Grid Noise and Entropy Growth in PIC Codes

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- Theory overview
- Grid and particle collisions in 3d and 2d (bunches + FODO)
- Noise and rms entropy in equilibrium
- Application to resonant/unstable processes
- Conclusions

Acknowledgments:
O. Boine-Frankenheim (co-worker)
J. Struckmeier (discussions)

Motivation

Why do we study collisions and noise in high intensity simulation?

- „usual“ approach: let us increase N, grid rsolution, time steps → convergence
- in linacs so far we have lived well with this – questions arise for error studies (1000‘s of linacs) with „low“ N (~10^5)
- in circular machines 100.000‘s of turns – cross-check resonance trapping with space charge (noise-free simulations by G. Franchetti)
- CERN space charge workshop April 2013 triggered off new interest ..

3 papers give basis for „equilibrium“ beams:

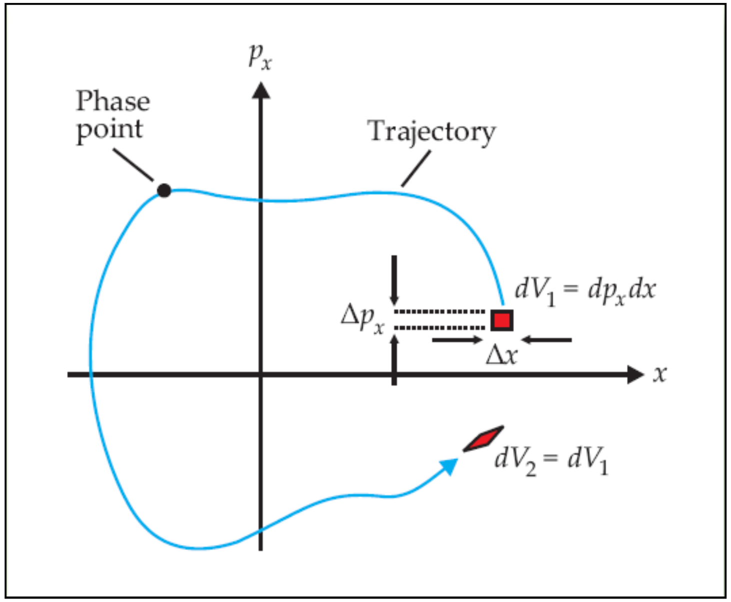
1. *Theory: J. Struckmeier, Part. Acc. (1994) & Phys. Rev. E (1996) & PRSTAB (2000)*
2. *3d-simulation: I. Hofmann and O. Boine-Frankenheim, to be published in PRSTAB (2014)*
3. *2d-simulation: O. Boine-Frankenheim et al. NIM (2014)*

Current study extends equilibrium discussion to (typical) dynamical phenomena (mismatch, resonances ...)

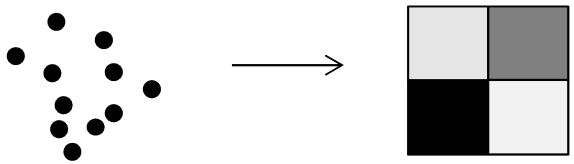
- are above noise concepts useful?

Entropy
Liouville - infinite resolution – coarse graining

Liouville



- Liouville: exact areas in 2d, 4d, 6d phase space invariant for Hamiltonian flow – no growth of „infinite resolution“ entropy
- How break this?
  - for „finite resolution“ self-consistent space charge potential on a grid (as in PIC) exactly Hamiltonian flow broken → growth of entropy
  - for exactly resolved motion of directly interacting particles (collisions) in 6d:
    - collisions break Hamiltonian flow in 6d → growth of entropy
    - „infinite resolution“ entropy in 6Nd phase space still invariant → Gibbs introduced coarse graining of phase space to obtain entropy growth



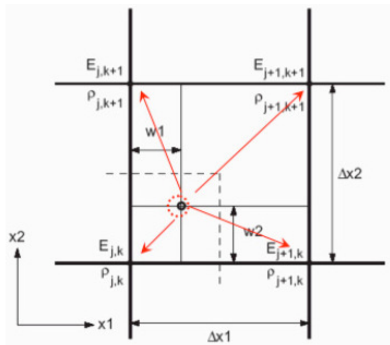
$$S_{CG}(\rho(X)) = -k \int \bar{\rho}(X)[\ln \bar{\rho}(X)] d\Gamma$$

$\bar{\rho}$ is averaged over a cell

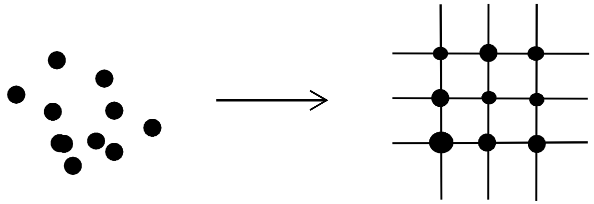
Poisson solver grid & noise

Grid induced noise:
- not included in original „collisional“ approach of Struckmeier
- assume several sources:
  - **non-Liouvillean effect by fluctuating charges on grid**
  - focussing modulation „fast“
  - coherent flow vs. incoherent „temperature“

area weigthing



PIC: replaces infinite resolution charge density by “grid distribution”



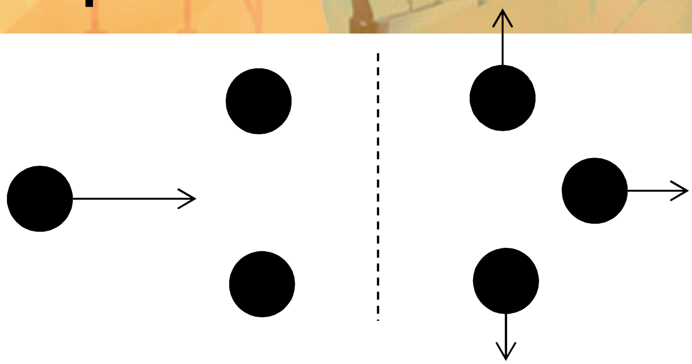
Phase space remains infinitely resolved

Averaging charges over cells:
- ✓ **loss of Hamiltonian character of phase space flow**
- ✓ **→ growth of entropy**

Is there a practically useful „reduced“ definition of entropy?

"Reduced" approach for beams:
J. Struckmeier suggested (1994 ff) to start from Fokker-Planck Equation in 6d phase space space

- Assuming Markov process for collisions of charged particles: dynamical friction
  - no correlation between several particles
  - memory extinction
- friction and diffusion terms



collisional interaction "beyond" Hamiltonian flow in 6d

$$\frac{df}{dt}=\frac{\partial f}{\partial t}+\sum_{i=1}^{3}\left(\dot{x}_i\frac{\partial f}{\partial x_i}+\dot{p}_i\frac{\partial f}{\partial p_i}\right)=\left[\frac{\delta f}{\delta t}\right]_{Non-Liou}$$

$$\left[\frac{\delta f}{\delta t}\right]_{Non-Liou}\equiv\sum_{i=1}^{3}\frac{\partial}{\partial p_i}\left\{\beta_{f;i}\,p_i\,f\right\}+\sum_{i,j=1}^{3}\frac{m^2\partial^2}{\partial p_i\partial p_j}\left\{D_{ij}(\vec{p},t)\,f\right\}$$

→ form second order moments

Second order moments of Vlasov – FP equation
→ rms based (emittance, "temperature", ...)

