Comparison of Symplectic PIC, Symplectic Gridless Particle, and Non-Symplectic PIC for Long Term Space-Charge Simulation

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A Symplectic Multi-Particle Tracking Model (1)

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

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

space-charge Coulomb potential

external focusing/acceleration

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

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

$$\frac{d\zeta}{ds} = -[H, \zeta]$$

A formal single step solution

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

$H = H_1 + H_2$

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

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

J. Qiang, "A Symplectic Multi-Particle Tracking Model for Self-Consistent Space-Charge Simulation," Phys. Rev. ST Accel. Beams 20, 014203 (2017).

A Symplectic Multi-Particle Tracking Model (2)

2nd order:

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

4th order:

$$\mathcal{M}(\tau) = \mathcal{M}_1(\frac{s}{2})\mathcal{M}_2(s)\mathcal{M}_1(\frac{\alpha s}{2})\mathcal{M}_2((\alpha-1)s)\mathcal{M}_1(\frac{\alpha s}{2})\mathcal{M}_2(s)\mathcal{M}_1(\frac{s}{2})$$

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

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

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

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

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

$$M_2 = \begin{pmatrix} I & 0 \\ L & I \end{pmatrix}$$

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)

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = -\frac{\rho}{\epsilon_0}$$

$$\begin{aligned} \phi(x=0,y) &= 0 \\ \phi(x=a,y) &= 0 \\ \phi(x,y=0) &= 0 \\ \phi(x,y=b) &= 0 \end{aligned}$$

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

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

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

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

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

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

Self-Consistent Space-Charge Transfer Map (2)

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

$$\phi^{lm} = \frac{4\pi}{\gamma_{lm}^2}\frac{4}{ab}\frac{1}{N_p}\sum_{j=1}^{N_p}\int_0^a\int_0^b S(x-x_j)S(y-y_j)\sin(\alpha_l x)\sin(\beta_m y)dxdy$$

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

$$\phi(x_i,y_i) = \int_0^a\int_0^b \phi(x,y)S(x-x_i)S(y-y_i)dxdy$$

$$\varphi(x_i,y_i,x_j,y_j) = 4\pi\frac{4}{ab}\frac{1}{N_p}\sum_{l=1}^{N_l}\sum_{m=1}^{N_m}\frac{1}{\gamma_{lm}^2}\int_0^a\int_0^b S(x-x_j)S(y-y_j)\sin(\alpha_l x)\sin(\beta_m y)dxdy$$
$$\int_0^a\int_0^b S(x-x_i)S(y-y_i)\sin(\alpha_l x)\sin(\beta_m y)dxdy$$

Self-Consistent Space-Charge Transfer Map (3)

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

Symplectic Gridless Particle Model

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

w is the particle charge weight

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

$\mathcal{M}_2$

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

Symplectic PIC Model (1)

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

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

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

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

Symplectic PIC Model (2)

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

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

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

Symplectic PIC Model (3)

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

$\mathcal{M}_2$ →

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

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

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

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

Non-Symplectic PIC Model

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

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

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

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

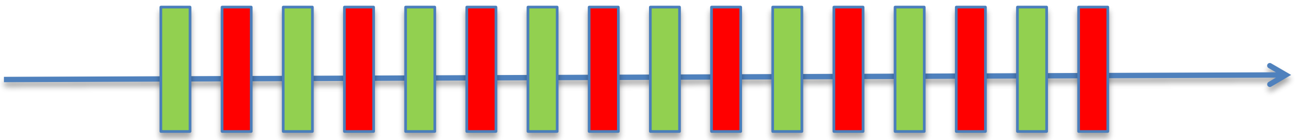
$$E_y(x_I, y_J) = -\sum_{l=1}^{N_l}\sum_{m=1}^{N_m} \beta_m \phi^{lm} \sin(\alpha_l x)\cos(\beta_m y)$$

