

# Analysis of Emittance Growth in a Gridless Spectral Poisson Solver for Fully Symplectic Multiparticle Tracking

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\*Work done in collaboration with Ji Qiang



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# Outline

- *Introduction to a symplectic spectral space charge algorithm*
- *Probabilistic model of computed field error*
- *Analysis of emittance growth on a single step*
- *Numerical emittance growth in a FODO channel*
- *Conclusions*

# Introduction and Motivation

- Interest has grown in variational (Lagrangian) or “multi-symplectic” (Hamiltonian) algorithms that preserve the geometric properties of the **collective** self-consistent equations of motion for plasmas<sup>1</sup> or beams<sup>2</sup>.
- Do such algorithms exhibit a non-physical increase in phase space volume due to the presence of numerical errors? If the physical system possesses one or more dynamical invariants, does the numerical system possess “nearby” invariants?
- Models of numerical emittance growth often treat this effect as a form of collisional Coulomb scattering. Grid heating (for PIC algorithms) significantly complicates this picture.
- Symplectic gridless spectral solvers<sup>2</sup> are sufficiently simple that perhaps numerical noise and its contribution to emittance growth can be understood in more complete detail.

[1] B. Shadwick et al, Physics of Plasmas 21, 055708 (2014), S. Webb, Plasma Phys. Control. Fusion 58, 034007 (2016),  
[2] J. Qiang, Phys. Rev. AB 20, 014203 (2017), previous talks by Thomas Planche and Paul Jung.

# Numerical Hamiltonian of a coasting beam with space charge + external focusing (using particles and modes)

Assume that the collective Hamiltonian of the  $N_p$ -particle system is given as the sum of a contribution due to external fields and a contribution due to space charge:

$$H = \sum_{j=1}^{N_p} H_{\text{ext}}(\vec{r}_j, \vec{p}_j, s) - \frac{n}{N_p} \frac{1}{2} \sum_{j=1}^{N_p} \sum_{k=1}^{N_p} \sum_{l=1}^{N_l} \frac{1}{\lambda_l} e_l(\vec{r}_j) e_l(\vec{r}_k).$$

All quantities are computed in the laboratory frame. Each numerical step in the path length coordinate  $s$  is obtained by applying a second-order operator splitting to  $H$ .

$\Omega$	bounded domain (1-2D)
$e_l, \lambda_l$	$l$ th mode and eigenvalue
$N_p$	number of particles
$N_l$	number of modes
$n$	space charge intensity

Eigenmodes of the Laplacian

$$\nabla^2 e_l = \lambda_l e_l \quad e_l|_{\partial\Omega} = 0 \quad (\lambda_l < 0)$$

Symplectic map for a single step:

$$\mathcal{M}(\tau) = \mathcal{M}_{\text{ext}}(\tau/2) \mathcal{M}_{SC}(\tau) \mathcal{M}_{\text{ext}}(\tau/2) + O(\tau^3)$$

# Numerical Hamiltonian of a coasting beam with space charge + external focusing (using particles and modes)

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Thus, each particle moves in response to the *smooth* space charge potential and force:

$$U(\vec{r}) = -\frac{n}{N_p} \sum_{l=1}^{N_l} \sum_{j=1}^{N_p} \frac{1}{\lambda_l} e_l(\vec{r}) e_l(\vec{r}_j) \quad \vec{F}(\vec{r}) = \frac{n}{N_p} \sum_{l=1}^{N_l} \sum_{j=1}^{N_p} \frac{1}{\lambda_l} e_l(\vec{r}_j) \nabla e_l(\vec{r})$$

where  $\nabla^2 U = -\rho$ ,  $U|_{\partial\Omega} = 0$ ,  $\rho = \frac{n}{N_p} \sum_{l=1}^{N_l} \sum_{j=1}^{N_p} e_l(\vec{r}_j)$ .

# Probabilistic model of computed field error



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**ATAP** The logo for Accelerator Technology & Applied Physics Division, featuring the acronym ATAP with a stylized wave graphic.

# Statistical properties of the system of particles

Suppose we sample the *smooth beam phase space density*  $P$  using  $N_p$  macroparticles. The macroparticle coordinates  $\{(\vec{r}_j, \vec{p}_j) : j = 1, 2, \dots, N_p\}$  are treated as i.i.d. random variables described by the probability density  $P$  on the single-particle phase space.

More precisely, the full beam is (initially) described by the joint probability density:

$$P_N(\vec{r}_1, \vec{p}_1, \dots, \vec{r}_{N_p}, \vec{p}_{N_p}) = P(\vec{r}_1, \vec{p}_1)P(\vec{r}_2, \vec{p}_2)\dots P(\vec{r}_{N_p}, \vec{p}_{N_p})$$

Given a function  $a$  on the single-particle phase space, we denote its *beam average*:

$$\langle a \rangle = \frac{1}{N_p} \sum_{j=1}^{N_p} a(\vec{r}_j, \vec{p}_j) \quad \Delta a = a - \langle a \rangle .$$

Given functions  $F$  and  $G$  defined on the  $N_p$ -particle phase space (depending on all particle coordinates within the beam), we define statistics with respect to  $P_N$ :

$$\mathbb{E}[F] = \int F dP_N, \quad \text{Cov}[F, G] = \mathbb{E}[FG] - \mathbb{E}[F]\mathbb{E}[G] .$$



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# Statistical properties of the density and computed field

We may now evaluate the statistical properties of the various modes of the (spatial) beam density. Here  $\delta\rho = \rho - \rho_{\text{exact}}$ . It follows that the first and second moments of the mode coefficients of  $\delta\rho$  are given by:

$$\mathbb{E}[\delta\rho^l] = 0, \quad \text{Cov}[\delta\rho^l, \delta\rho^m] = \frac{n^2}{N_p} \text{Cov}[e_l, e_m].$$

This allows us to evaluate the statistical moments of the error in the various modes of the computed field. Here  $\delta\vec{F} = \vec{F} - \vec{F}_{\text{exact}}$ . The second moments are given by:

$$\mathbb{E}[\delta F^l \delta F^m] = \frac{1}{N_p} \frac{n^2}{\sqrt{\lambda_l \lambda_m}} \text{Cov}[e_l, e_m] \quad (l, m \leq N_l) \quad (\text{modes below cutoff})$$

$$\mathbb{E}[\delta F^l \delta F^m] = \frac{n^2}{\sqrt{\lambda_l \lambda_m}} \mathbb{E}[e_l] \mathbb{E}[e_m] \quad (l, m > N_l) \quad (\text{modes above cutoff})$$



