Entropy Growth

(in Computer Simulations of Hamiltonian Systems)

J. Struckmeier

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Outline

- Review: Properties of Hamiltonian dynamics
  - Liouville's theorem
  - Reversibility
  - Symplecticity
- Non-reversibility in computer simulations
- Continuous description of reversible and irreversible phase-space dynamics: Vlasov equation, Fokker-Planck equation
- Moment analysis of the Vlasov-Fokker-Planck equation
- Fluctuation-dissipation theorem, beam temperatures
- Entropy and emittance growth rates
- Numerical examples
- Conclusions

Properties of Hamiltonian dynamics

1. Liouville's theorem (proper) states that the volume element $d\Gamma$

$$d\Gamma = d\boldsymbol{x}_1 d\boldsymbol{v}_1 \ldots d\boldsymbol{x}_N d\boldsymbol{v}_N = d\boldsymbol{x}'_1 d\boldsymbol{v}'_1 \ldots d\boldsymbol{x}'_N d\boldsymbol{v}'_N$$

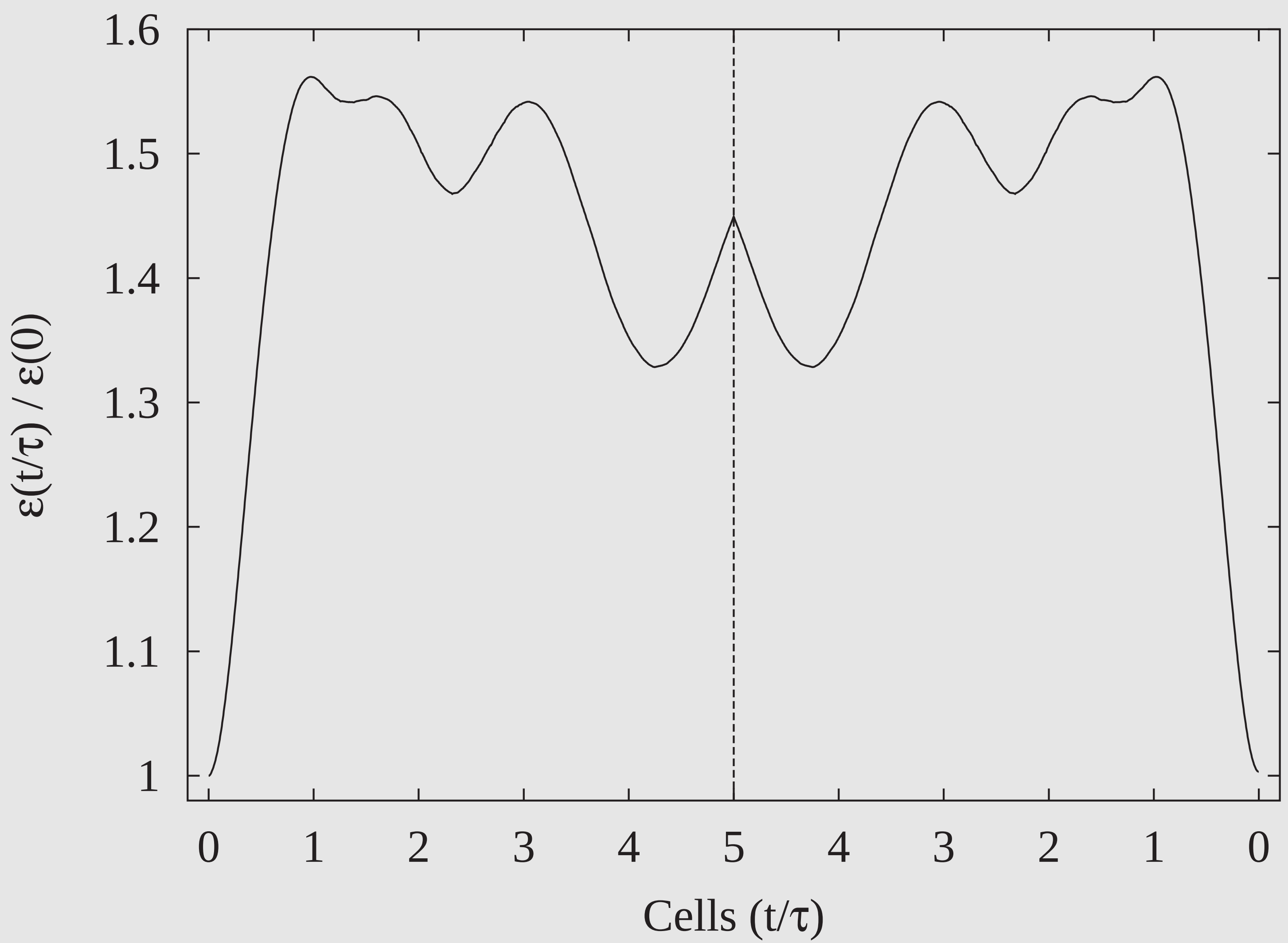
   of a Hamiltonian N particle system is *invariant* with respect to *canonical transformations* — in particular with respect to the system's time evolution.