$$\frac{d}{dt}\left\langle x_i^2 \right\rangle = \int x_i^2 \frac{\partial f}{\partial t} d\tau$$

$$\varepsilon_i^2(s) \equiv \left\langle x_i^2 \right\rangle\left\langle x_i'^2 \right\rangle - \left\langle x_i x_i' \right\rangle^2 \qquad s = \beta c t$$

negligible transient effects associated with initially non-matched self-fields
(*I. Hofmann and J. Struckmeier, Part. Acc.1987*)

$$\frac{1}{\left\langle x_i^2 \right\rangle}\frac{d}{ds}\varepsilon_i^2(s) = \frac{2q}{mc^2\beta^2\gamma^3}\left(\left\langle x_i' E_i \right\rangle - \frac{\left\langle x_i x_i' \right\rangle}{\left\langle x_i^2 \right\rangle}\left\langle x_i E_i \right\rangle\right) - 2\left(\frac{\beta_{f;i}}{c\beta\gamma}\frac{\varepsilon_i^2(s)}{\left\langle x_i^2 \right\rangle} - \frac{\left\langle D_{ii} \right\rangle}{c^2\beta^3\gamma^3}\right).$$

$$\frac{kT_i}{mc^2\beta^2\gamma} = \frac{\varepsilon_i^2(s)}{\left\langle x_i^2 \right\rangle}; \qquad T_{eq} = \frac{1}{3}\sum_{i=1}^{3} T_i$$

$$D \equiv \left\langle D_{ii} \right\rangle; \qquad \beta_f \equiv \beta_{f;i}; \quad k_f \equiv \beta_f / c\beta\gamma \quad D = \beta_f \gamma k T / m \quad \text{(Einstein relation)}$$

$$\frac{d}{ds}\ln\varepsilon_x^2 = k_f\left[\frac{T_y(s)}{T_x(s)} - 1\right] \qquad \frac{d}{ds}\ln\varepsilon_y^2 = k_f\left[\frac{T_x(s)}{T_y(s)} - 1\right] \qquad \text{(one decreasing, one increasing)}$$

$$\frac{d}{ds}\ln\varepsilon_x^2\varepsilon_y^2 = k_f\left[\frac{(T_x - T_y)^2}{T_x T_y}\right] \geq 0 \quad \text{or in 6d} \quad \frac{d}{ds}\ln\varepsilon_x^2\varepsilon_y^2\varepsilon_z^2 = \frac{2}{3}k_f\left[\frac{(T_x - T_y)^2}{T_x T_y} + \frac{(T_x - T_z)^2}{T_x T_z} + \frac{(T_z - T_y)^2}{T_z T_y}\right] \geq 0$$

Resulting in an rms entropy law

$$S_{6d,rms} \equiv \ln \varepsilon_x \varepsilon_y \varepsilon_z \qquad \varepsilon_{6d,rms} \equiv \varepsilon_x \varepsilon_y \varepsilon_z$$

$$\frac{d}{ds} S_{6d,rms} = \frac{1}{3} k_f \left[\frac{(T_x - T_y)^2}{T_x T_y} + \frac{(T_x - T_z)^2}{T_x T_z} + \frac{(T_y - T_z)^2}{T_y T_z} \right] \geq 0$$

$$= 0, \text{ if } T_x = T_y = T_z \text{ (equipartitioned)}$$

never decreasing – under the assumptions of its validity!

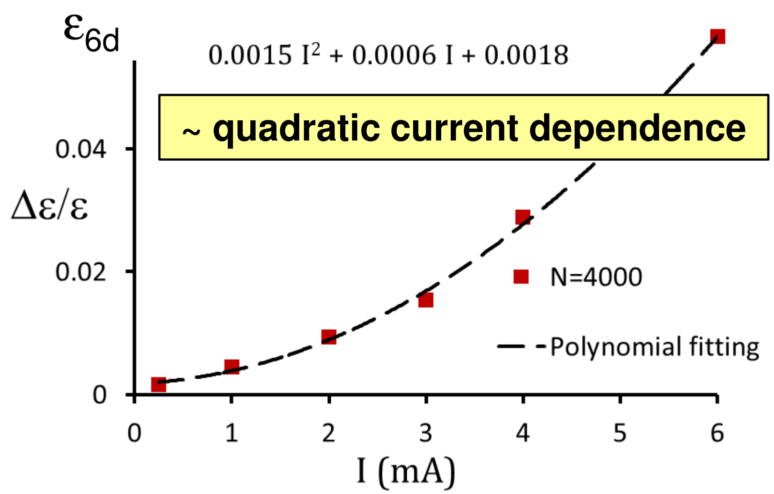
heuristic justification:

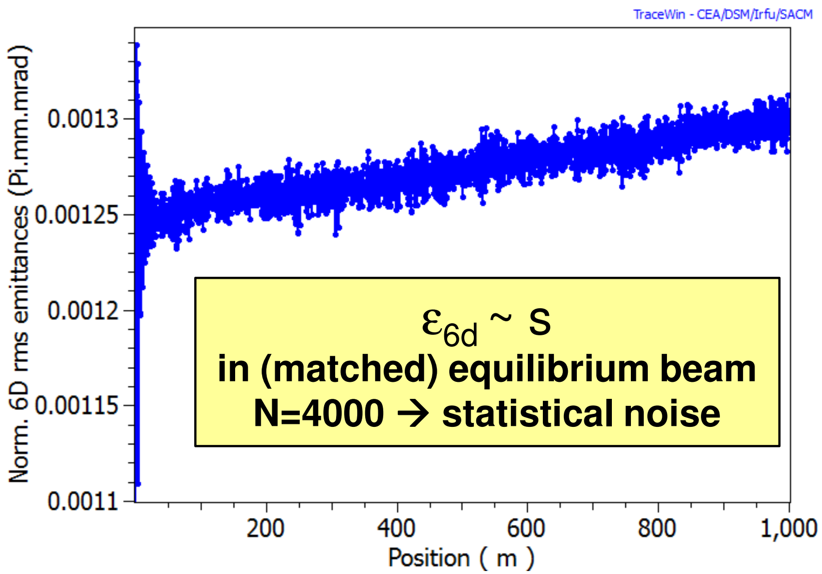
- emittances ~ "probabilities" in phase space
- → product of probabilities for "independent" events
- entropies should be additive for ~ decoupled probabilities (→ ln)
- → coupling between degrees of freedom only on microscopic level
- should be non-decreasing
- **rms approximation – no higher order correlations resolved !!!**

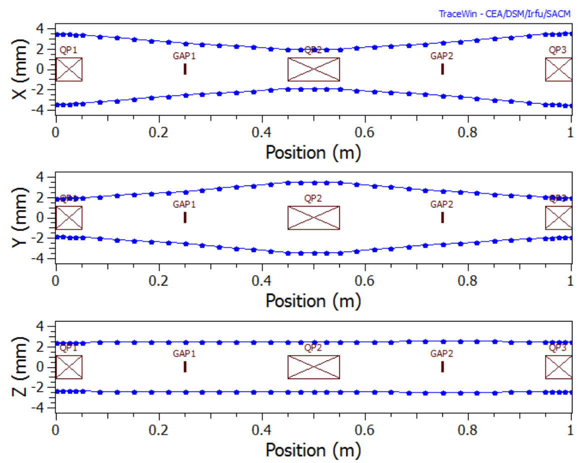
TRACEWIN simulations: matched equilibrium

„Confirms“ ε_{6d} – as rms entropy concept

- spherical bunch:
- $k_{0x,y,z}$=60° and $\varepsilon_z = \varepsilon_{xy}$
- $k_{x,y,z}$=32°/32°/32° (xyz Poisson solver)
- 1000 cells as reference base
- no acceleration – only RF gaps