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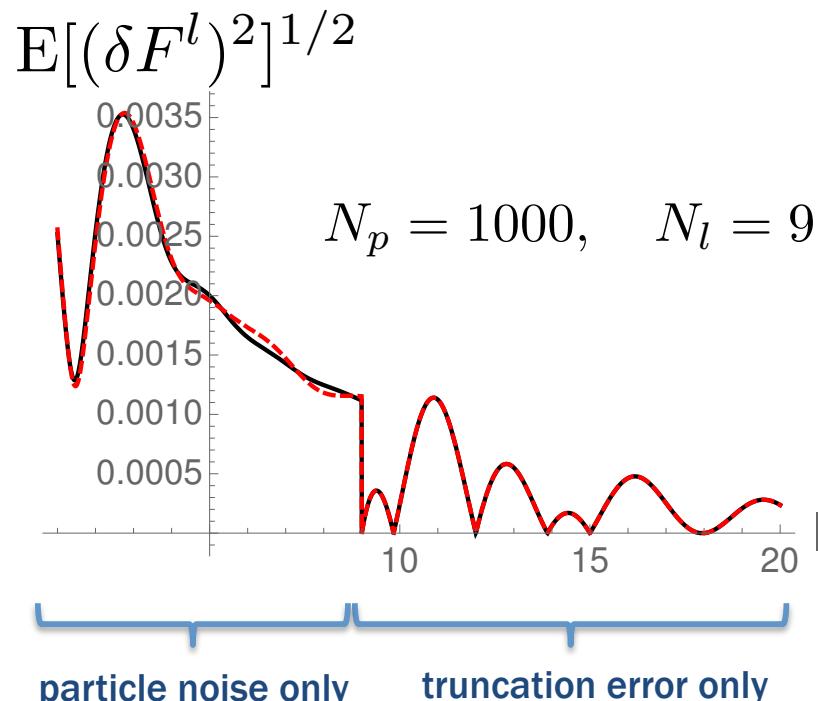
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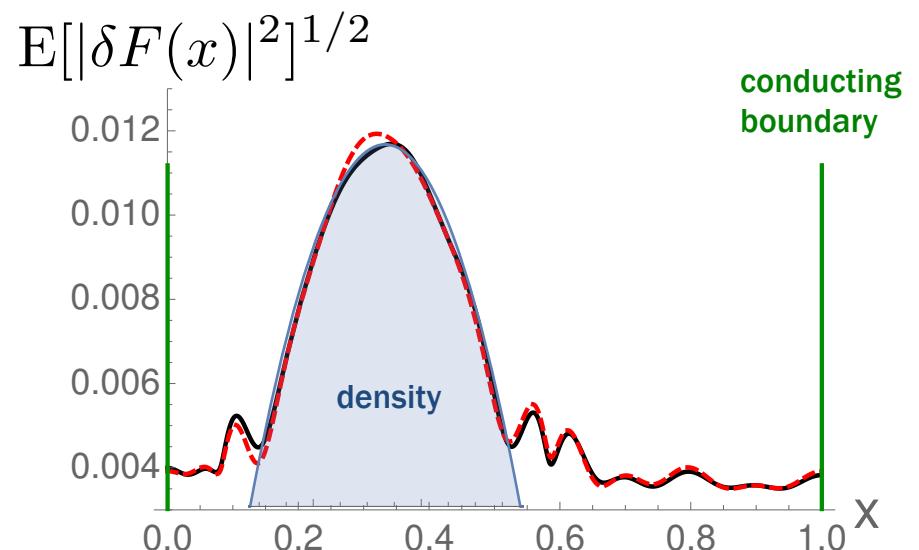


# 1D Example: Errors in the Spectral and Spatial Domains for a parabolic beam distribution

RMS error vs. mode number



RMS error vs. position



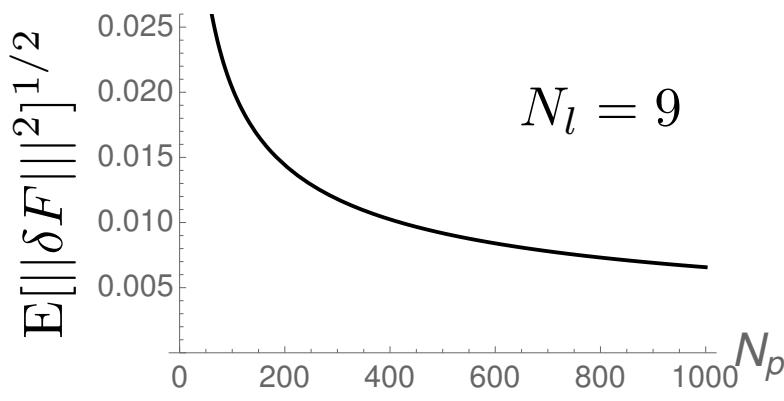
- Absolute error is largest in the beam core.
- Gibbs ringing near the edges of the beam.

- Analytical prediction of the rms error in the computed field  
--- Statistically computed rms field error using 200 random seeds

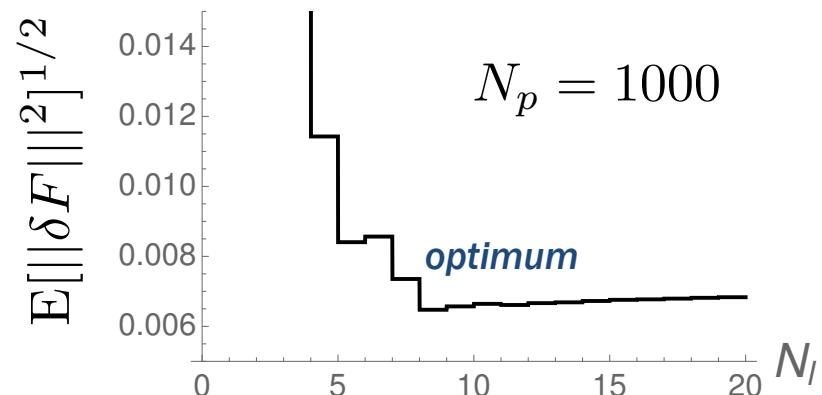
# Expected $L^2$ norm of the field error and its minimization

The mean-squared value of the  $L^2$  norm of the error over the domain  $\Omega$  is given by:

## RMS error vs. number of particles



## *RMS error vs. number of modes*



# Expected $L^2$ norm of the field error and its minimization

The mean-squared value of the  $L^2$  norm of the error over the domain  $\Omega$  is given by:

$$\mathbb{E}[||\delta \vec{F}||^2] = -\frac{1}{N_p} \sum_{l \in S} \frac{n^2}{\lambda_l} \text{Var}[e_l] - \sum_{l \notin S} \frac{n^2}{\lambda_l} \mathbb{E}[e_l]^2$$



- Here  $S$  denotes the set of indices for all numerically computed modes.
- Every mode contribution is nonnegative, and the  $L^2$  error is globally optimized when we enforce the condition that  $l \in S$  if and only if:

$$\frac{\mathbb{E}[(\delta F^l)^2]}{(F_{\text{exact}}^l)^2} = \frac{\text{Var}[\delta \rho^l]}{(\rho_{\text{exact}}^l)^2} = \frac{1}{N_p} \frac{\text{Var}[e_l]}{\mathbb{E}[e_l]^2} \leq 1$$

- A tighter condition on the variance of computed modes helps with emittance growth<sup>1</sup>.

