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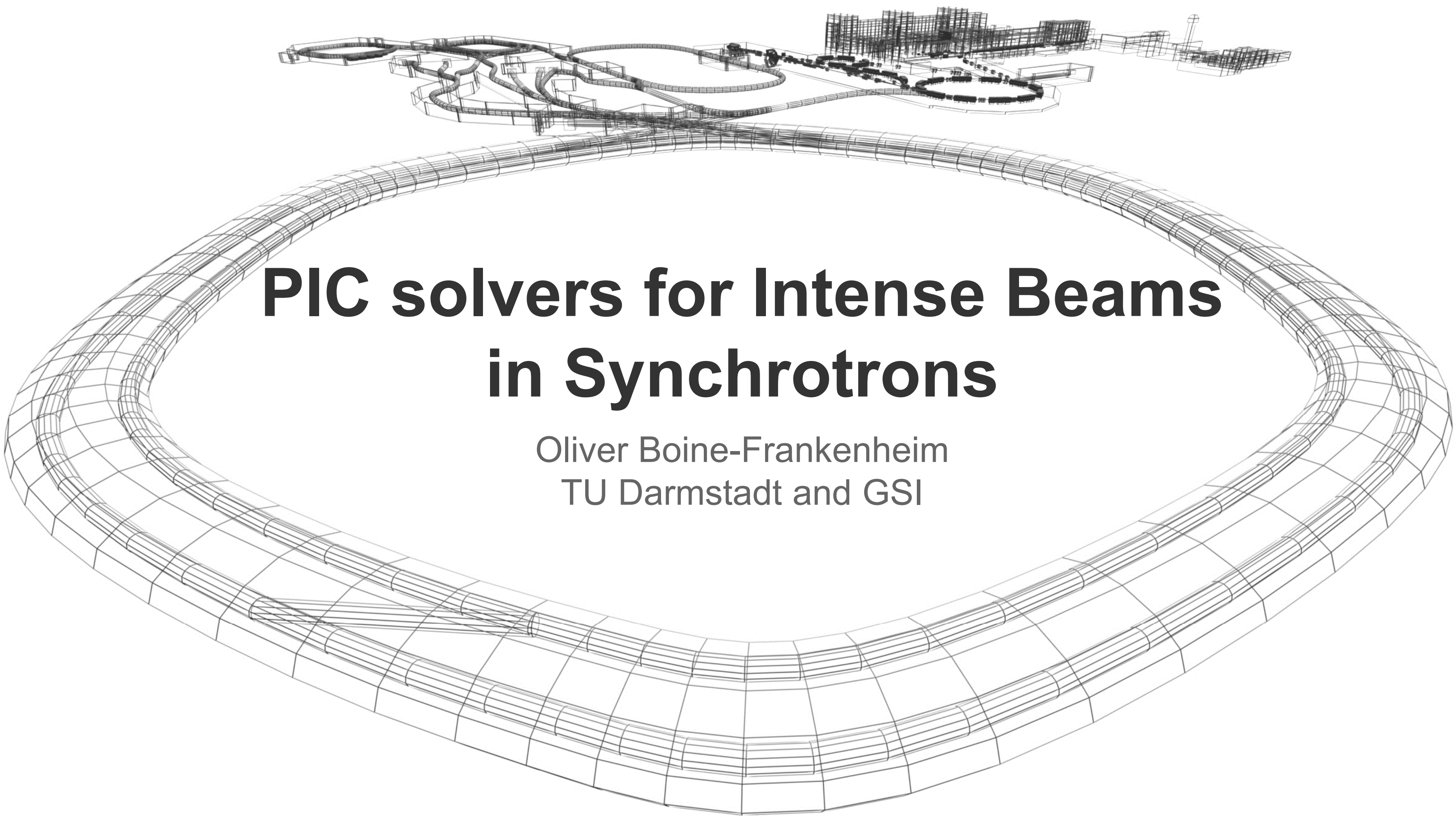

PIC solvers for Intense Beams in Synchrotrons

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Contents

- Application and challenges for beam simulations with space charge
- 2D electrostatic Particle-In-Cell (PIC) simulation scheme for beams
- Review: Numerical noise in PIC codes and related emittance growth
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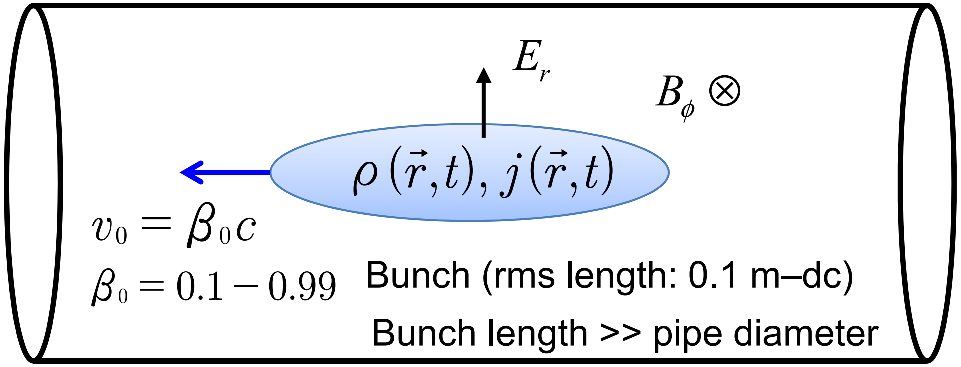
- Summary and Outlook

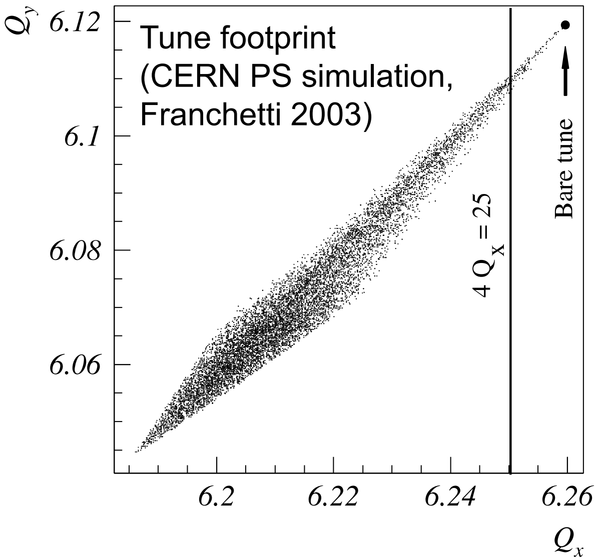
Space Charge Simulations in Synchrotrons

$$\varepsilon_0 \nabla \cdot \vec{E} = \rho$$

(in the rest system of the beam)

Space charge tune shift: $\Delta Q_y^{sc} \propto -\frac{q^2}{m}\frac{N}{B_f}\frac{4}{\varepsilon \beta_0^2 \gamma_0^3}$





The transverse space charge force is the main intensity limiting effect in in the FAIR synchrotrons at GSI and in other high current synchrotrons.