2. The coded canonical equations are always *reversible*. Example:

$$m\ddot{\vec{x}}_i - \vec{F}_{\text{ext}}(\vec{x}_i, t) - q\big(\vec{E}_i + \dot{\vec{x}}_i \times \vec{B}_i\big) = 0\,, \qquad i = 1, \ldots, N^{\,\text{sim}}\,.$$

3. The simulation algorithm must maintain the symplectic nature of Hamiltonian systems in order to avoid unphysical results.

   Note: Linear lens transformations and (non-linear) lumped "space-charge kick" transformations are always symplectic.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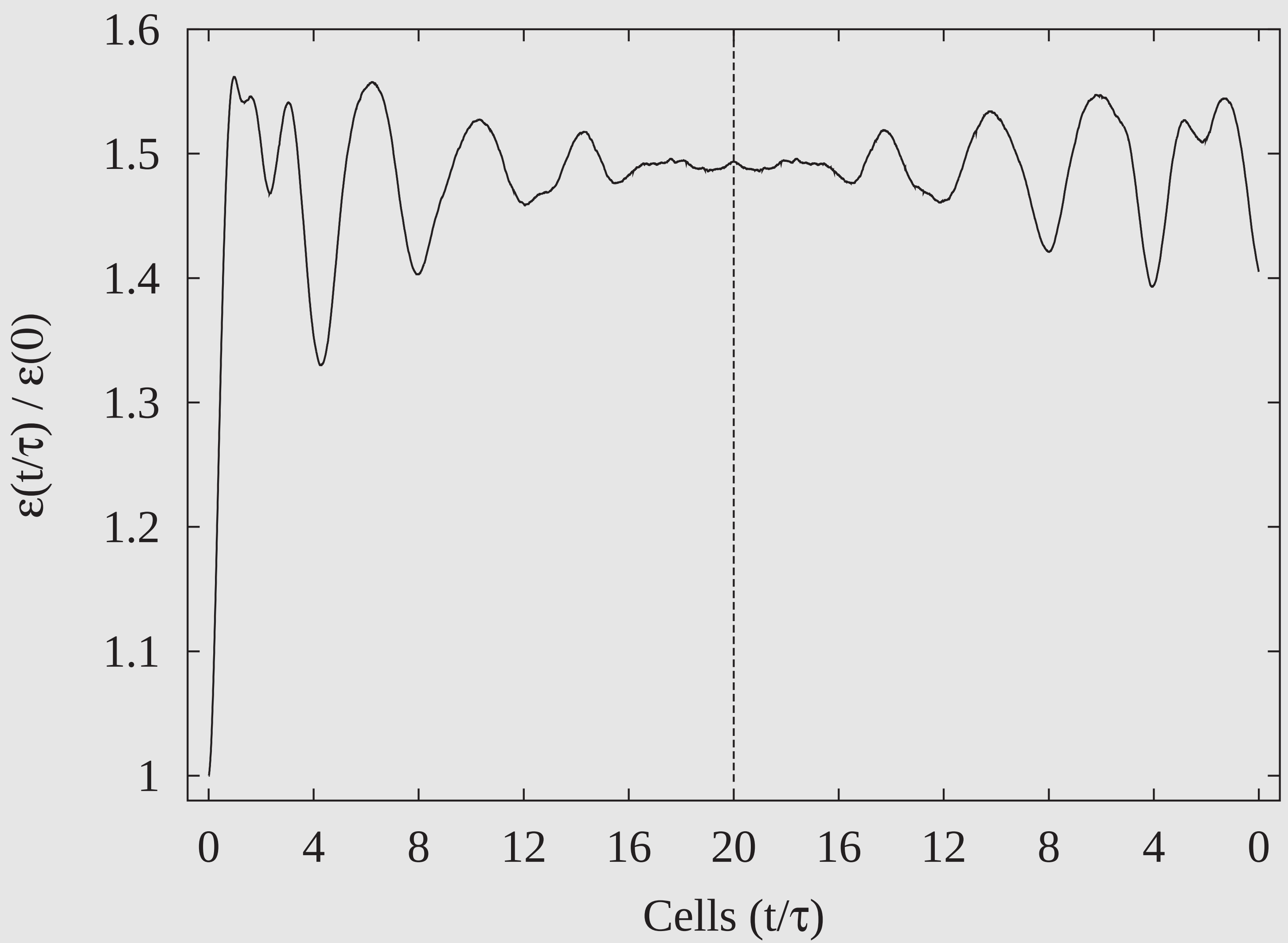
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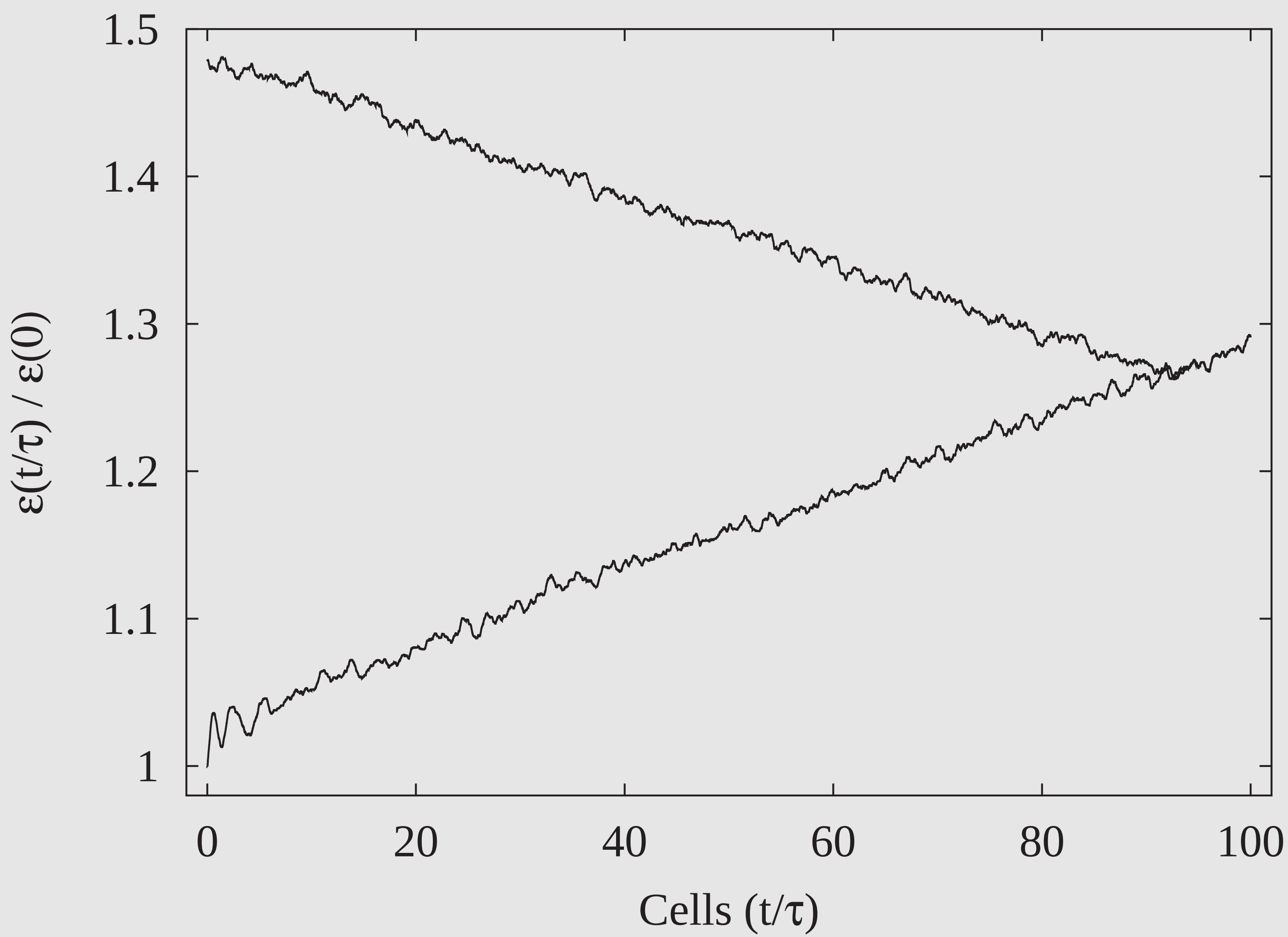
1.5
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ε(t/τ) / ε(0)
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Cells (t/τ)

Continuous description of phase-space dynamics

We define a 6-dimensional phase-space probability density function

$$f = f(\boldsymbol{x}, \boldsymbol{v}, t)$$

$\rightsquigarrow$ $f \, d\boldsymbol{x} \, d\boldsymbol{v}$ provides the probability of finding a particle inside the volume $d\boldsymbol{x} \, d\boldsymbol{v}$ around the phase-space point $(\boldsymbol{x}, \boldsymbol{v})$ at time t.

$\rightsquigarrow$ f is a smooth function of the phase-space variables.