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

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

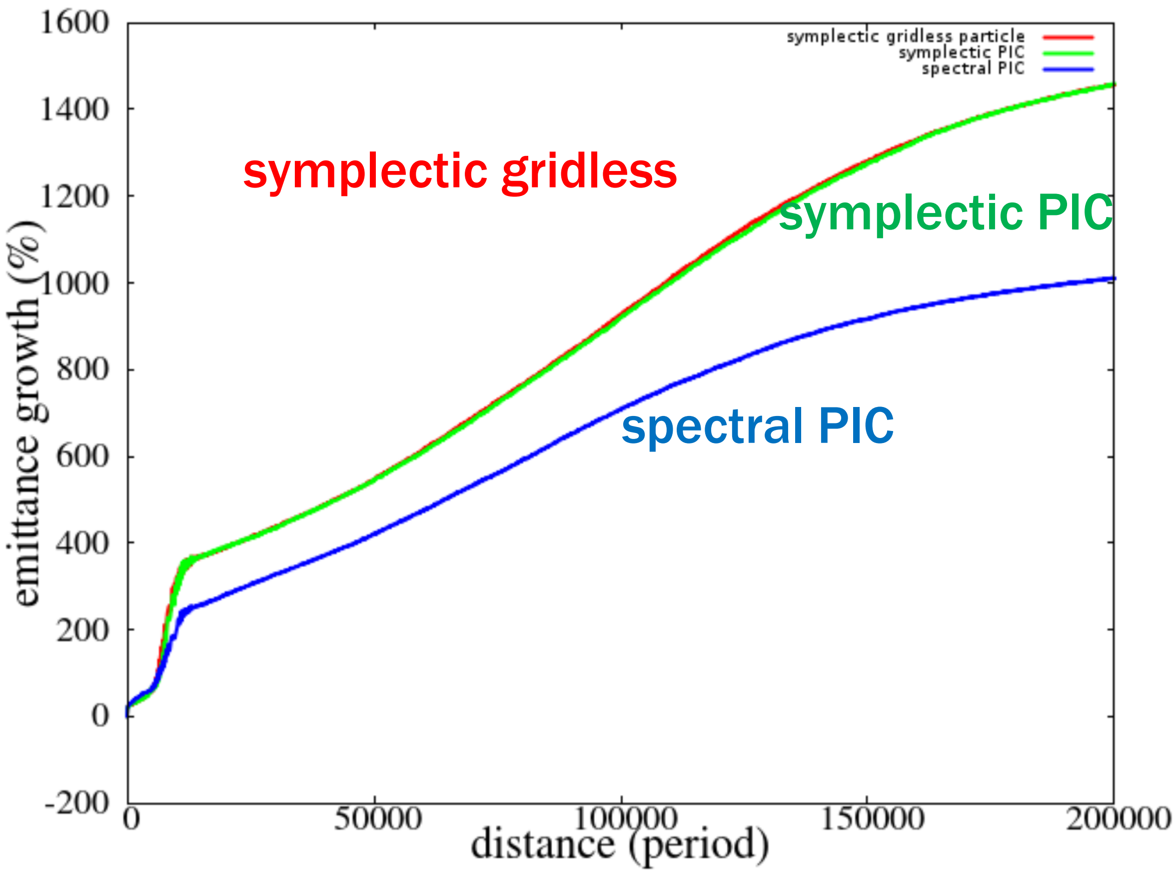
$$\mathbf{r}(\tau)_i = \mathbf{r}(\tau/2)_i + \frac{1}{2}\tau\mathbf{p}_i(\tau)$$

Benchmark Case 1: FODO Lattice, Below 2nd Order Envelop Instability



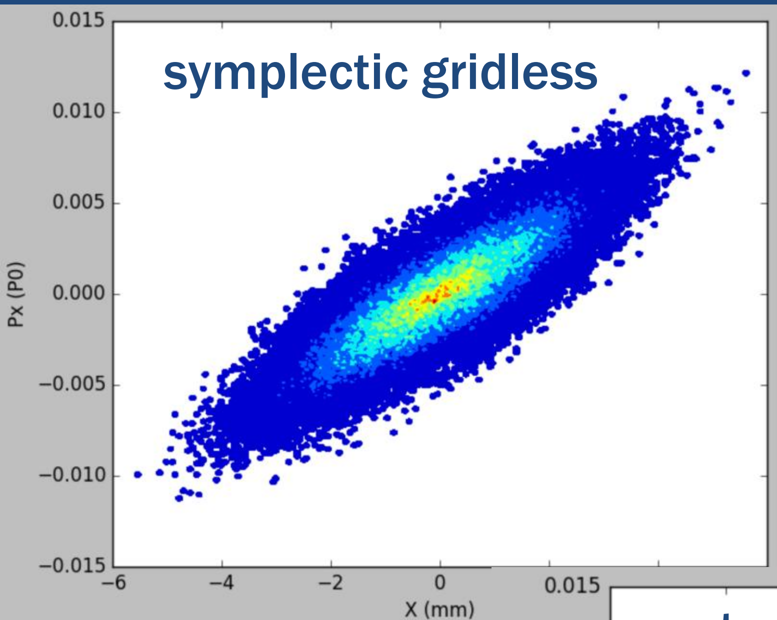
- 1 GeV proton beam
- FODO lattice
- 0 current phase advance: 85 degrees
- Initial 4D Gaussian distribution

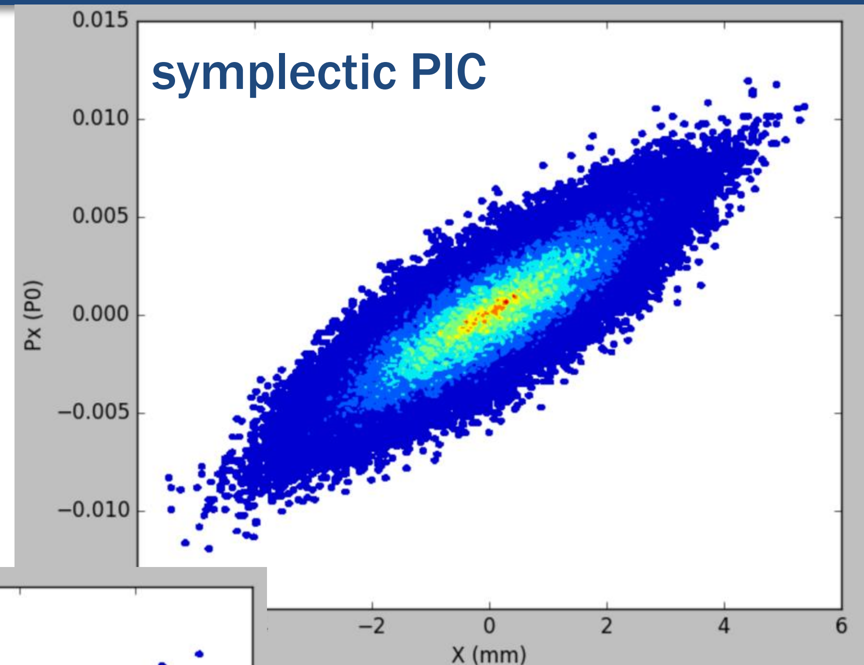
Significant Difference in Final 4D Emittances Between the Symplectic and the Non-Symplectic Methods (Strong Space-Charge: Phase Advance Change 85 -> 42)

