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ANALYSIS OF PARTICLE NOISE IN A GRIDLESS SPECTRAL POISSON SOLVER FOR SYMPLECTIC MULTIPARTICLE TRACKING

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Abstract

Gridless symplectic methods for self-consistent modeling of space charge in intense beams possess several advantages over traditional momentum-conserving particle-in-cell methods, including the absence of numerical grid heating and the presence of an underlying multi-particle Hamiltonian. Despite these advantages, there remains evidence of irreversible entropy growth due to numerical particle noise. For a class of such algorithms, a first-principles kinetic model of the numerical particle noise is obtained and applied to gain insight into noise-induced entropy growth and thermal relaxation.

INTRODUCTION

Distinguishing between physical and numerical emittance growth observed in long-term tracking of beams with space charge is critical to understanding beam performance at high intensities. Numerical emittance growth has been modeled as a collisional increase of the beam phase space volume driven by random noise caused by the use of a small number of macroparticles, and intimately related to the beam entropy [1]. Recently, several authors have developed methods for multiparticle tracking (in plasmas or beams) using variational or explicitly symplectic algorithms designed to preserve the geometric properties of the self-consistent equations of motion [2–4]. The multi-particle symplectic algorithm described in [4] is sufficiently simple that field fluctuations and emittance growth on a single numerical step can be studied analytically [5]. In this paper, we develop a kinetic formalism to better understand the dynamical evolution of particle noise in this and similar algorithms.

SYMPLECTIC SPECTRAL ALGORITHM

We extend the algorithm described in Section III of [4] to treat the Poisson equation in a general bounded domain $\Omega \subset \mathbb{R}^d$ $(d \leq 2)$ with conducting boundary $\partial\Omega$. The symplectic map describing a numerical step in the path length coordinate t is performed by applying second-order operator splitting to the following multi-particle Hamiltonian:

$$H_N = \sum_{j=1}^{N} H_{\text{ext}}(\vec{r}_j, \vec{p}_j, t) + \frac{1}{2N}\sum_{j,k=1}^{N} G(\vec{r}_j, \vec{r}_k). \quad (1)$$

Here H_{ext} is the single-particle Hamiltonian in the external applied fields, N denotes the number of simulation particles, and G denotes a two-body interaction potential, given by:

$$G(\vec{r}, \vec{r}\,') = -\sum_{l=1}^{M} \frac{n}{\lambda_l} e_l(\vec{r}) e_l(\vec{r}\,'), \quad (2)$$

where M denotes the number of computed modes and n is a space charge intensity parameter. The smooth functions e_l $(l = 1, 2, \ldots)$ form an orthonormal basis for the space of square-integrable functions on the domain Ω, and satisfy:

$$\nabla^2 e_l = \lambda_l e_l, \quad e_l|_{\partial\Omega} = 0, \quad (\lambda_l < 0). \quad (3)$$

It follows from (1-3) that each particle moves in response to a space charge potential U satisfying the Poisson equation:

$$\nabla^2 U = -\rho, \quad U|_{\partial\Omega} = 0, \quad (4)$$

where ρ is a particle-based approximation to the beam density, given by taking the first M modes:

$$\rho = \sum_{l=1}^{M} \rho^l e_l, \quad \rho^l = \frac{n}{N}\sum_{j=1}^{N} e_l(\vec{r}_j). \quad (5)$$

Due to the factorized form of the interaction (2), the computational complexity of each timestep is $\sim O(NM)$.

STATISTICAL APPROACH

Neglecting the error due to finite timestep, and holding the number of modes M fixed, the system of particles is described by the N-body Hamiltonian (1). For simplicity, consider a constant focusing system, so that H_{ext} in (1) is independent of t. Assume that initial particle coordinates $z_j = (\vec{r}_j, \vec{p}_j)$, $j = 1, \ldots, N$ are randomly sampled from a probability density f_0 on the single-particle phase space. The joint probability density on the N-body phase space describing the particles at $t = 0$ is:

$$P_N(z_1, \ldots, z_N; 0) = \prod_{j=1}^{N} f_0(z_j). \quad (6)$$

The evolution of the joint probability density is governed by the Liouville equation $\partial P_N/\partial t + \{P_N, H_N\} = 0$, and we are interested in the single-particle density function f:

$$f(z, t) = \int P_N(z, z_2, \ldots, z_N; t) dz_2 \ldots dz_N. \quad (7)$$

This can be obtained from the BBGKY hierarchy obtained from (1), or by studying the Klimontovich density:

$$f_K(z, t) = \frac{1}{N}\sum_{j=1}^{N} \delta(z - z_j(t)), \quad (8)$$

where $(z_1(t), \ldots, z_N(t))$ is an orbit of (1) with random initial condition sampled from (6). It follows that $f = \mathrm{E}[f_K]$.