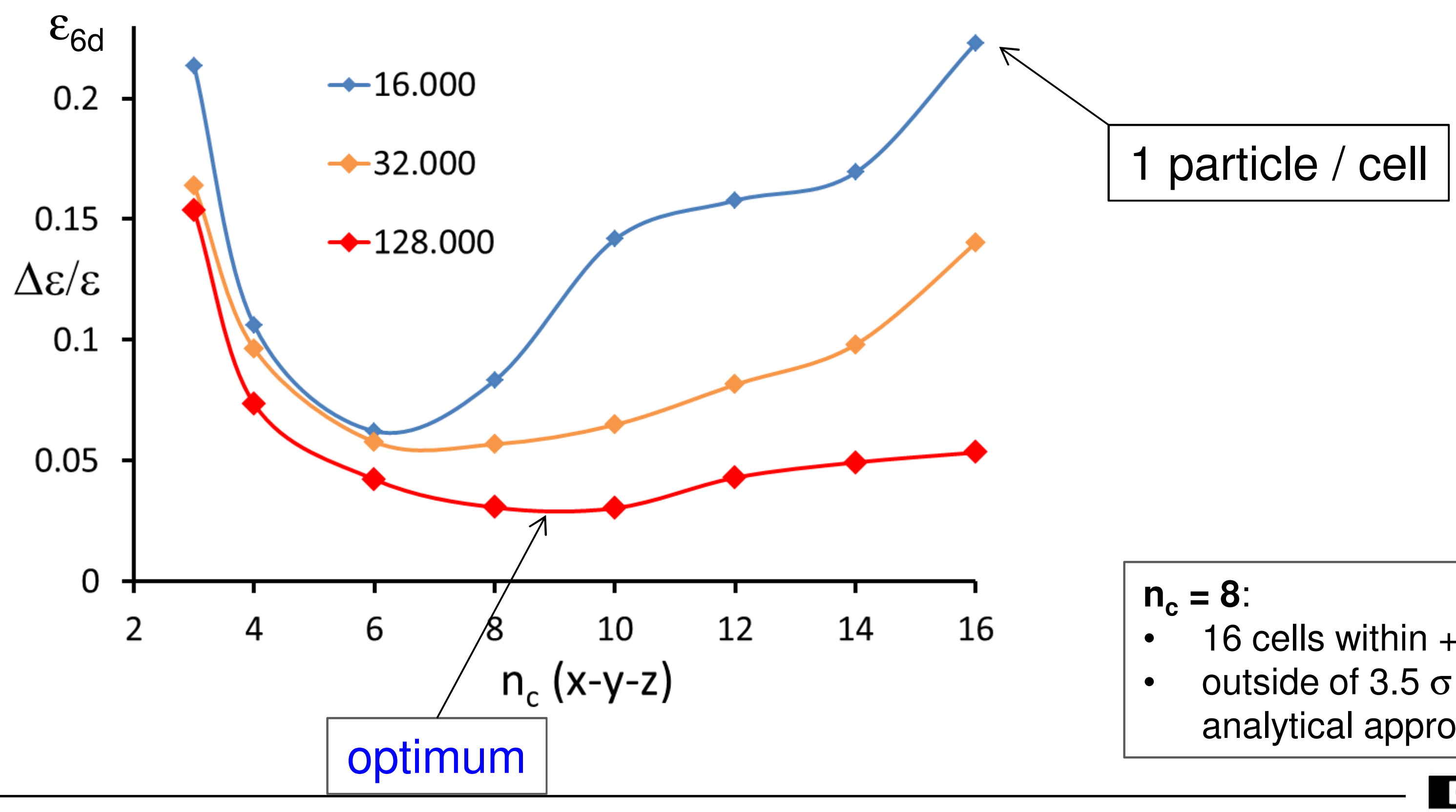
$\Delta\varepsilon_{6d}/\varepsilon_{6d}$ growth as function of # grid cells n_c

Minimizing rms entropy growth → determine optimum grid/particle resolution

Fully isotropic (spherical) bunch

grid dominated
- not resolving Gaussian profile -

collision dominated
- charge ~1/N -



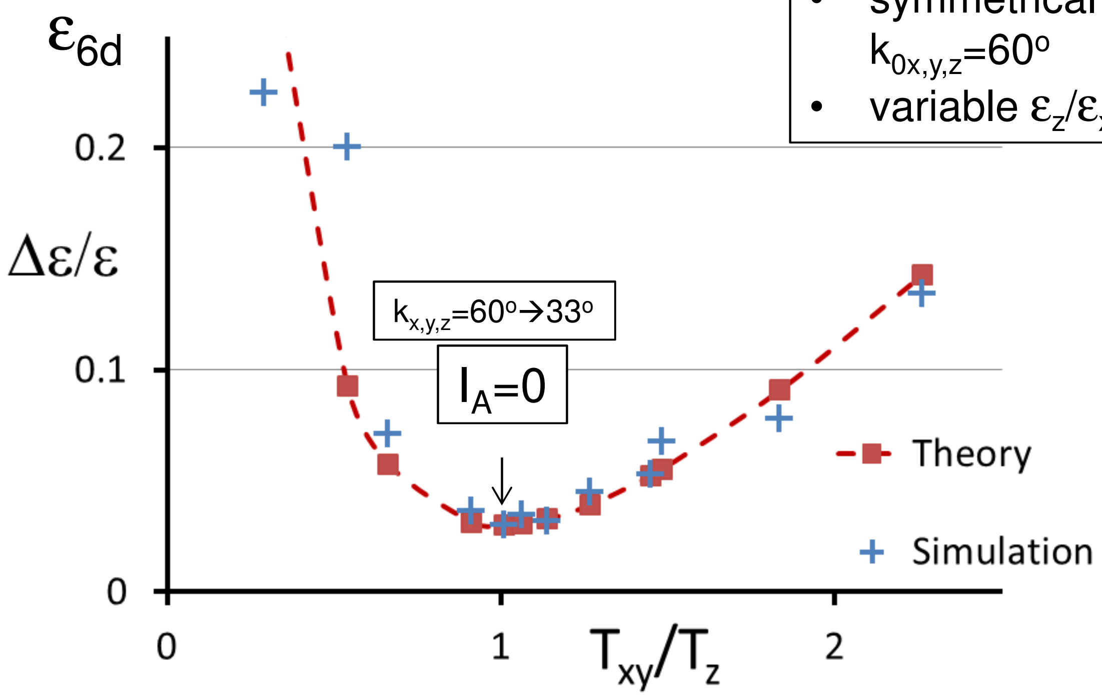
n_c = 8:

- 16 cells within +/- 3.5 σ
- outside of 3.5 σ boundary analytical approximation

Anisotropy and grid effect

→ fits to theory with I_{GN} and k_f^* fitted to data

- symmetrical external focussing $k_{0x,y,z}$=60°
- variable $\varepsilon_z/\varepsilon_{xy}$