Time scales: 1000-10^6 turns (1 ms - 1 s)
-> Emittance growth, Beam loss (< 1%)

Challenge: Control of numerical emittance growth !

'Space charge' collaboration
(CERN, GSI, FNAL, SNS, KEK,…)
- Codes for long-term simulations
  -> Effect of stochastic noise !
- (PIC) codes used for FAIR at GSI: pyORBIT, Micromap, PATRIC

PIC simulation scheme (for 2D beams)

q: beam particle charge

$Q = q\dfrac{N}{M}$: macro particle charge

N: number of beam particles

$M \ll N$: number of macro-particles

$$x_i'' - \kappa(s)x_i - \frac{qE_x(x_i, y_i, s)}{\gamma_0 m v_0^2} = 0$$

$$y_i'' + \kappa(s)y_i - \frac{qE_y(x_i, y_i, s)}{\gamma_0 m v_0^2} = 0$$

2.5D electric fields:
bunches are long (m)
Compared to their
transverse width (cm).

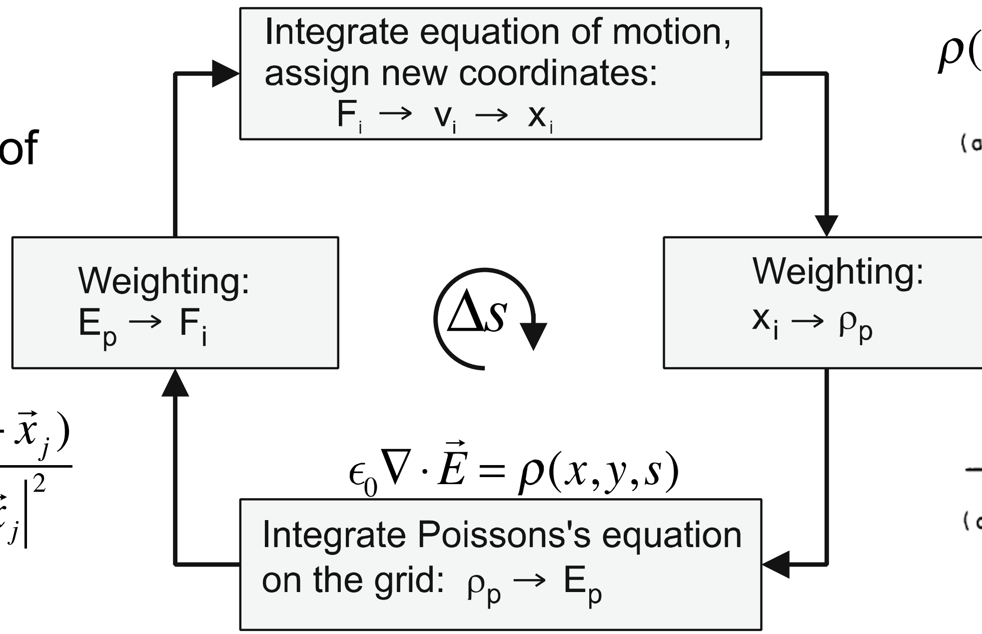
'Error' sources:
1) 'artificial' collisions of macro-particles Q and test particles q.

(Coulomb's law)

$$\vec{F}_i = \sum_{j=0}^{M} \frac{qQ' S(\vec{x}_i - \vec{x}_j)(\vec{x}_i - \vec{x}_j)}{2\pi\epsilon_0 \gamma_0 m v_0^2 \left|\vec{x}_i - \vec{x}_j\right|^2}$$

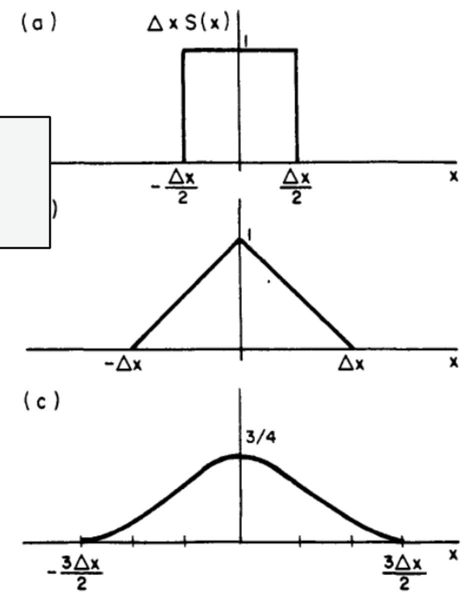
-> energy conserving.

2) Grid/stochastic heating



$$\epsilon_0 \nabla \cdot \vec{E} = \rho(x, y, s)$$

$$\rho(x,y,s) = Q\sum_{i=0}^{M} S(\vec{x} - \vec{x}_i)$$



Depending on particle shape S the macro-particles have a finite width: $\Delta \approx \Delta x$

What physics system does a PIC code represent ?

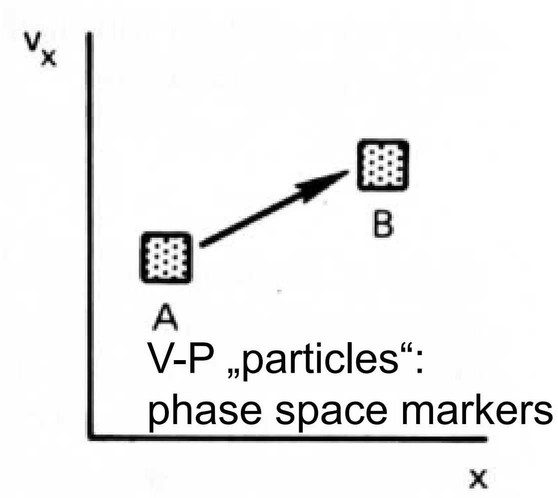
The system we would like to solve: **Collision-free Vlasov-Poisson (V-P) system**

$$\frac{\partial f}{\partial t} + \boldsymbol{x}' \frac{\partial f}{\partial \boldsymbol{x}} + \boldsymbol{F}_\perp \frac{\partial f}{\partial \boldsymbol{x}'} = 0$$