[1] J. Qiang, "Long-term simulation of space charge fields," submitted NIMA (2018).

# Analysis of emittance growth on a single step



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# Change in RMS emittance after a single space charge step

A single space charge kick of step size  $\tau$  of the form  $(x, p) \rightarrow (x, p + \tau F(x))$  induces a change of RMS emittance given exactly by:

$$\epsilon^2 - \epsilon_0^2 = 2\tau A + \tau^2 B \quad \text{where}$$



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$$A = \langle \Delta x^2 \rangle \langle \Delta p \Delta F \rangle - \langle \Delta x \Delta p \rangle \langle \Delta x \Delta F \rangle = \langle \Delta x^2 \rangle \langle \Delta p_u \Delta F_u \rangle$$

measures the size of nonlinear correlations between  $p$  and  $F$

variable sign

Here  $F_u$  and  $p_u$  denote  $F$  and  $p$  after subtracting linear correlations with  $x$ .



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measures the size of nonlinear correlations between  $p$  and  $F$

variable sign

$$B = \langle \Delta x^2 \rangle \langle \Delta F^2 \rangle - \langle \Delta x \Delta F \rangle^2 = \langle \Delta x^2 \rangle \langle \Delta F_u^2 \rangle$$

measures the size of the nonlinear part of  $F$

always  
nonnegative

Here  $F_u$  and  $p_u$  denote  $F$  and  $p$  after subtracting linear correlations with  $x$ .



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# Statistical properties of emittance change after a single space charge step (1)

Our probabilistic model gives the statistics of  $A$  and  $B$  as sums over spectral modes:

$$\text{E}[A] = \sum_{l=1}^{N_l} \frac{n}{\lambda_l} A^l , \quad \text{Var}[A] = \sum_{l,m=1}^{N_l} \frac{n^2}{\lambda_l \lambda_m} A^{lm} ,$$

$$\text{E}[B] = \sum_{l,m=1}^{N_l} \frac{n^2}{\lambda_l \lambda_m} B^{lm} , \quad \text{Var}[B] = \sum_{l,m,l',m'=1}^{N_l} \frac{n^4}{\lambda_l \lambda_m \lambda_{l'} \lambda_{m'}} B^{lml'm'}$$

In the smooth beam limit  $N_p \rightarrow \infty$  we have nonzero emittance change given by\*:

$$A^l = \text{Var}[x] \text{Cov}[p, e'_l] \text{E}[e_l] , \quad A^{lm} = 0$$

$$B^{lm} = \text{Var}[x] \text{Cov}[e'_l, e'_m] \text{E}[e_l] \text{E}[e_m] , \quad B^{lml'm'} = 0$$

\*after removing linear correlations of  $p$  and  $e$ , with  $x$

# Statistical properties of emittance change after a single space charge step (2)

When we include corrections through order  $1/N_p$ , we introduce the effects of particle noise. Term A is simple when p and x have no nonlinear correlation:

$$\text{E}[A] = 0 , \quad \text{Var}[A] = \frac{1}{N_p} \text{Var}[x] \text{Var}[p] \text{E}[B] .$$

Term B is quite complicated, but can be determined via computer algebra. For example:

$$B^{lm} = \lim_{N_p \rightarrow \infty} B^{lm} + \frac{1}{2N_p} (T^{lm} + T^{ml}) ,$$

$$T^{l,m} =$$

$$\begin{aligned} & \text{Var}[x] \text{Cov}[e'_l, e'_m] \text{Cov}[e_l, e_m] - 3 \text{Var}[x] \text{Cov}[e'_l, e'_m] \text{E}[e_l] \text{E}[e_m] \\ & + 2 \text{Cov}[x^2, e_l] \text{Cov}[e'_l, e'_m] \text{E}[e_m] + 2 \text{Var}[x] \text{Cov}[e'_l e'_m, e_l] \text{E}[e_m] \end{aligned}$$



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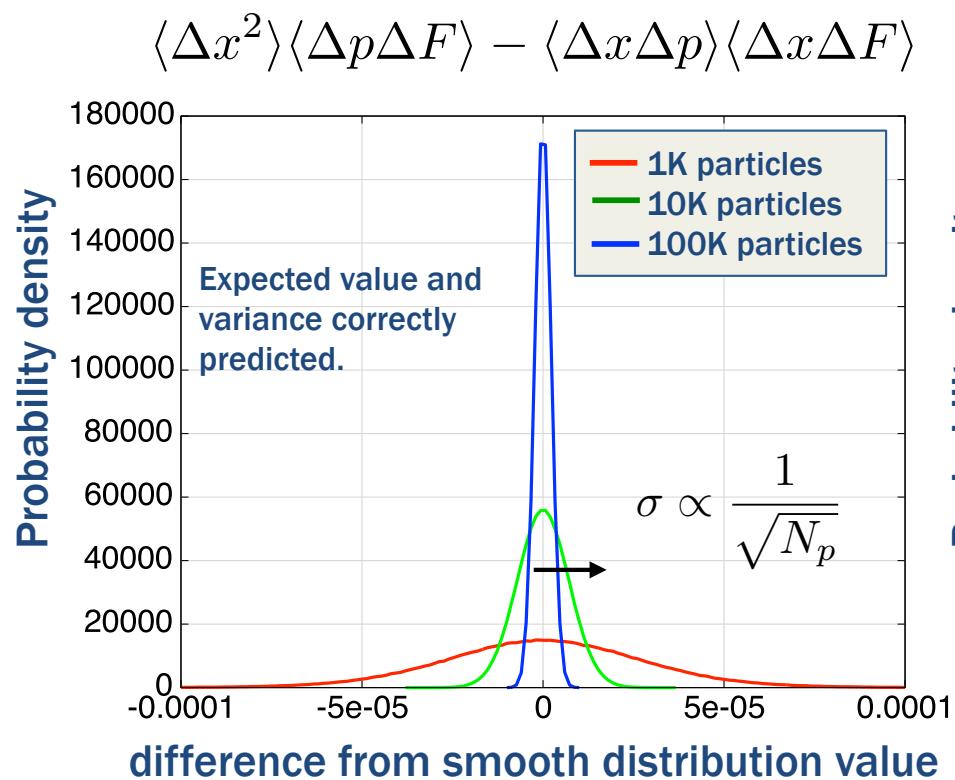
$$\begin{aligned} & \text{Var}[x] \text{Cov}[e'_l, e'_m] \text{Cov}[e_l, e_m] - 3 \text{Var}[x] \text{Cov}[e'_l, e'_m] \text{E}[e_l] \text{E}[e_m] \\ & + 2 \text{Cov}[x^2, e_l] \text{Cov}[e'_l, e'_m] \text{E}[e_m] + 2 \text{Var}[x] \text{Cov}[e'_l e'_m, e_l] \text{E}[e_m] \end{aligned}$$

This result is consistent with that of Kesting<sup>1</sup> if we keep only the first term.