$\rightsquigarrow$ f does *not* provide information on individual particles.

The "special" Liouville theorem

$$\frac{df}{dt} = 0$$

applies for systems with non-negligible Coulomb interaction only if

1. no particle losses $\Longleftrightarrow \int f \, d\boldsymbol{x} \, d\boldsymbol{v} = \text{const.}$
2. the system is described by a *continuous* Hamilton function.

$\rightsquigarrow$ This description cannot cover "numerical noise effects".

“Non Liouvillean” Effects

⇝ In order to describe “noise effects”, a generalization of the “special” Liouville theorem is necessary (Chandrasekhar (1943)):

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \vec{v} \cdot \vec{\nabla}_x f + \frac{1}{m}\left(\vec{F}_{\text{ext}} + q\vec{E}_{\text{ssc}}\right) \cdot \vec{\nabla}_v f = \left[\frac{\partial f}{\partial t}\right]_{\text{NL}} .$$

If the non-Liouvillean effects are small compared to the macroscopic forces (smooth space charge and external forces), we may describe them by the Fokker-Planck equation:

$$\left[\frac{\partial f}{\partial t}\right]_{\text{NL}} = -\sum_i \frac{\partial}{\partial v_i}\left\{F_i(\boldsymbol{v},t)\, f\right\} + \sum_{i,j} \frac{\partial^2}{\partial v_i \partial v_j}\left\{D_{ij}(\boldsymbol{v},t)\, f\right\} .$$

D_{ij} are referred to as elements of the “diffusion tensor” and the F_i as elements of the “drift vector” that describes the “dynamical friction forces”.

Description of irreversibility

We apply a transformation that reverses the direction of time flow

$$t \to -t \qquad \rightsquigarrow x_i \to x_i, \qquad v_i \to -v_i.$$

We may write the equation of motion for $f(\boldsymbol{x}, \boldsymbol{v}, t)$ in operator form and separate its components with respect to their behavior under time reversal

$$\frac{\partial f}{\partial t} = \boldsymbol{L} f\,, \qquad \boldsymbol{L} = \boldsymbol{L}_{\mathrm{rev}} + \boldsymbol{L}_{\mathrm{ir}}\,.$$

The “reversible” operator $\boldsymbol{L}_{\mathrm{rev}}$: terms that change sign under time reversal, hence leave $\partial f/\partial t = \boldsymbol{L}_{\mathrm{rev}} f$ invariant.

$\rightsquigarrow$ Earlier states are fully restored — just like a movie that is reversed at some instant of time t_0.

The *reversible* terms agree with the familiar Vlasov equation

$$\boldsymbol{L}_{\mathrm{rev}} = \sum_{i=1}^{3} \left[-\frac{\partial}{\partial x_i} v_i - \frac{1}{m} \frac{\partial}{\partial v_i} \left(F_{\mathrm{ext},i} + q E_{\mathrm{ssc},i} \right) \right] .$$

The components $\boldsymbol{L}_{\mathrm{ir}}$ that do not change sign are given by the Fokker-Planck terms

$$\boldsymbol{L}_{\mathrm{ir}} = \sum_{i=1}^{3} \frac{\partial}{\partial v_i} \left[-\frac{F_{\mathrm{fr},i}(v_i,t)}{m} + \frac{\partial}{\partial v_i} D_{ii}(v_i,t) \right] ,$$

as the friction forces $F_{\mathrm{fr},i}$ must always be decelerating

$$F_{\mathrm{fr},i}(v_i) = -F_{\mathrm{fr},i}(-v_i) \quad , \quad \rightsquigarrow D_{ii}(v_i) = D_{ii}(-v_i) \, .$$

$\boldsymbol{L}_{\mathrm{ir}}$ describes those effects that do *not* depend on the direction of time flow. In other words, it describes the *irreversible* aspects of the particle motion.

Real system: mixture of reversible and irreversible behavior.

We observe:

- The coupled set of Vlasov, Poisson, and Fokker-Planck equations provides the equation of motion for f that includes the description of irreversible effects.
- This equation is too costly to solve directly.
- We do not really want to know $f(\boldsymbol{x}, \boldsymbol{v}, t)$ in detail.
- We must switch to more global quantities.

Moment analysis of the Vlasov-Fokker-Planck equation

The usual way to switch to even more global physical quantities is to consider "moments" of $f(\boldsymbol{x}, \boldsymbol{v}, t)$ (F. Sacherer, P. Lapostolle (1970)):

$$\langle x_i^2 \rangle = \int x_i^2 \, f(\boldsymbol{x}, \boldsymbol{v}, t) \, d\boldsymbol{x} d\boldsymbol{v} \, , \quad i = 1, 2, 3 \, .$$

$\sqrt{\langle x_i^2 \rangle}$ is proportional to the actual beam width in x_i.

