

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

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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 plasmas¹ or beams².
- 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 solvers² 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 .

Ω	bounded domain (1-2D)
e_l, λ_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:

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

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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

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*:

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

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 :

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

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:

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

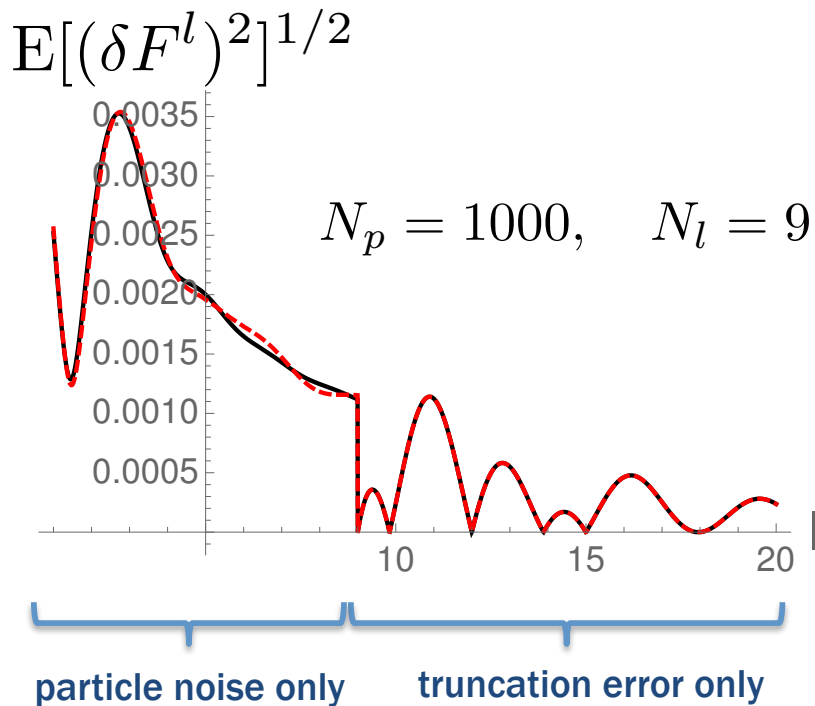
This allows us to evaluate the statistical moments of the error in the various modes of the computed field. Here $\delta\vec{F} = \vec{F} - \vec{F}_{\text{exact}}$. The second moments are given by:

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

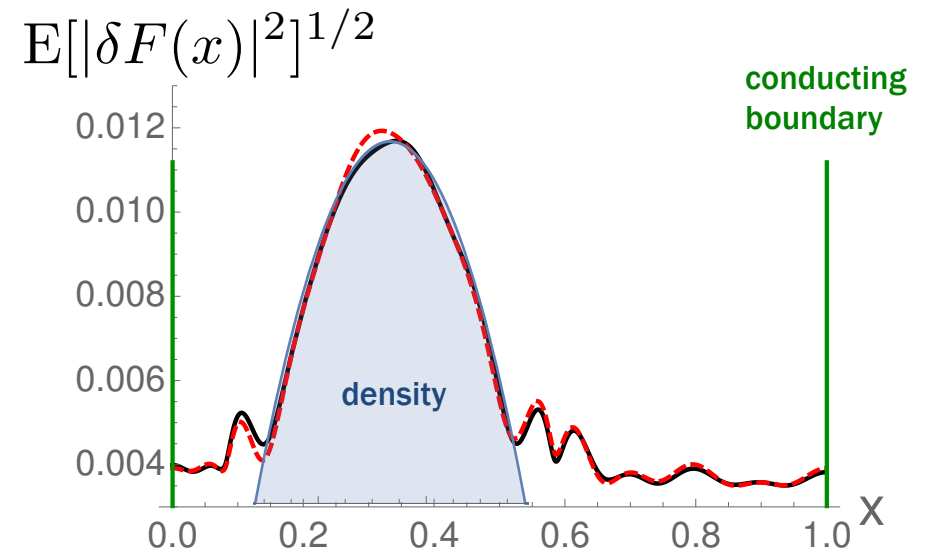
$$\mathbb{E}[\delta F^l \delta F^m] = \frac{n^2}{\sqrt{\lambda_l \lambda_m}} \mathbb{E}[e_l] \mathbb{E}[e_m] \quad (l, m > N_l) \quad \text{(modes above cutoff)}$$

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.