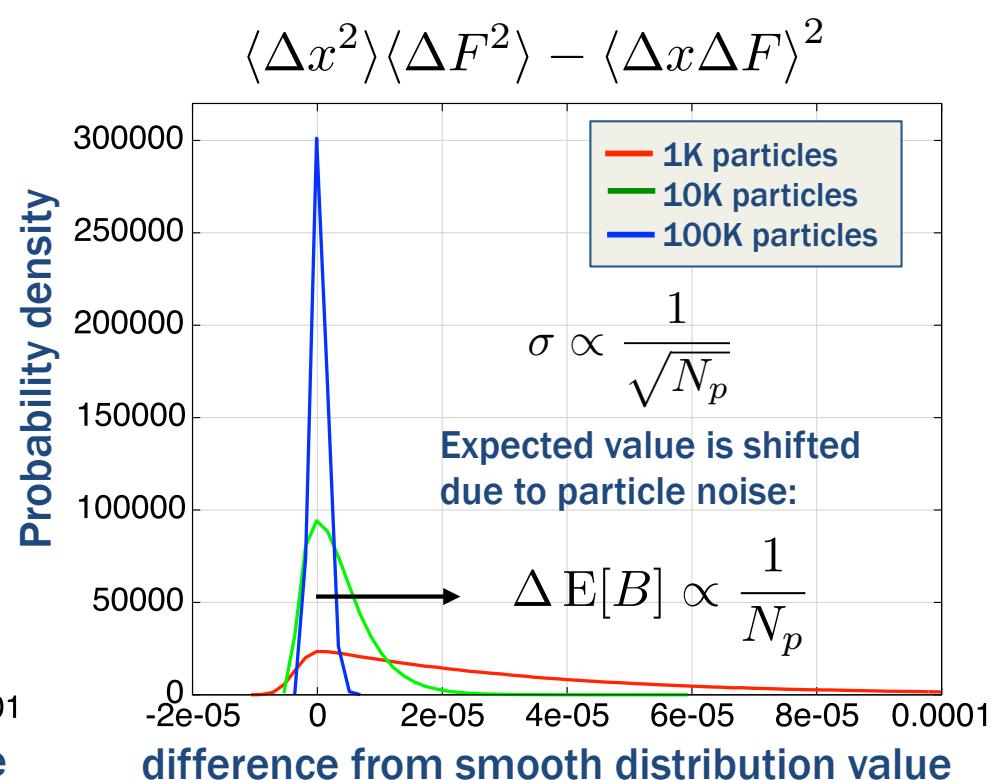
# Statistical properties of excess emittance growth on a single numerical step (uniform beam w/ x-p correlation)

1D uniform beam using 15 spectral modes, using 1M random seeds

*term A*



*term B*



# Numerical emittance growth in a FODO channel



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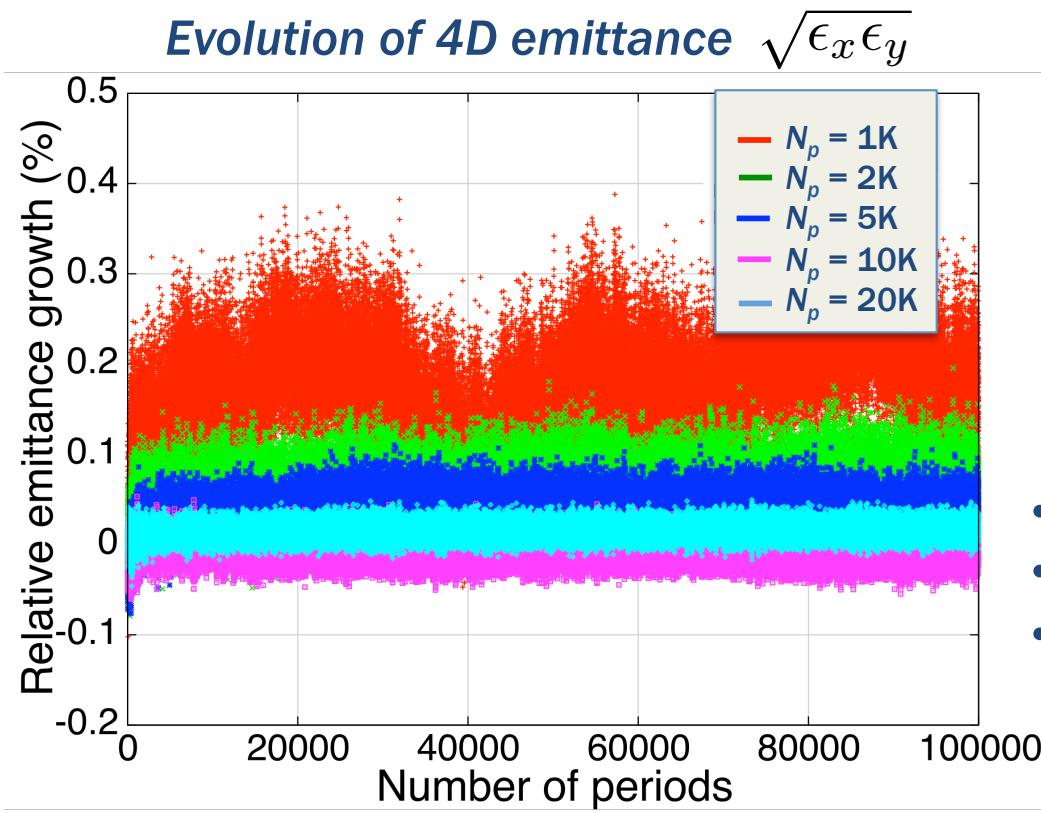
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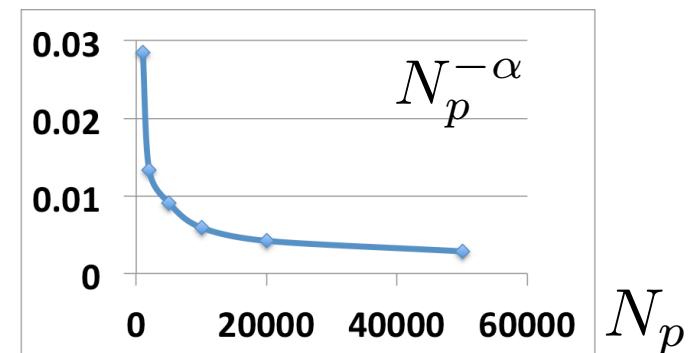
# Matched KV Beam in a FODO Channel