(Vlasov equation)

$$\epsilon_0 \nabla \phi = \rho(x, y)$$

(Poisson equation)



$$\rho(x, y) = q \int f(\boldsymbol{x}, \boldsymbol{x}') d^2 x$$

(charge density)

$$\boldsymbol{F}_\perp = \kappa_{x,y}(s)\boldsymbol{x} - \frac{q}{\gamma_0 m v_0^2} \nabla \phi(x, y, s)$$

(AG focusing) (space charge)

$$\Rightarrow \quad S = -k \int f \ln f d\boldsymbol{x} d\boldsymbol{x}' = \text{const.}$$ (Entropy)

What in fact we solve is (forget about the grid for a moment):

$$\frac{\partial F}{\partial t} + \boldsymbol{x}' \frac{\partial F}{\partial \boldsymbol{x}} + \boldsymbol{F}_\perp \frac{\partial F}{\partial \boldsymbol{x}'} = 0$$

(Klimontovich equation)

-> Artificial collisions and related noise.
-> Noise level is much stronger than the Schottky noise in real beams.

$$F(x, x') = \sum_{j=0}^{M} S(x - x_j)\delta(x' - x'_j) \quad \Rightarrow \quad S_{4M} = -k \int F \ln F d\boldsymbol{x} d\boldsymbol{x}' = \text{const.}$$ (Entropy)

[1] Winjum et al., *Verification and convergence properties of PIC codes* (2014)

Artificial collisions in a 2D computer beam

In a 2D beam the beam macro-particles are rods: **Collision angle independent on b !**

All particles with relative velocities less than

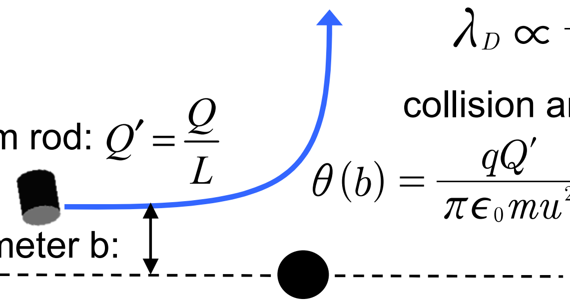
$$v_{\perp}^{2} = \frac{qQ'}{2\pi\epsilon_0 m}$$ are deflected by angles > 90^0.

Debye length:

$$\lambda_D \propto \frac{1}{\sqrt{N}}$$

collision angle:

$$\theta(b) = \frac{qQ'}{\pi\epsilon_0 m u^2}\arccos\frac{b}{\lambda_D}$$



$$F = \frac{qQ'}{2\pi\varepsilon_0 r}$$

(2D 'Coulomb' force)

Friction force on a test particle:

$$F_p(\vec{v}) = m\nu\vec{v} = m\int d^2v\,db\,u^2 f(\vec{v})\sin^2(\theta/2)$$

$$\nu \propto \frac{N^2}{M}\left(1-\frac{\Delta}{\lambda_D}\right)$$ (2D collision rate for finite -sized macro particles)

$$\nu \propto \frac{N^2}{M}\ln\left(\frac{\lambda_D}{\Delta}\right)$$ (3D collision rate)

$\Delta \approx \Delta x$ (grid spacing)

Relation between friction and diffusion in a system with energy conservation:

$$D = \nu\frac{k_B T}{m}$$ (Einstein relation)

$$T(s) = \left(T_x + T_y\right)/2 \qquad k_B T_x \propto mc^2\frac{\varepsilon_x}{\hat{\beta}_x}$$

[1] Boine-Frankenheim, Hofmann, Struckmeier, Appel, NIMA (2015)

Entropy and emittance growth due to artificial collisions in computer beams

J. Struckmeier, *Stochastic effects in real and simulated charged particle beams*, Phys. Rev. ST-AB 2000

Entropy/Emittance growth for anisotroptic beams: $T_x \neq T_y$

$$D = \nu \frac{k_B T}{m} \Rightarrow \frac{1}{\varepsilon}\frac{d\varepsilon}{dt} = \frac{1}{2} k_B \nu \frac{(T_x - T_y)^2}{T_x T_y} \qquad \varepsilon = \varepsilon_x \varepsilon_y$$

(4D emittance)

-> Emittance growth due to AG focusing in a FODO channel !

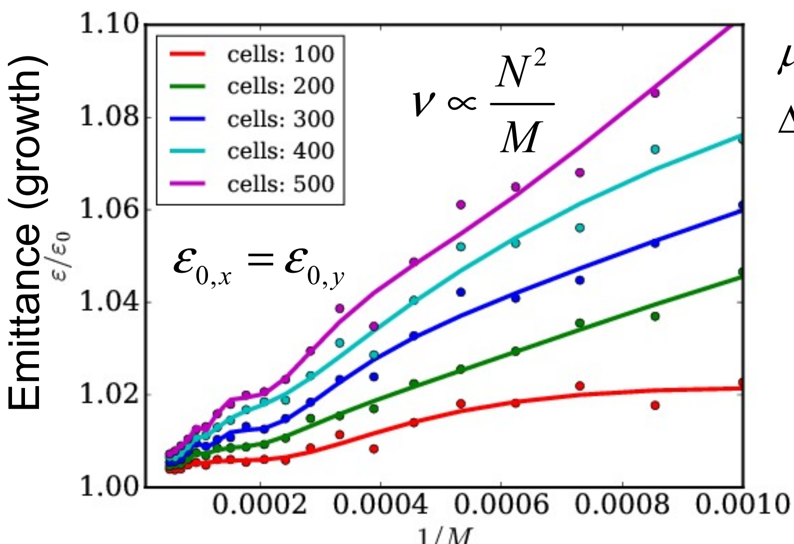
-> No growth for constant focusing (CF) and for FODOXX channels.

