

A New RFQ Model and Symplectic Multi-Particle Tracking in the IMPACT Code Suite

Ji Qiang

HB 2016, July 3-9, Malmo, Sweden



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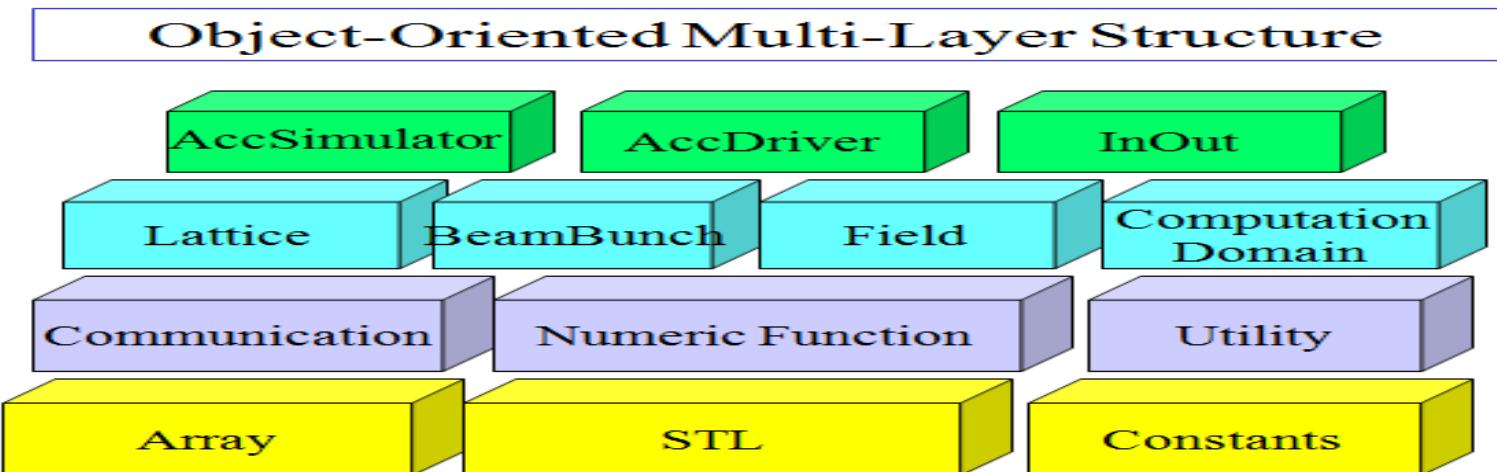
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Outline

- **Introduction**
- **A new RFQ model (in collaboration with Z. Wang and H. P. Li of Peking University)**
- **Symplectic multi-particle tracking for space-charge simulation**
- **Conclusions**

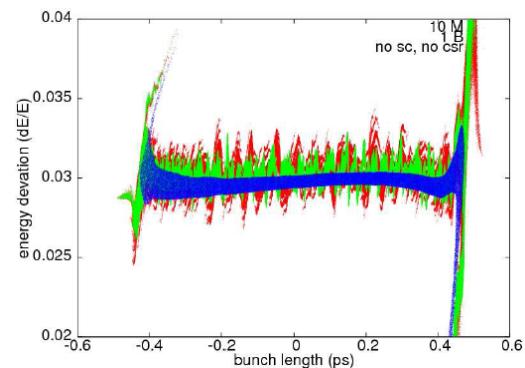
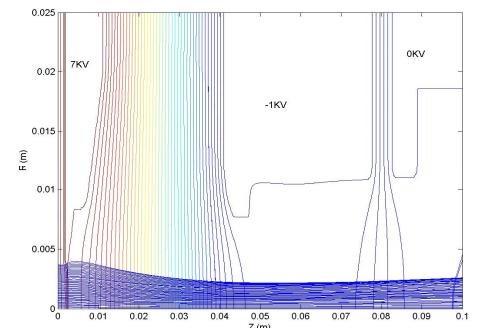
IMPACT: Integrated Map and Particle Tracking Code

- The IMPACT(-Z depend.) started around middle of 90s (R. Ryne) including:
 - Drift, Quadrupole, RF linear transfer map
 - one 3D space-charge solver with open BCs
 - a few thousand lines of High Performance Fortran (HPF) code
- Redesign of the IMPACT code around the end of 90s (J. Qiang):
 - object-oriented design and implementation using F90
 - domain decomposition parallelization using MPI
 - multiple 3D space-charge solvers with open BCs, periodic BCs, conducting pipes



IMPACT: Recent Advances

- Current Features (with >100,000 lines of code) include:
 - Z dependent and T dependent tracking
 - Detailed 3D RF accelerating and focusing model, dipole, solenoid, multipole, ...
 - Multiple charge states, multiple bunches
 - 3D shifted-integrated Green's function space-solver
 - 3D spectral finite difference multigrid space-solver
 - Structure + resistive wall wakefields
 - CSR/ISR
 - Gas ionization
 - Photo-electron emmission
 - Machine errors and steering
- Can be used to model beam dynamics in:
 - Photoinjectors
 - Ion beam formation and extraction
 - RF linacs
 - Rings



J. Qiang et al., Computer Physics Communications, vol. 175, 416, (2006).

J. Qiang et al., Phys. Rev. ST Accel. Beams, 12, 100702 (2009).



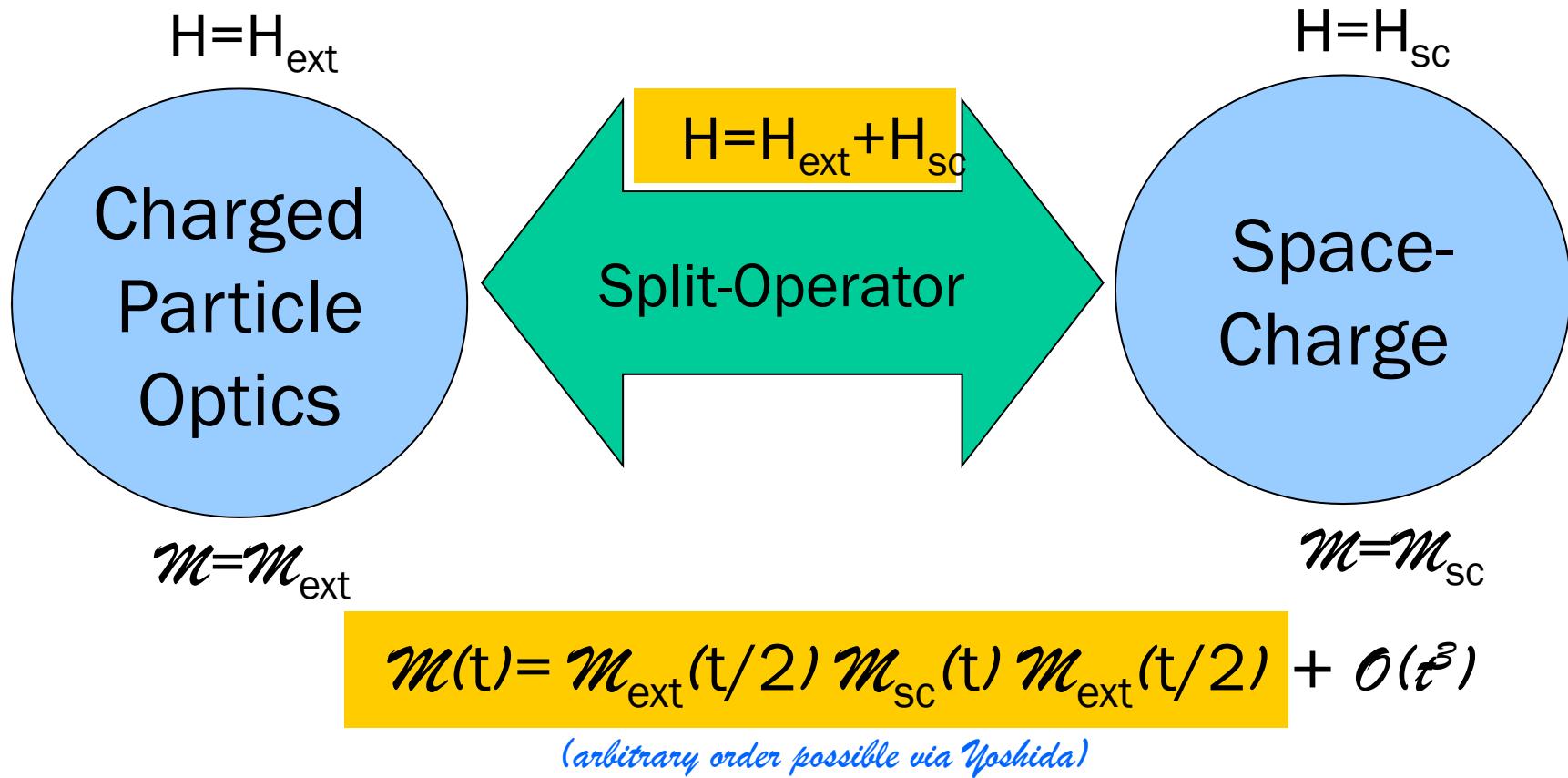
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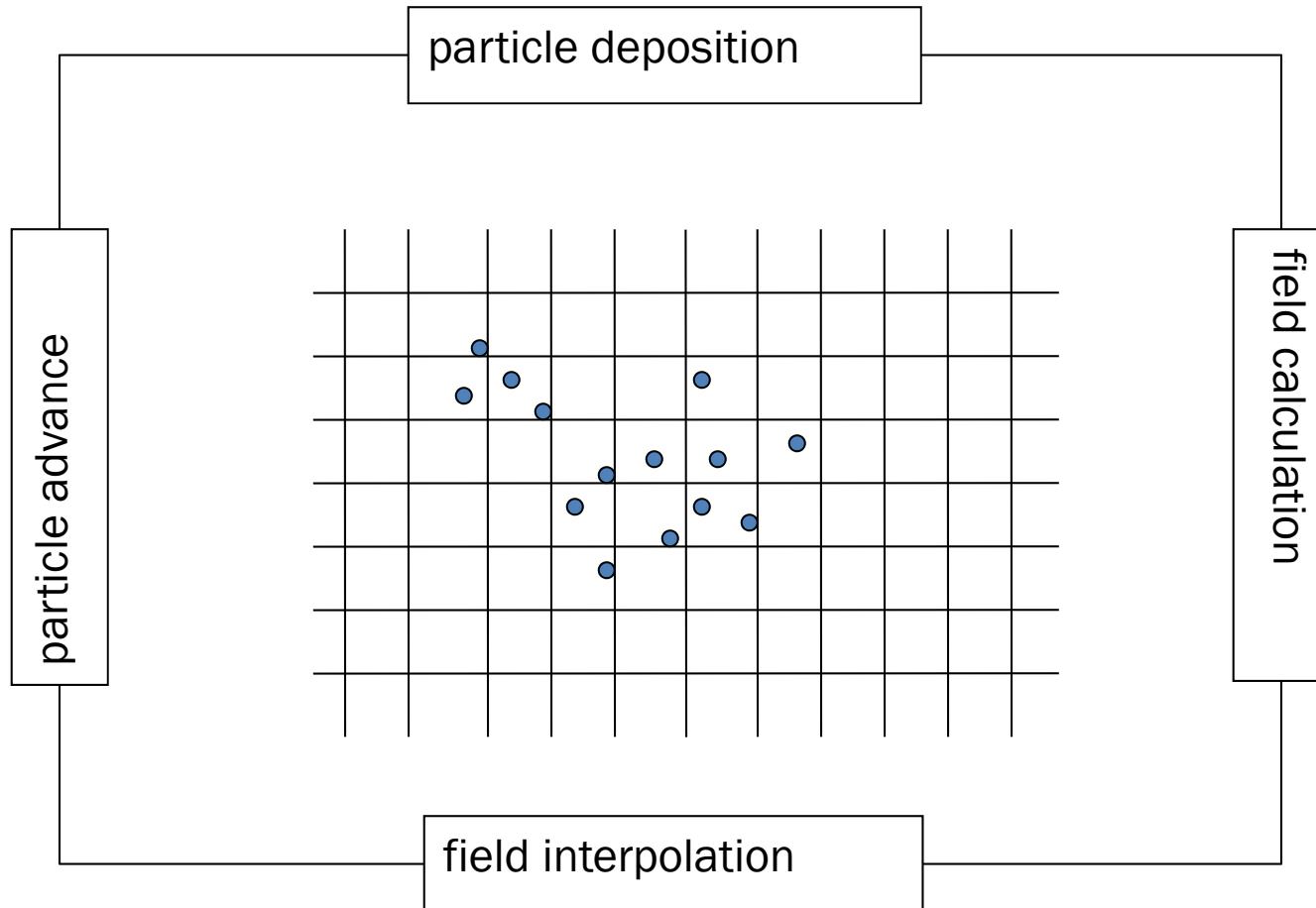
Split-Operator Method