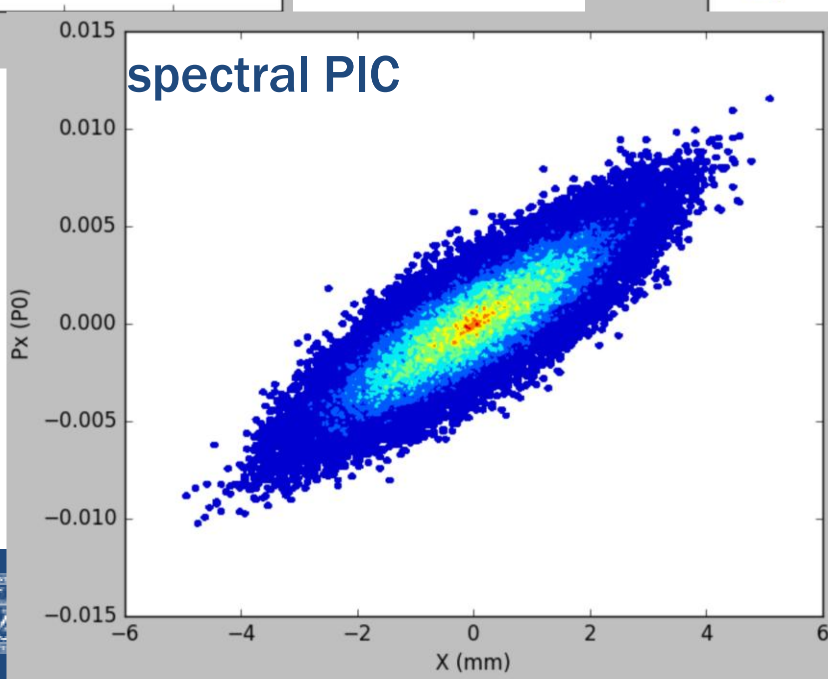


Two symplectic approaches show good agreement.

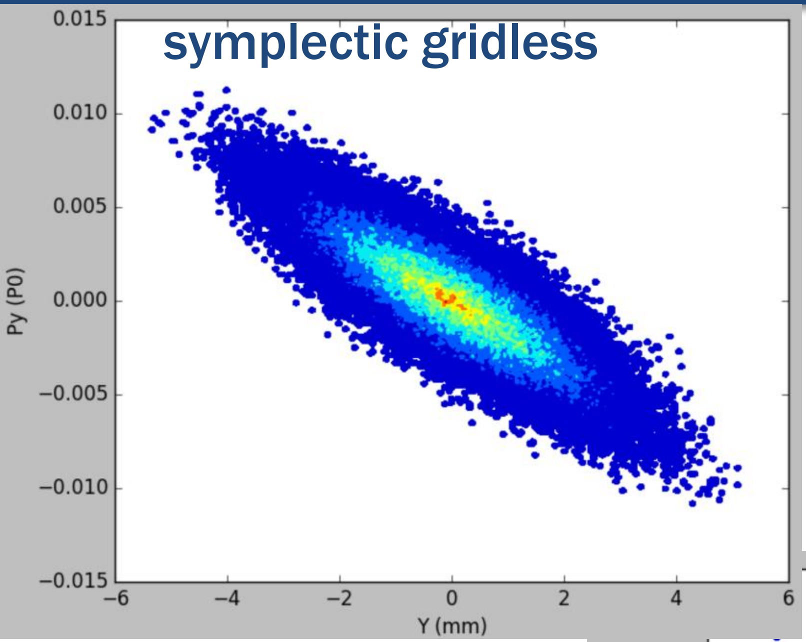
Final Beam X-Px Phase Spaces Have Similar Shapes
Non-Symplectic Model Has Smaller Area