FODOXX: $\kappa_x(s) = \kappa_y(s) \Rightarrow \hat{\beta}_x = \hat{\beta}_y$

CF: $\kappa_x = \kappa_y = \text{const.}$

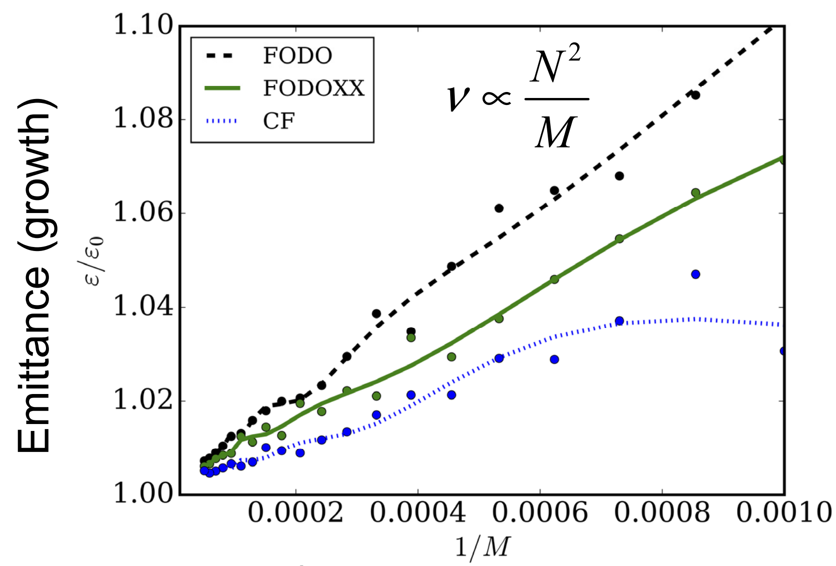
PATRIC (2D PIC):

Emittance growth after 100-500 FODO cells



$\mu_0 = 60^o$

$\Delta\mu_x^{sc} = -10^o$



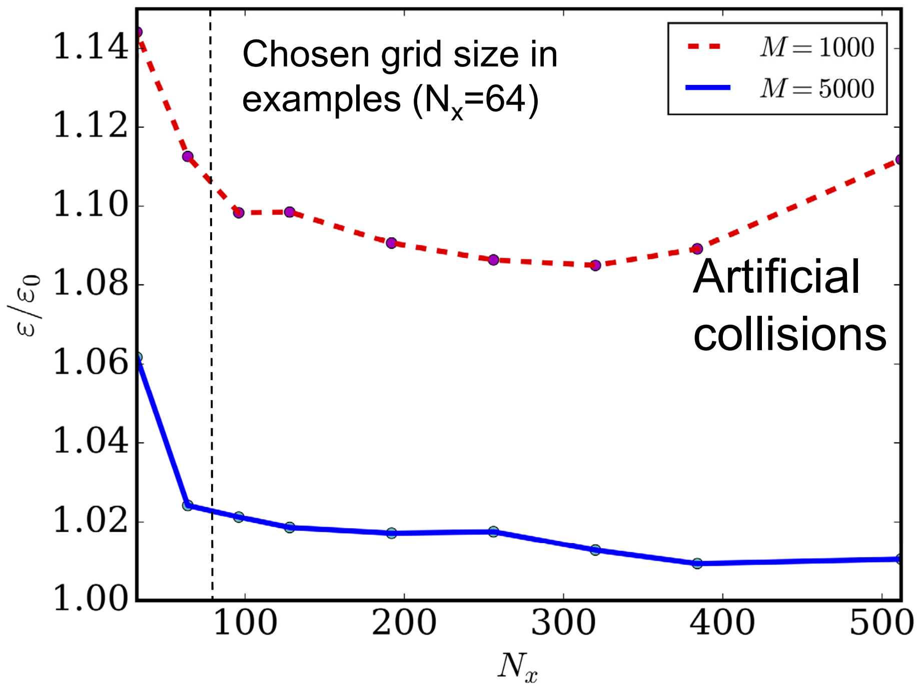
Emittance growth in CF/FODOXX channels.

-> Obviously there is additional heating !

[1] Hofmann, Boine-Frankenheim, PRAB (2015)

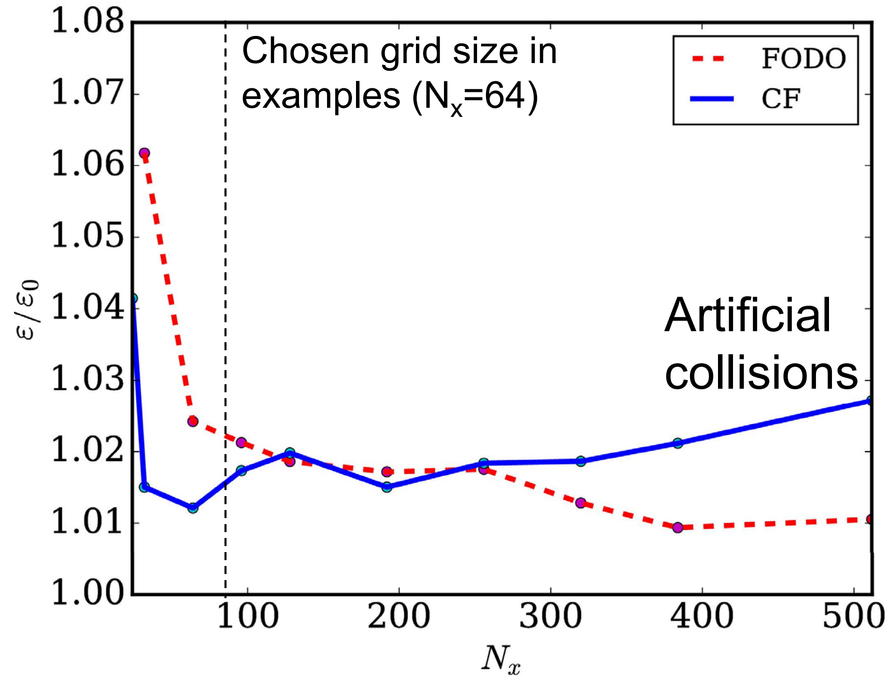
Short comment on the effect of the grid spacing on emittance growth

PATRIC (2D PIC):
Emittance growth after 100-500 FODO cells



(grid points)

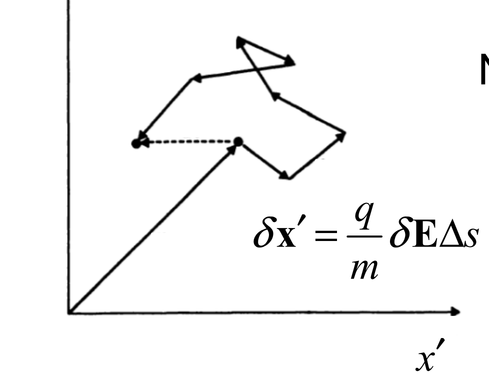
PATRIC (2D PIC):
FODO vs. CF



(grid points)