- Rapidly varying s-dependence of external fields is decoupled from slowly varying space charge fields

One Step Particle-In-Cell Method to Model Space-Charge Effects

$$f(\vec{r}, \vec{p}, t) = \sum w \delta(\vec{r} - \vec{r}_p) \delta(\vec{p} - \vec{p}_p)$$



A New RFQ Module

- Time as independent variable
- The 8-term expression for RFQ fields
- Longitudinal quasi-periodic boundary condition

$$V(r, \theta, z) = \frac{V_0}{2} \left\{ A_0 \left(\frac{r}{r_0} \right)^2 \cos(2\theta) + A_1 \left(\frac{r}{r_0} \right)^6 \cos(6\theta) + A_{10} I_0(kr) \sin(kz) + A_{12} I_4(kr) \cos(4\theta) \sin(kz) + A_{21} I_2(2kr) \cos(2\theta) \sin(2kz) + A_{23} I_6(2kr) \cos(6\theta) \sin(2kz) + A_{30} I_0(3kr) \sin(3kz) + A_{32} I_4(3kr) \cos(4\theta) \sin(3kz) \right\}$$

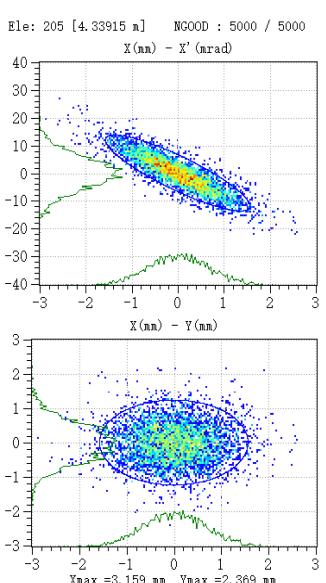
3D space-charge model:
includes space-charge
forces from the bunch
itself and from
neighboring bunches



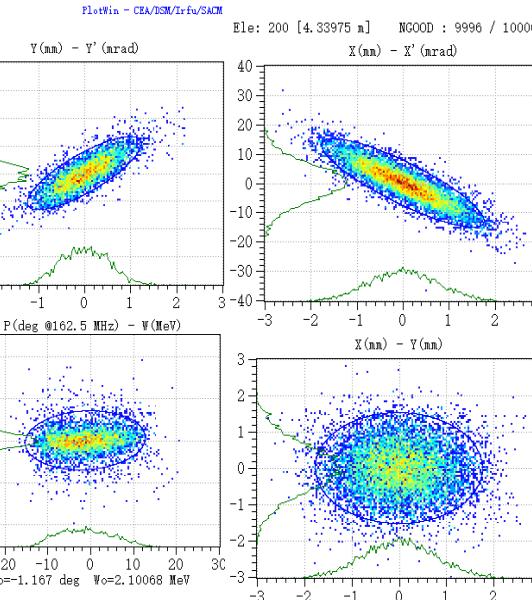
Good Agreement among Three Codes: Simulation Results— PIP-II RFQ

PIP-II RFQ (proton, 5mA@2.1MeV) simulation results given by Impact-T, Parmteqm and Toutatis at the end of the RFQ:

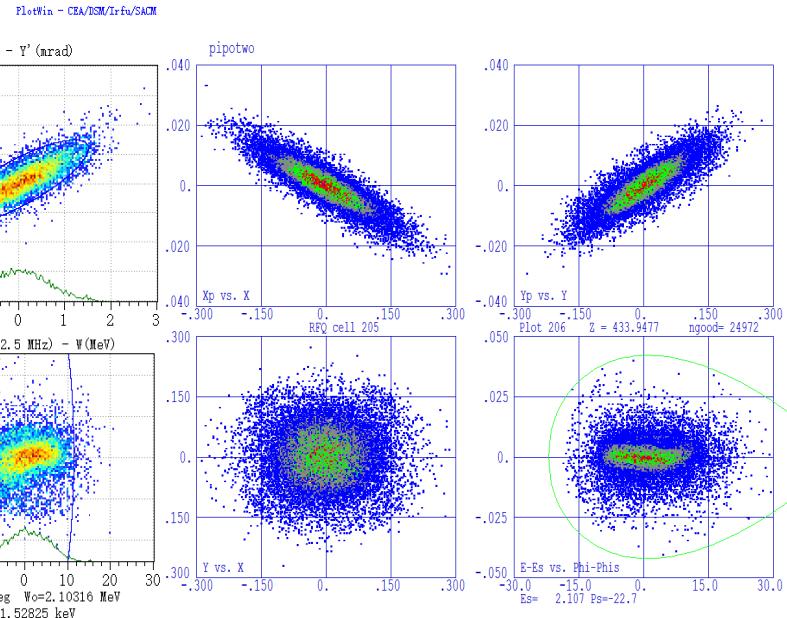
IMPACT-T



TOUTATIS



PARMTEQM



H. P. Li and Z. Wang

- Final emittances are within 10%
- Final transmissions are nearly the same (~100%)



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Contrast of Non-Symplectic and Symplectic Integrator

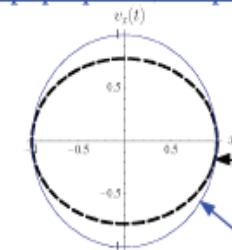
Example: Contrast of Non-Symplectic and Symplectic Advances

Contrast: Numerical and Actual Orbit for a Simple Harmonic Oscillator

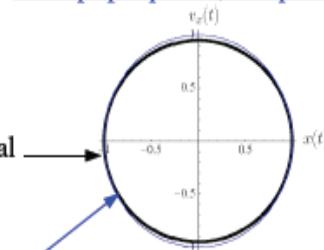
use scaled coordinates (max extents unity for analytical solution)

Symplectic Leapfrog Advance:

5 steps per period, 100 periods



10 steps per period, 100 periods



Cosine-type initial conditions

Sine-type initial conditions

Numerical Orbit

Actual Orbit

75

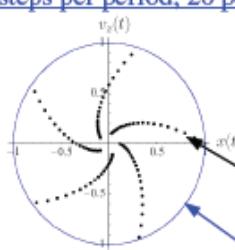
SM Lund, USPAS, June 2008

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

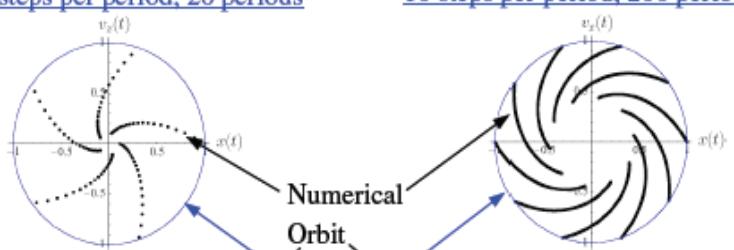
Contrast: Numerical and Actual Orbit for a Simple Harmonic Oscillator

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

5 steps per period, 20 periods



10 steps per period, 200 periods



Cosine-type initial conditions

Sine-type initial conditions

Numerical Orbit

Actual Orbit

Simulation Techniques 77

SM Lund, USPAS, June 2008

Courtesy of S. Lund



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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
Coulomb potential

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

external focusing/acceleration

A formal single step solution

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

$$H = H_1 + H_2$$

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

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

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

A Symplectic Multi-Particle Tracking Model (2)

2nd order:

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

4th 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:

$$\mathcal{M}_{2n+2}(\tau) = \mathcal{M}_{2n}(z_0\tau)\mathcal{M}_{2n}(z_1\tau)\mathcal{M}_{2n}(z_0\tau)$$

$$\text{where } z_0 = 1/(2 - 2^{1/(2n+1)}) \text{ and } z_1 = -2^{1/(2n+1)} / (2 - 2^{1/(2n+1)})$$

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.