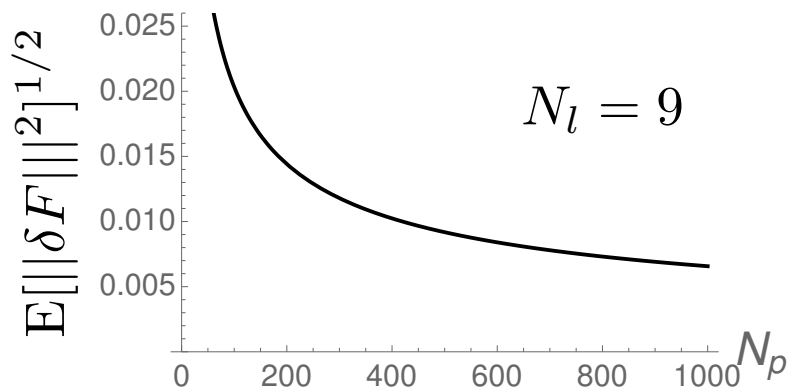
- Analytical prediction of the rms error in the computed field
- - - Statistically computed rms field error using 200 random seeds

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

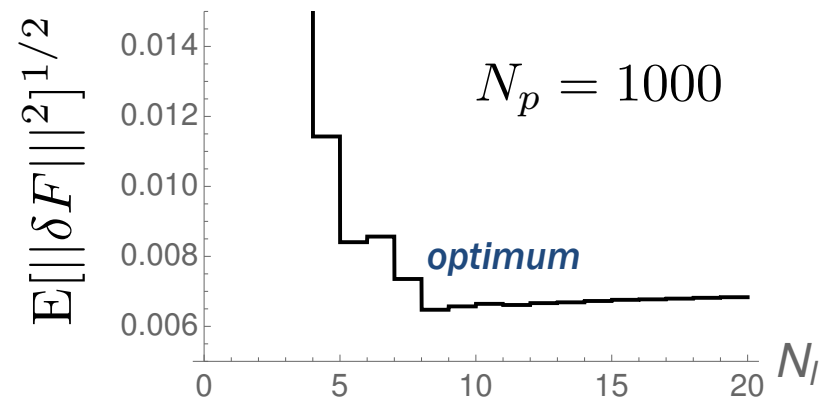
The mean-squared value of the L^2 norm of the error over the domain Ω is given by:

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

RMS error vs. number of particles



RMS error vs. number of modes



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

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- 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 growth¹.

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

Analysis of emittance growth on a single step

Change in RMS emittance after a single space charge step

A single space charge kick of step size τ 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 .

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:

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

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

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

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

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

*after removing linear correlations of p and e_l 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:

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

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

$$B^{lm} = \lim_{N_p \rightarrow \infty} B^{lm} + \frac{1}{2N_p} (T^{lm} + T^{ml}) ,$$
$$T^{l,m} =$$
$$\text{Var}[x] \text{Cov}[e'_l, e'_m] \text{Cov}[e_l, e_m] - 3 \text{Var}[x] \text{Cov}[e'_l, e'_m] E[e_l] E[e_m]$$
$$+ 2 \text{Cov}[x^2, e_l] \text{Cov}[e'_l, e'_m] E[e_m] + 2 \text{Var}[x] \text{Cov}[e'_l e'_m, e_l] E[e_m]$$

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

This result is consistent with that of Kesting¹ if we keep only the first term.