Stochastic or grid heating (‚inelastic collisions‘)

Random walk in grid induced error fields:

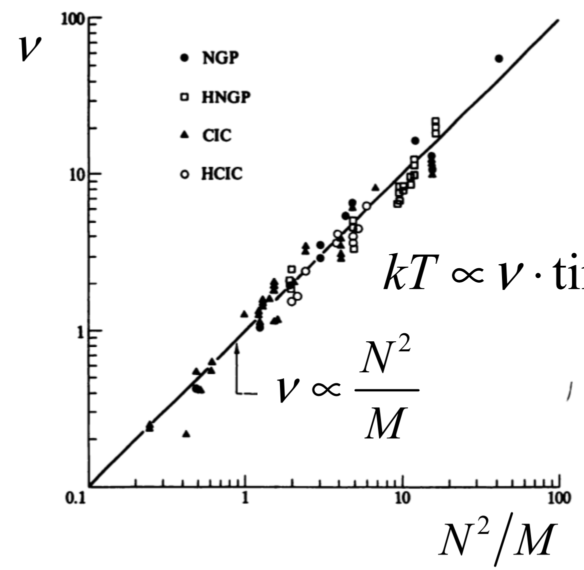


$$\delta \mathbf{x}' = \frac{q}{m}\,\delta \mathbf{E}\,\Delta s$$

$$kT \approx n\frac{1}{2}\frac{q^2}{m}(\delta\mathbf{E})^2(\Delta s)^2$$

Numerical heating due to grid !

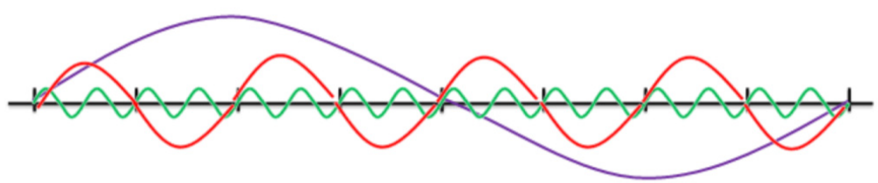
$$D > \nu\frac{k_B T}{m}$$



$$kT \propto \nu \cdot \text{time steps}$$

$$\nu \propto \frac{N^2}{M}$$

$\delta\mathbf{E}$ Random grid induced electrical error field: rounding, time step, finite differences,…



A non-conservative force (-> heating) is introduced by **grid undersampling**.

-> Standard PIC integrators are non-symplectic

‚Noise is not bad, the grid (undersampling) is‘

Stochastic heating in computer plasmas:

[1] Hockney, *Measurement of collision and heating times in a 2D computer plasma,* J. Comput. Phys. (1971)

Application to computer beams:

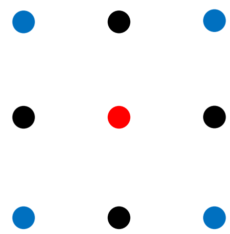
[2] Kesting, Franchetti, *Propagation of numerical noise in PIC*, PRAB (2015)

Digital filters for PIC

+ Reduce noise at short wavelengths (smoothing of the charge density).
+ Relatively fast.
- Can lead to non-physical results and numerical instabilities
- (Non-) Energy conservation (e.g. damping of modes)

$$\rho_{i,k} = \frac{M\rho_{i,k} + S(\textbf{side terms}) + K(\textbf{corner terms})}{M + 4(S+K)}$$

$(M, S, K) =$ Middle, side and corner weights



(grid points)

Examples:

Hollow 8-point filter (0,1,1): Studied in [2]. Has negative spectral representation.
Binomial 9-point filter (4,2,1): Proposed for PIC codes in [1].

Digital filters:

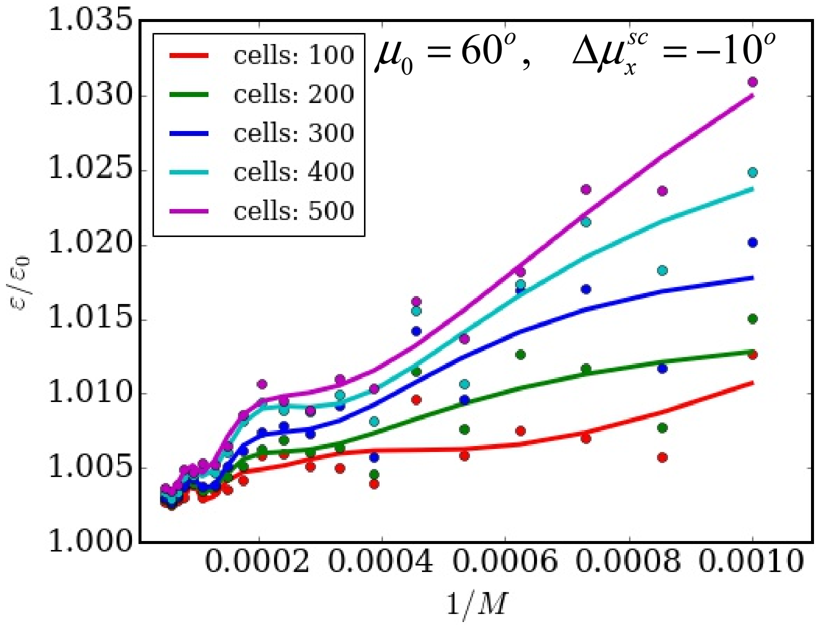
[1] Birdsall, Langdon, *Plasma Physics via Computer Simulation* (2004)
[2] Hockney, Eastwood, *Computer Simulation using Particles* (1988)
[3] Verboncoeur, *PIC for plasmas: Review and Advances*, Plasma Phys. Control. Fusion (2005)
[4] Vay et al., *Numerical methods for instability mitgation in* …, J. Comput. Phys. (2011)

Wavelet denoising:

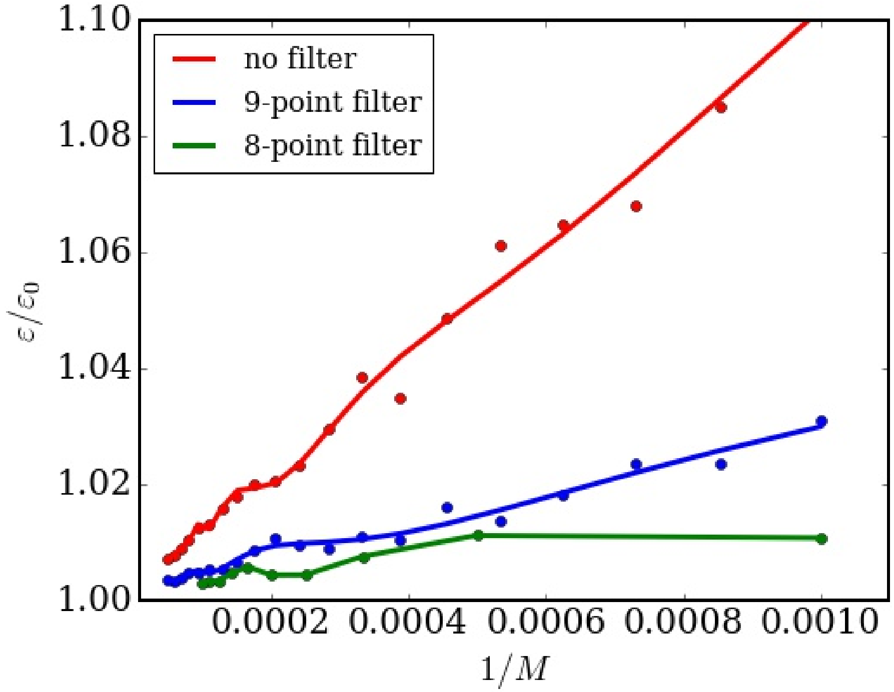
[4] Gassama, Sonnendrücker, *Wavelet denoising for postprocessing of 2D PIC codes*, ESAIM (2007)
[5] Terzic et al., *PIC simulations with a wavelet based Poisson s*olver, PRAB (2007)

Example results for FODO channel with filters

PATRIC 2D: Numerical emittance growth in a FODO channel after 100-500 cells with 9-point filter



After 500 cells: no filter vs. with filter



With digital filters:
-> Emittance growth rate is slower (approx. factor 10).
-> However, emittance growth is not the only benchmark -> resonances,…

‘Symplectic Particle-In-Cell’

Conventional PIC: Total momentum is conserved, but not energy (grid heating).
‚Energy conserving‘ PIC [3]: Momentum is not conserved (self-force on the grid).
-> PIC codes are usually not symplectic

An ideal beam particle integrator with space charge would conserve:
Phase space (Symplectic), Emittance, Entropy, Energy (only for constant focusing)

‘Multi-symplectic’ integrators offer bounded variations of those constants.

Starting point is usually the Lagrangian (here for a 2D beam with space charge):

$$L = \int dx_0 dy_0 dx_0' dy_0' f(x_0, y_0, x_0', y_0') \left(\frac{1}{2}\left((x')^2 + (y')^2\right) - \frac{1}{2}\kappa\left(x^2 - y^2\right) - \frac{q}{E_0 \gamma_0^2 \beta_0^2} \phi(x) \right) - \frac{\varepsilon_0}{E_0 \gamma_0^2 \beta_0^2} \int dx dy \nabla\phi \cdot \nabla\phi$$

Equations of motion (for particles and fields) from Euler-Lagrange equations:

$$\frac{\partial L}{\partial \xi} - \frac{d}{ds}\frac{\partial L}{\partial \xi'} = 0 \quad \Rightarrow \quad x'' + \kappa(s) x = -\frac{q}{E_0 \gamma_0^2 \beta_0^2}\frac{\partial \phi}{\partial x} \qquad y'' - \kappa(s) x = -\frac{q}{E_0 \gamma_0^2 \beta_0^2}\frac{\partial \phi}{\partial y} \qquad \varepsilon_0 \Delta\phi = -\rho$$

[1] Webb, *A spectral canonical electrostatic algorithm*, Plasma Phys. Control. Fusion (2016)
[2] Shadwick et al., *Variational formulation of macro-particle plasma simulation algo.*, PoP (2014)
[3] Langdon, *„Energy-Conserving“ plasma simulation algorithms,* J. Comput. Phys. (1973)
[4] Qin, et al., *Canonical symplectic PIC method for long term simulations..* , arxiv 1503.08334 (2015)

Spectral (grid-less) computer beam Lagrangian

Beam macro-particle distribution:

$$f(\boldsymbol{x},\boldsymbol{x}') = w\sum_{j=0}^{M} S(\boldsymbol{x}-\boldsymbol{x}_j)\delta(\boldsymbol{x}'-\boldsymbol{x}'_j)$$

Spectral space charge potential

$$\phi(\boldsymbol{x}) = \sum_{\boldsymbol{k}} \phi_{\boldsymbol{k}} \exp(i\boldsymbol{k}\cdot\boldsymbol{x})$$

Resulting discrete Lagrangian: $L_D = W_k - W_{AG} - W_{sc} - W_{\text{field}}$

$$W_k = w\sum_{j=0}^{M}\frac{1}{2}(\boldsymbol{x}')^2$$

(kinetic)

$$W_{sc} = w\frac{q}{E_0\gamma_0^2\beta_0^2}\sum_{j=0}^{M}\sum_{\boldsymbol{k}} S(\boldsymbol{k})\phi_{\boldsymbol{k}}\exp(i\boldsymbol{k}\cdot\boldsymbol{x}_j)$$

(space charge potential)

$$W_{\text{field}} = \frac{1}{E_0\gamma_0^2\beta_0^2}\sum_{\boldsymbol{k}}\sum_{\boldsymbol{k}'} kk'\phi_{\boldsymbol{k}}\phi_{\boldsymbol{k}'}$$

(space charge field energy)

Equations for macro-particles and spectra field) from Euler-Lagrange equations:

$$\frac{\partial L_D}{\partial \xi_j} - \frac{d}{ds}\frac{\partial L_D}{\partial \xi'_j} = 0 \quad \Rightarrow \quad \boldsymbol{x}''_j + \kappa(s)\boldsymbol{x}_j = -\frac{iq}{E_0\gamma_0^2\beta_0^2}\sum_{\boldsymbol{k}} \boldsymbol{k}\phi_{\boldsymbol{k}} S(\boldsymbol{k}) e^{i\boldsymbol{k}\cdot\boldsymbol{x}_j} \qquad \varepsilon_0 k^2\phi_{\boldsymbol{k}} = \rho_{\boldsymbol{k}}$$