Given any density function h on the single-particle phase space, we define a single-particle Hamiltonian $H_{MF}[h]$ by:

$$H_{MF}[h] = H_{\text{ext}} + H_{SC}[h], \quad (9a)$$

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where $H_{SC}[h]$ is the mean-field potential associated with h, given in terms of the interaction (2) by:

$$H_{SC}[h](\vec{r}) = \int G(\vec{r},\vec{r}\,')h(z')dz', \quad \vec{r} \in \Omega. \tag{9b}$$

It follows from (1) and Hamilton's equations that f_K in (8) satisfies:

$$\frac{\partial f_K}{\partial t} + \{f_K, H_{MF}[f_K]\} = 0. \tag{10}$$

Note that (10) is interpreted to hold after integrating against a smooth test function of compact support [6].

KINETIC EQUATIONS

We desire an equation for the single-particle density f. Denote $f = \mathrm{E}[f_K]$ and $\delta f = f_K - f$. It follows from (10) that:

$$\frac{\partial f}{\partial t} + \{f, H_{MF}[f]\} = \mathrm{E}\{H_{SC}[\delta f], \delta f\}. \tag{11}$$

Note that (11) corresponds to the lowest-order equation in the BBGKY hierarchy. It is exact, but it is not closed due to the appearance of δf.

The hierarchy can be closed [7, 8] by noting that for long-range interactions, $\delta f \sim O(1/\sqrt{N})$. Defining $g = \sqrt{N}\delta f$, subtracting (10) from (11), and evaluating the resulting equation for g to leading order in $1/N$ gives the coupled pair of kinetic equations:

$$\frac{\partial f}{\partial t} + \{f, H_{MF}[f]\} = \frac{1}{N}\mathrm{E}\{H_{SC}[g], g\}, \tag{12a}$$

$$\frac{\partial g}{\partial t} + \{g, H_{MF}[f]\} + \{f, H_{SC}[g]\} = 0, \tag{12b}$$

where g is the Gaussian random field satisfying at $t = 0$:

$$\mathrm{E}[g_0] = 0, \quad \mathrm{E}[g_0(z)g_0(z')] = \delta(z - z')f_0(z) - f_0(z)f_0(z').$$

The system (12) is our fundamental model. In the limit $N \to \infty$, we recover the Vlasov equation for the interaction (2). The term on the right-hand side of (12a) describes the effect of the fluctuation g associated with the initial random sampling, which propagates according to the linearized Vlasov equation (12b). The statistics of g_0 follow from (6).

Perturbation Around Vlasov Equilibrium

Let f_1 denote a stationary solution of (12a) with $N \to \infty$ (a Vlasov equilibrium). We analyze (12) perturbatively by taking $f = f_1 + \frac{1}{N}f_2 + \ldots$ and $g = g_1 + \frac{1}{N}g_2 + \ldots$. Using these expressions in (12) and equating terms of like order in $1/N$ gives a sequence of *linear* equations for the f_j, g_j, $j = 1, 2, \ldots$ describing deviations from Vlasov equilibrium of successively higher order in $1/N$. In particular, let L denote the linear operator:

$$Lh = \{h, H_{MF}[f_1]\} + \{f_1, H_{SC}[h]\}. \tag{13}$$

Then the leading correction f_2 is obtained by solving:

$$\frac{\partial f_2}{\partial t} + Lf_2 = \mathrm{E}\{H_{SC}[g_1], g_1\}, \quad \frac{\partial g_1}{\partial t} + Lg_1 = 0, \tag{14}$$

with initial conditions $f_2 = 0$ and $g_1 = g_0$ at $t = 0$.