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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

A Coasting Beam in a Rectangular Conducting Pipe (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 $\beta_m = m\pi/b$

$$\boxed{\phi^{lm} = \frac{\rho^{lm}}{\epsilon_0 \gamma_{lm}^2}}$$

where $\gamma_{lm}^2 = \alpha_l^2 + \beta_m^2$



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A Coasting Beam in a Rectangular Conducting Pipe (2)

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

w is the particle charge weight

$$\phi^{lm} = \frac{1}{\epsilon_0 \gamma_{lm}^2} \frac{4}{ab} w \sum \sin(\alpha_l x_j) \sin(\beta_m y_j)$$

$$\phi(x, y) = \frac{1}{\epsilon_0} \frac{4}{ab} w \sum_j \sum_l \sum_m \frac{1}{\gamma_{lm}^2} \sin(\alpha_l x_j) \sin(\beta_m y_j) \sin(\alpha_l x) \sin(\beta_m y)$$

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

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

M₂ →

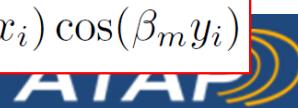
$$p_{yi}(\tau) = p_{yi}(0) - \tau \frac{1}{\epsilon_0} \frac{4}{ab} w \sum_j \sum_l \sum_m \frac{\beta_m}{\gamma_{lm}^2} \sin(\alpha_l x_j) \sin(\beta_m y_j) \sin(\alpha_l x_i) \cos(\beta_m y_i)$$



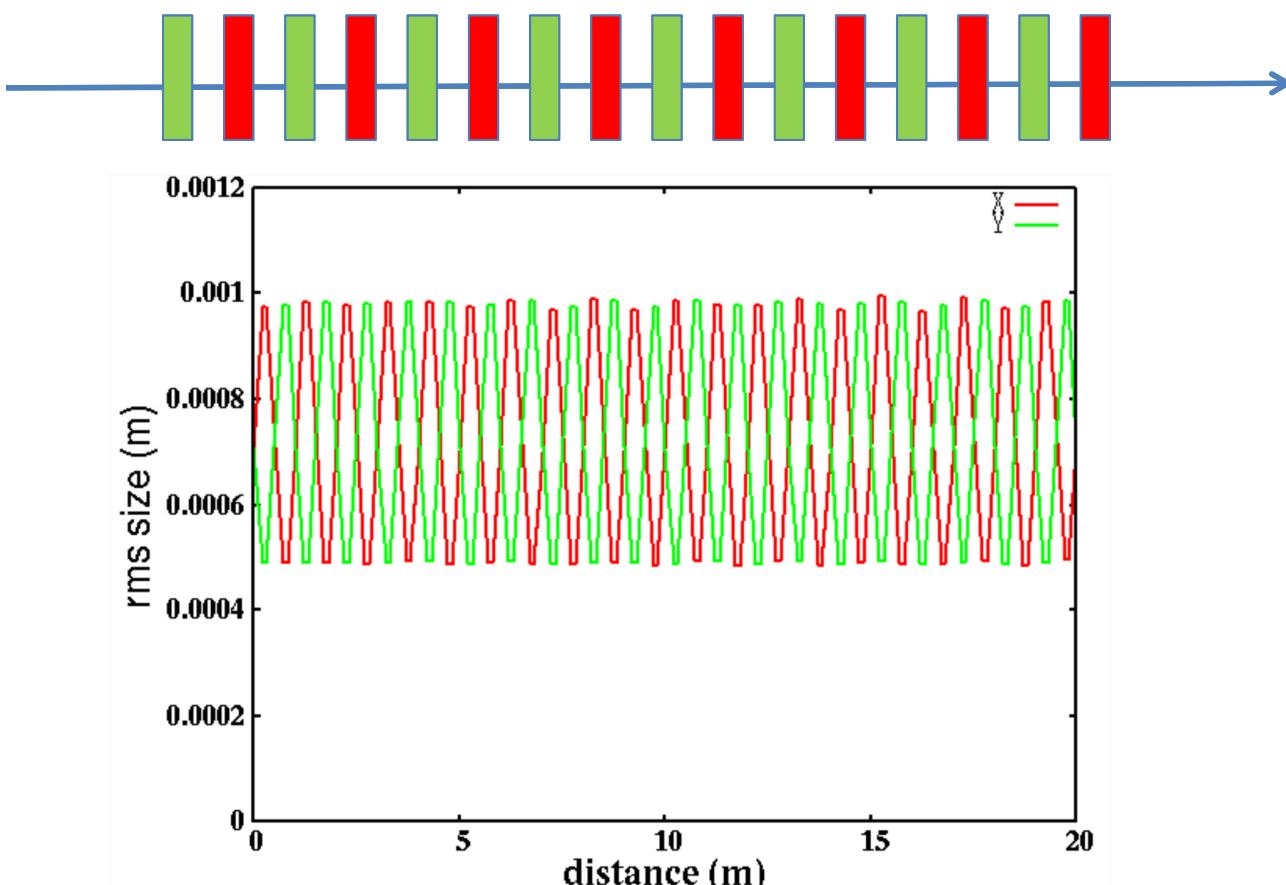
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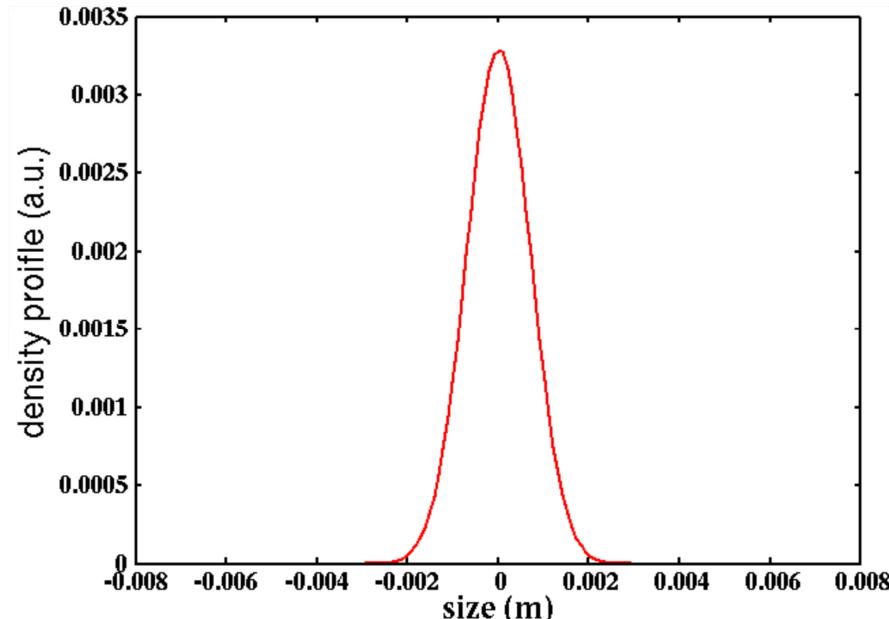
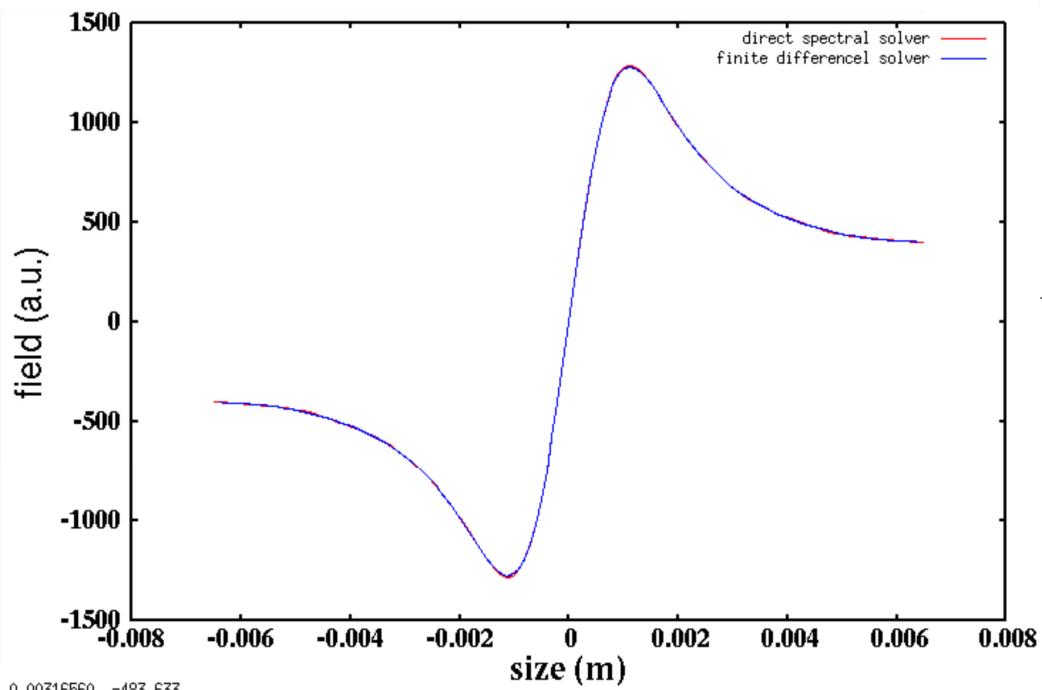
An Illustration Example