Spectral (grid-less) PIC for plasmas:

[1] Webb, *A spectral canonical electrostatic algorithm*, Plasma Phys. Control. Fusion (2016)
[2] Decyk, *Spectral PIC codes,* ISSS (2011)
[3] Huang et al., *Grid instability and spectral fidelity of ES PIC codes,* arxiv:1508.03360 (2016)

Spectral algorithm for 2D beams

Spectral charge density: $\rho_{\boldsymbol{k}} = wS(\boldsymbol{k})\sum_j e^{-i\boldsymbol{k}\cdot\boldsymbol{x}_j}$

Space charge potential: $\varepsilon_0 k^2 \phi_{\boldsymbol{k}} = \rho_{\boldsymbol{k}}$

Space charge kick:

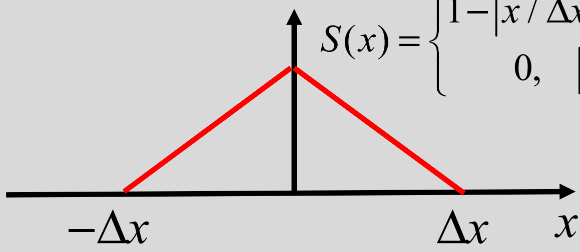
$$\Delta x'_n = -\Delta s \frac{iq}{E_0\gamma_0^2\beta_0^2}\sum_k k_x \phi_{\boldsymbol{k}} S^*(\boldsymbol{k}) e^{ik_x\cdot x_j^n}$$

Time step (Δs):

$$\begin{pmatrix} x_j \\ x'_j \\ y_j \\ y'_j \end{pmatrix}_{n+1} = M(s_n, s_{n+1}) \begin{pmatrix} x_j \\ x'_j + \Delta x'_j \\ y_j \\ y'_j + \Delta y'_j \end{pmatrix}_n$$

'Tent' particles shape:

$$S(x) = \begin{cases} 1 - |x/\Delta x|, & |x| \le \Delta x \\ 0, & |x| > \Delta x \end{cases}$$



$$S(k) = \frac{1}{\sqrt{2\pi}}\int dx S(x)\exp(-ikx)$$

2D spectral particle shape:

$$\Rightarrow \quad S(\boldsymbol{k}) = \mathrm{sinc}^2(\Delta x k_x / 2)\mathrm{sinc}^2(\Delta y k_y / 2)$$

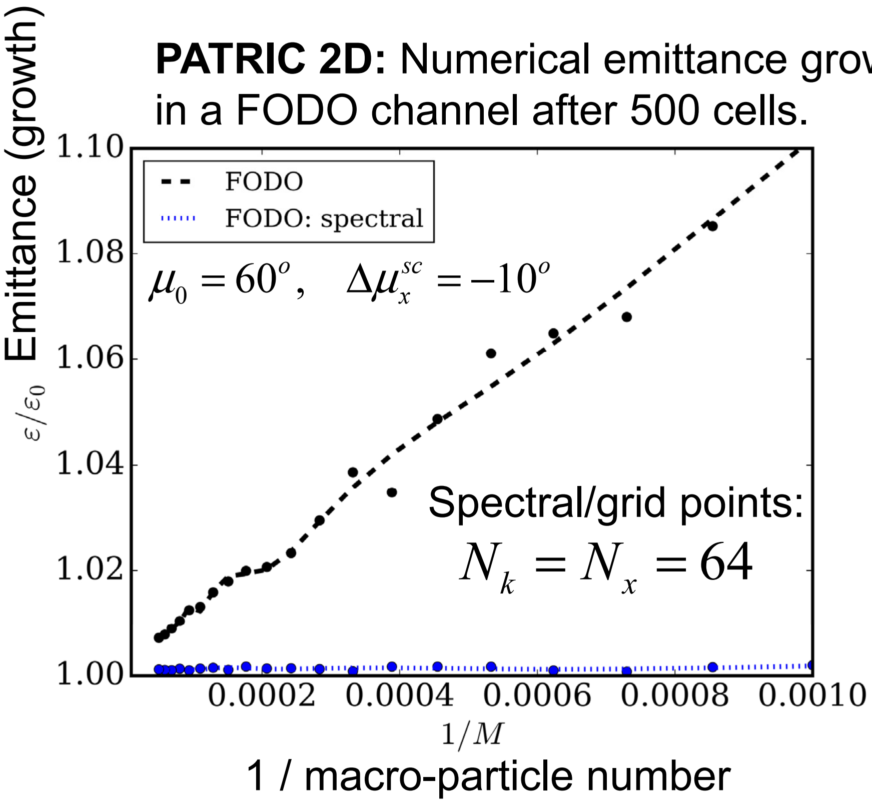
Algorithm derived from a grid-less macro-particle Lagrangian.

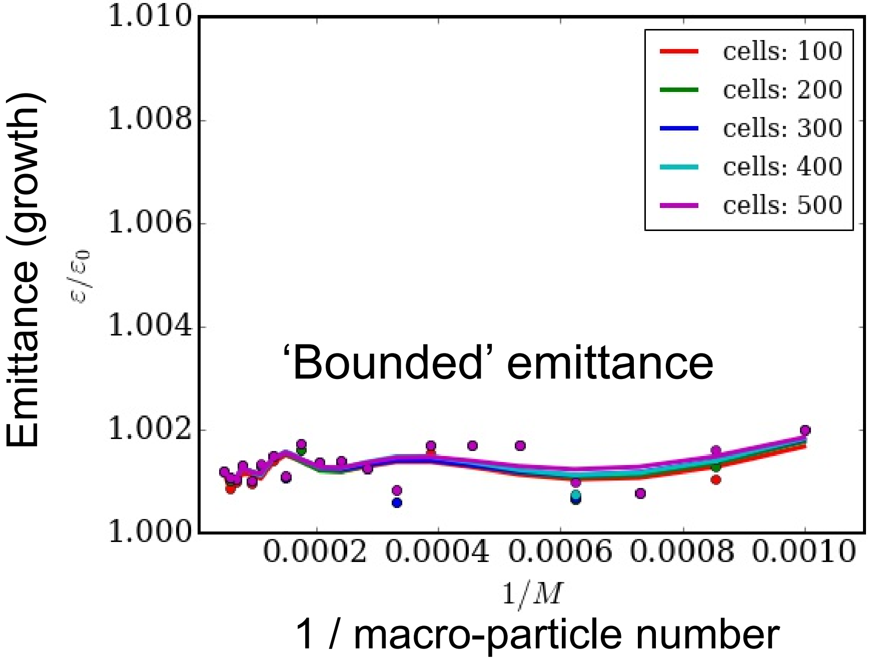
We expect the system to follow: $D \approx \nu \frac{k_B T}{m}$

Tests: Spectral PIC vs. Conventional PIC

PATRIC 2D: Numerical emittance growth in a FODO channel after 500 cells.