In some cases, the solution of the rightmost equation in (14) is known explicitly. For a clear 1D example with applications to particle noise, see [9]. In this case, we write $g_1(t) = e^{-tL}g_0$, suppressing the dependence on z. Then f_2 is given by:

$$f_2(t) = \int_0^t e^{-(t-\tau)L}\,\mathrm{E}\{H_{SC}[e^{-\tau L}g_0], e^{-\tau L}g_0\}d\tau. \tag{15}$$

Energy, Entropy, and Observables

Under the assumption that H_{ext} is independent of t, the Hamiltonian (1) is an invariant of N-body motion. Taking the limit H_N/N as $N \to \infty$ gives the statistical energy:

$$Q = \int H_{\text{ext}}(z)f(z)dz + \frac{1}{2}\int f(z)G(\vec{r},\vec{r}\,')f(z')dzdz'. \tag{16}$$

Likewise, the Boltzmann entropy is defined as [1]:

$$S = -k_B \int f(z)\ln f(z)dz. \tag{17}$$

Using (14), we obtain the following expression for the growth rate of the beam entropy, valid to first order in $1/N$:

$$\frac{dS}{dt} = \frac{k_B}{N}\int \mathrm{E}\{H_{SC}[e^{-tL}g_0], e^{-tL}g_0\}\ln f_1 dz. \tag{18}$$

If ϕ is a function on the single-particle phase space, we let $\langle\phi\rangle = \frac{1}{N}\sum_{j=1}^N \phi(z_j)$. Then $\mathrm{E}[\langle\phi\rangle] = \int \phi(z)f(z)dz$.

RELAXATION TO EQUILIBRIUM

The unique f maximizing (17) for fixed (16) is the self-consistent Boltzmann distribution $f_{eq} \propto e^{-H_{MF}[f_{eq}]/k_BT}$. We study relaxation to f_{eq} for a beam initially described by a self-consistent waterbag distribution of the form:

$$f_0 \propto \Theta(H_0 - H_{MF}[f_0]), \tag{19}$$

in a constant-focusing channel $H_{\text{ext}} = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}k^2(x^2 + y^2)$. Note that (19) is a stationary solution of (12a) in the limit $N \to \infty$. A 2.5 MeV proton beam with 120 mA current is used, with k and H_0 chosen to give $\epsilon_{x,n} = \epsilon_{y,n} = 0.6$ μm and $\sigma_x = \sigma_y = 3.8$ mm. 5-20K particles initially sampled from (19) are tracked with space charge using 128×128 spectral modes in a rectangular domain Ω of side 3.4 cm.

To study relaxation of the distribution, we use a momentum kurtosis parameter, as used in [10]:

$$\kappa = \frac{\langle p_x^4\rangle + \langle p_y^4\rangle}{2(k_BT)^2} - 2, \qquad k_BT = \frac{\langle p_x^2\rangle + \langle p_y^2\rangle}{2}, \tag{20}$$

where $\kappa \approx 0.21$ for f_0 (waterbag) and $\kappa = 1$ for f_{eq} (Boltzmann). Fig. 1 shows the evolution of κ as a function of t (in betatron periods $L = 2\pi/k$) for $N = 5$K. The growth to saturation is reasonably described by $\kappa(t) = 1 - e^{-t/\tau}(1 - \kappa_0)$ for relaxation time $\tau = 4,750$ (blue). Fig. 2 illustrates the initial and final particle distributions in momentum space.

The relaxation rate is given in terms of the beam moments near $t = 0$ by:

$$\frac{1}{\tau} = \frac{1}{1-\kappa}\left(\frac{1}{(k_BT)^2}\frac{d}{dt}\langle p_x^4\rangle - \frac{2}{k_BT}(\kappa + 2)\frac{d}{dt}\langle p_x^2\rangle\right)\Bigg|_{t=0},$$

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where we have used the isotropy of the momentum distribution. Using (14-15), one may obtain an expression for the rate of change of an observable ϕ to leading order in $1/N$:

$$\frac{d}{dt}\langle\phi\rangle\Big|_{t=0} = \frac{1}{N}\int \mathrm{E}\{\phi, H_{SC}[g_0]\}(z) g_0(z) dz. \quad (21)$$

Using the expression for g_0 and applying (2) gives:

$$\frac{d}{dt}\langle\phi\rangle\Big|_{t=0} = \frac{1}{N}\sum_{l=1}^{M}\frac{n}{\lambda_l}\int\{f_0,\phi\}\left(\rho_0^l e_l - \frac{1}{2}e_l^2\right) dz, \quad (22)$$

where ρ_0^l denotes the coefficient of mode l in the initial spatial density. Using (22) in the expression for $1/\tau$ gives a contribution from each spectral mode that scales linearly with space charge intensity n and inversely with the number of simulation particles N. The prediction that $\tau \propto N$ is consistent with numerical tracking, as shown in Fig. 3.