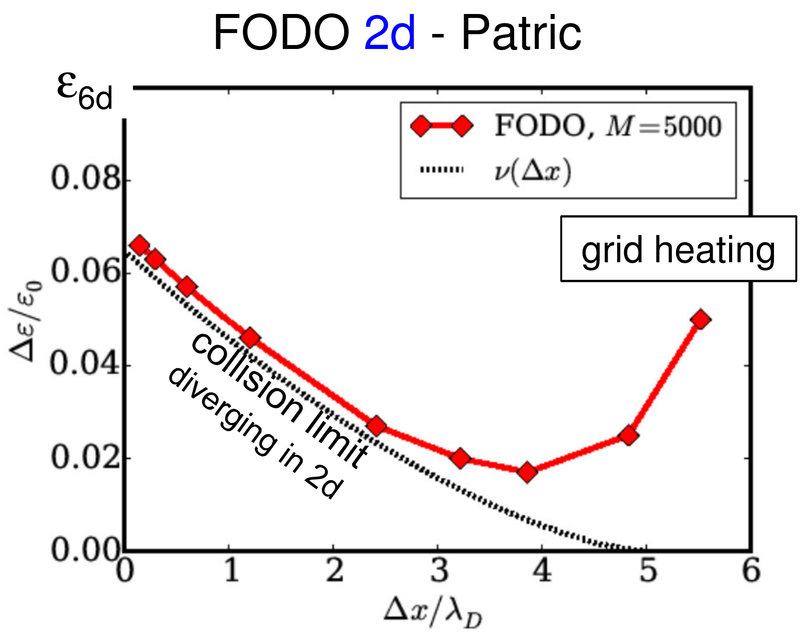
$$\frac{d}{ds}\ln\,\epsilon_x(s)\epsilon_y(s)\epsilon_z(s) = \frac{k_f}{3}\,I_A = \frac{k_f}{3}\left(\frac{(1-r_{xy})^2}{r_{xy}} + \frac{(1-r_{xz})^2}{r_{xz}} + \frac{(1-r_{yz})^2}{r_{yz}}\right) \geq 0$$

→

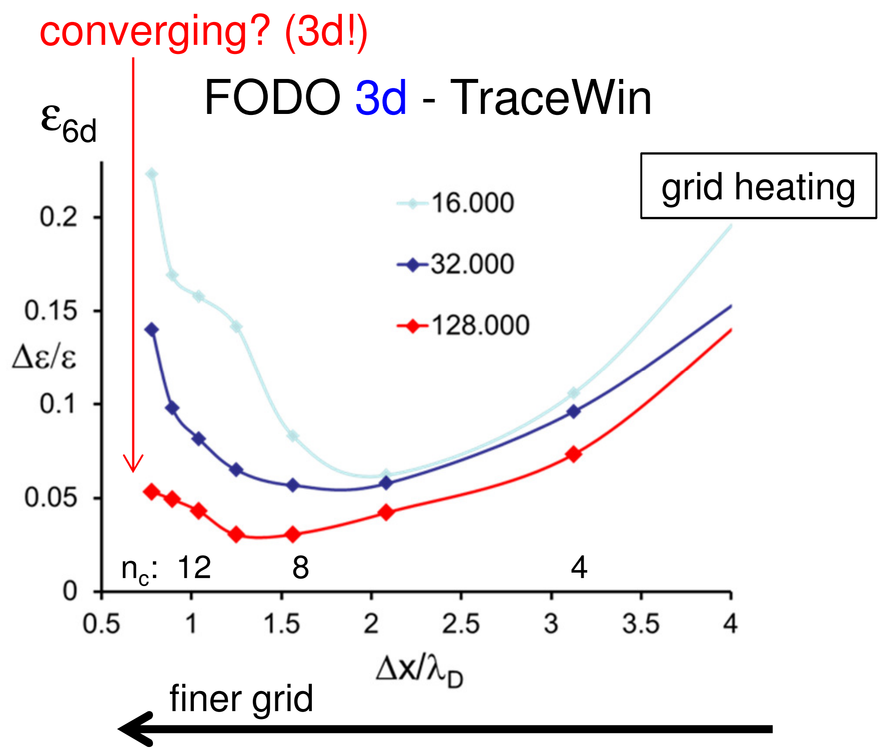
$$\frac{d}{ds}\ln\,\epsilon_x(s)\epsilon_y(s)\epsilon_z(s) = \frac{k_f^*}{3}\,(I_A + I_{GN})\,.$$

$$\frac{1}{k}\Delta S = \frac{\Delta\epsilon_{6d}}{\epsilon_{6d}} = \Delta s\frac{k_f^*}{3}\,(I_A + I_{GN})$$

Comparison of 3d with 2d results



Source: *O. Boine-Frankenheim et al., NIM 2014*



A. B. Langdon, Effect of the spatial grid in simulation plasmas, J. Comput. Phys. (1970)

→ Artificial heating if grid is too coarse: $\Delta x \gtrsim \lambda_D$ (Debye length)

In 2d enhanced collisions if grid too fine → larger N

From matched equilibrium beams → mismatched, resonances, ...

1. Can we apply our models of noise vs. N and/or n_c to dynamical situations with resonant effects? Use for optimization?
2. Are there transient/resonant/unstable phenomena, which require a more refined measure for noise/entropy than $\varepsilon_{6d,rms}$?
3. Do we need more theory efforts, or are phemenological studies the only way?

Non-stationary (non-equilibrium) beams

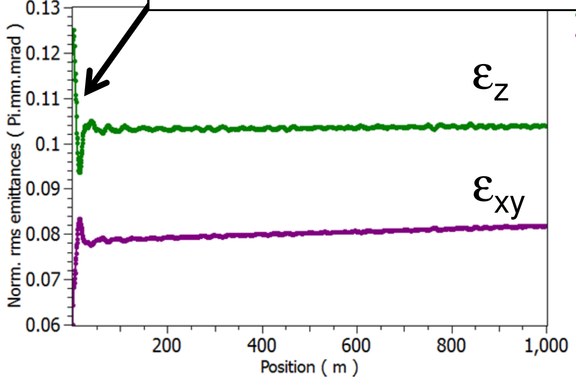
- fast emittance exchange on $2k_z$-$2k_{xy}$=0 resonance (space charge octupole)

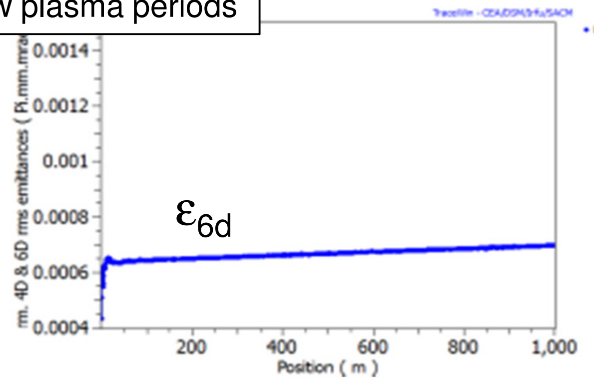
exchange practically unaffected by noise

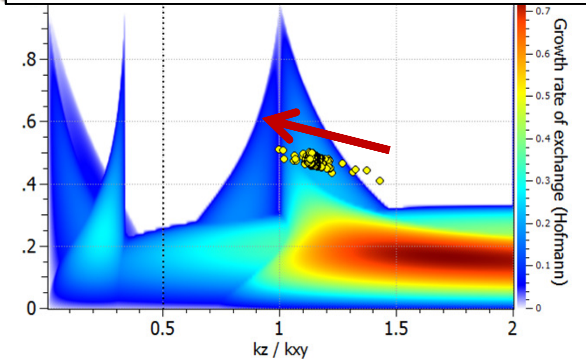
$N=10^5$

fast emittance exchange: ~ few plasma periods

- $k_{0x,y,z}$=60/60/60° and $\varepsilon_z/\varepsilon_{xy}$=2
- $k_{x,y,z}$=26°/26°/35°