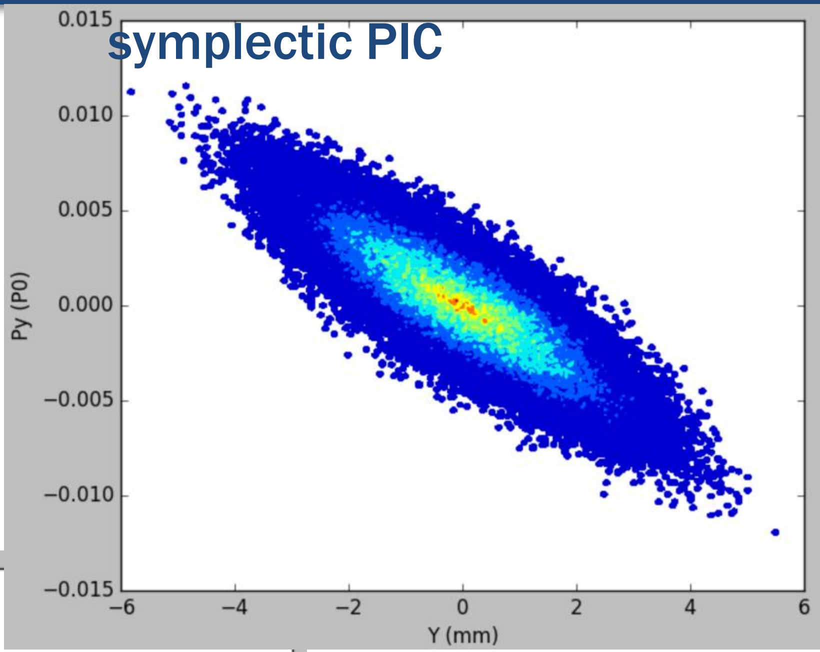


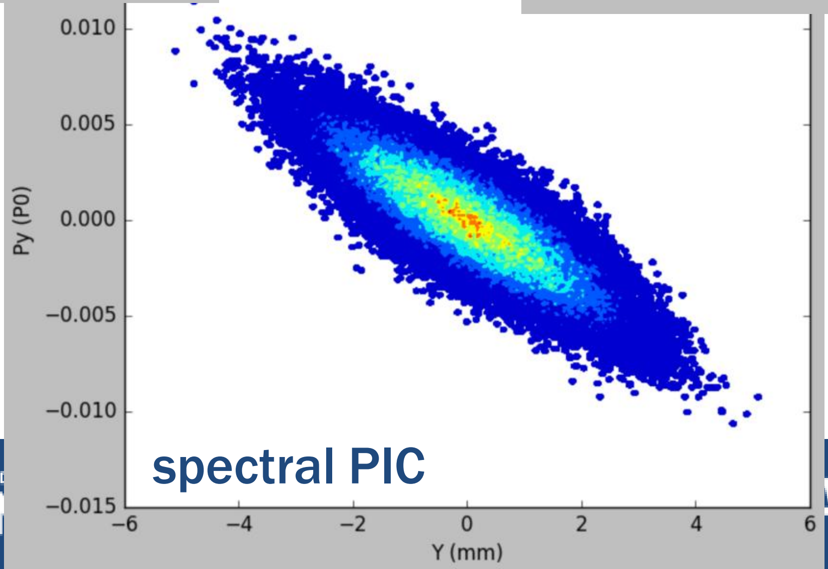




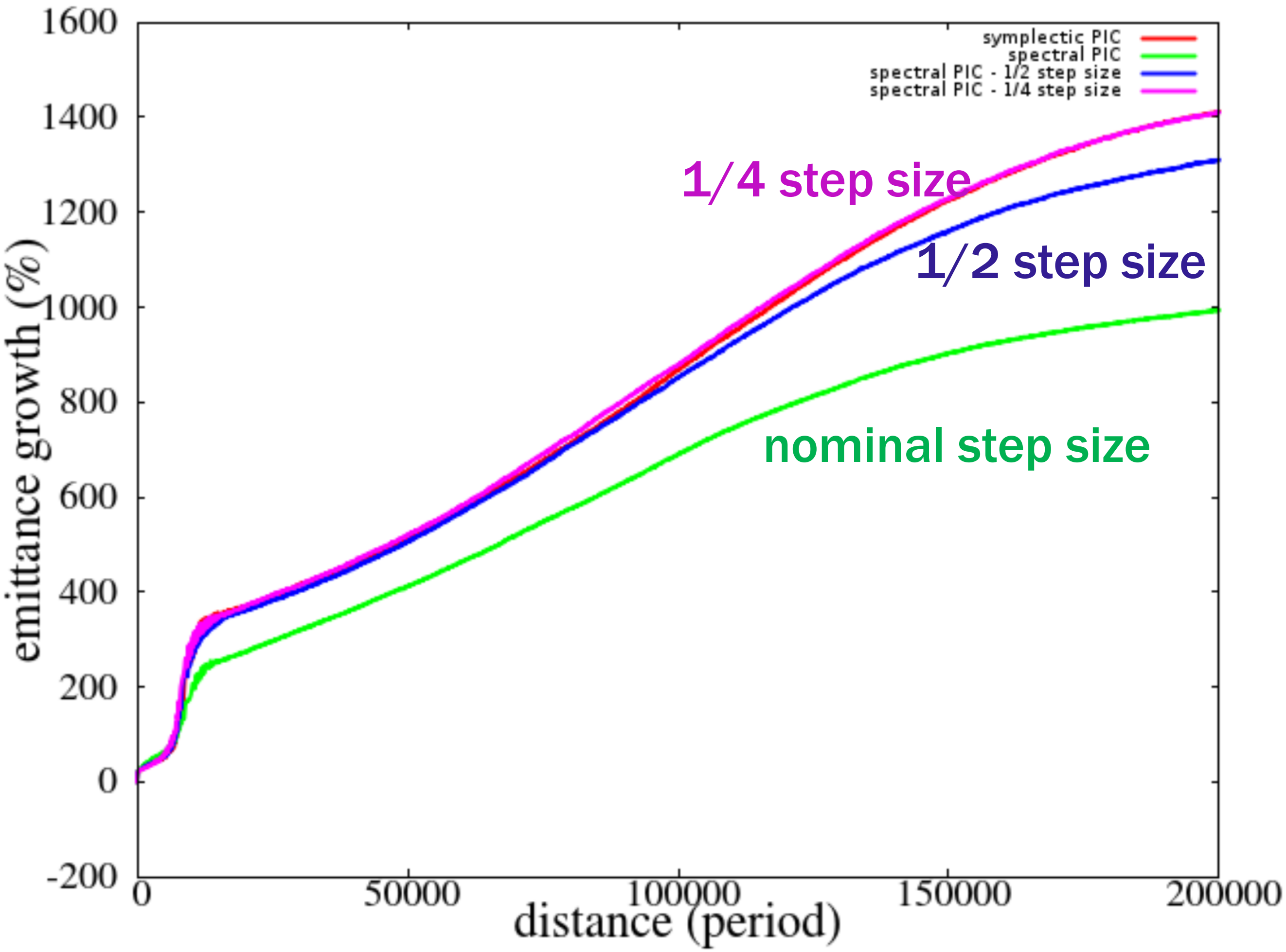
Final Y-Py Phase Space Show Similar Shapes