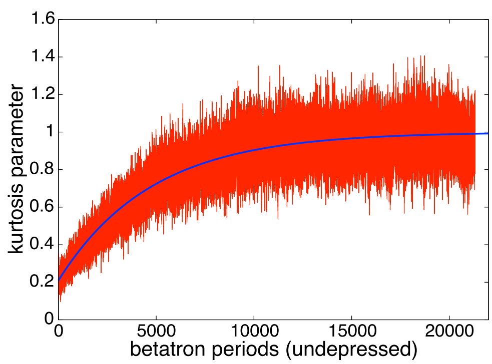

Figure 1: Evolution of (20) showing relaxation of a waterbag beam to Boltzmann equilibrium in a constant-focusing channel in the presence of numerical particle noise.

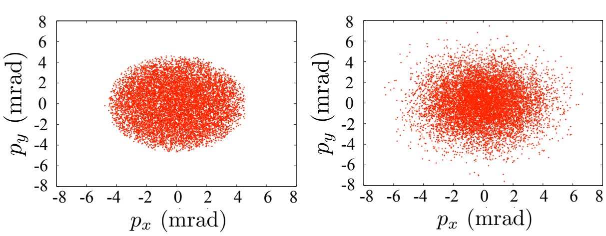

Figure 2: Initial (left) and final (right) distributions in momentum space, illustrating the transition from waterbag to Boltzmann equilibrium due to numerical particle noise.

CONCLUSION

A kinetic formalism was developed to describe particle noise in a gridless multi-symplectic space charge algorithm [4], resulting in a generalized Lenard-Balescu model with long-range interaction (2). In a constant focusing channel, we observe relaxation of a beam initialized in a waterbag Vlasov equilibrium to a Boltzmann (thermal) equilibrium.

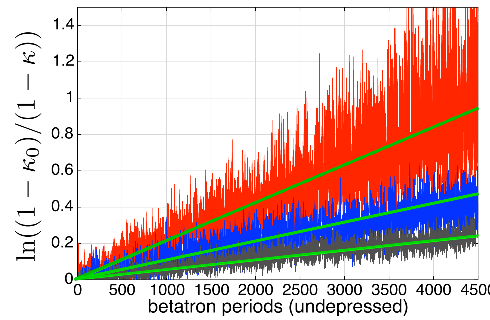

Figure 3: Comparison of kurtosis evolution for $N = 5$K, 10K, 20K. Slope of each fitted green curve gives the relaxation rate $1/\tau$, illustrating that τ scales linearly with N.

The relaxation rate, which scales as $1/N$, could be evaluated explicitly in special cases where solution of the linearized Vlasov equation about the equilibrium is known exactly (such as [9]). This is a topic of future research.

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REFERENCES

[1] J. Struckmeier, *Phys. Rev. ST Accel. Beams*, vol. 3, p. 034202, 2000.

[2] B. A. Shadwick, A. B. Stamm, and E. G. Evstatiev, *Physics of Plasmas*, vol.21, p. 055708, 2014.

[3] S. D. Webb, *Plasma Phys. Control. Fusion*, vol. 58, p. 034007, 2016.

[4] Ji Qiang, *Phys. Rev. Accel. Beams*, vol. 20, p. 014203, 2017.

[5] C. Mitchell and J. Qiang, "Analysis of Emittance Growth in a Gridless Spectral Poisson Solver for Fully Symplectic Multiparticle Tracking", in *Proc. ICAP'18*, Key West, Florida, USA, Oct. 2018, pp. 335–340.

[6] H. Spohn, *Large Scale Dynamics of Interacting Particles*, Berlin, Germany, Springer-Verlag, 1991.

[7] A. Campa *et al*, *Physics of Long-Range Interacting Systems*, NY, USA, Oxford University Press, 2014.

[8] P. Chavanis, *Physica A*, vol. 377, pp. 469-486, 2007 and *Eur. Phys. J. Plus*, vol. 127, p. 19, 2012.

[9] G. Bassi, J. Ellison, and K. Heinemann, "Equilibrium Fluctuations in an N-Particle Coasting Beam: Schottky Noise Effects", in *Proc. PAC'07*, Albuquerque, NM, USA, Jun. 2007, paper FRPMN099, pp. 4318–4320.

[10] C. Benedetti, S. Rambaldi, and G. Turchetti, *Physica A*, vol. 364, pp. 197-212, 2006.