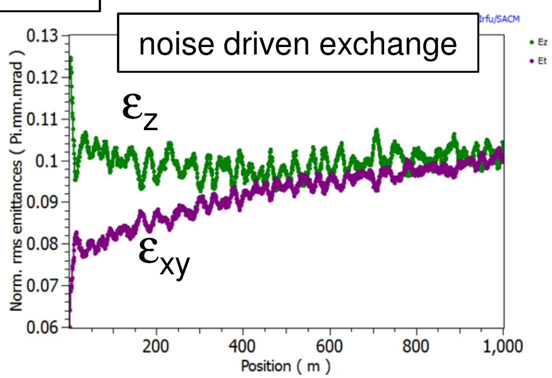


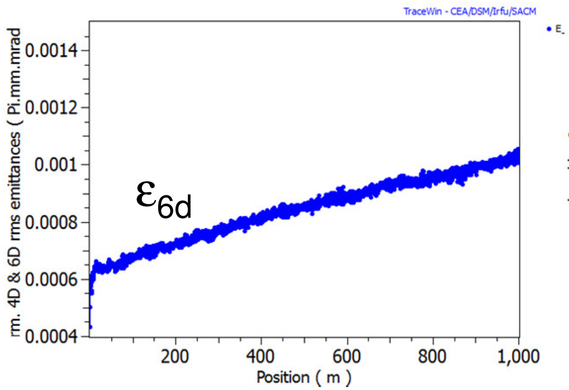


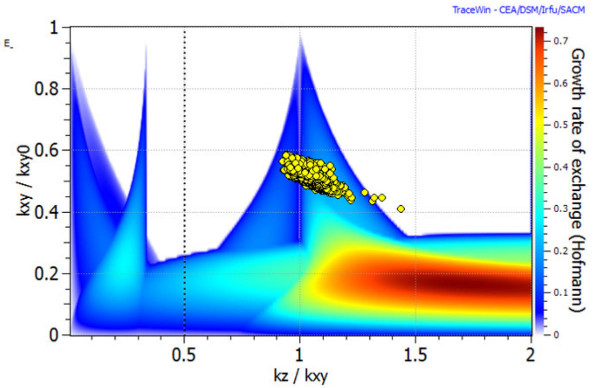
n_c=6

$N=10^3$

noise driven exchange

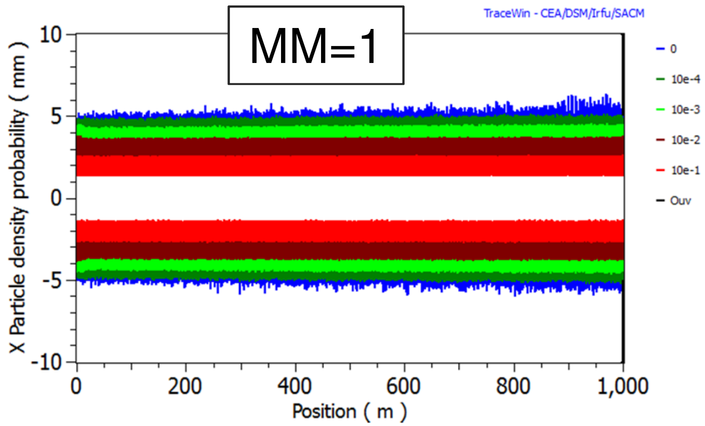


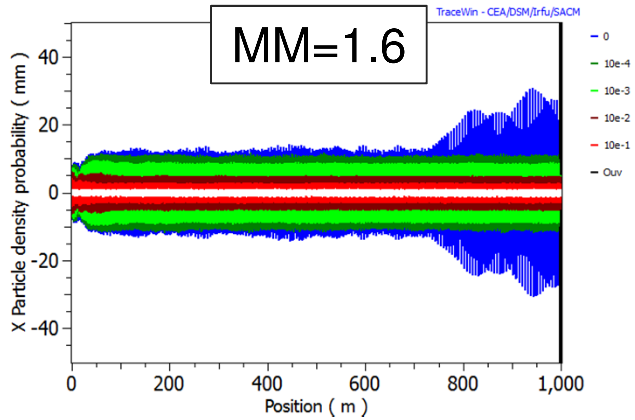


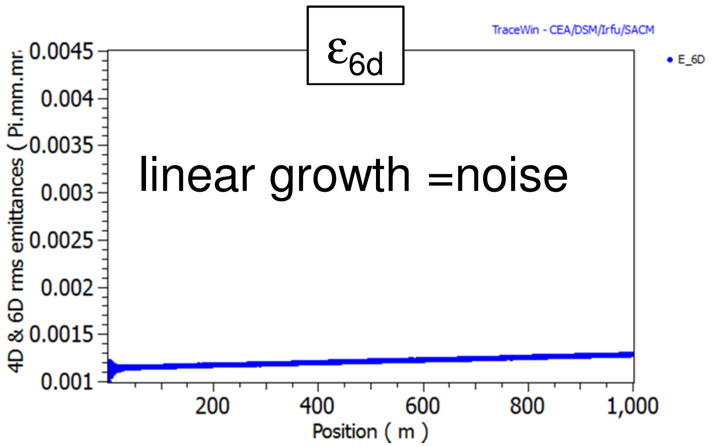


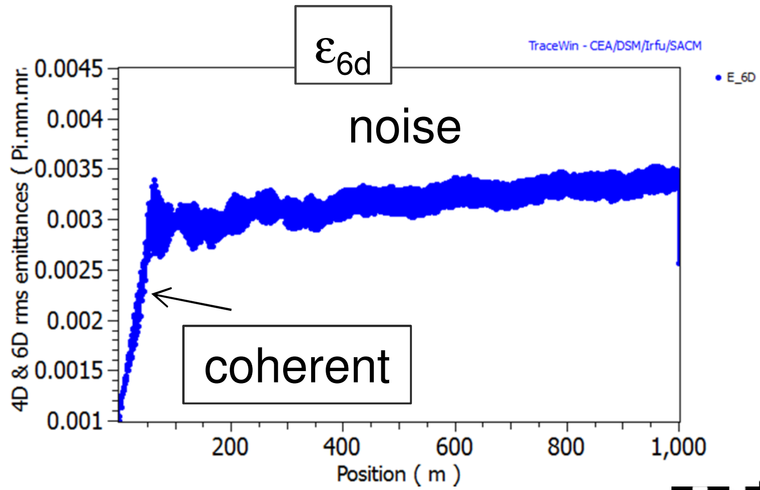
Mismatched beams → halo formation

chose large MM factor in x,y and z & N=10^5