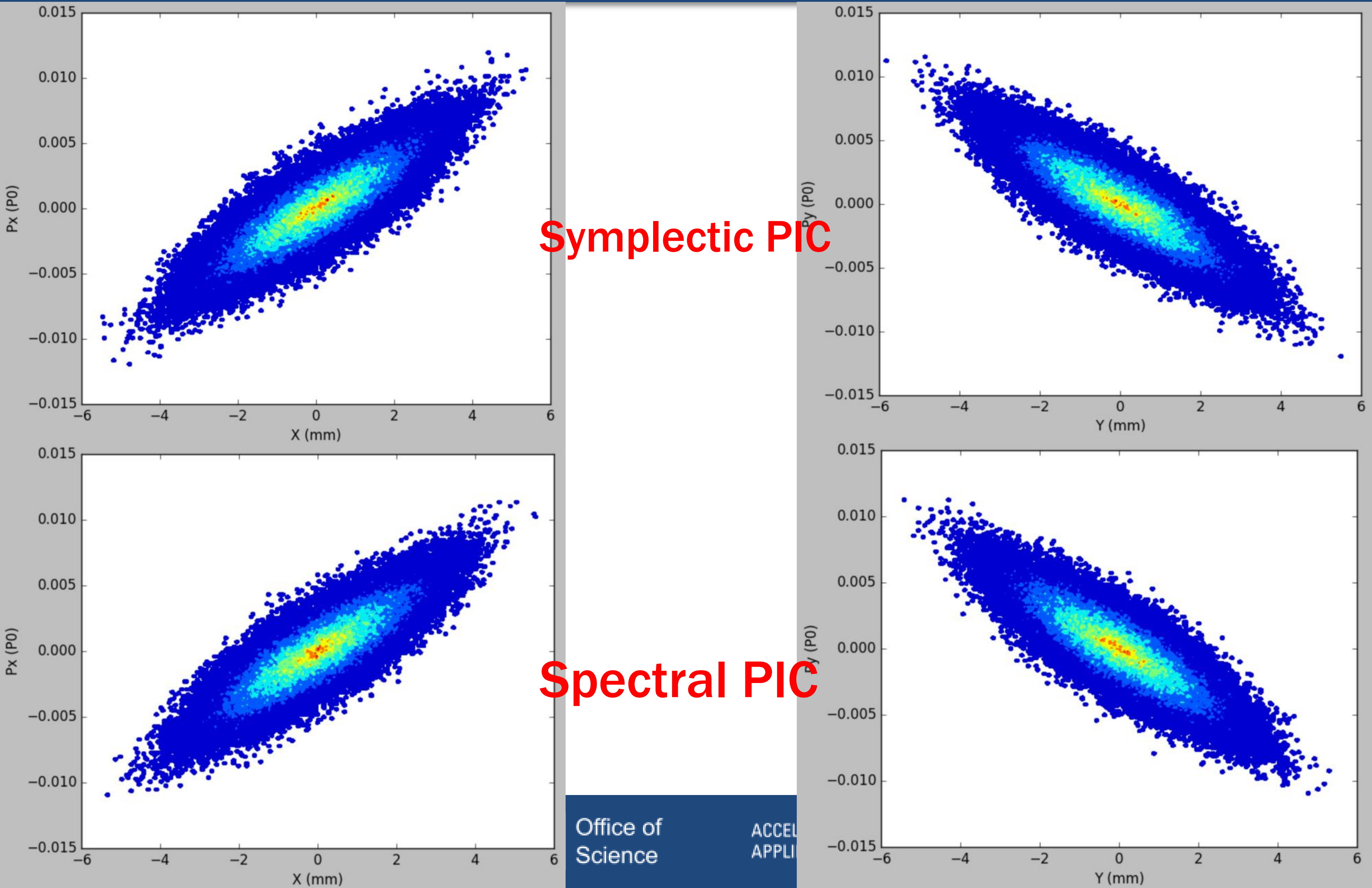




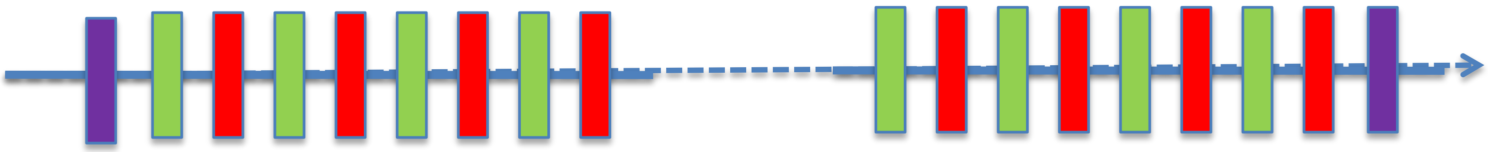
Finer Step Size Needed for Non-Symplectic PIC (Symplectic PIC vs. Non-Symplectic PIC)