- 0 current phase advance: 87 degrees
- phase advance with current: 74 degrees

A Small Number of Modes Are Needed in the Gridless Spectral Solver

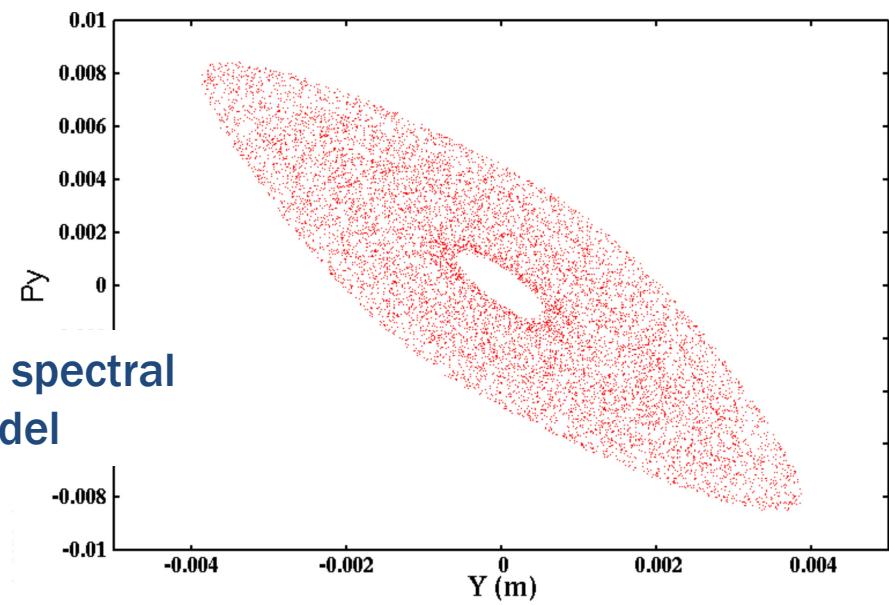
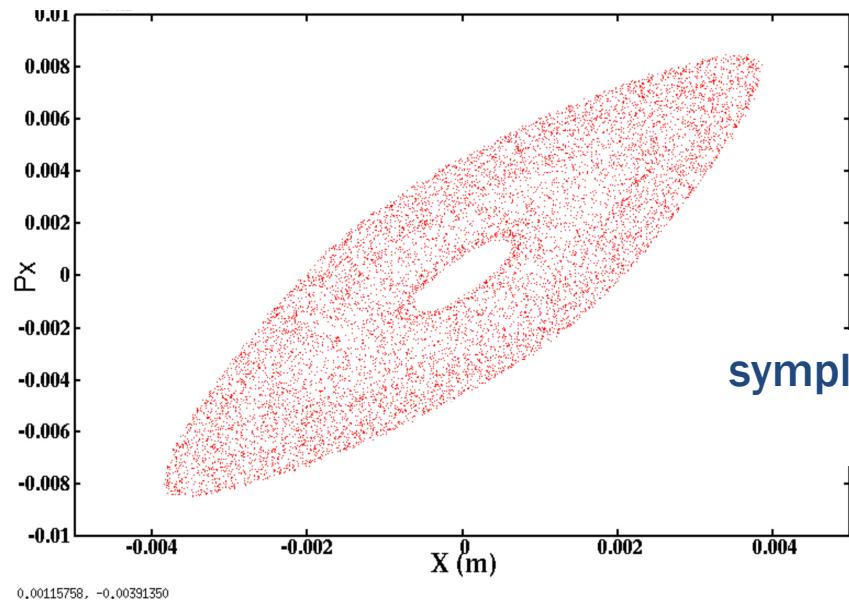
on-axis electric fields from the spectral solver with 15×15 modes and the 2nd finite difference solver with 129×129 grid points



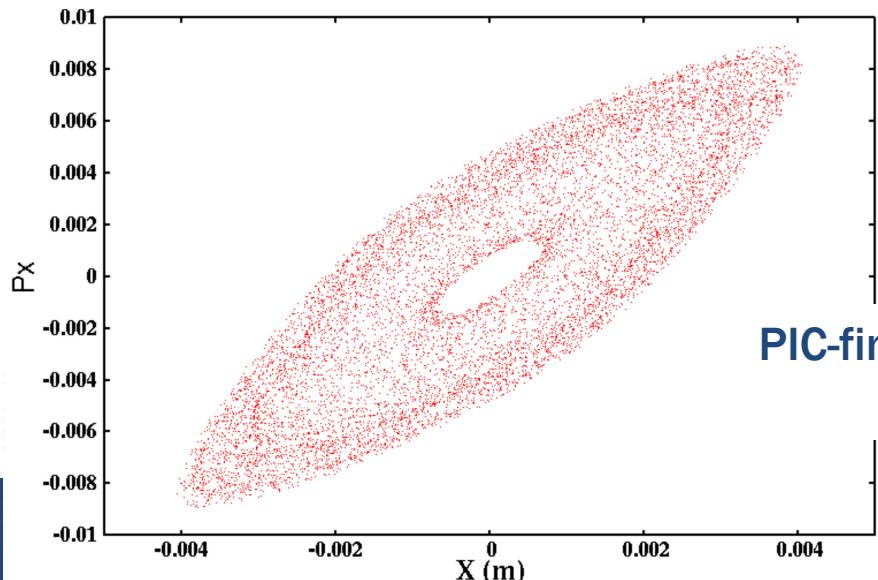
Gaussian density distribution

A Stroboscopic Plot of a Single Particle Phase Space (1)

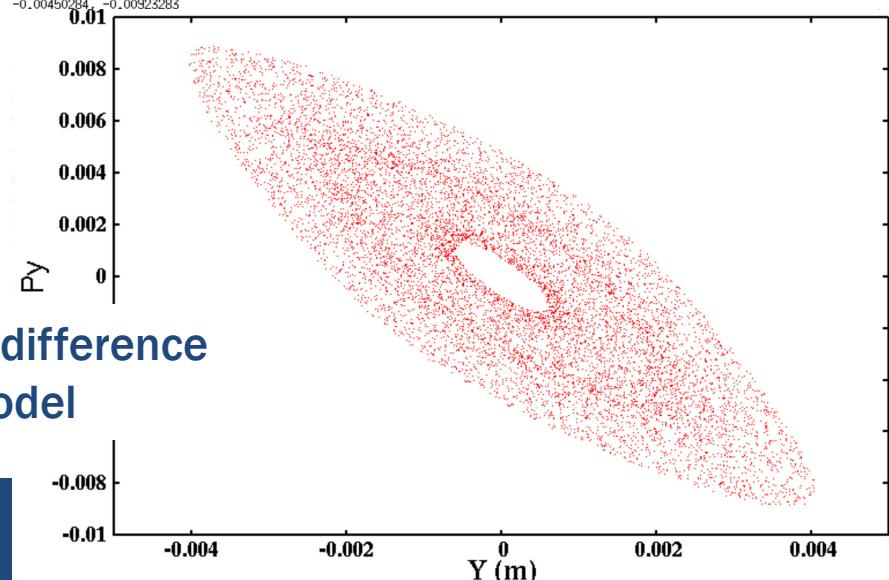
(similar shape but somewhat different phase structure)



symplectic spectral
model



PIC-finite difference
model

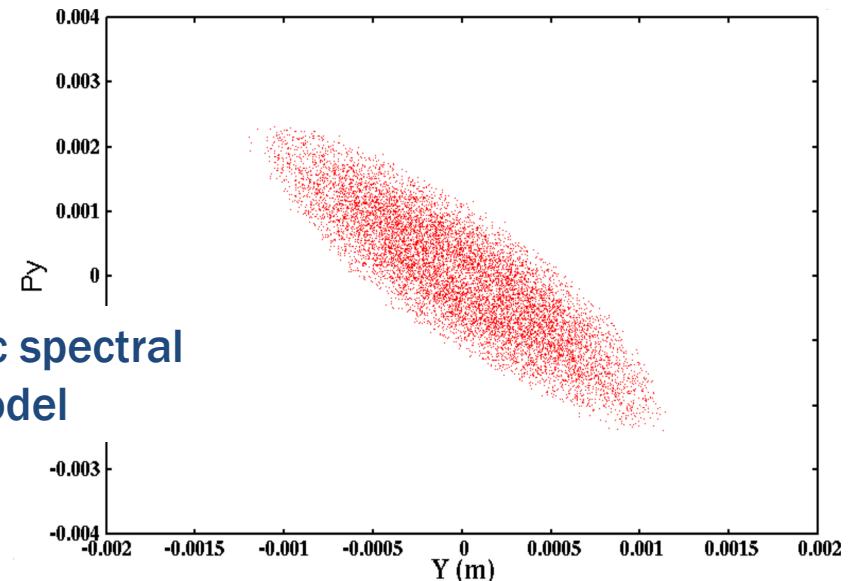
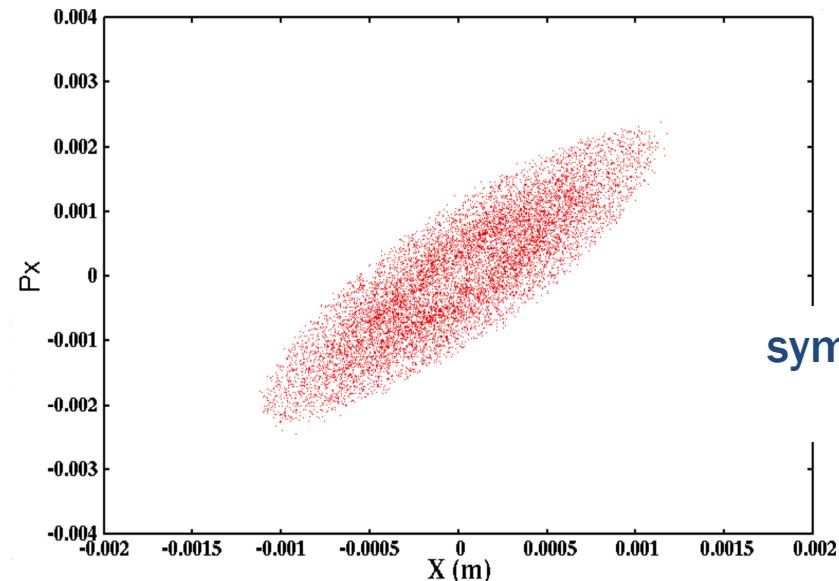


-0.00635227, -0.00856223

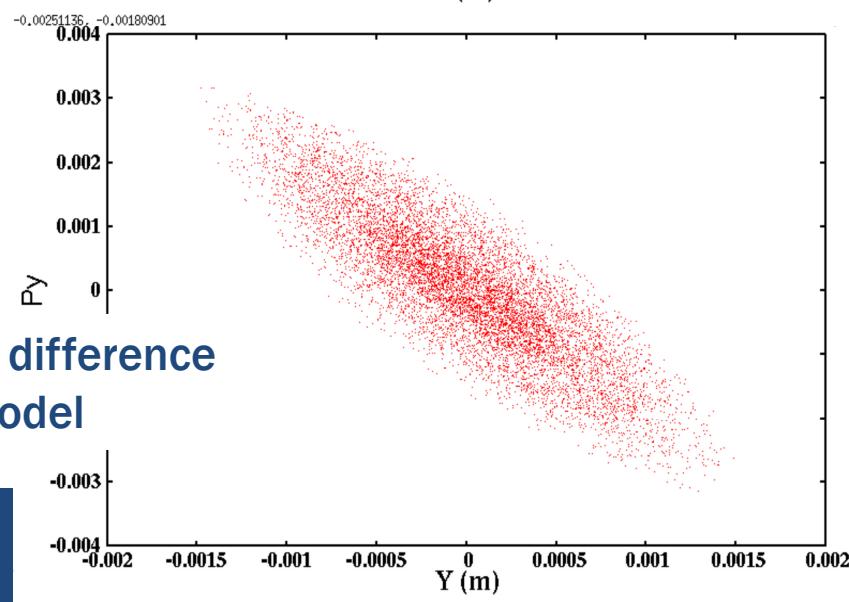
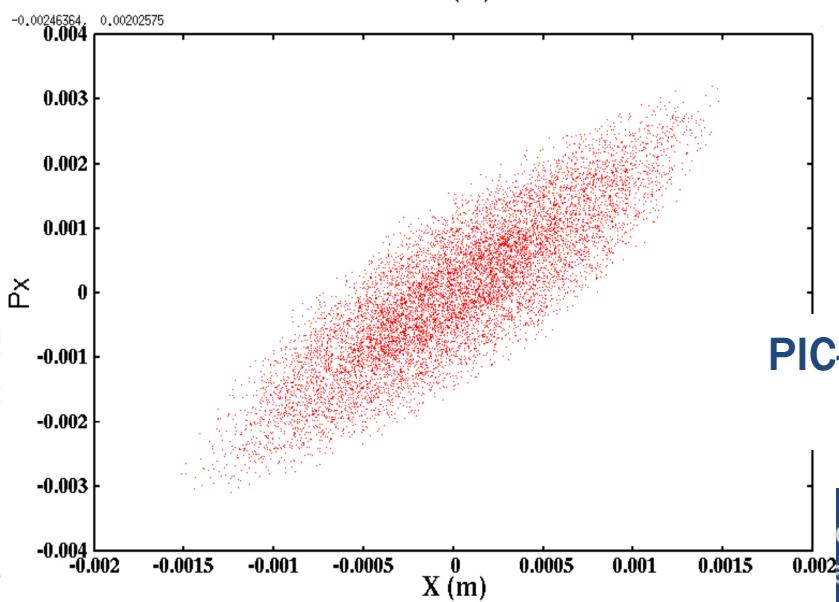
-0.00414489, -0.00256974

