Calculations for Non-Uniform Cathode Distributions

Martin Dohlus, 23. Jan. 2017

see also: September 2016
http://www.desy.de/xfel-beam/s2e/talks/2016_09_12/GUN.pdf
http://www.desy.de/xfel-beam/s2e/talks/2016_09_12/gun.avi

there is nothing new:
it is just the conventional tracking with Poisson "space charge" fields;
it is implemented in 3D while Astra is "rz" at cathode;
problems with the ode-solver: time dependent mesh and birth/death of particles
my dirty solutions for that

- Poisson solver for free space (fields without "history")
- tracking of particles without birth and death
- EM fields and Lorentz force with mirror charges
- mirror charges in rest frame
- birth: my simple injection model
- tracking with birth
- example

Poisson solver for free space (fields without "history")

Lorentz transformation
particle mesh method:
particles $\{q_\nu, \mathbf{r}_\nu\}$ are binned to cells of an equidistant mesh

$\rightarrow q_{ijk}$ = charge in cell i,j,k

$G(\mathbf{r})$ = potential of a mesh cell with charge = 1 C
(analytic formula)

$g_{ijk} = G(\mathbf{r}_{ijk})$ discrete Green's function

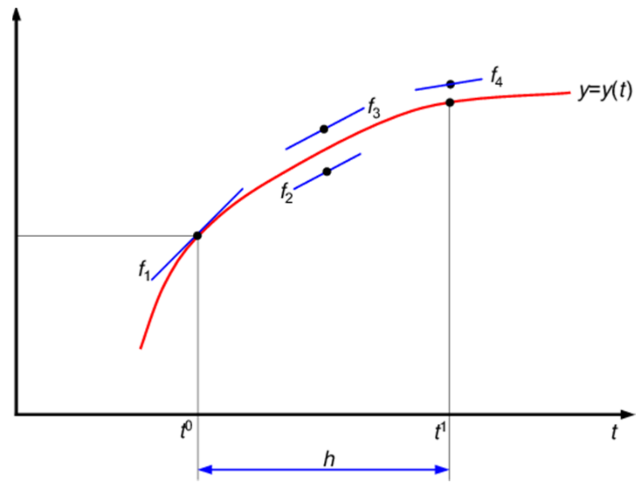
$v_{ijk} = q_{ijk} \otimes g_{ijk}$ potential at cell centers
(fast convolution)

$\rightarrow E_{xyz,ijk}$ E-field on staggered grid

inverse Lorentz transformation
interpolation to particle positions $\mathbf{E}(\mathbf{r}_\nu)$

numerical effort

tracking of particles without birth and death



this is Runge-Kutta, 4th order,
it needs 4 evaluations per step

or Dormand-Prince of 5th order needs 6 evaluations

or other methods …

a single evaluation: $\frac{d}{dt}\{\mathbf{r}_\nu,\mathbf{p}_\nu\} = f\left(t,\{\mathbf{r}_\nu,\mathbf{p}_\nu\}\right)$ equation of motion

$$= \{\mathbf{v}_\nu(\mathbf{p}_\nu), q_0(\mathbf{E}(\mathbf{r}_\nu,t) + \mathbf{v}_\nu(\mathbf{p}_\nu)\times\mathbf{B}(\mathbf{r}_\nu,t))\}$$

$$\mathbf{E},\mathbf{B} = \mathbf{E}^{(\mathrm{external})},\mathbf{B}^{(\mathrm{external})} + \underbrace{\mathbf{E}^{(\mathrm{self})},\mathbf{B}^{(\mathrm{self})}}$$

needs one Poisson computation per step

but this is not the only problem!

not the only problem:

the mth order accuracy is reached if the right hand side $f(t,\{\cdots\})$ is sufficiently smooth

this is the case for many external fields (described by analytic functions or field maps)