Final Transverse Phase Space: Symplectic PIC vs. Spectral PIC

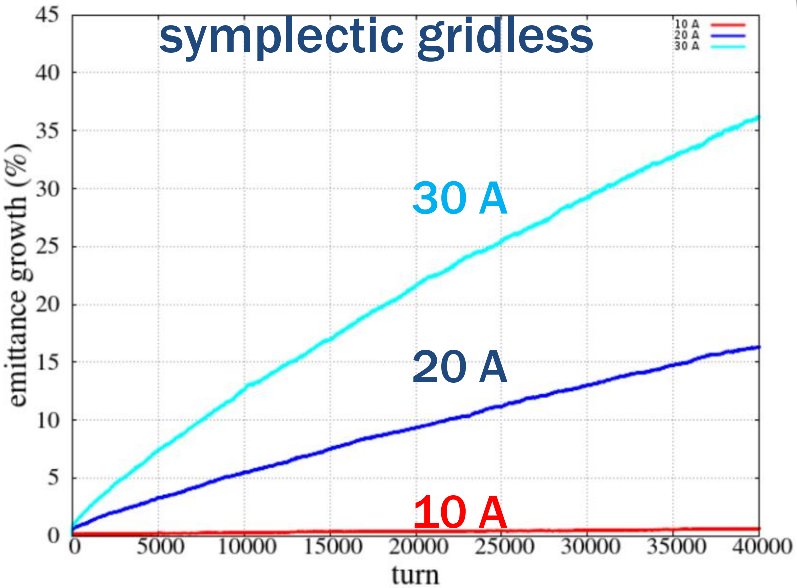


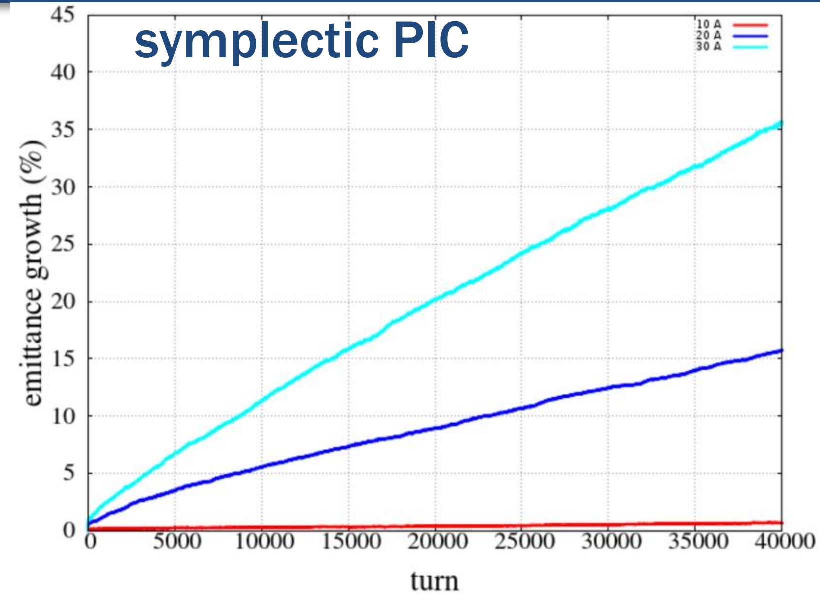
Benchmark Case 2: 1 Turn = 10 FODOs + 1 Sextupole