Spectral PIC only.





Noise still present (in k-space), but no emittance growth.

However, spectral PIC is (still) much slower:

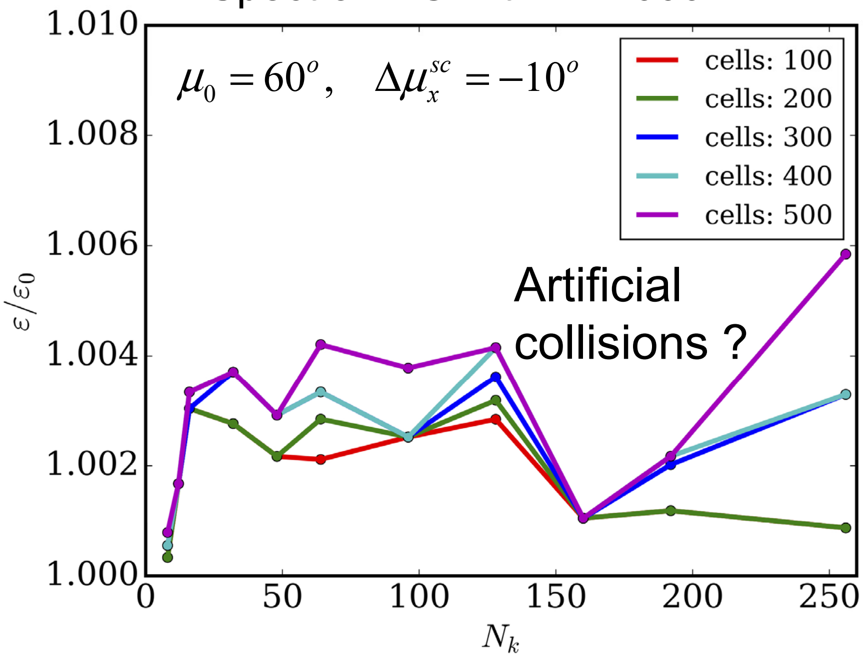
$$T \propto \alpha \cdot M \cdot \text{cells} \qquad \frac{\alpha_{spectral}}{\alpha_{grid}} \approx 20-50$$

Remark: For a python/numpy/cython implementation and on a Mac Pro. Process running on one core.

Spectral PIC: More results for FODO channel

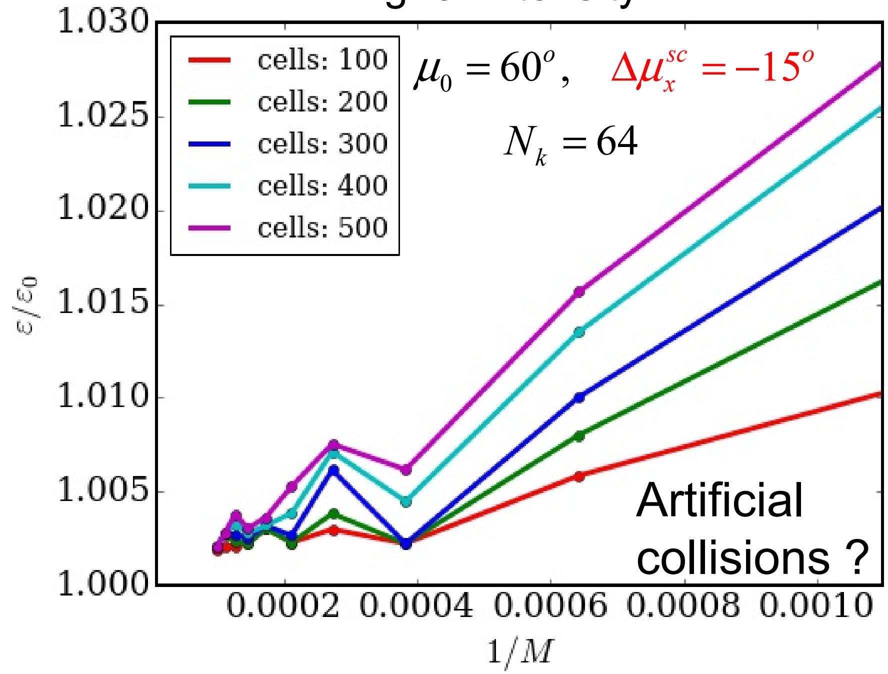
Numerical emittance growth in a FODO channel after 100-500 cells.

Spectral PIC with M=1000.



(Spectral resolution)

Higher intensity.



1 / macro-particle number

Because ‘symplectic’ PIC solves a macro-particle model, collisions should be present and the emittance should growth in AG focusing according to (still to be shown) :

$$D = \nu \frac{k_B T}{m} \Rightarrow \quad \frac{1}{\varepsilon}\frac{d\varepsilon}{dt} = \frac{1}{2} k_B \nu \frac{(T_x - T_y)^2}{T_x T_y}$$

Conclusions and Outlook

Numerical emittance growth is a concern for long-term PIC particle tracking simulations with space charge in synchrotrons.

Two sources of numerical emittance growth:

1) Artificial collisions (or 'numerical IBS'): Emittance growth in AG focusing

2) Stochastic or grid heating ('inelastic collisions') -> dominant in conventional PIC

Collision rate: $\nu \propto \frac{N^2}{M}$ $D > \nu \frac{k_B T}{m}$ (diffusion, not balanced by friction -> heating)

Counter measures to decrease the growth rate: Larger M, particle shapes, filters, ….

'Symplectic' PIC:

+ Still collisional (we don't solve the Vlasov-Poisson equations) !

+ Noise/collisions do not cause emittance growth -> Bounded emittance $D \approx \nu \frac{k_B T}{m}$

- Usually slower than conventional PIC.

To do:

-> optimized implementations, e.g. using a properly chosen S(x) one a grid.

-> check other benchmarks: Resonances, Landau damping and echoes,…..

-> compare with other approaches, like symplectic Vlasov-Poisson solvers