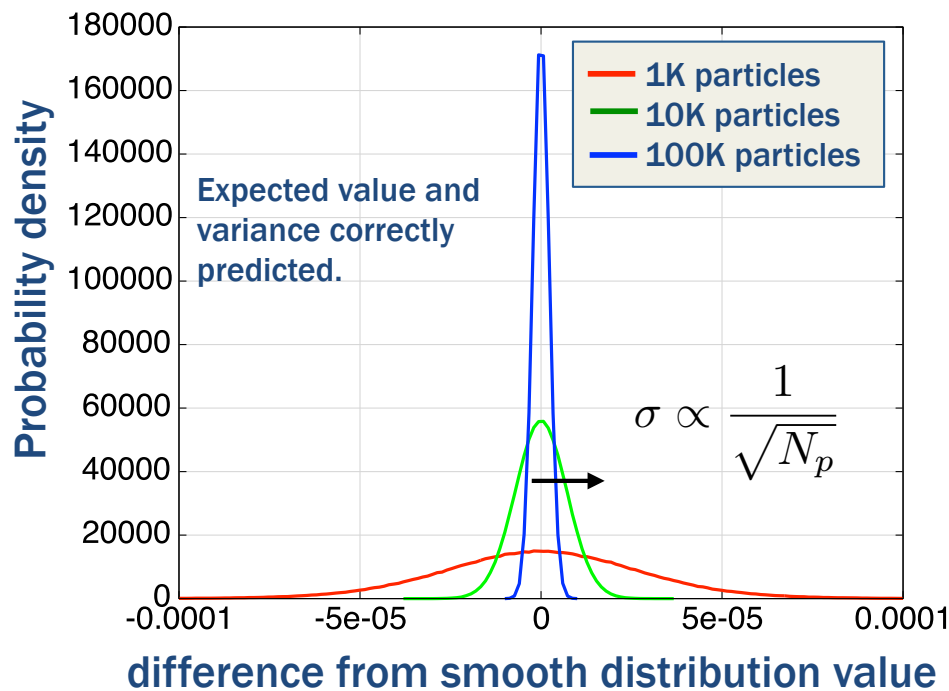
[1] F. Kesting and G. Franchetti, PRAB 18, 114201 (2015).

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

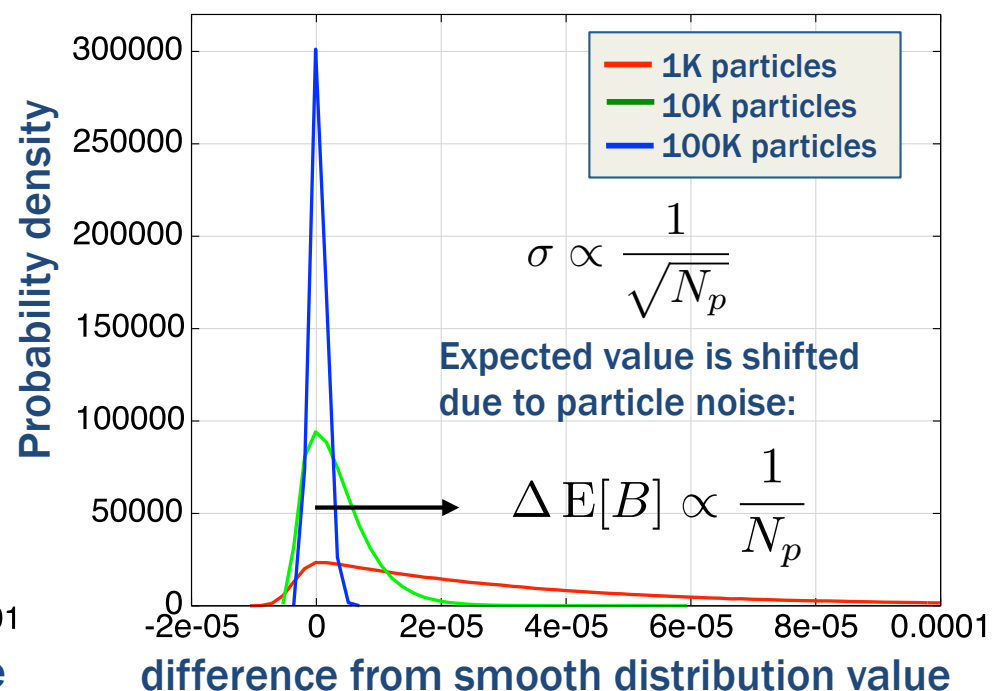
term A

$$\langle \Delta x^2 \rangle \langle \Delta p \Delta F \rangle - \langle \Delta x \Delta p \rangle \langle \Delta x \Delta F \rangle$$



term B

$$\langle \Delta x^2 \rangle \langle \Delta F^2 \rangle - \langle \Delta x \Delta F \rangle^2$$