Idea: Instead of solving the equation of motion for f, we are going to set up and solve the equations of motion for the second beam moments.

The derivatives of the moments are calculated according to

$$\frac{d}{dt} \langle x_i^2 \rangle = \int x_i^2 \, \frac{\partial f}{\partial t} \, d\boldsymbol{x} d\boldsymbol{v} \, ,$$

inserting $\partial f / \partial t$ from the Vlasov-Fokker-Planck equation.

Integrating by parts, we obtain for each phase-space plane i a coupled set of "moment" equations

$$\frac{d}{dt}\left\langle x_i^2\right\rangle - 2\left\langle x_i v_i\right\rangle = 0$$

$$m\frac{d}{dt}\left\langle x_i v_i\right\rangle - m\left\langle v_i^2\right\rangle - \left\langle x_i F_{\mathrm{ext},i}\right\rangle - q\left\langle x_i E_{\mathrm{ssc},i}\right\rangle = \left\langle x_i F_{\mathrm{fr},i}\right\rangle$$

$$m\frac{d}{dt}\left\langle v_i^2\right\rangle - 2\left\langle v_i F_{\mathrm{ext},i}\right\rangle - 2q\left\langle v_i E_{\mathrm{ssc},i}\right\rangle = 2\left\langle v_i F_{\mathrm{fr},i}\right\rangle + 2m\left\langle D_{ii}\right\rangle$$

As usual, we define the rms emittance $\varepsilon_i(t)$ as

$$\varepsilon_i^2(t) = \left\langle x_i^2\right\rangle\left\langle v_i^2\right\rangle - \left\langle x_i v_i\right\rangle^2 .$$

The time derivative of the rms emittance may be arranged as

$$\frac{d}{dt}\varepsilon_i^2(t) = \left.\frac{d}{dt}\varepsilon_i^2(t)\right|_{\mathrm{ext}} + \left.\frac{d}{dt}\varepsilon_i^2(t)\right|_{\mathrm{ssc}} + \left.\frac{d}{dt}\varepsilon_i^2(t)\right|_{\mathrm{fp}} .$$

$\frac{d}{dt}\varepsilon_i^2(t)\Big|_{\text{ext}}$ and $\frac{d}{dt}\varepsilon_i^2(t)\Big|_{\text{ssc}}$ describe the emittance change due to non-linear external focusing forces and smooth non-linear electric self-fields

$$\begin{aligned}\frac{m}{2}\frac{d}{dt}\varepsilon_i^2(t)\Big|_{\text{ext}} &= \left\langle x_i^2\right\rangle \left\langle v_i F_{\text{ext},i}\right\rangle - \left\langle x_i v_i\right\rangle \left\langle x_i F_{\text{ext},i}\right\rangle \\ &= 0 \quad \Longleftrightarrow \quad F_{\text{ext},i} \propto x_i \\ \frac{m}{2}\frac{d}{dt}\varepsilon_i^2(t)\Big|_{\text{ssc}} &= q\left[\left\langle x_i^2\right\rangle \left\langle v_i E_{\text{ssc},i}\right\rangle - \left\langle x_i v_i\right\rangle \left\langle x_i E_{\text{ssc},i}\right\rangle\right] .\end{aligned}$$

The third contribution to the change of the emittance emerges from the terms of Fokker-Planck equation

$$\frac{m}{2}\frac{d}{dt}\varepsilon_i^2(t)\Big|_{\text{fp}} = \left\langle x_i^2\right\rangle \left\langle v_i F_{\text{fr},i}\right\rangle - \left\langle x_i v_i\right\rangle \left\langle x_i F_{\text{fr},i}\right\rangle + m\left\langle x_i^2\right\rangle \left\langle D_{ii}\right\rangle .$$

$\leadsto$ The emittance growth depends on both the Fokker-Planck coefficients *and* and the specific shape of the envelope functions.

The fluctuation-dissipation theorem relates the Fokker-Planck coefficients $F_{\mathrm{fr},i}$ and D_{ii}.

Systems in dynamical equilibrium are governed by

- diffusion: effect that drives a quantity off its steady-state value,
- friction (dissipation): effect that causes the decay of this deviation from the steady-state value.

The diffusion process and friction effects dependent on each other.

$\leadsto$ Both effects are related by a fluctuation-dissipation theorem

$\leadsto$ Isotropic process, which applies here: Einstein relation

$$F_{\mathrm{fr},i} = -\beta_f m v_i \,, \qquad D \equiv D_{ii} = \beta_f \, \frac{k_B T_{\mathrm{eq}}}{m} \,.$$

$\leadsto$ We are left with β_f as the only free parameter in our description of "numerical noise" effects.