1 GeV proton beam, 100 A current  
Zero current phase advance: 87°  
Depressed phase advance: 74°

Initial rms emittance: 1  $\mu\text{m}$   
2D domain: [0,6.5]  $\times$  [0,6.5] mm  
Number of modes: 15  $\times$  15



*Emittance fluctuation (rms) vs.  $N_p$*

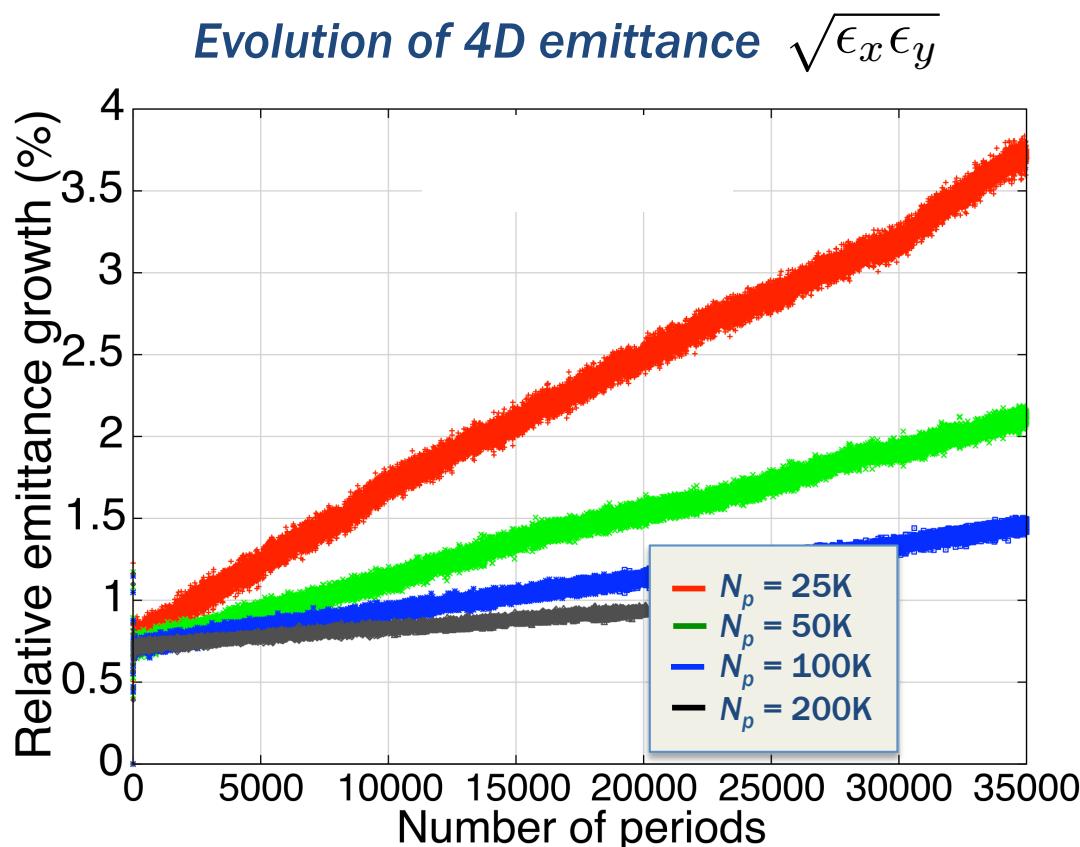


- Emittance is well-preserved.
- Fluctuations scale w/power  $\alpha = 0.57$
- Based on model of a single step:

$$\sigma_{\Delta\epsilon} \propto \text{Var}[A]^{1/2} \propto \frac{n}{\sqrt{N_p}}$$

# Matched Gaussian Beam in a FODO Channel

1 GeV proton beam, 100 A current  
Zero current phase advance: 87°  
Depressed phase advance: 74°



Initial rms emittance: 1  $\mu\text{m}$   
2D domain: [0,6.5]  $\times$  [0,6.5] mm  
Number of modes: 32  $\times$  32

- Emittance growth rate  $N_p^{-\beta}$
- Emittance fluctuations  $N_p^{-\alpha}$   
 $\beta = 0.996, \quad \alpha = 0.58$
- Based on model of a single step:

$$E \left[ \frac{d\epsilon}{ds} \right] \propto E[B] \propto \frac{n^2}{N_p}$$

- Driven by collisional heat exchange between degrees of freedom<sup>1</sup>:

$$\frac{dS}{dt} = \frac{1}{2} k_B \beta_f \frac{(T_x - T_y)^2}{T_x T_y}$$

# Conclusions

- *The properties of “symplecticity” and “collisionlessness” in particle-based space charge tracking codes are distinct.*
- Symplecticity (in the  $N_p$ -particle sense) eliminates non-Hamiltonian artifacts from the numerical integrator, but does *not* imply that the system of macroparticles is collisionless. Additional techniques (particle shapes, noise filtering) can be used.
- This symplectic spectral algorithm is simple enough that probabilistic models of the numerical field error and emittance growth on a numerical step can be applied.
- Two emittance driving terms:  $A$  (drives fluctuations),  $B$  (nonnegative, drives growth).
- A first-principles treatment of emittance growth due numerical collisions *with dynamics* would take the complete approach:

Numerical  $N_p$ -particle Hamiltonian  $\rightarrow$  BBGKY hierarchy  $\rightarrow$  kinetic equation (Vlasov-Fokker-Planck-like)  $\rightarrow$  moment equations (*a la* Struckmeier)



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## Backup material



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# Spectral approach to the Poisson equation on bounded domains

Let  $\Omega$  be a bounded, open domain in  $\mathbb{R}^d$ . Consider the Poisson eq. in the form:

$$\nabla^2 U = -\rho \quad U|_{\partial\Omega} = 0 .$$

There exists an orthonormal basis  $\{e_l : l = 1, 2, \dots\}$  for the Hilbert space of square-integrable functions on  $\Omega$  such that each  $e_l$  is a smooth eigenfunction of the Laplace operator:

$$\nabla^2 e_l = \lambda_l e_l \quad e_l|_{\partial\Omega} = 0 \quad (\lambda_l < 0) .$$