A Stroboscopic Plot of a Single Particle Phase Space (2)

(similar shape but different phase structure)



symplectic spectral
model

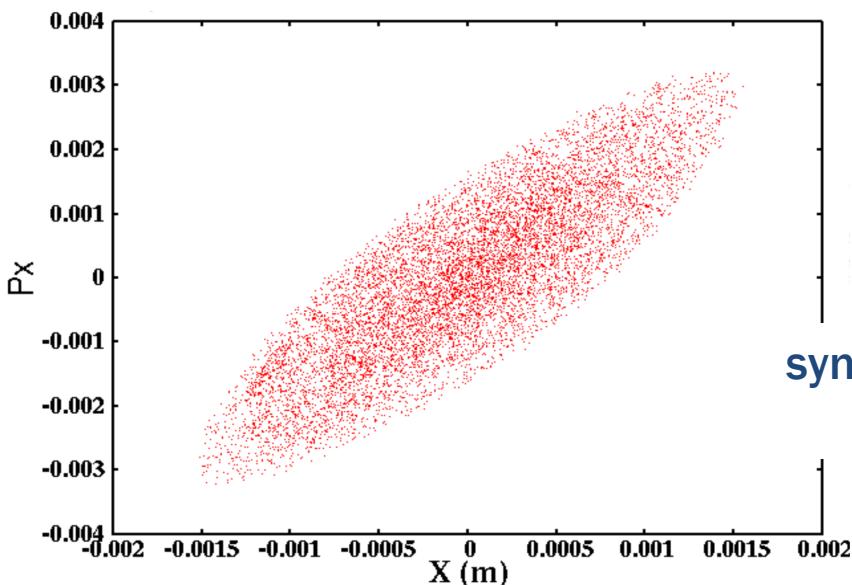


PIC-finite difference
model

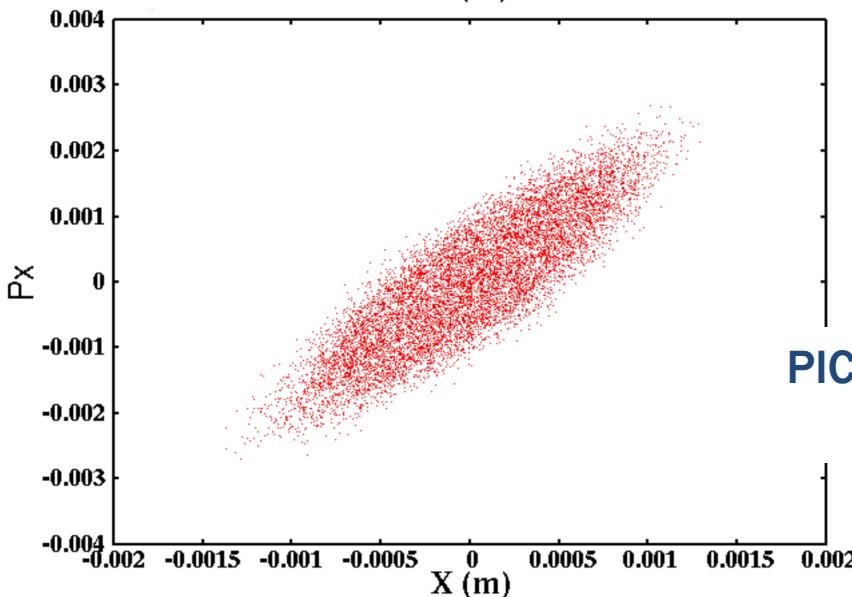
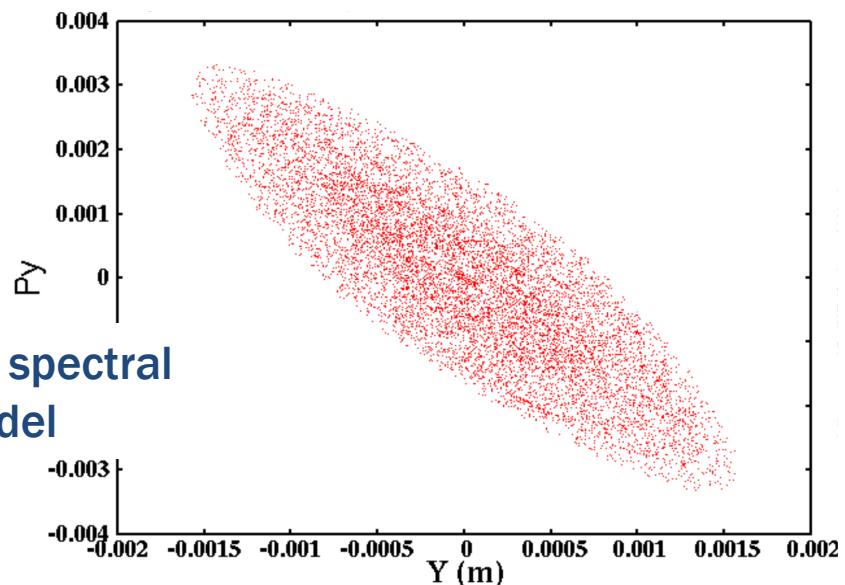
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A Stroboscopic Plot of a Single Particle Phase Space (3)

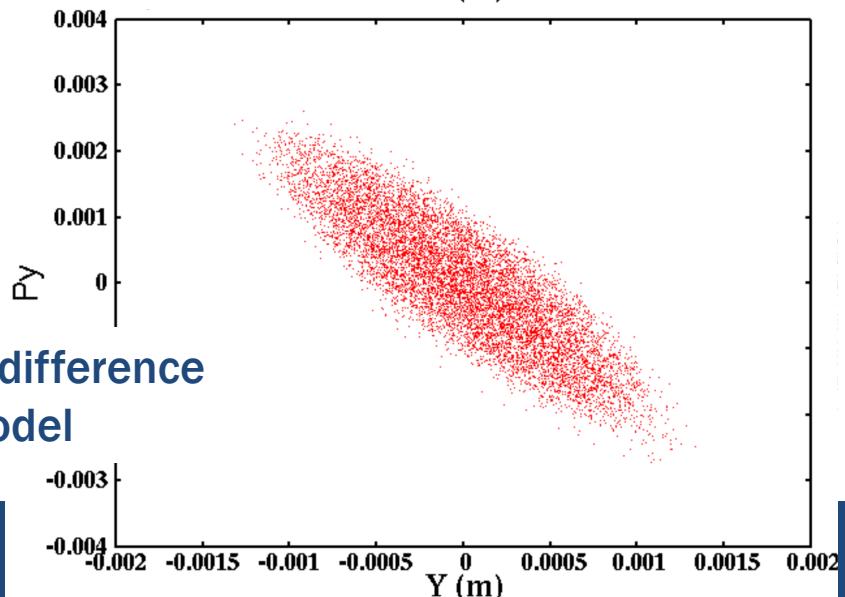
(similar shape but different phase structure)