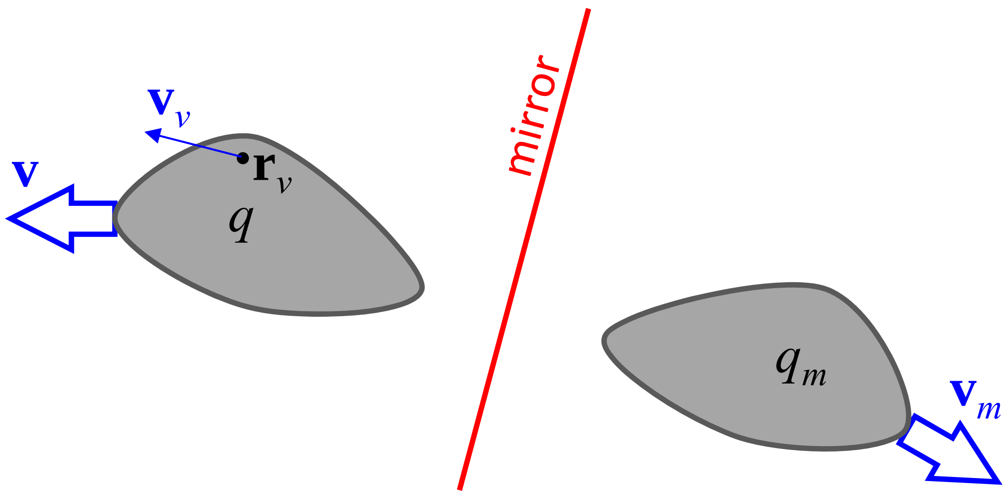
external fields (magnets, cavities) can be strong and need high accuracy

“beam dynamics” uses hard edged models; they are not smooth
$\rightarrow$ (i) use soft fields (as in nature) or (ii) special treatment of edges

particle-mesh methods calculate the self field on a mesh
self fields are usually weak or moderate and need less accuracy
not in the gun: self fields may be larger than external fields (f.i. SC limit)

but: particle distribution changes shape even in one track step; therefore the binning changes and the source term is not necessarily continuous in time; this may spoil the accuracy of higher order integrators; try everything to avoid this:
$\rightarrow$ (i) do not change mesh properties in one step; if possible: move mesh with beam; change mesh between steps to avoid systematic mesh artefacts ($\rightarrow$ μB effects)
(ii) use better methods to calculate continuous source distributions from discrete particles

EM fields and Lorentz force with mirror charges



field of q in original rest frame $\mathbf{E}_0(\mathbf{r}) \xrightarrow{LT} \mathbf{E}(\mathbf{r},t) = \mathbf{E}(\mathbf{r} - \mathbf{v}t)$

field of q_m in mirror rest frame $\tilde{\mathbf{E}}_0(\mathbf{r}) \xrightarrow{LT_m} \tilde{\mathbf{E}}(\mathbf{r},t) = \tilde{\mathbf{E}}(\mathbf{r} - \mathbf{v}_m t)$

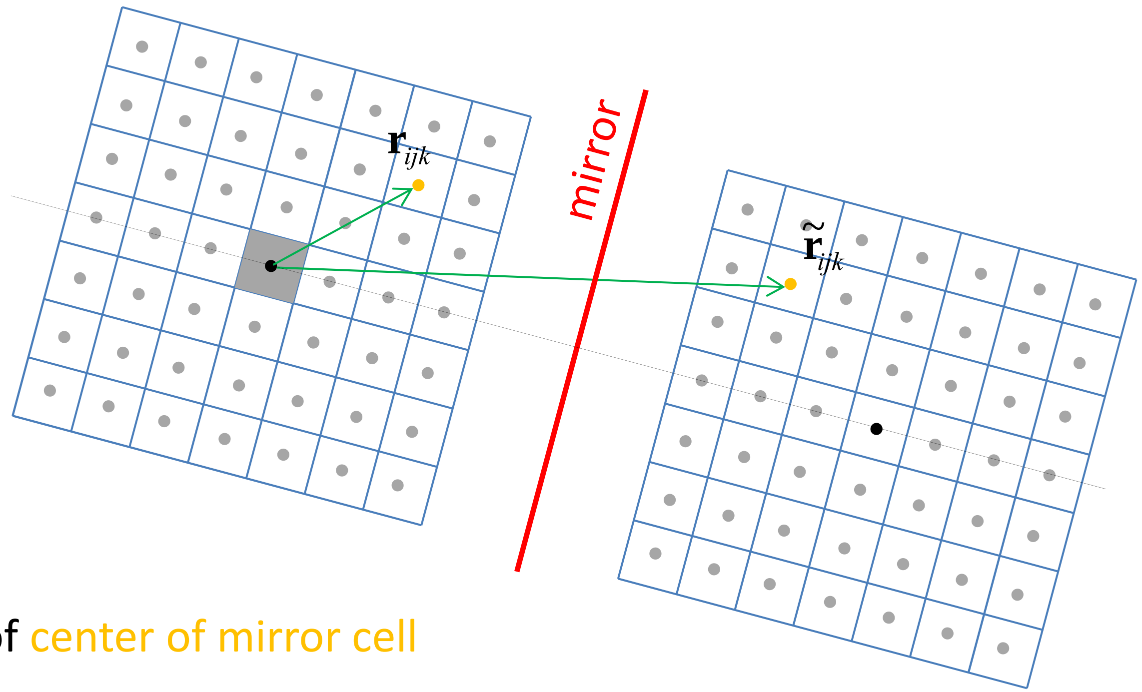
fields in lab-frame

Lorentz force $\mathbf{F}_\nu$ to particle at $\mathbf{r}_\nu$ with velocity $\mathbf{v}_\nu$