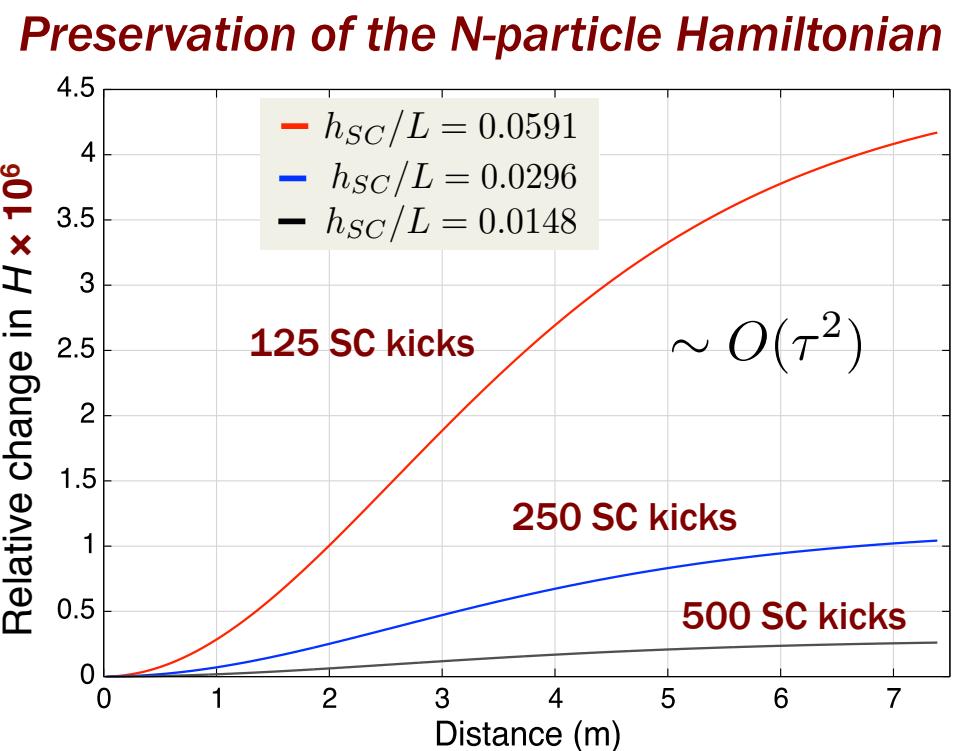
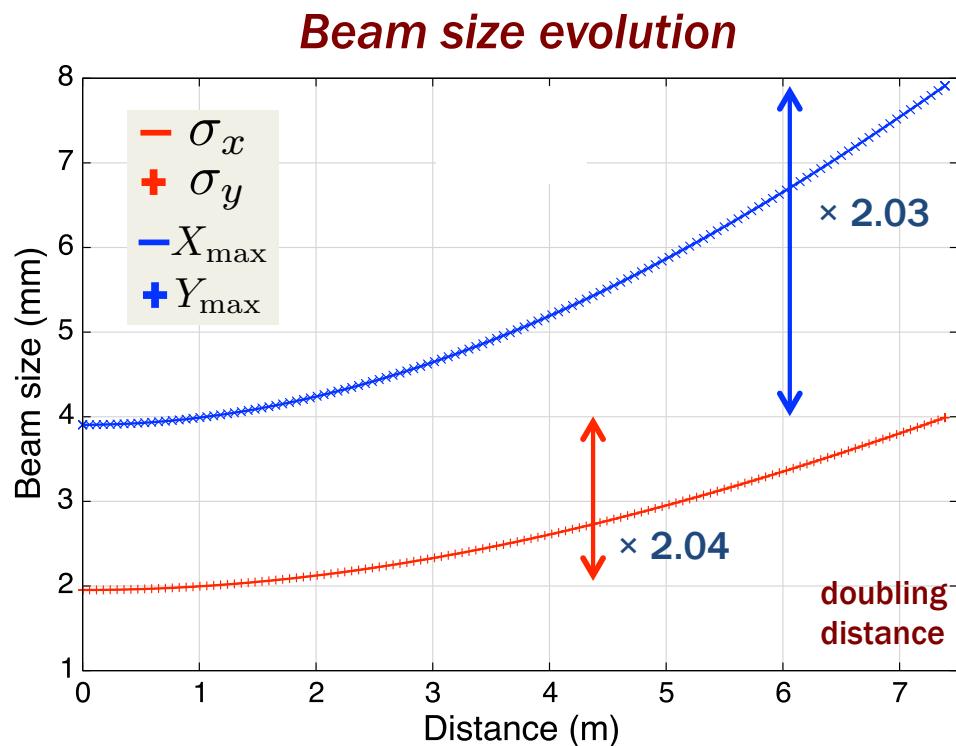
We denote the coefficient of mode  $l$  of any square-integrable function  $f$  on  $\Omega$  as  $f^l$ .

The following vector-valued functions can be extended to an orthonormal basis:

$$\vec{e}_l = \frac{1}{\sqrt{-\lambda_l}} \nabla e_l \quad (l = 1, 2, \dots) .$$

The modes of  $U$  and  $\vec{F} = -\nabla U$  satisfy:  $U^l = -\rho^l / \lambda_l$ ,  $F^l = -\sqrt{-\lambda_l} U^l$ .

# Benchmark: Expansion in a drift space of a cold uniform cylinder beam with 2D transverse space charge



$KE = 2.5 \text{ MeV } p$   
 $R_0 = 3.905 \text{ mm}$   
 $I = 4.113 \text{ mA}$   
 $a = b = 5 \text{ cm}$

2D rectangular domain  
 $\Omega = (0, a) \times (0, b)$

Similar behavior for the beam emittance evolution.

# Systematic removal of correlations with $x$

Note that term A and term B are each invariant under any transformation of the form:

$$x \rightarrow x + c, \quad p \rightarrow p + ax + b, \quad F \rightarrow F + gx + h$$

for any constants a, b, c, g, and h. It follows that we can replace  $x$ ,  $p$ , and  $e$ , using

$$x = E[x] + x_u \quad p = E[p] + \frac{\text{Cov}[x, p]}{\text{Var}[x]}(x - E[x]) + p_u$$

$$e'_l = E[e'_l] + \frac{\text{Cov}[x, e'_l]}{\text{Var}[x]}(x - E[x]) + e'_{l,u}$$

The final result is then made significantly simpler, since we may assume w.l.o.g. that:

$$E[x] = 0, \quad E[p] = 0, \quad E[e_l] = 0, \quad \text{Cov}[x, p] = 0, \quad \text{Cov}[x, e'_l] = 0$$

provided we replace  $x$ ,  $p$ , and  $e$ , with their uncorrelated values.