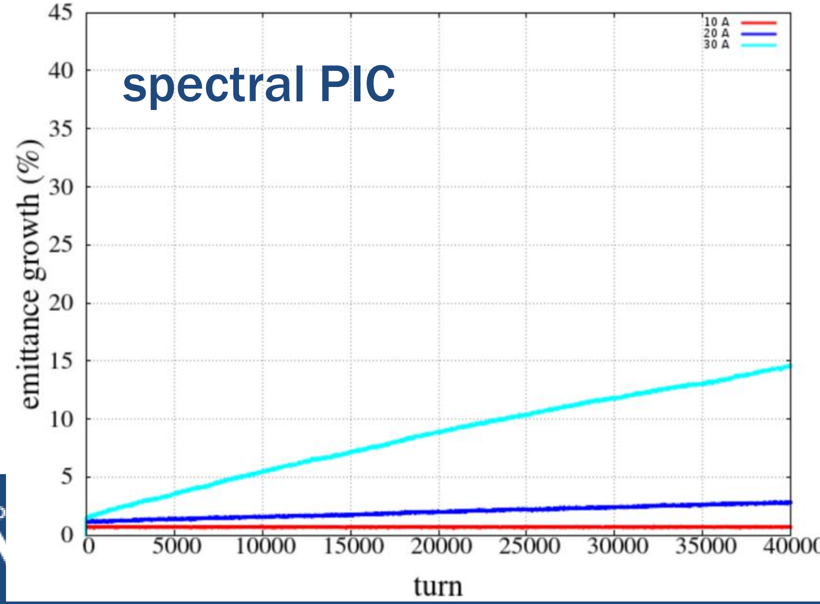


- 0 current tune 2.417
- sextupole KL = 10 T/m/m

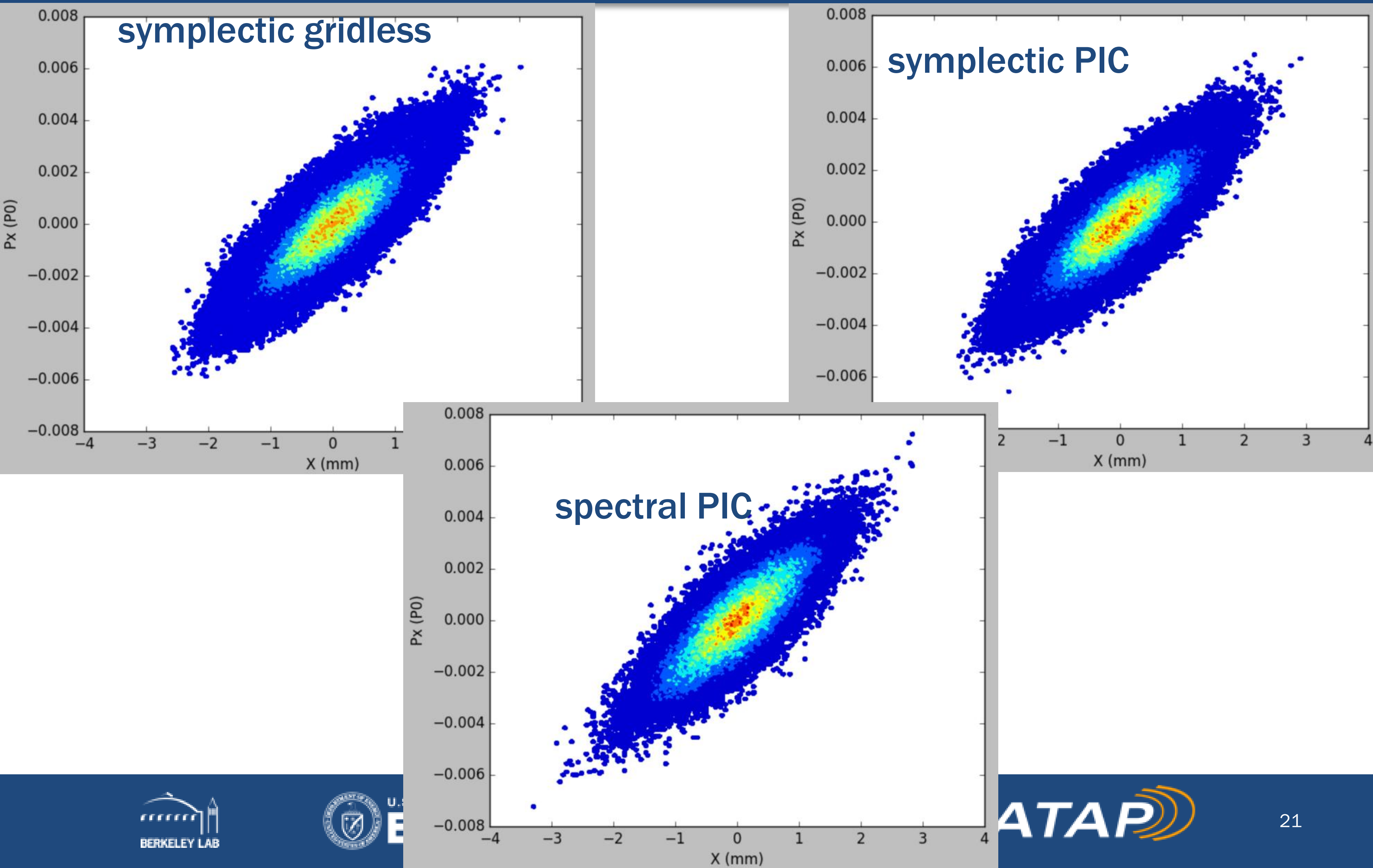
Non-Symplectic PIC Shows Much Less Emittance Growth Compared with Two Symplectic Models (4D Emittance Evolution with Different Currents)