Beam "Temperatures"

Non-equilibrium temperature:

For charged particle beams, we define the generalized, non-equilibrium "temperature" $k_B T_i$ as the instantaneous *incoherent* part of the kinetic energy of the beam particles in the i-th degree of freedom:

$$k_B T_i \equiv m \left\langle \left(v_i^{\text{inc}}\right)^2 \right\rangle , \qquad v_i^{\text{inc}} = v_i - x_i \frac{\langle x_i v_i \rangle}{\langle x_i^2 \rangle} .$$

Non-equilibrium "temperature" $k_B T_i$ of the i-th degree of freedom

$$k_B T_i(t) = m \frac{\varepsilon_i^2(t)}{\langle x_i^2 \rangle} .$$

For $\delta(t - t')$-correlated noise, we may approximate the equilibrium temperature T_{eq} by

$$\frac{k_B T_{\text{eq}}}{m} = \frac{k_B}{3m} \left(T_x + T_y + T_z\right) = \frac{1}{3} \left(\frac{\varepsilon_x^2}{\langle x^2 \rangle} + \frac{\varepsilon_y^2}{\langle y^2 \rangle} + \left\langle \left(\Delta v_{z,b}\right)^2 \right\rangle \right) .$$

Emittance growth rates

With the temperature relations, the above formula for the F-P related emittance growth is obtained for the x-direction as

$$\frac{1}{\langle x^2 \rangle} \frac{d}{dt} \varepsilon_x^2(t) \bigg|_{\mathrm{fp}} = -\frac{2\beta_f}{3} \left(\frac{2\varepsilon_x^2(t)}{\langle x^2 \rangle} - \frac{\varepsilon_y^2(t)}{\langle y^2 \rangle} - \left\langle (\Delta v_{z,b})^2 \right\rangle \right) ,$$

or equivalently with the temperature ratios $r_{xy} = T_y(t)/T_x(t)$, $r_{xz} = T_z(t)/T_x(t)$, and $r_{yz} = T_z(t)/T_y(t)$

$$\frac{d}{dt} \ln \varepsilon_x^2(t) \bigg|_{\mathrm{fp}} = \frac{2\beta_f}{3} \left(r_{xy} + r_{xz} - 2 \right) .$$

$\leadsto$ The change of the emittance may be positive as well as negative.

Summing over all three degrees of freedom, we get

$$\frac{d}{dt} \ln \varepsilon_x^2 \varepsilon_y^2 \varepsilon_z^2 \bigg|_{\mathrm{fp}} = \frac{2\beta_f}{3} \left(\frac{(1 - r_{xy})^2}{r_{xy}} + \frac{(1 - r_{xz})^2}{r_{xz}} + \frac{(1 - r_{yz})^2}{r_{yz}} \right) \geq 0 \,.$$

$\rightsquigarrow$ The total change of all emittances is always positive.

With the entropy definition

$$S(t) = -k_B \int f \, \ln f \, d\tau \,,$$

we may show the total fp-related emittance growth exactly reflects the increase of entropy $S(t)$

$$\frac{1}{k_B} \frac{dS(t)}{dt} = \frac{d}{dt} \ln \varepsilon_x^2 \varepsilon_y^2 \varepsilon_z^2 \bigg|_{\mathrm{fp}} \geq 0 \,.$$

Final result: we integrate the emittance equation over one focusing period T to obtain the emittance e-folding time $\tau_{\rm ef}$ of the total emittance $\varepsilon = \sqrt[3]{\varepsilon_x \varepsilon_y \varepsilon_z}$

$$\tau_{\rm ef}^{-1} = \tfrac{1}{9}\, \beta_f \left(I_{xy} + I_{xz} + I_{yz} \right),$$

with the "temperature imbalance integrals" I_{xy}, I_{xz}, I_{yz} defined as

$$I_{xy} = \frac{1}{T} \int_0^T \frac{\left[1 - r_{xy}(t)\right]^2}{r_{xy}(t)}\, dt \qquad , \qquad r_{xy}(t) = \frac{\varepsilon_y^2}{\langle y^2 \rangle} \frac{\langle x^2 \rangle}{\varepsilon_x^2} \, .$$