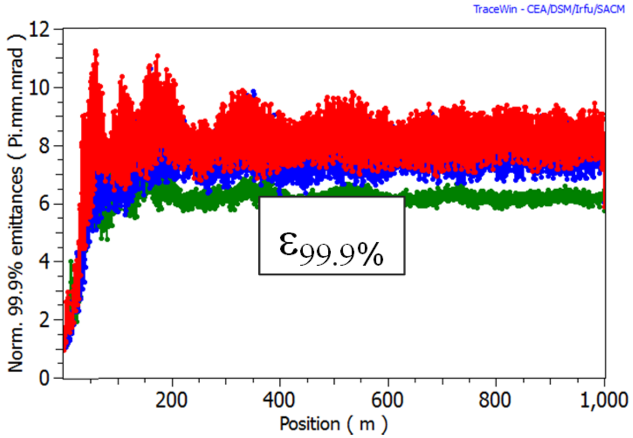


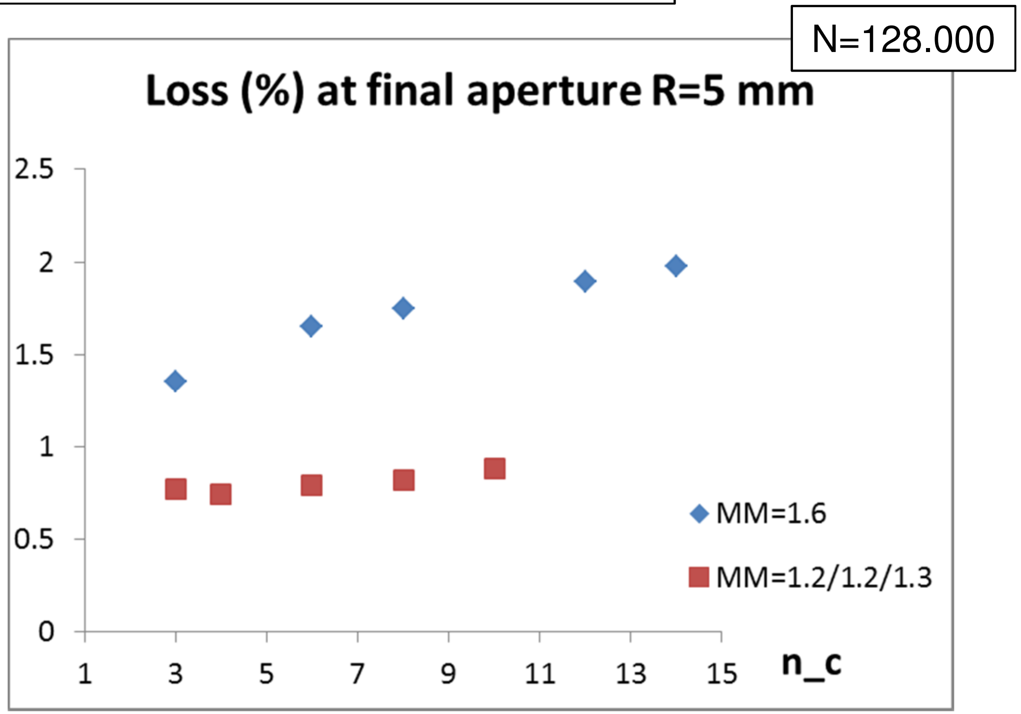


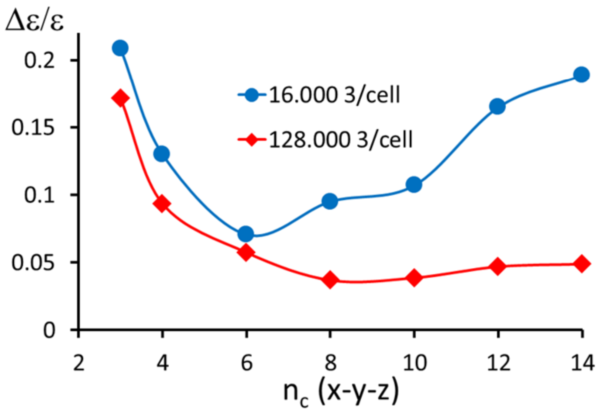


Mismatch → halo ~ 50 turns

fast conversion into halo → noise has no effect on this!

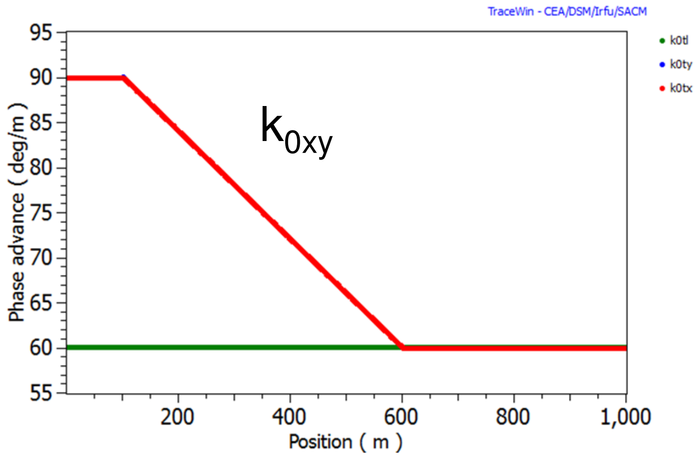


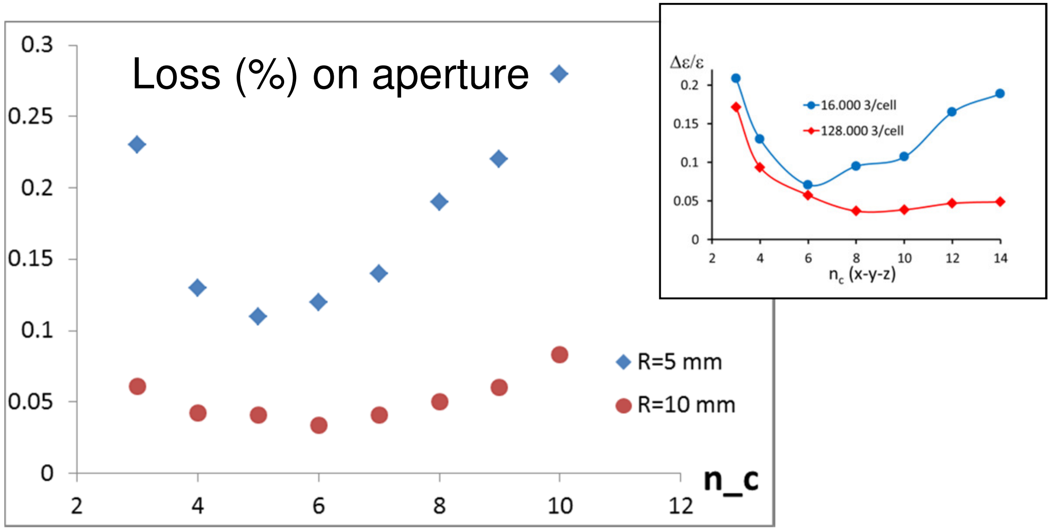


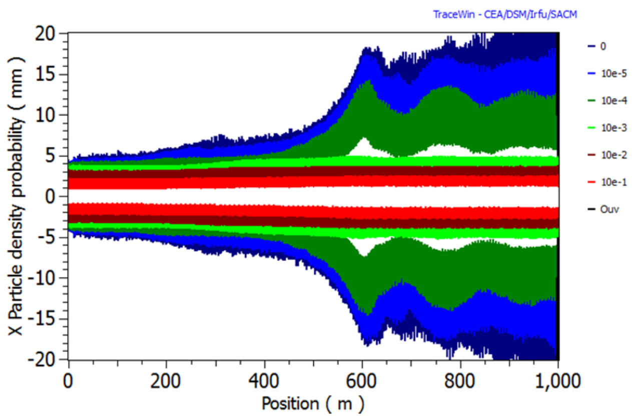


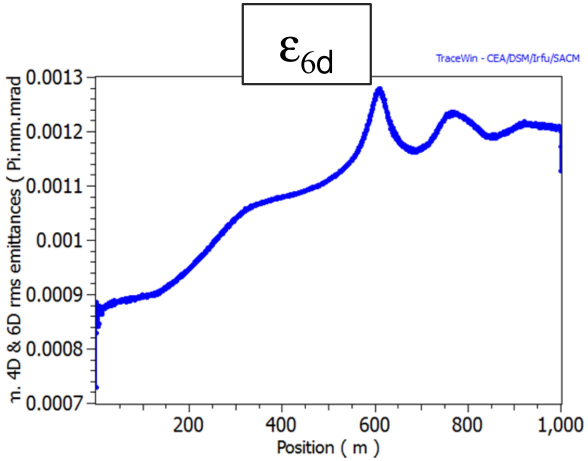
Crossing of space charge driven resonances