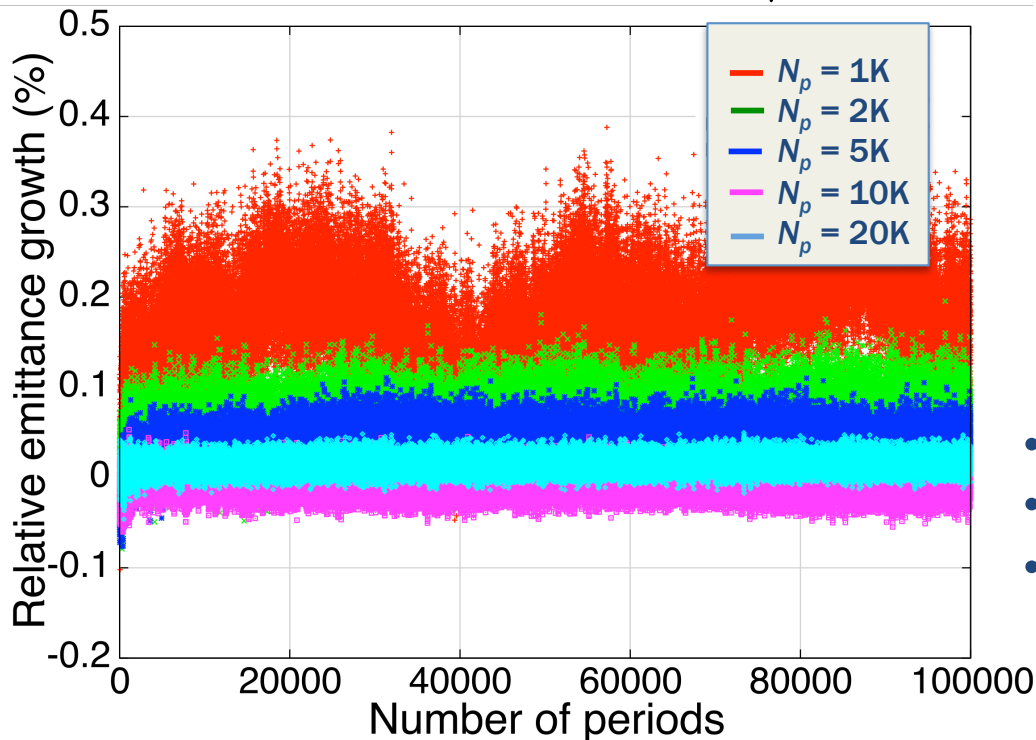
Numerical emittance growth in a FODO channel

Matched KV Beam in a FODO Channel

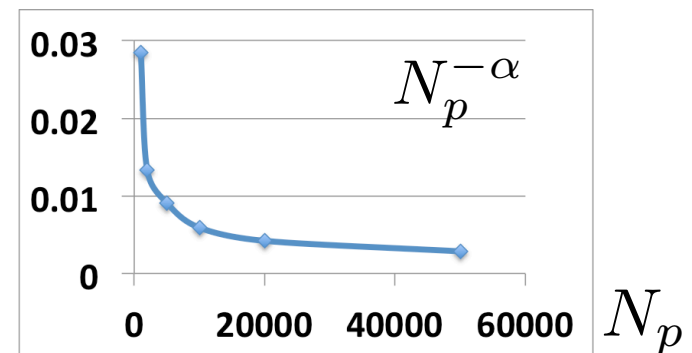
1 GeV proton beam, 100 A current
 Zero current phase advance: 87°
 Depressed phase advance: 74°