This means for "coasting beams" in "trace space" notation

$$\tau_{\mathrm{ef}}^{-1} = \tfrac{1}{4}\, \beta_f \, I_{xy} \,,$$

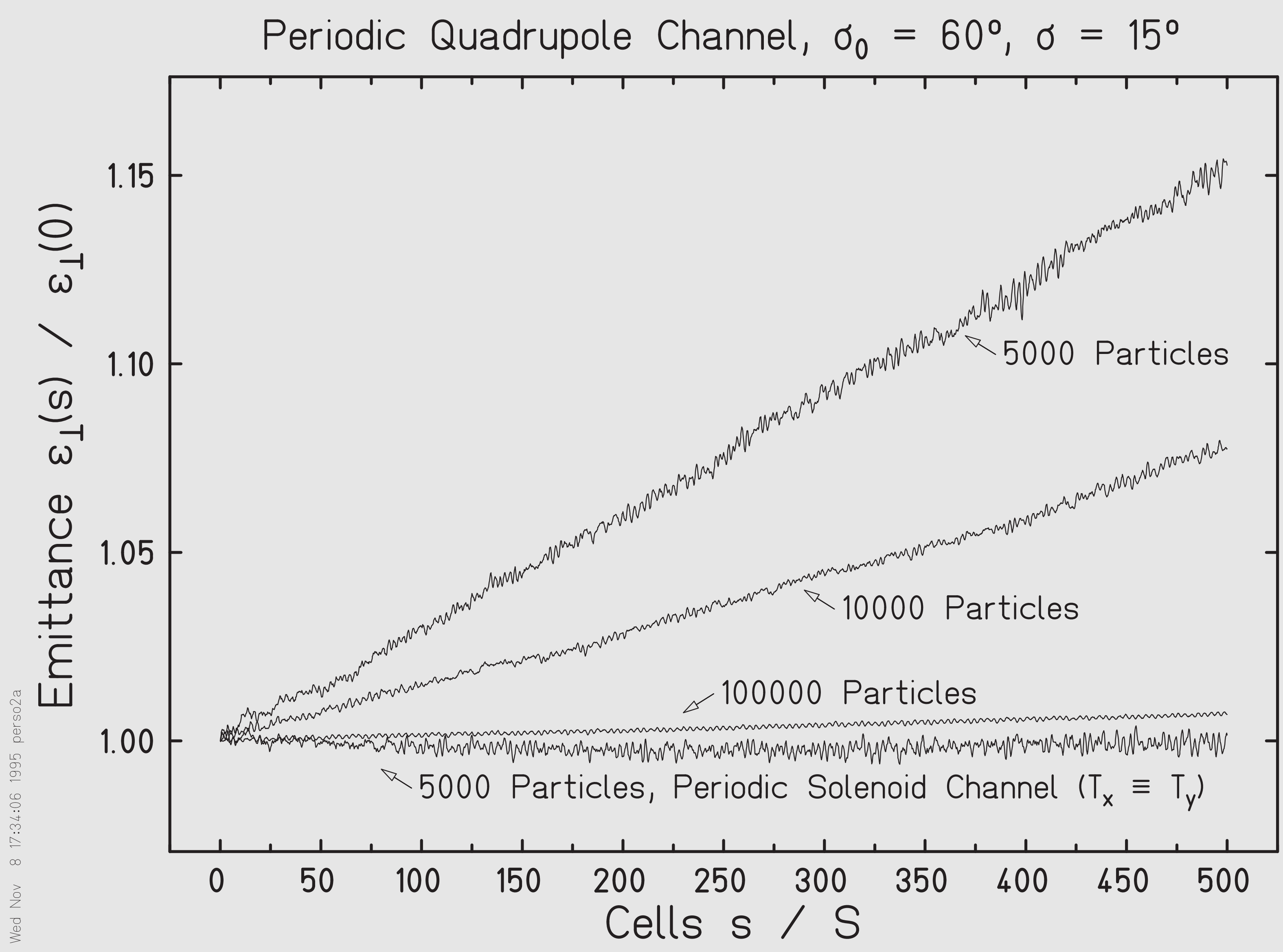
with I_{xy} defined as

$$I_{xy} = \frac{1}{S} \int_0^S \frac{\left[1 - r_{xy}(s)\right]^2}{r_{xy}(s)}\, ds \qquad , \qquad r_{xy}(s) = \frac{\varepsilon_y^2}{\langle y^2 \rangle} \frac{\langle x^2 \rangle}{\varepsilon_x^2} \,.$$

If the number of macro-particles used in the simulation is increased, the system get "smoother", hence β_f becomes smaller whereas I_{xy} is kept constant.

If the system is modified and the number of macro-particles is kept constant, β_f remains unchanged whereas I_{xy} is varied.

$\Rightarrow$ If either β_f becomes very small or if I_{xy} vanishes, we do not expect any fp-related emittance growth.