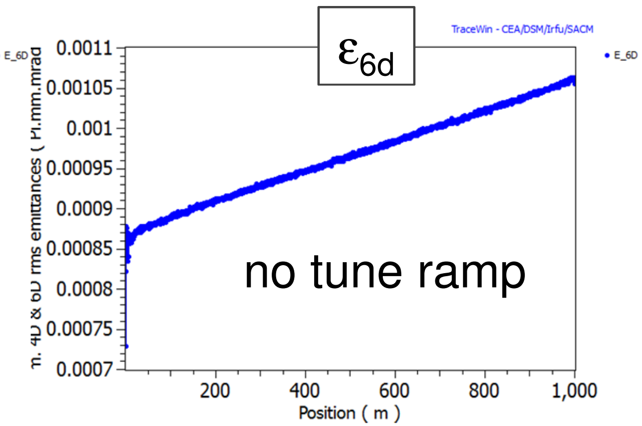
$k_{0xy}=90^0 \rightarrow 60^0$ / 500 cells







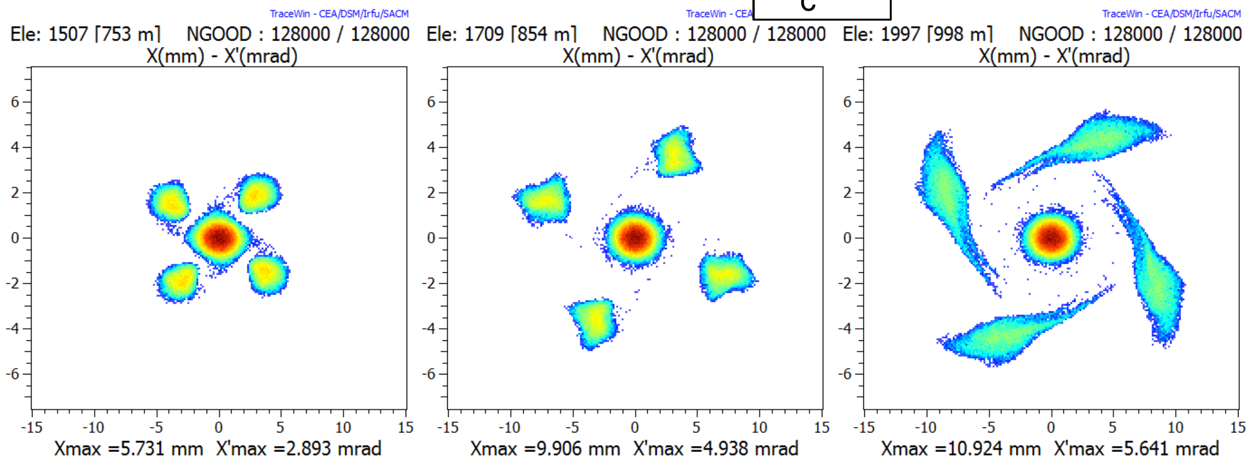


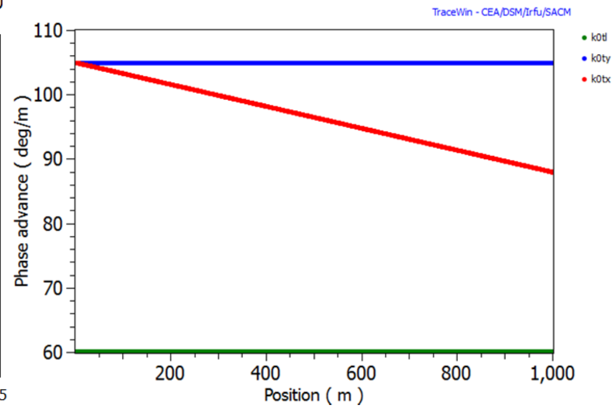


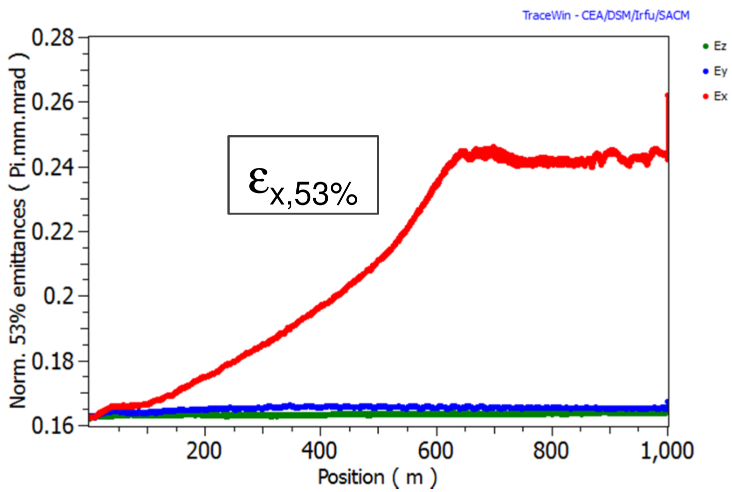
Crossing of 90^0 (4^{th} order) space charge driven resonance $k_{0x}=105^0 \rightarrow 88^0$ / 1000 cells ($k_{0y}=105^0$ fixed)

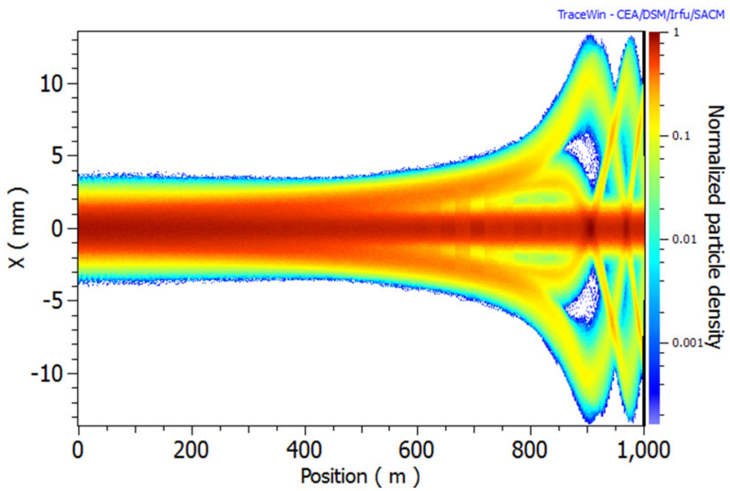
128 k particles, n_c=4-6: find 4 „identical“ islands pushed outwards