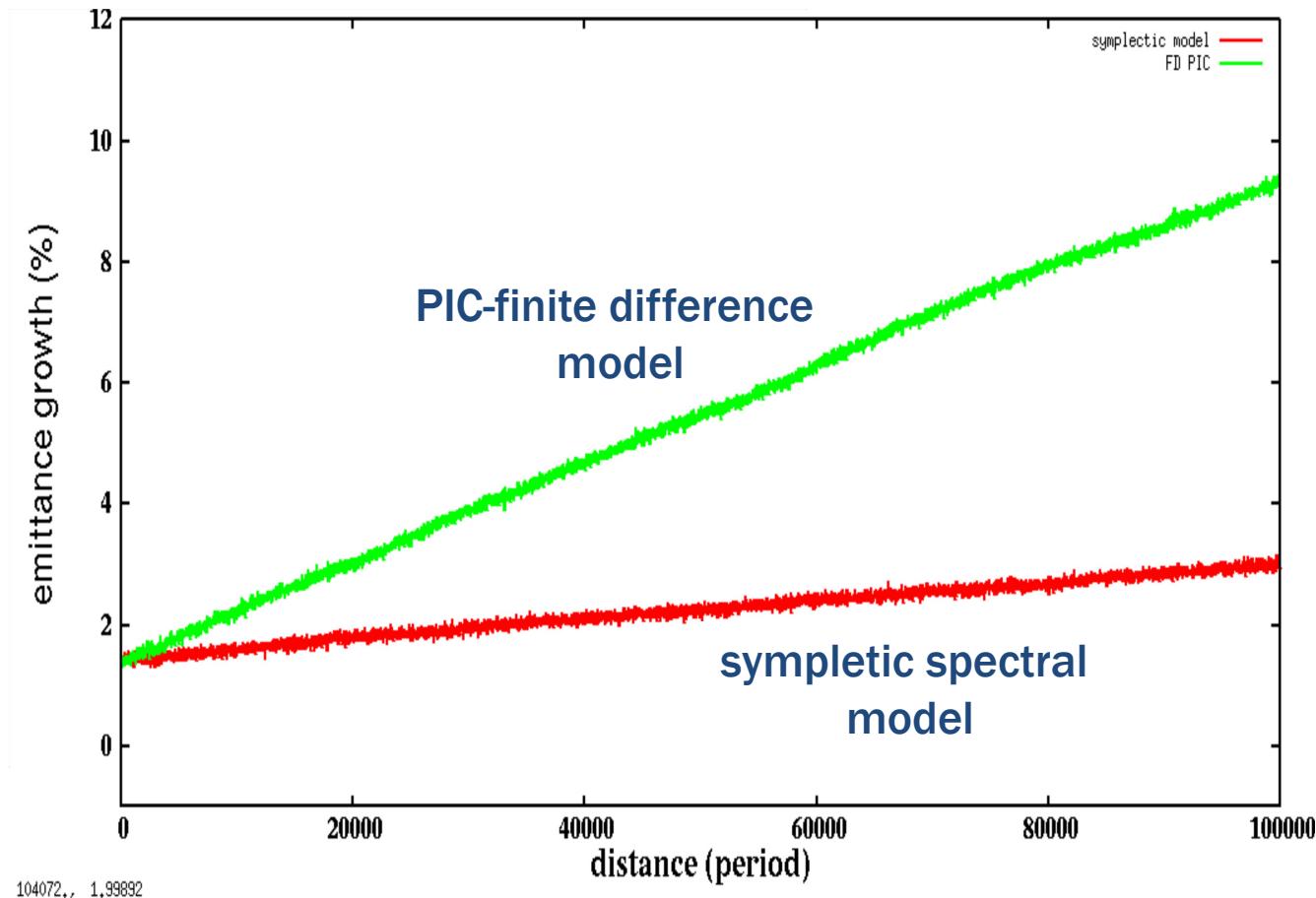
symplectic spectral
model



PIC-finite difference
model

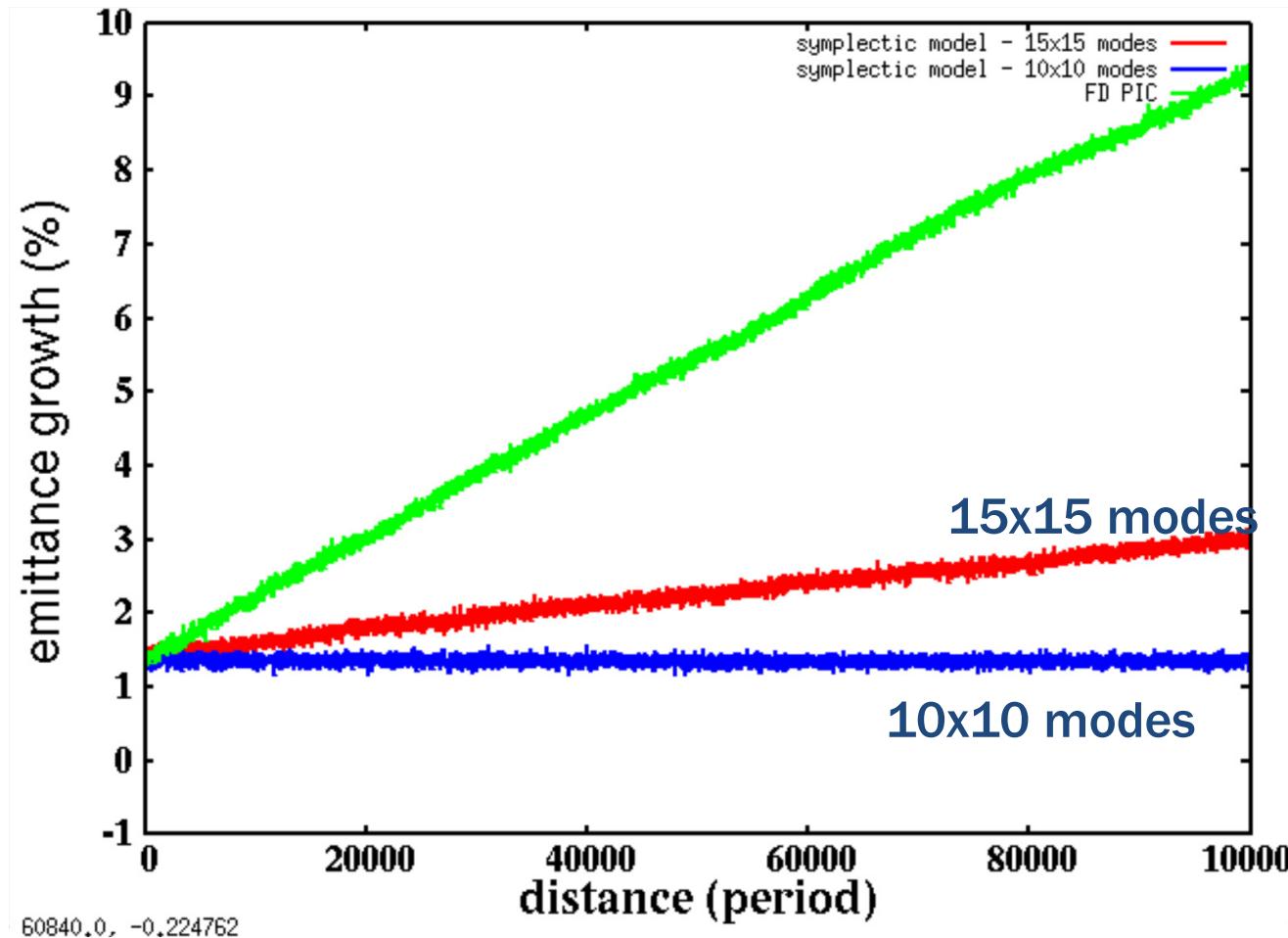


Much Less Four Dimensional Emittance Growth Using the Symplectic Spectral Model (1)



104072., 1.99892

Much Less Four Dimensional Emittance Growth Using the Symplectic Spectral Model (2)



Computational Complexity

Symplectic Gridless Spectral Model

- $O(N_{\text{modes}} \times N_{\text{particles}})$

PIC Finite Difference Model

- $O(N_{\text{particles}}) + O(N_{\text{grid}} \log N_{\text{grid}})$

PIC model is faster than the symplectic model on a single processor

However ->



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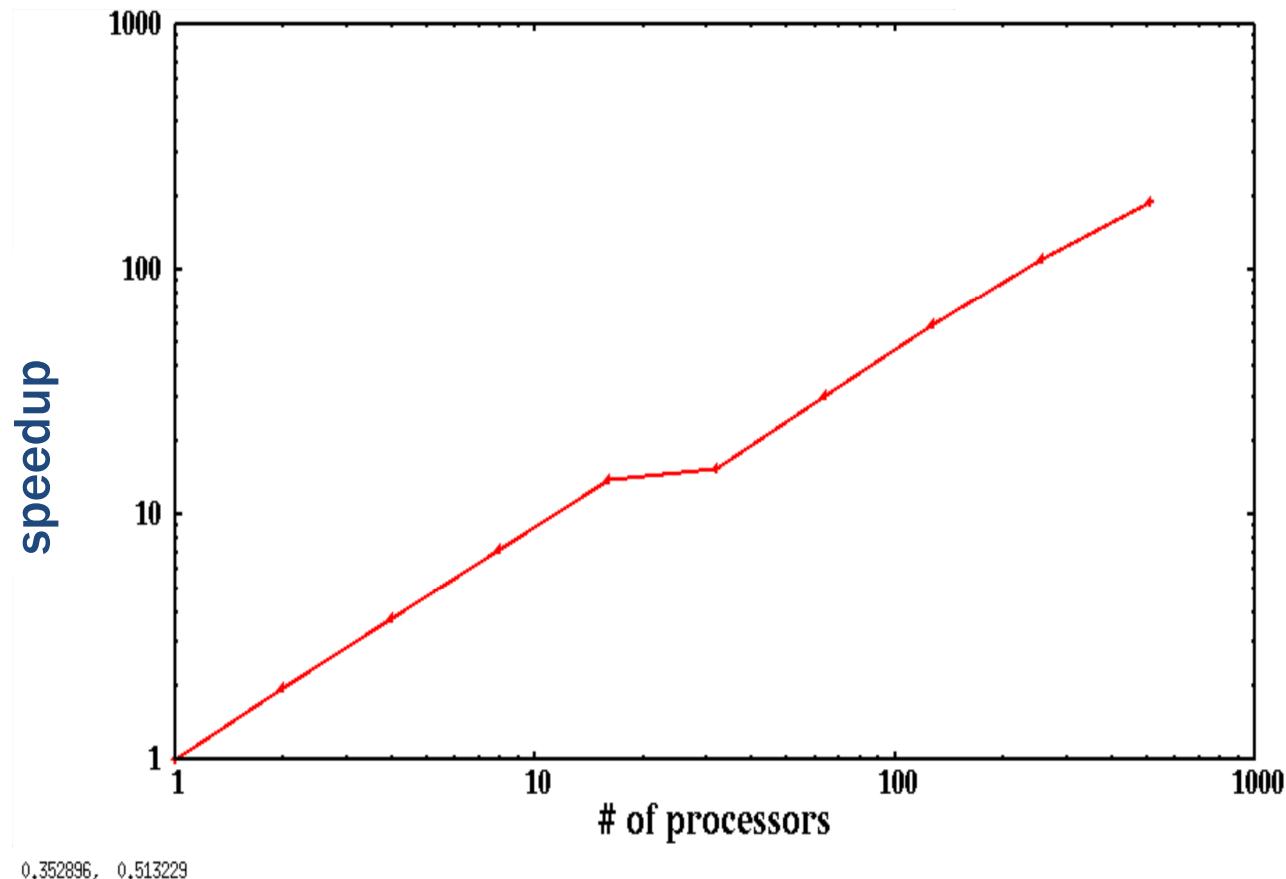
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The Symplectic Gridless Spectral Model Has a Good Parallel Scalability

The symplectic model scales very well on multi-processor computer



Coulomb Potential in a 3D Bunched Beam (1)

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

$$\rho(x, y, z) = \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \sum_{n=1}^{N_n} \rho^{lmn} \sin(\alpha_l x) \sin(\beta_m y) \sin(\gamma_n z)$$

$$\phi(x, y, z) = \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \sum_{n=1}^{N_n} \phi^{lmn} \sin(\alpha_l x) \sin(\beta_m y) \sin(\gamma_n z)$$

$$\rho^{lmn} = \frac{8}{abc} \int_0^a \int_0^b \int_0^c \rho(x, y, z) \sin(\alpha_l x) \sin(\beta_m y) \sin(\gamma_n z) dx dy dz$$

$$\phi^{lmn} = \frac{8}{abc} \int_0^a \int_0^b \int_0^c \phi(x, y, z) \sin(\alpha_l x) \sin(\beta_m y) \sin(\gamma_n z) dx dy dz$$