Periodic Quadrupole Channel, σ0 = 60°, σ = 15°
Emittance εT(s) / εT(0)
1.15
1.10
1.05
1.00
5000 Particles
10000 Particles
100000 Particles
5000 Particles, Periodic Solenoid Channel (Tx ≡ Ty)
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Cells s / S
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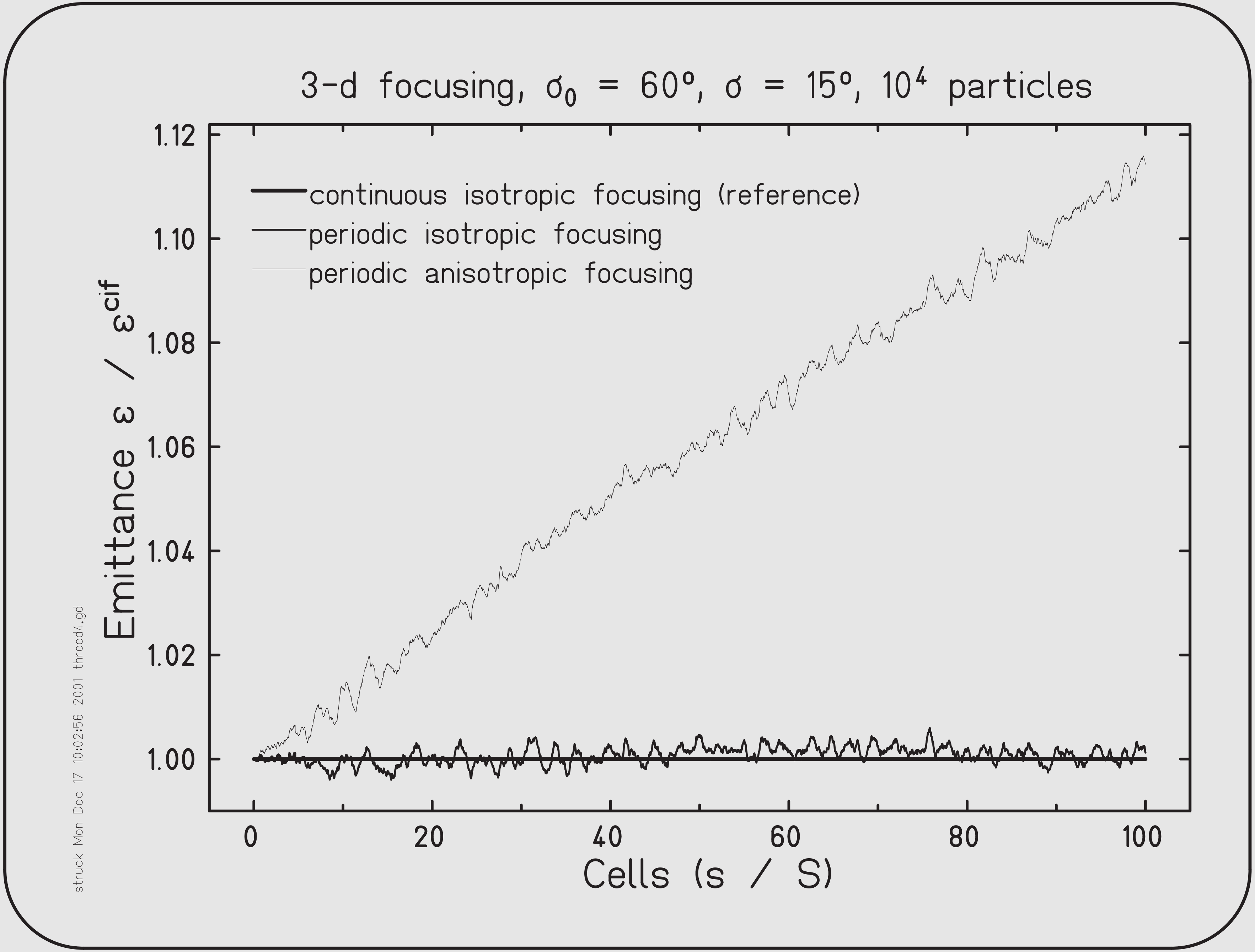
3-d focusing, σ0 = 60°, σ = 15°, 10^4 particles
continuous isotropic focusing (reference)
periodic isotropic focusing
periodic anisotropic focusing
Emittance ε / ε^cif
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1.10
1.08
1.06
1.04
1.02
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Cells (s / S)
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Conclusions

- “Numerical noise” effects inevitably emerge in computer simulations of dynamical systems.
- The actual time evolution of the simulated system always comprises irreversible aspects — even if the actually coded equations of motion are strictly reversible.
- A computer simulation based on individual particles can never be an *exact* realization of a solution of the canonical equations.
- The results of the computer simulation may be modeled as an *exact* solution of a Vlasov-Fokker-Planck equation.
- The crucial point for the correct interpretation of computer simulations is to keep in mind that the noise-related emittance growth depends on both the magnitude of the noise “forces” *and* the time averaged temperature anisotropy induced by the lattice.