n_c=6



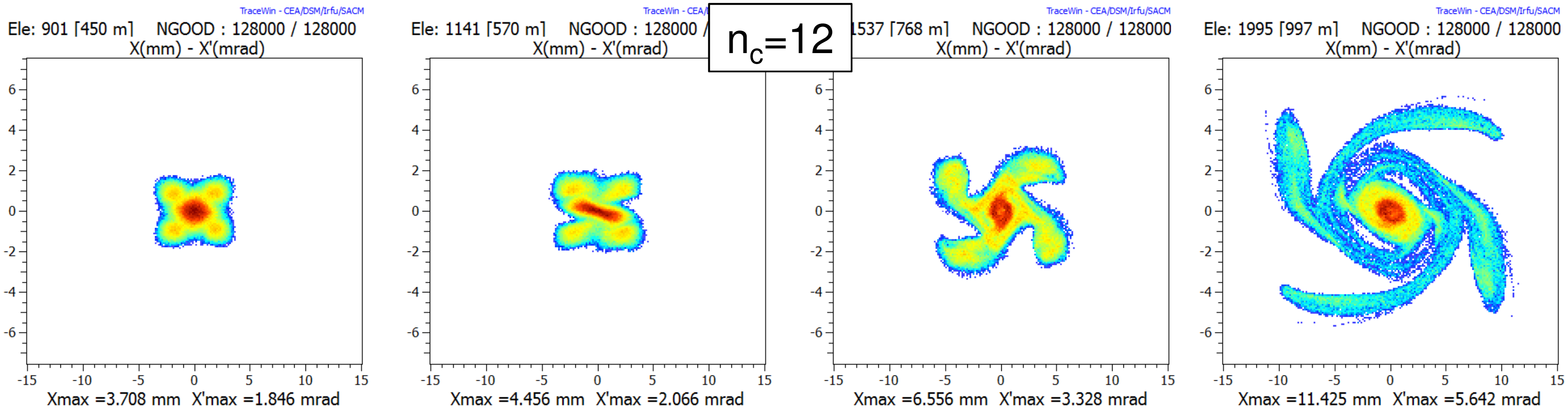


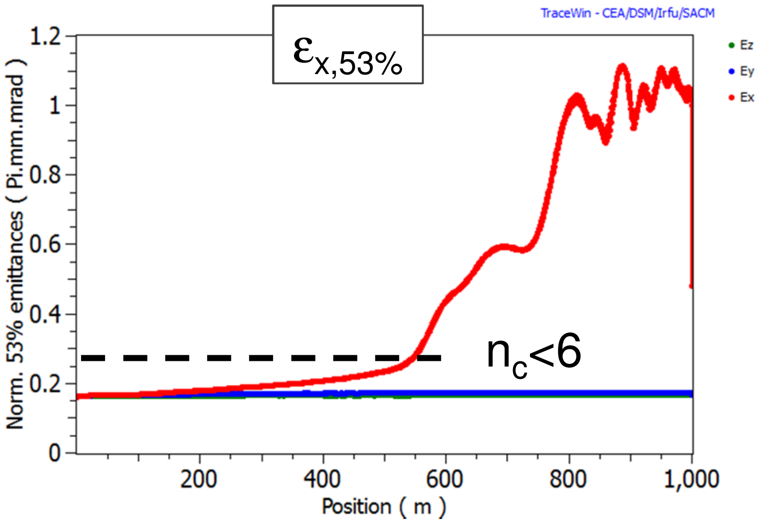


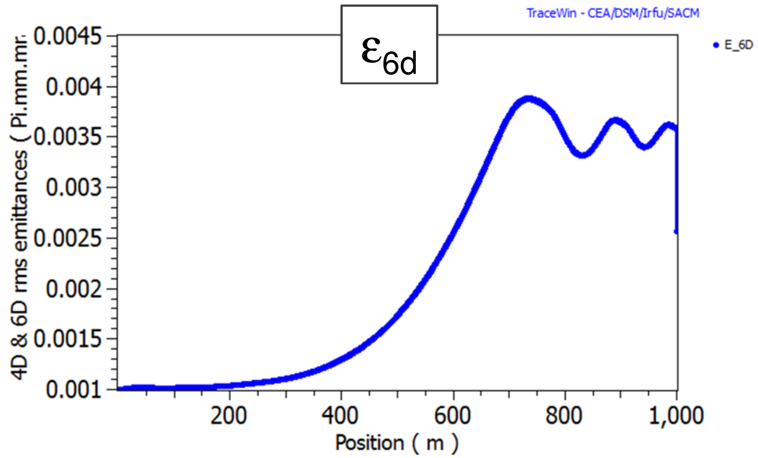


cont‘d crossing $k_{0x}=105^0 \rightarrow 88^0$ /1000 cells

128 k particles, n_c=7-12: find breaking of four-fold symmetry > 500 cells
envelope instability (h=2) on top of h=4?

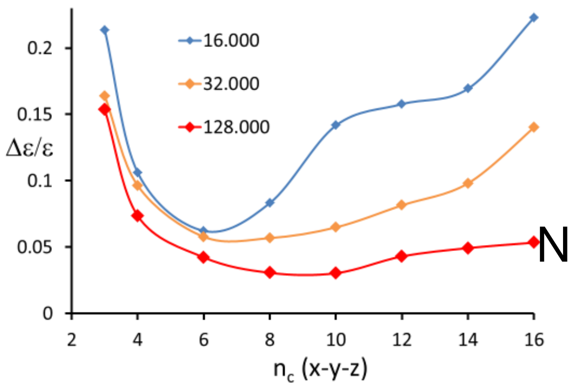




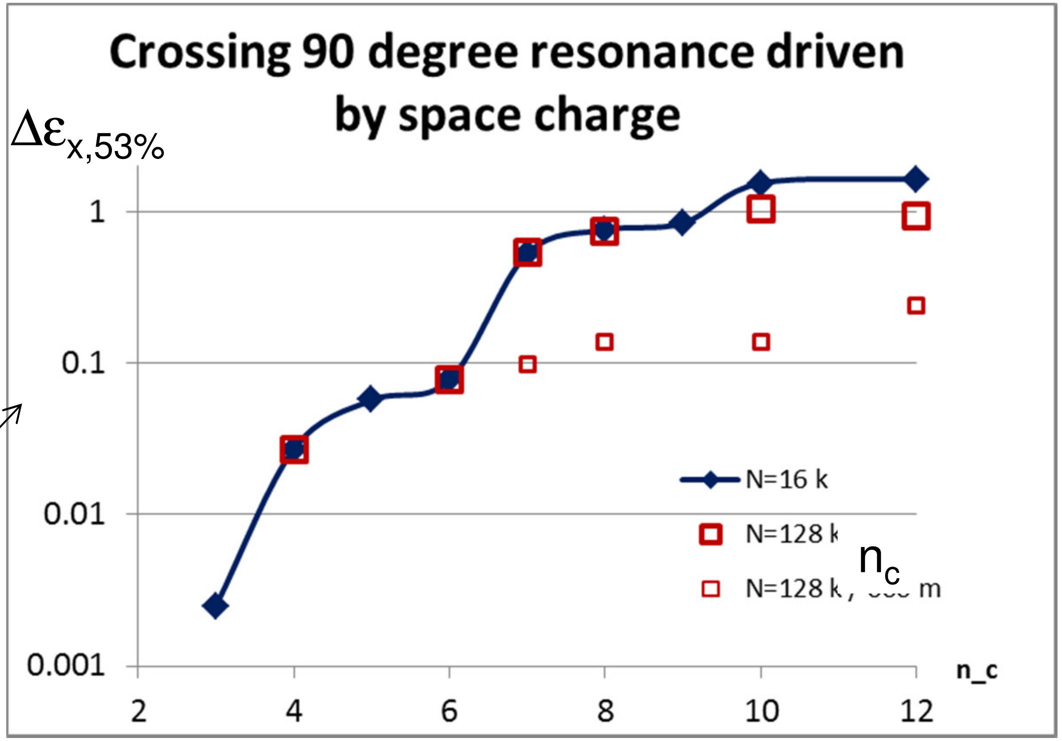


Summary: crossing $k_{0x}=105^0 \rightarrow 88^0$ /1000 cells

question: why more growth for finer grid, if additional mode is only 2nd order?



N=10^5



Summary

- ✓ 3 d noise by grid well represented by rms entropy in equilibrium beam
- ✓ Grid heating (n_c<5) or collisional heating (n_c>10) for small/large number of grid cells n_c → optimum n_c for given N
- ✓ Anisotropy effect in „good“ agreement with theory
- ✓ Dynamical problems:
  - ✓ our noise modelling seems irrelevant for fast processes – „no“effect of noise
  - ✓ slow resonance crossing: retrieve noise dependence on grid, but different for island trapping → much increased halo for larger n_c ?
- ✓ → needs more work especially towards resonance (collective) effects