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Coulomb Potential in a 3D Bunched Beam (2)

$$\phi^{lmn} = \frac{\rho^{lmn}}{\epsilon_0 \Gamma_{lmn}^2}$$

$$\text{where } \Gamma_{lmn}^2 = \alpha_l^2 + \beta_m^2 + \gamma_n^2$$

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

$$\phi^{lmn} = \frac{1}{\epsilon_0 \Gamma_{lmn}^2} \frac{8}{abc} w \sum_j \sin(\alpha_l x_j) \sin(\beta_m y_j) \sin(\gamma_n z_j)$$

$$\phi(x, y, z) = \frac{1}{\epsilon_0} \frac{8}{abc} w \sum_j \sum_l \sum_m \sum_n \frac{1}{\Gamma_{lmn}^2} \sin(\alpha_l x_j) \sin(\beta_m y_j) \sin(\gamma_n z_j) \sin(\alpha_l x) \sin(\beta_m y) \sin(\gamma_n z)$$



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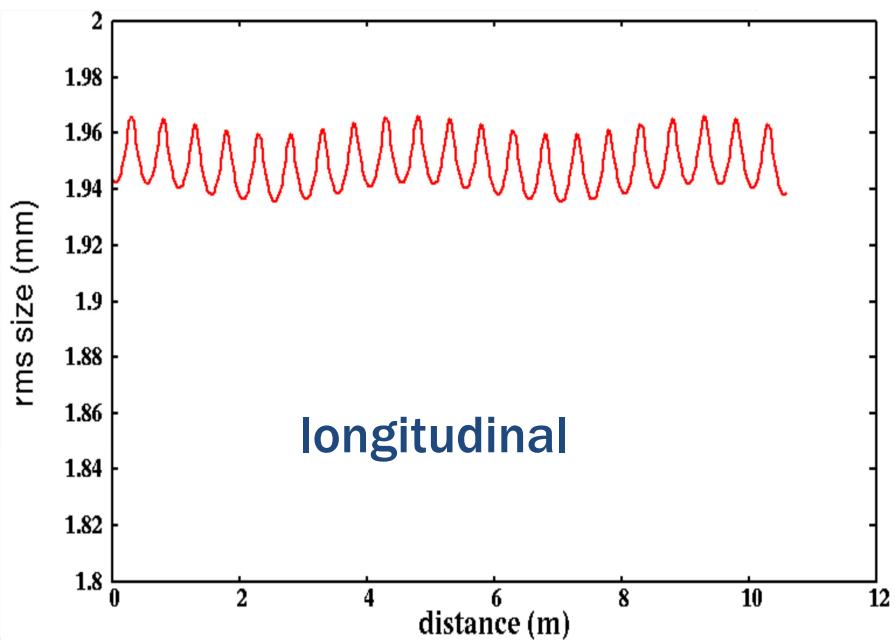
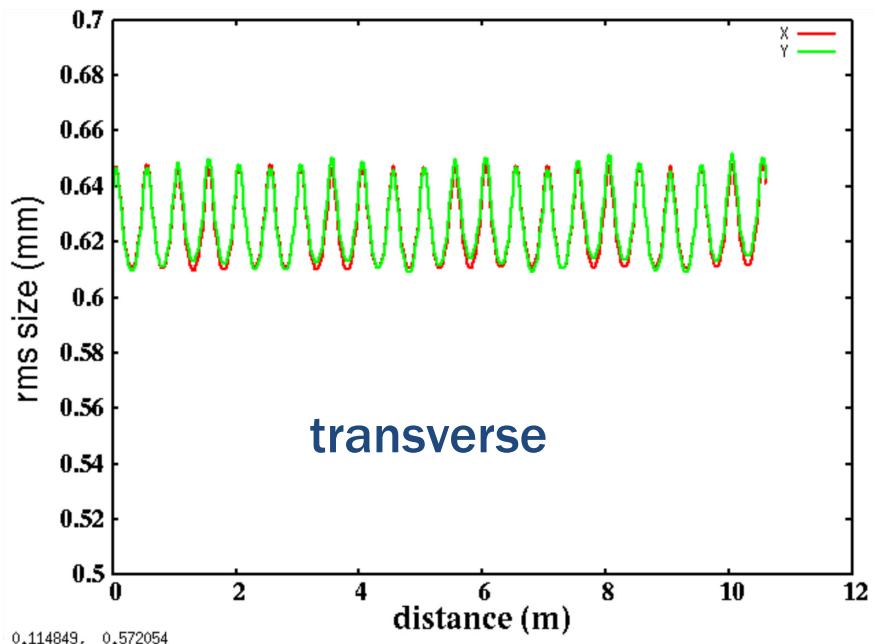
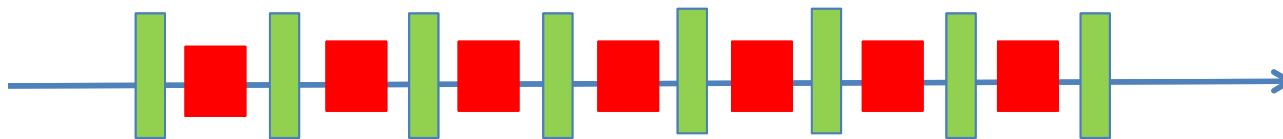
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Single Step Symplectic Map for H_2

$$H_2 = \frac{1}{2\epsilon_0} \frac{8}{abc} w \sum_i \sum_j \sum_l \sum_m \sum_n \frac{1}{\gamma_{lmn}^2} \sin(\alpha_l x_j) \sin(\beta_m y_j) \sin(\gamma_n z_j) \sin(\alpha_l x_i) \sin(\beta_m y_i) \sin(\gamma_n z_i)$$

$$\begin{aligned} p_{xi}(\tau) &= p_{xi}(0) - \tau \frac{1}{\epsilon_0} \frac{8}{abc} w \sum_j \sum_l \sum_m \sum_n \frac{\alpha_l}{\Gamma_{lmn}^2} \\ &\quad \sin(\alpha_l x_j) \sin(\beta_m y_j) \sin(\gamma_n z_j) \cos(\alpha_l x_i) \sin(\beta_m y_i) \sin(\gamma_n z_i) \\ p_{yi}(\tau) &= p_{yi}(0) - \tau \frac{1}{\epsilon_0} \frac{8}{abc} w \sum_j \sum_l \sum_m \sum_n \frac{\beta_m}{\Gamma_{lmn}^2} \\ &\quad \sin(\alpha_l x_j) \sin(\beta_m y_j) \sin(\gamma_n z_j) \sin(\alpha_l x_i) \cos(\beta_m y_i) \sin(\gamma_n z_i) \\ p_{zi}(\tau) &= p_{zi}(0) - \tau \frac{1}{\epsilon_0} \frac{8}{abc} w \sum_j \sum_l \sum_m \sum_n \frac{\gamma_n}{\Gamma_{lmn}^2} \\ &\quad \sin(\alpha_l x_j) \sin(\beta_m y_j) \sin(\gamma_n z_j) \sin(\alpha_l x_i) \sin(\beta_m y_i) \cos(\gamma_n z_i) \end{aligned}$$

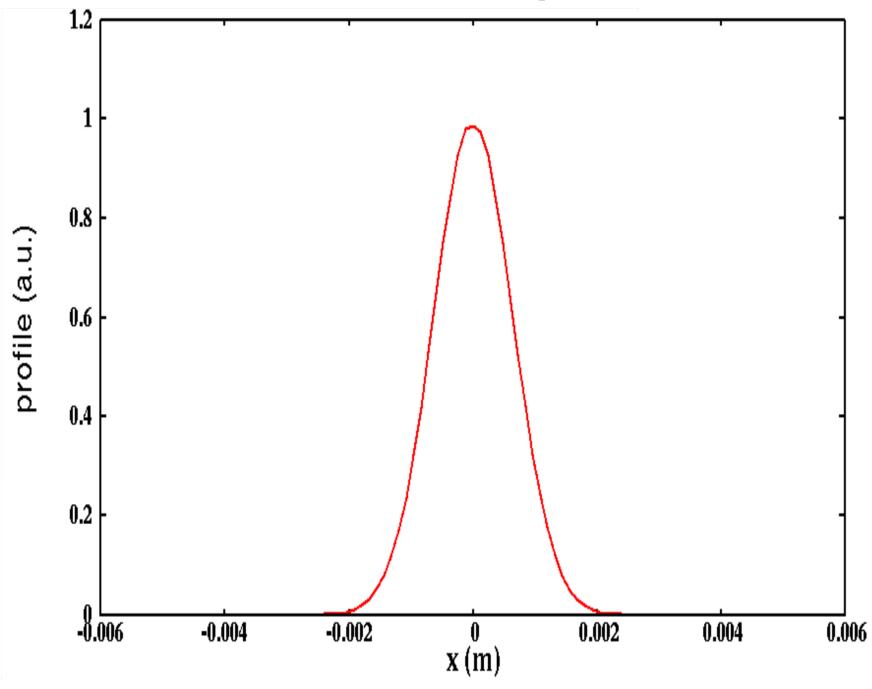
Another Illustration Example (in progress) (3D Bunched Beam)



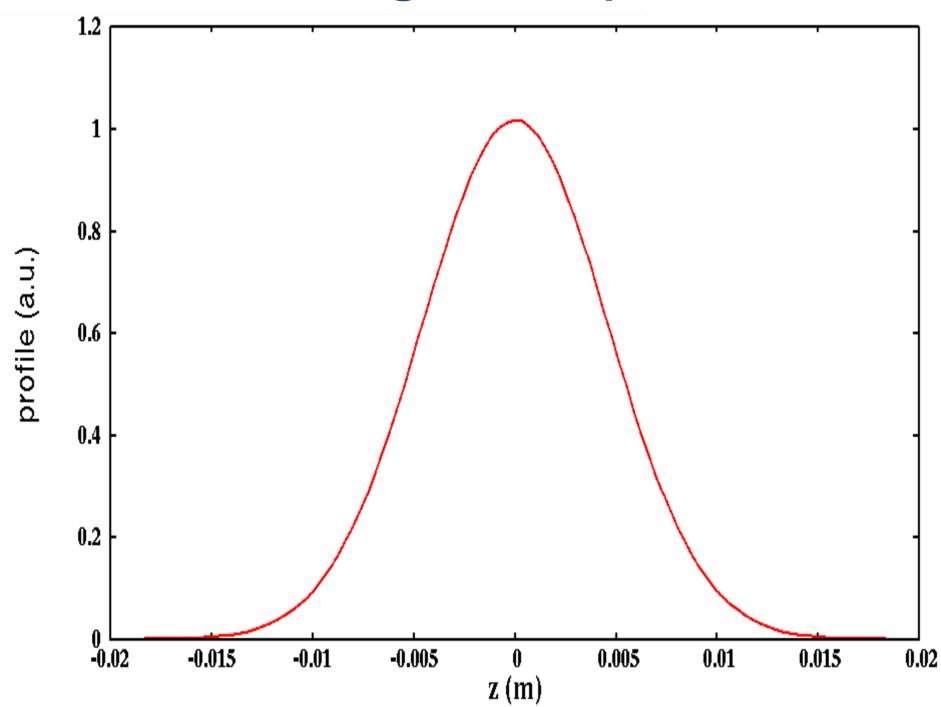
0 current phase advances: trans. 86, long. 40 degrees
phase advances with current: trans. 81, long. 39 degrees

