errors

# Predefined Maximum Fraction and Four Sigma Threshold Filtering Yields Similar Emittance Growth

sextupole KL = 10, current = 30 A, 25 k macroparticles



## Maximum Fraction

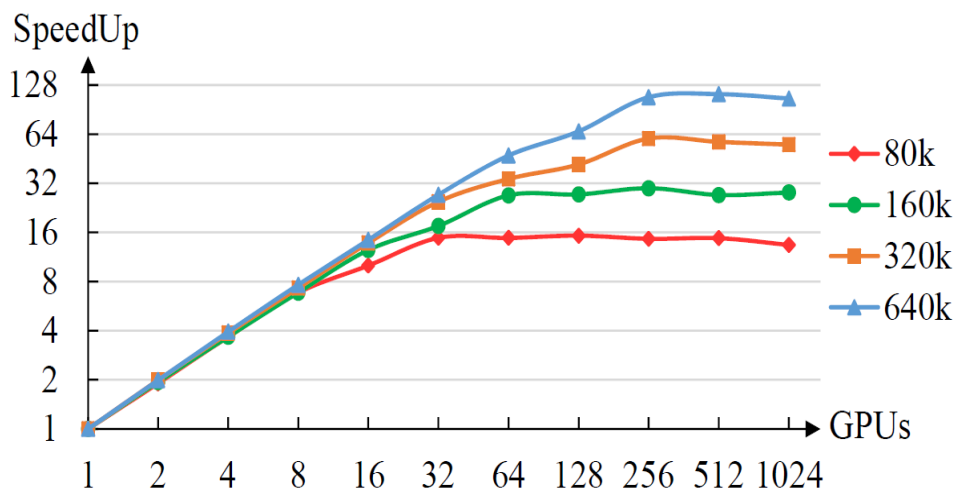
- Pro – easy to calculate the threshold value
- Con – another hyperparameter

## Standard Deviation

- Pro – calculate the threshold value dynamically
- Con – computationally expensive

# Computational Complexity

- Symplectic PIC/Spectral PIC:  $O(N_p) + O(N_g \log(N_g))$ , parallelization can be a challenge
- Symplectic gridless particle:  $O(N_m N_p)$ , easy parallelization



Z. Liu and J. Qiang, “Symplectic multi-particle tracking on GPUs,”  
Computer Physics Communications, 226, 10 (2018).

# Summary

- Symplectic space-charge model will help improve the accuracy of simulation for long-term simulation.
- Numerical emittance growth from finite macroparticle sampling can be mitigated using threshold filtering in frequency domain.
- For small number of modes and particles used, the symplectic gridless particle model can be computationally efficient; otherwise, the symplectic PIC model would be more efficient.