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

Evolution of 4D emittance $\sqrt{\epsilon_x \epsilon_y}$



Emittance fluctuation (rms) vs. N_p



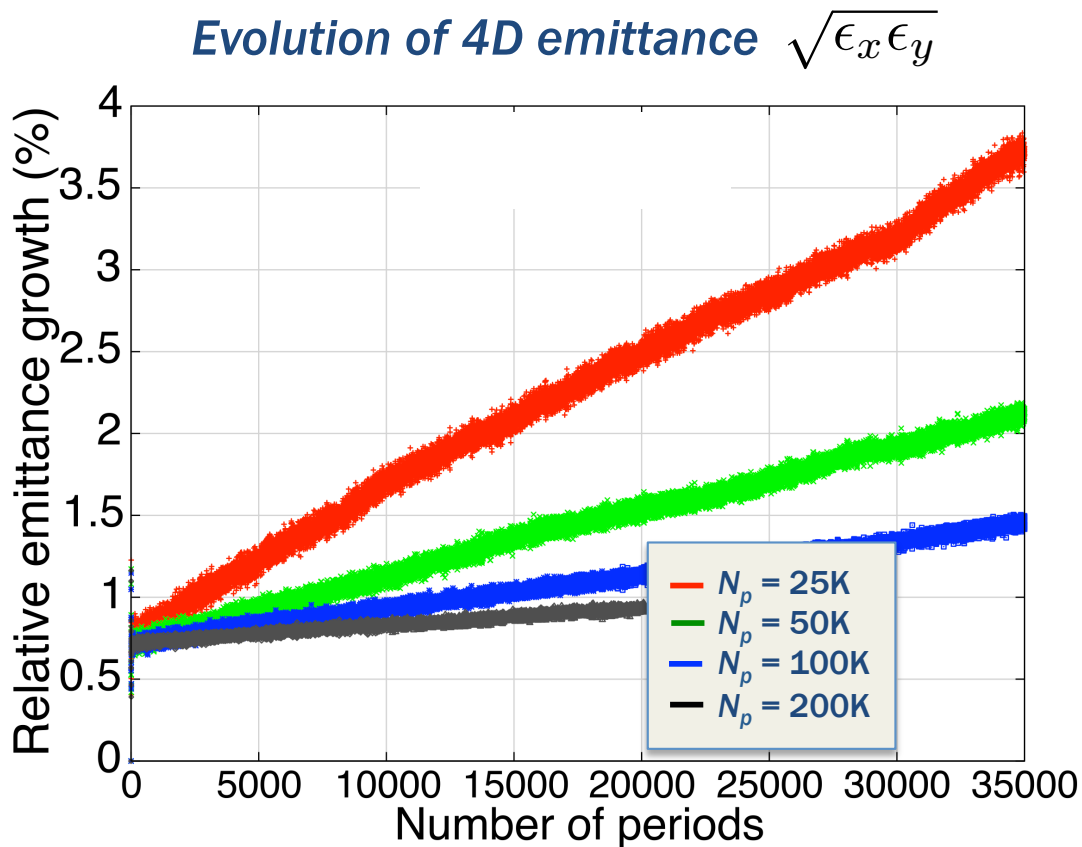
- Emittance is well-preserved.
- Fluctuations scale w/power $\alpha = 0.57$
- Based on model of a single step:

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

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: $[0,6.5] \times [0,6.5] \text{ mm}$
 Number of modes: 32×32



- 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 freedom¹:

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

[1] J. Struckmeier, Phys. Rev. E 54, 830 (1996).

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)

Backup material



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Spectral approach to the Poisson equation on bounded domains

Let Ω 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 Ω 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 Ω as f^l .

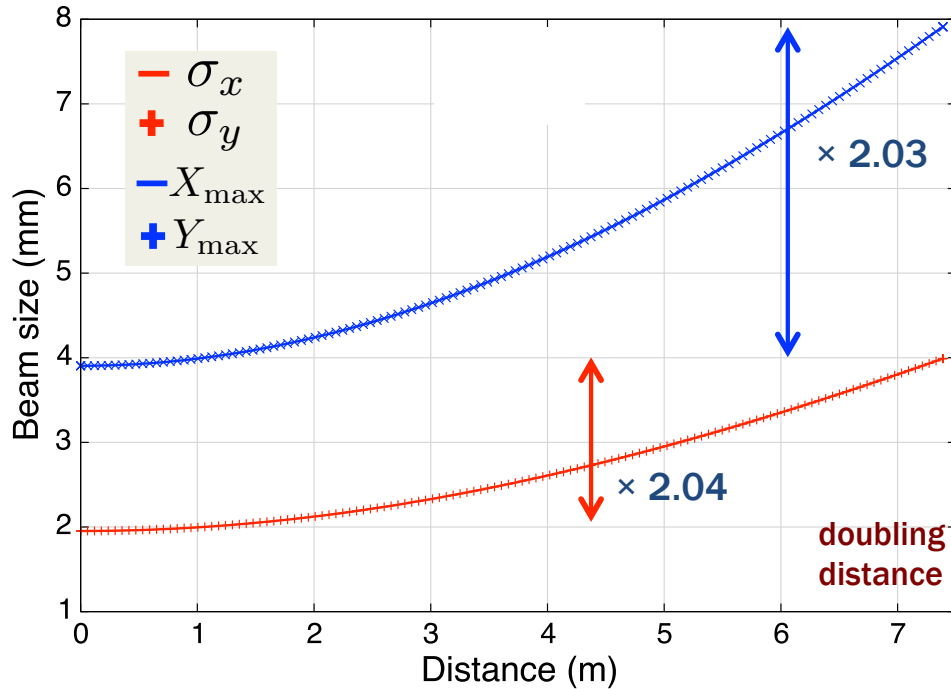
The following vector-valued functions can be extended to an orthonormal basis:

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

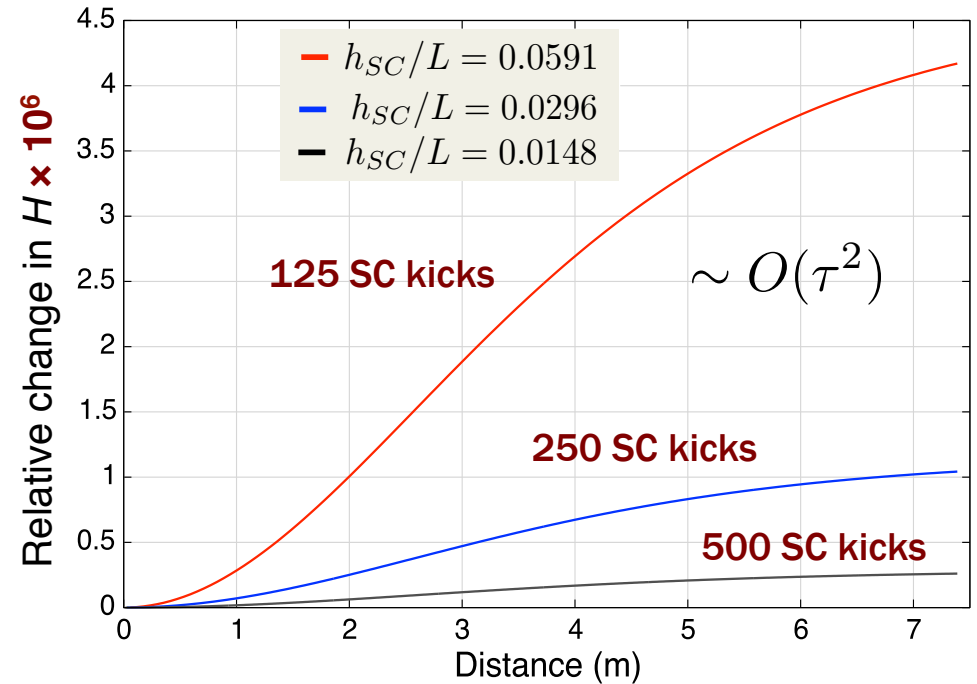
The modes of U and $\vec{F} = -\nabla U$ satisfy: $U^l = -\rho^l / \lambda_l$, $F^l = -\sqrt{-\lambda_l} U^l$.