Transverse and Longitudinal Density Profiles

transverse profile

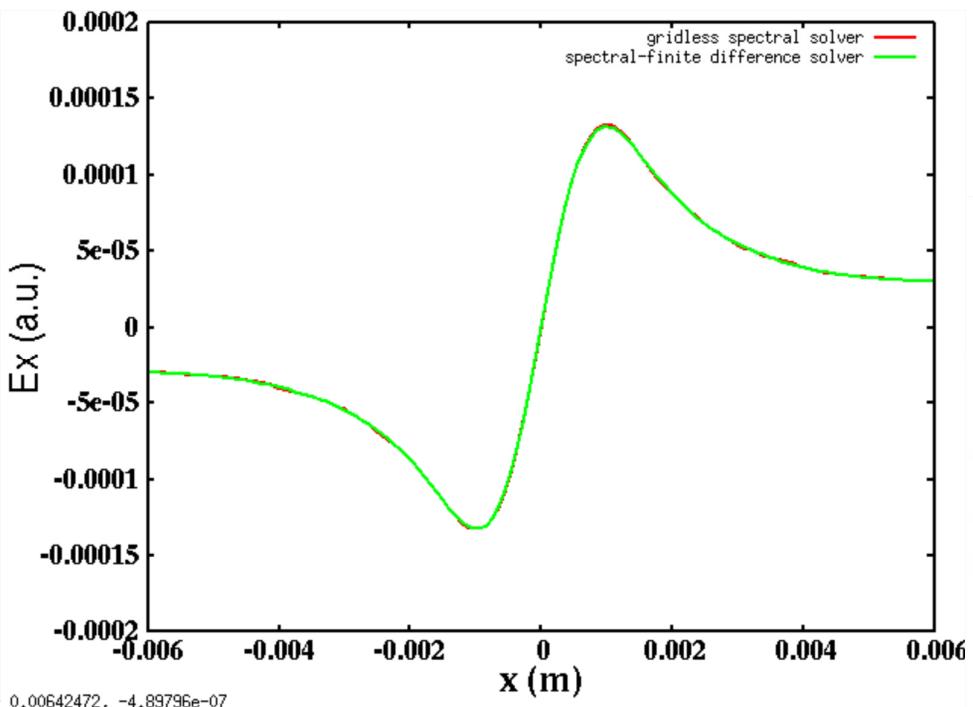


longitudinal profile



A Small Number of Modes Are Needed in the Gridless Spectral Solver for 3D Bunched Beam

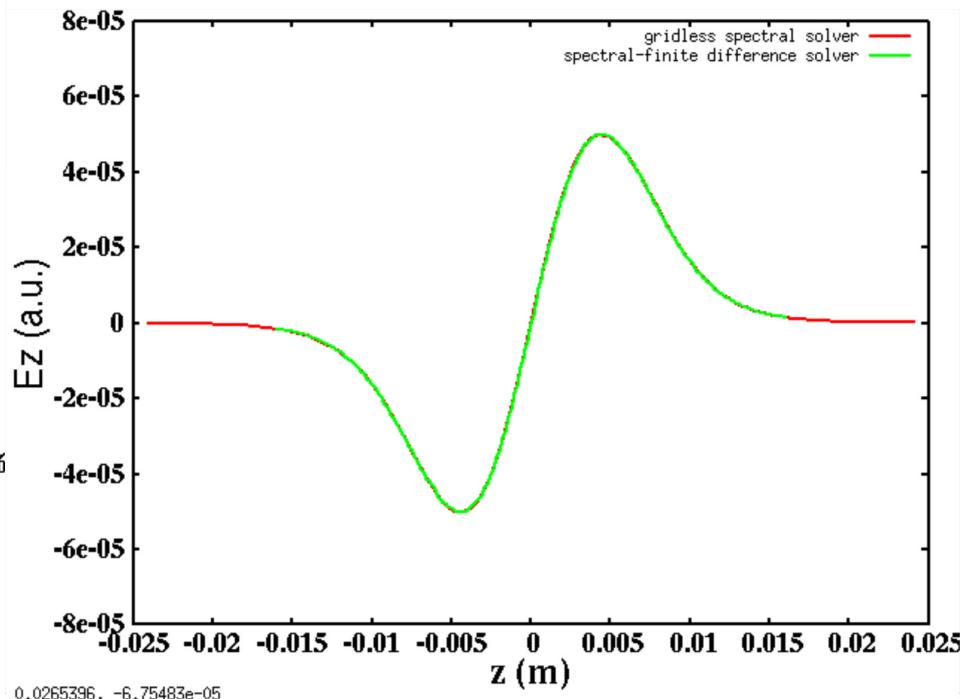
Ex vs. X



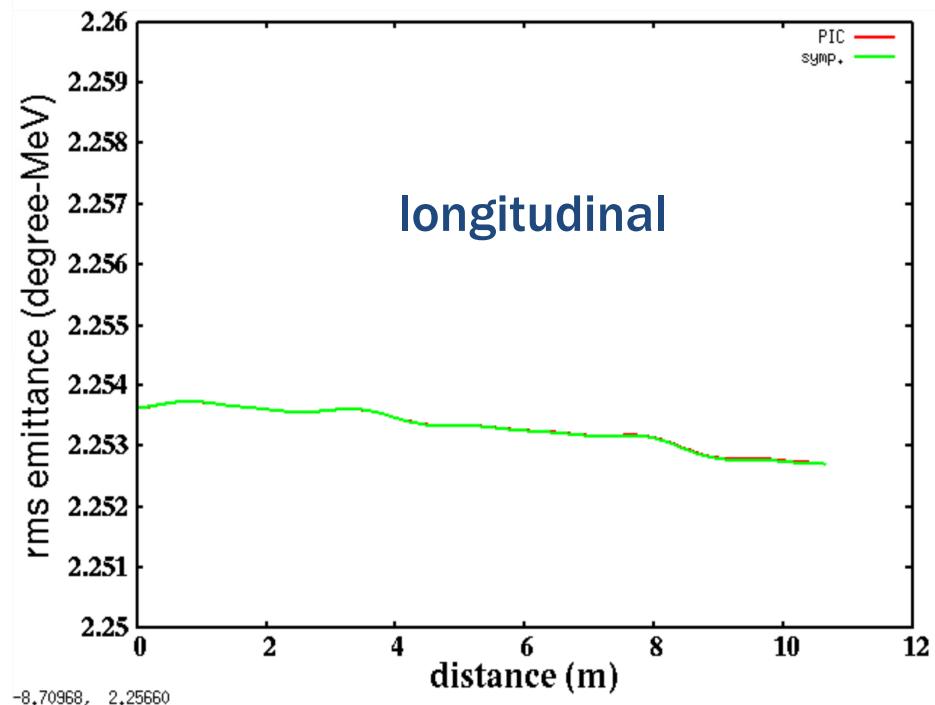
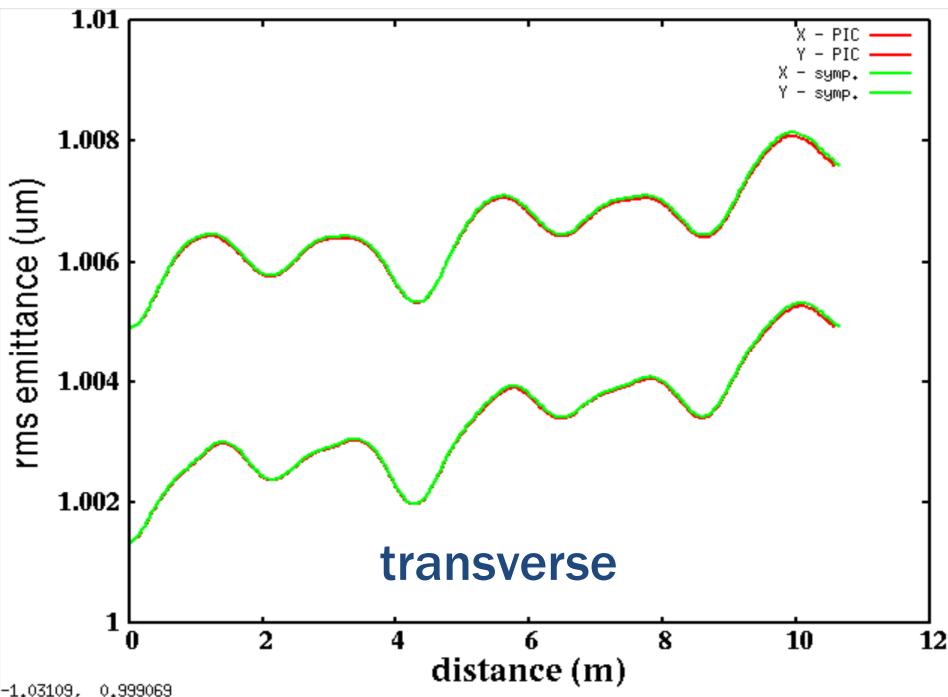
of modes: $15 \times 15 \times 15$

of grid points: $129 \times 129 \times 257$

Ez vs. z



Good Agreement in the Short-Term Emittance Evolution (Symplectic Gridless Spectr.vs. PIC Spectral-Finite Diff.)



Conclusions

- A new RFQ model expands the capability of the IMPACT code suite for start-to-end simulation
- Fully 4N and 6N dimensional symplectic multi-particle gridless spectral enables the IMPACT code suite for long term tracking
 - No errors associated with numerical grid (e.g. grid heating)
 - Much less numerical emittance growth than the PIC-finite difference model
 - Small number of modes due to spectral accuracy
 - Space-charge field accuracy can be further improved
 - Easy implementation and parallelization
 - Good parallel scalability