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# Statistical analysis of emittance growth during two numerical steps (numerical tests)

- 1) Randomly generate a beam consisting of particle data ( $x, p$ ).
  - 2) Take  $\frac{1}{2}$  step in the external fields (here, a drift).
  - 3) Compute space charge force  $F(x)$  at all particle locations using the 1-D symplectic spectral algorithm.
  - 4) Compute the statistical quantities appearing on Slide 2 (averaging over the beam).
  - 5) Take 1 full step in the space charge fields.
  - 6) Take  $\frac{1}{2}$  step in the external fields (here, a drift).
  - 7) Take  $\frac{1}{2}$  step in the external fields (here, a drift).
  - 8) Compute space charge force  $F(x)$  at all particle locations using the 1-D symplectic spectral algorithm.
  - 9) Compute the statistical quantities appearing on Slide 2 (averaging over the beam).
  - 10) Take 1 full step in the space charge fields.
  - 11) Take  $\frac{1}{2}$  step in the external fields (here, a drift).
  - 12) Repeat 1)-5) for  $N_{seed}$  distinct random seeds.
  - 13) Compute statistical moments of quantities computed in 4) and 9) (averaging over random seeds).
- step 1**      **term A, term B  
(kick 1)**
- step 2**      **term A, term B  
(kick 2)**

**Each step:**  $\mathcal{M}(\tau) = \mathcal{M}_{ext}(\tau/2)\mathcal{M}_{SC}(\tau)\mathcal{M}_{ext}(\tau/2) + O(\tau^3)$



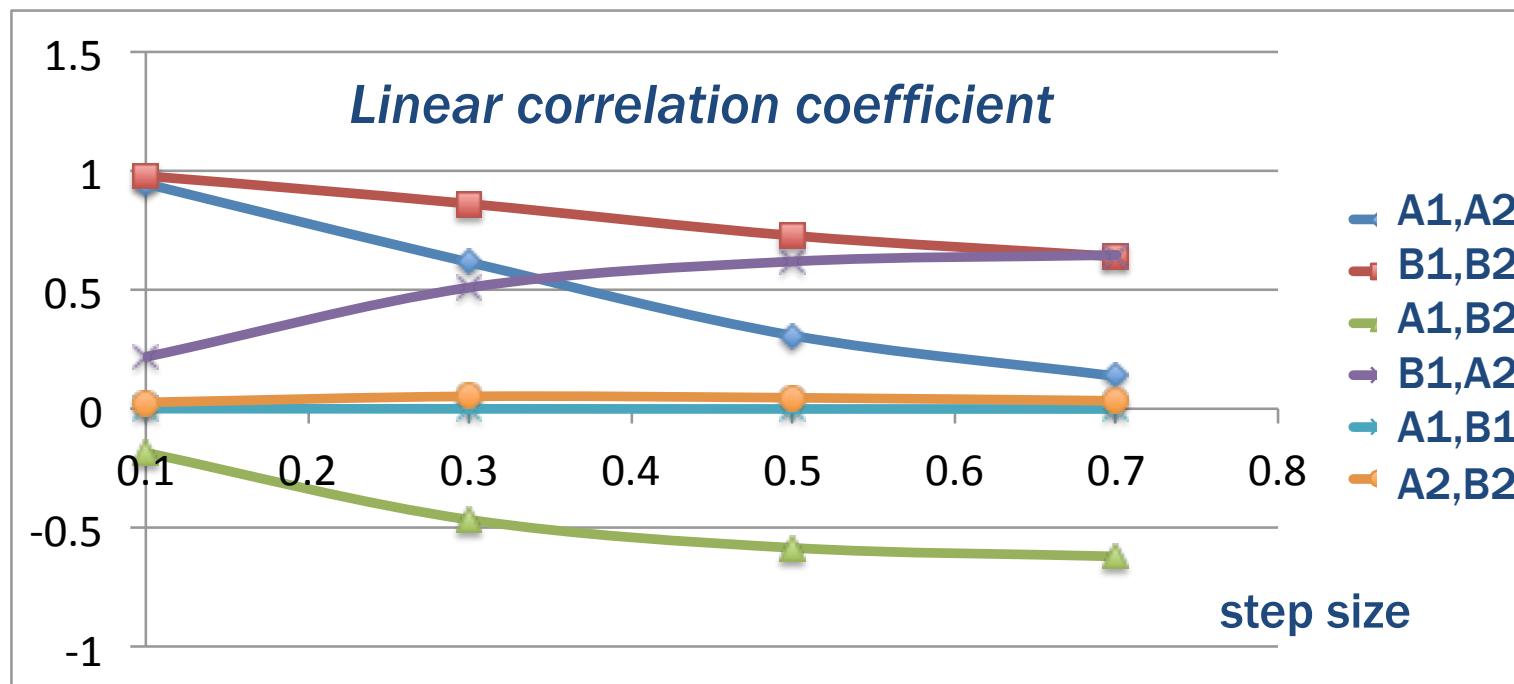
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# Statistical correlations between two successive steps for the Gaussian beam numerical example

*Correlations between terms A and B – successive steps*

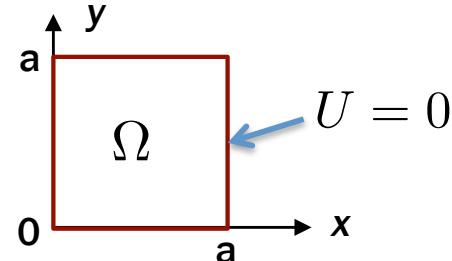


# Choosing the Optimal Number of Modes (to Minimize Norm of the Field Error) – 2D Example

Domain:  $\Omega = (0, a) \times (0, a)$

Orthonormal basis eigenmodes:

$$e_{lm} = \frac{2}{a} \sin\left(\frac{l\pi x}{a}\right) \sin\left(\frac{m\pi y}{a}\right) \quad \nabla^2 e_{lm} = \lambda_{lm} e_{lm}, \quad e_{lm}|_{\partial\Omega} = 0$$