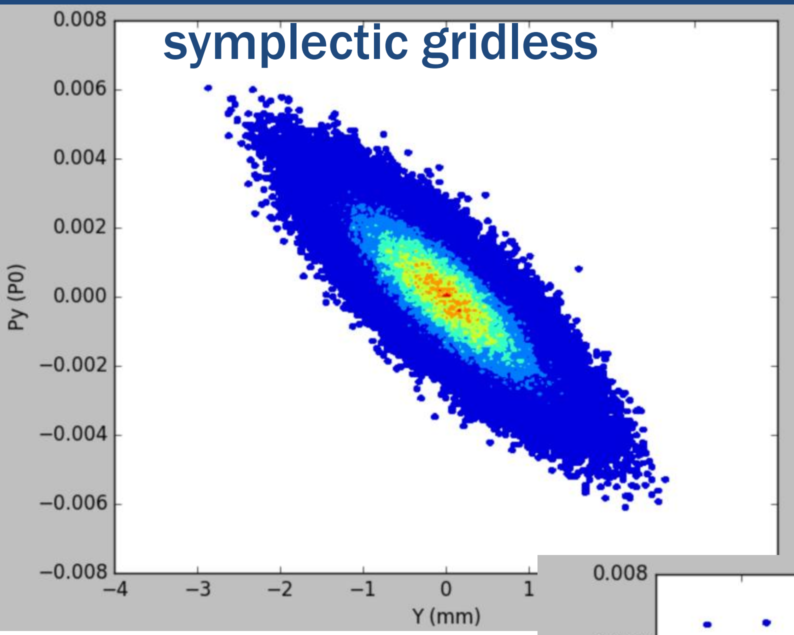


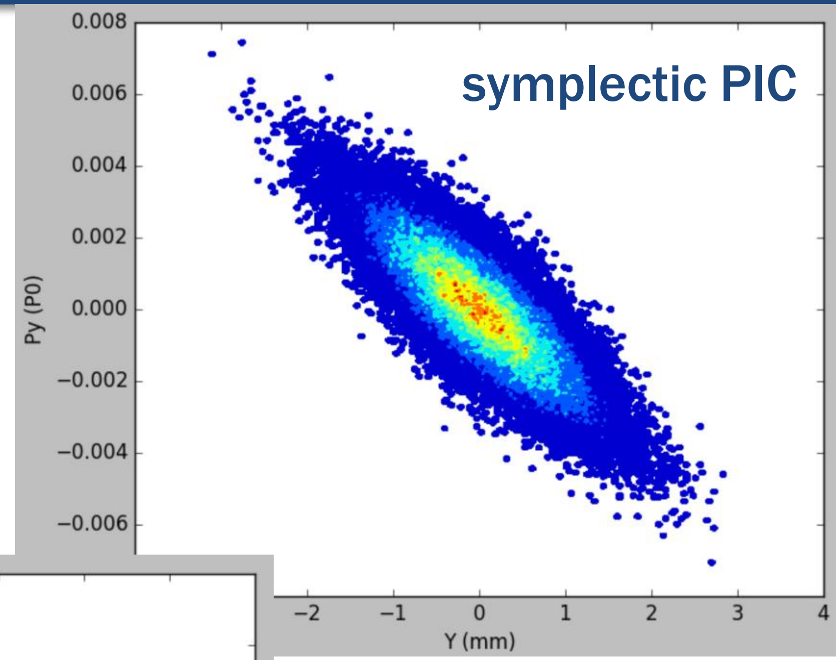


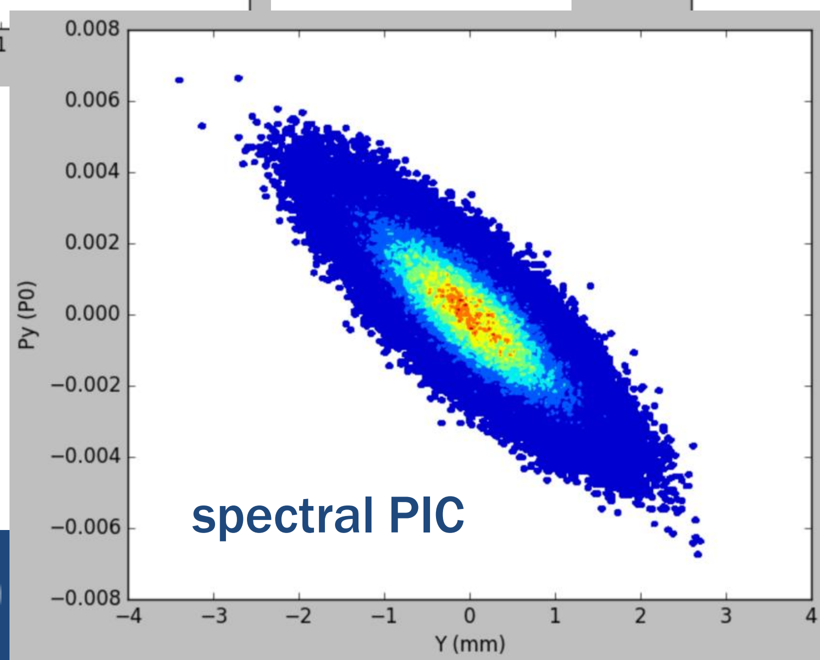
Final Beam X-Px Phase Spaces Have Similar Shapes



Final Beam Y-Py Phase Spaces Have Similar Shapes

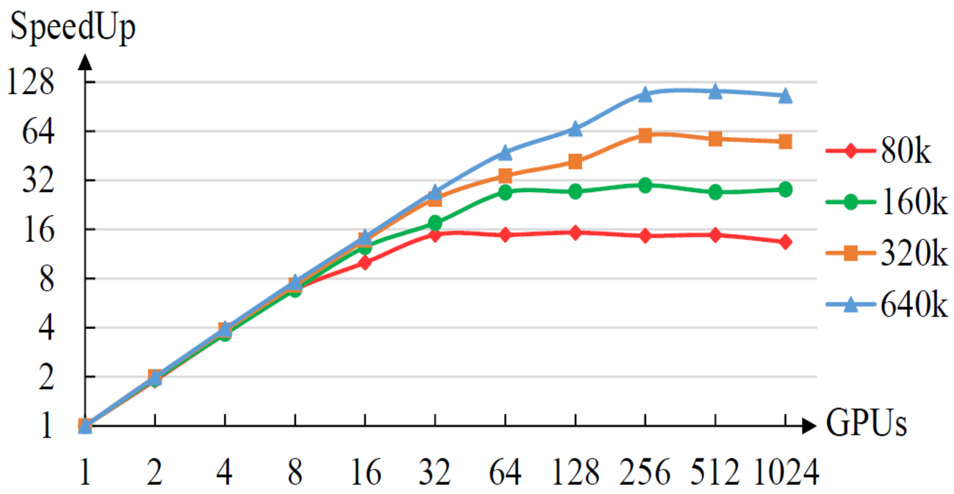






Computational Complexity

- Symplectic PIC/Spetral PIC: O(Np) + O(Ng log(Ng)), parallelization can be a challenge
- Symplectic gridless particle: O(Nm Np), easy parallelization



Z. Liu and J. Qiang, "Symplectic multi-particle tracking on GPUs," submitted to Computer Physics Communications, 1997.

Summary

- Using the same step size, same number of modes, with sufficient grid points, the symplectic PIC and the symplectic gridless particle model agree with each other very well.
- Using same step size, the non-symplectic PIC yields significantly different emittance growth.
- All three models show similar final phase space shapes.
- Using sufficient small step size, all three methods converge to the similar emittance growth (Is this too optimistic?)
- 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.

Thank You!