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

Beam size evolution



Preservation of the N-particle Hamiltonian



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

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_l using

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



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

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

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

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

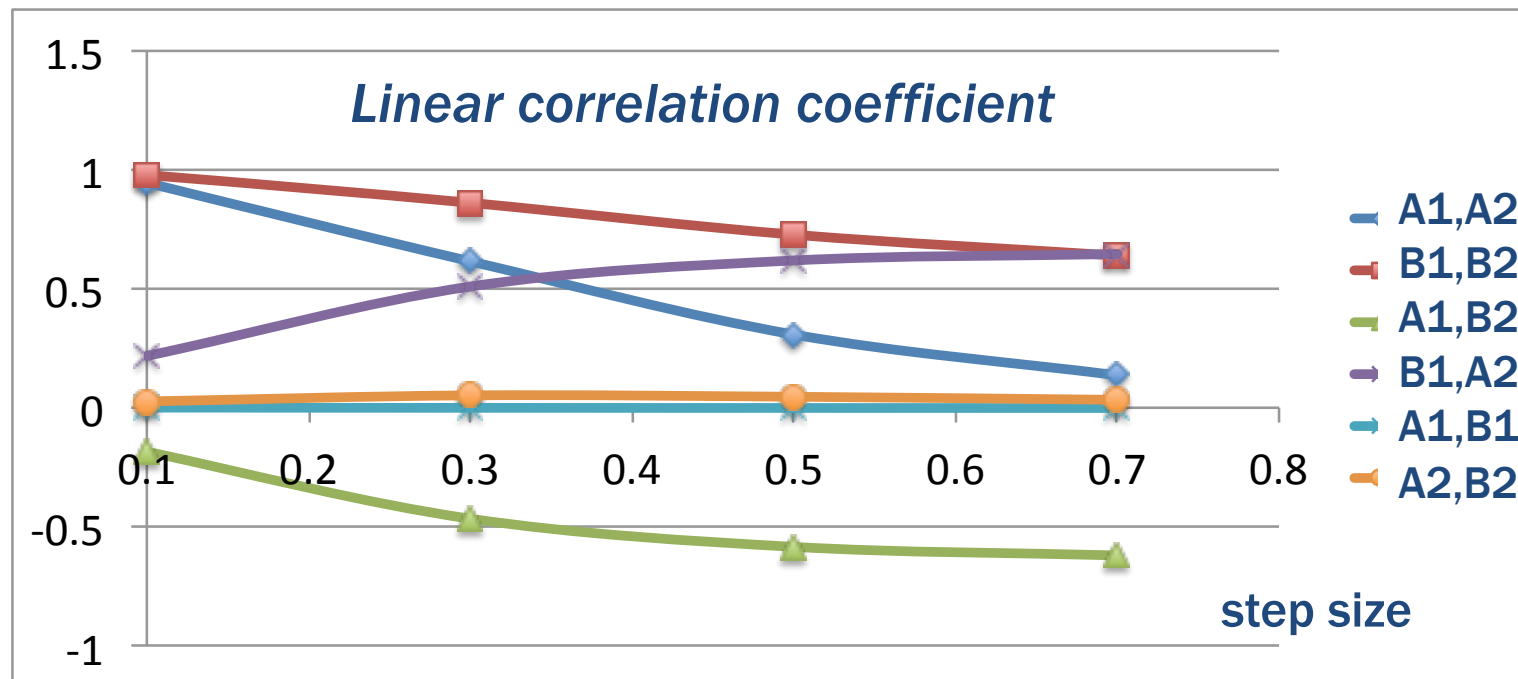
Statistical analysis of emittance growth during two numerical steps (numerical tests)

- step 1**
- 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).  **term A, term B (kick 1)**
 - 5) Take 1 full step in the space charge fields.
 - 6) Take $\frac{1}{2}$ step in the external fields (here, a drift).
- step 2**
- 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).  **term A, term B (kick 2)**
 - 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).

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

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:

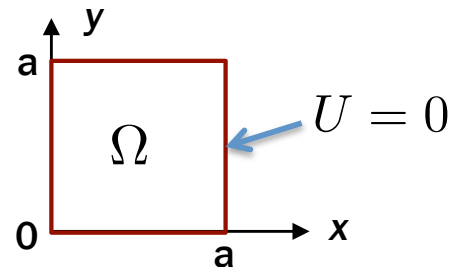
$$e_{lm} = \frac{2}{a} \sin\left(\frac{l\pi x}{a}\right) \sin\left(\frac{m\pi y}{a}\right) \quad \nabla^2 e_{lm} = \lambda_{lm} e_{lm}, \quad e_{lm}|_{\partial\Omega} = 0$$

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.

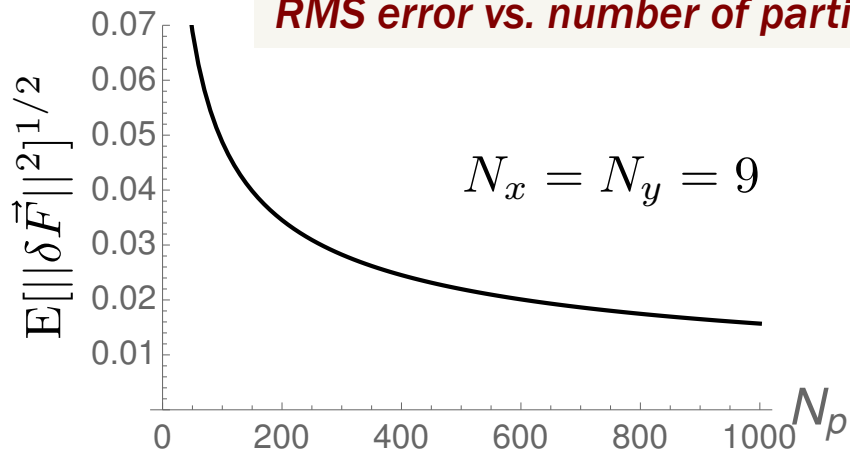
Density:

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

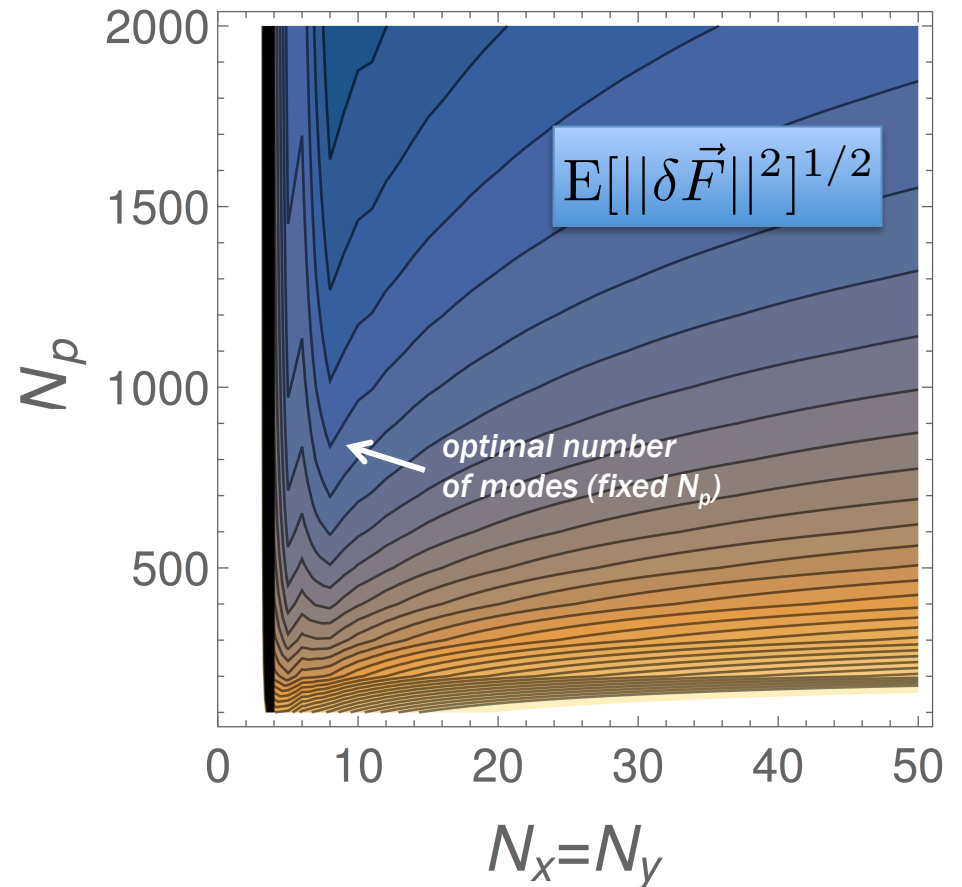


Choosing the Optimal Number of Modes (to Minimize Norm of the Field Error) – 2D Example

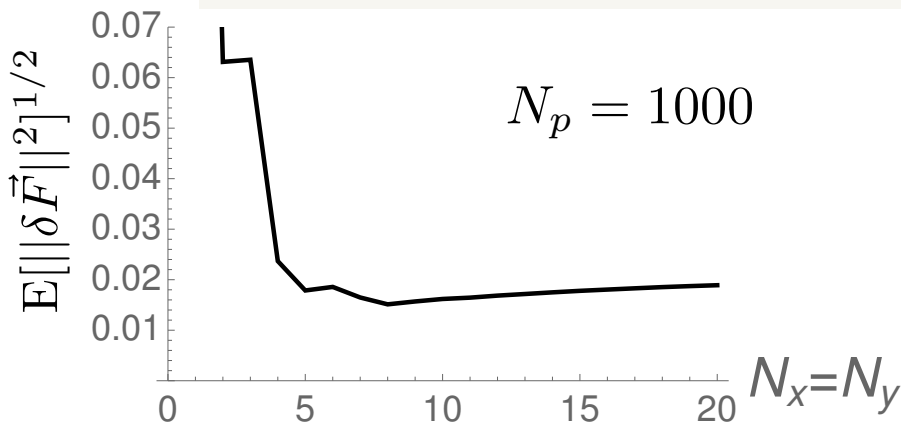
RMS error vs. number of particles



Contours of RMS error



RMS error vs. number of modes



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:

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

Using the linearity of \mathbb{E} and 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.