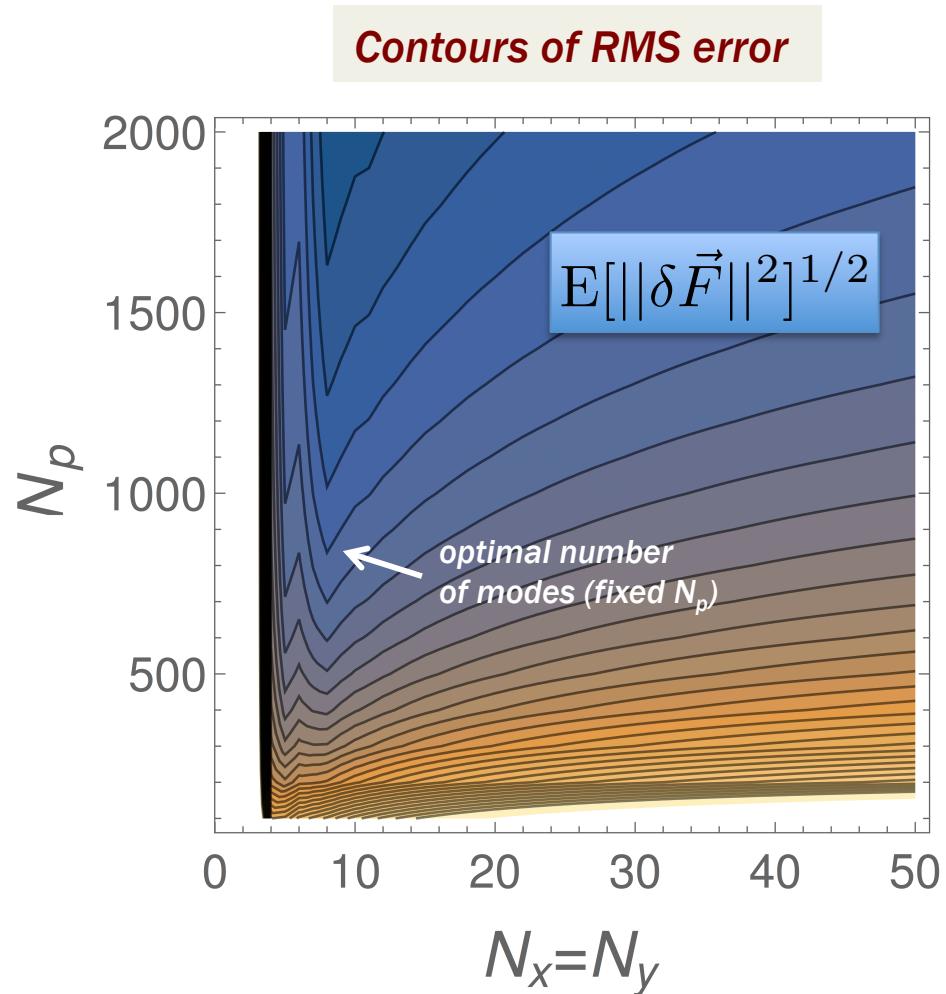
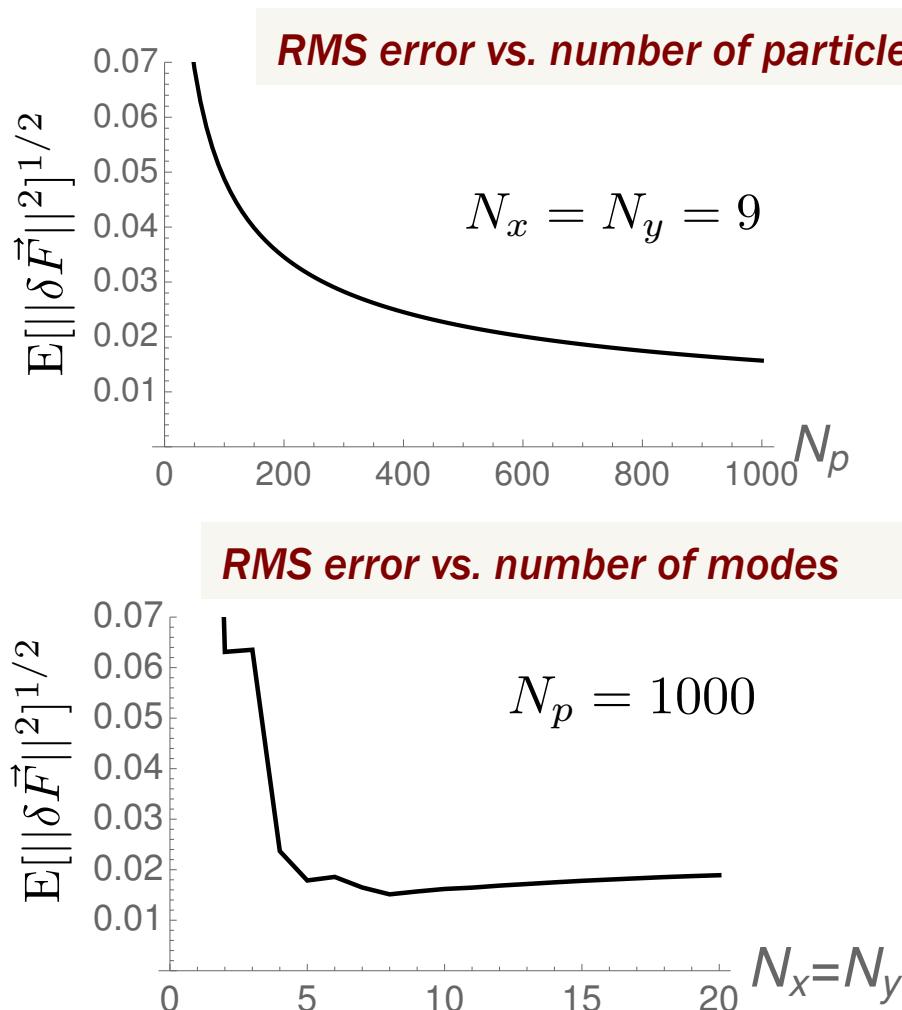
Eigenvalues:  $\lambda_{lm} = -\left(\frac{l\pi}{a}\right)^2 - \left(\frac{m\pi}{a}\right)^2 \quad (l, m = 1, 2, \dots)$

Each 2D mode is a tensor product of 1D modes. For simplicity, we truncate the mode sum such that the max horizontal 1D mode index = the max vertical 1D mode index.

Density:

$$P(x, y) = \frac{9}{16h^2} \left(1 - \frac{(x - d)^2}{h^2}\right) \left(1 - \frac{(y - d)^2}{h^2}\right) \quad |x - d| \leq h, \quad |y - d| \leq h$$

# Choosing the Optimal Number of Modes (to Minimize Norm of the Field Error) – 2D Example



# Probabilistic model of particle noise (identities)

If  $a_j$  ( $j=1, \dots, N$ ),  $b_k$  ( $k=1, \dots, M$ ) are single-particle dynamical variables, some work gives:

$$E \left[ \prod_{j=1}^N \langle a_j \rangle \right] = \prod_{j=1}^N E[a_j] + \frac{1}{N_p} \sum_{\substack{j,k=1 \\ j < k}}^N \text{Cov}[a_j, a_k] \prod_{\substack{n=1 \\ n \neq j \\ n \neq k}}^N E[a_n] + O\left(\frac{1}{N_p^2}\right)$$

$$\text{Cov} \left[ \prod_{j=1}^N \langle a_j \rangle, \prod_{k=1}^M \langle b_k \rangle \right] = \frac{1}{N_p} \sum_{j=1}^N \sum_{k=1}^M \prod_{r \neq j}^N E[a_r] \prod_{s \neq k}^M E[b_s] \text{Cov}[a_j, b_k] + O\left(\frac{1}{N_p^2}\right)$$

Using the linearity of  $E$  and  $\text{Cov}$ , these results allow us to determine the statistics of any quantity that is given as a *polynomial* when expressed using beam-based averages on the single-particle phase space.

This covers all cases of interest here. Higher-order terms in  $1/N_p$  are neglected.



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