$$\mathbf{F}(\mathbf{r}_\nu,t) = q_0\left\{\mathbf{E}(\mathbf{r}_\nu,t) + \tilde{\mathbf{E}}(\mathbf{r}_\nu,t) + \mathbf{v}_\nu \times \left(\mathbf{B}(\mathbf{r}_\nu,t) + \mathbf{B}(\mathbf{r}_\nu,t)\right)\right\}$$

$$\mathbf{F}(\mathbf{r}_\nu,t) = q_0\left\{1 + \frac{\mathbf{v}_\nu \times \mathbf{v} \times}{c^2}\right\}\mathbf{E}(\mathbf{r}_\nu,t) + q_0\left\{1 + \frac{\mathbf{v}_\nu \times \mathbf{v}_m \times}{c^2}\right\}\tilde{\mathbf{E}}(\mathbf{r}_\nu,t)$$

mirror charges in rest frame



$\tilde{\mathbf{r}}_{ijk} = \mathbf{M}\{\mathbf{r}_{ijk}\}$	location of center of mirror cell
$\tilde{g}_{ijk} = G(\tilde{\mathbf{r}}_{ijk})$	potential of source cell at mirror points
$\tilde{v}_{ijk} = q_{ijk} \otimes \tilde{g}_{ij(-k)}$	potential of source distribution at mirror points
$\hat{v}_{ijk} = -q_{ijk} \otimes \tilde{g}_{ij(-k)}$	potential of mirror charges at original points
$\rightarrow \tilde{\mathbf{E}}_0(\mathbf{r}_\nu)$	contribution of mirror charges to field in rest frame

birth: my simple injection model

particle "ν" is born (injected) at time t_ν with initial conditions $\mathbf{r}_\nu^{(i)}, \mathbf{p}_\nu^{(i)}$

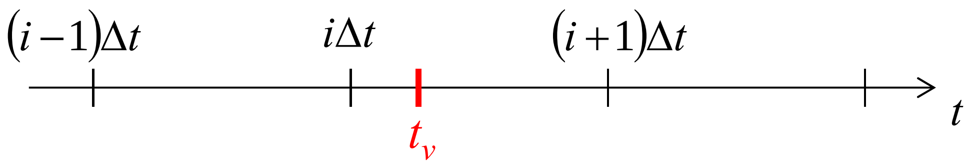
a random generator is used to generate these initial conditions $\{t_\nu, \mathbf{r}_\nu^{(i)}, \mathbf{p}_\nu^{(i)}\}$ before the simulation

be careful with Hammersly distributions !!!

in principle it is possible to generate particles "on the fly" with a probability that depends also depends on the local electric field

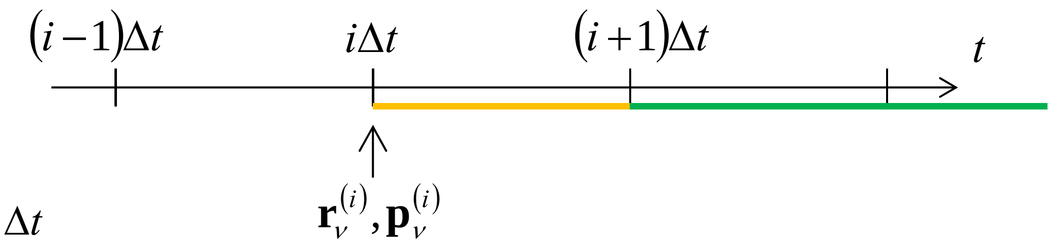
tracking with birth

particle "v" is born (injected) at time t_v with initial conditions $\mathbf{r}_v^{(i)}, \mathbf{p}_v^{(i)}$



it is not possible to choose the track steps so that the particles are injected between steps; there are too many particles to be started!

there are a couple of dirty tricks to start particles inside of an integration step; I used the following:



start at $t = i\,\Delta t$

for $t = i\Delta t \rightarrow (i+1)\Delta t$:
neglect contribution of "v" to space charge field in the injection step
modify equation of motion for this particle for this step: $\frac{d}{dt}(\mathbf{r}_v, \mathbf{p}_v) = \left(i + 1 - \frac{t_v}{\Delta t}\right) f(t, (\mathbf{r}_v, \mathbf{p}_v))$

for $t > (i+1)\Delta t$: consider "v" and track as usual

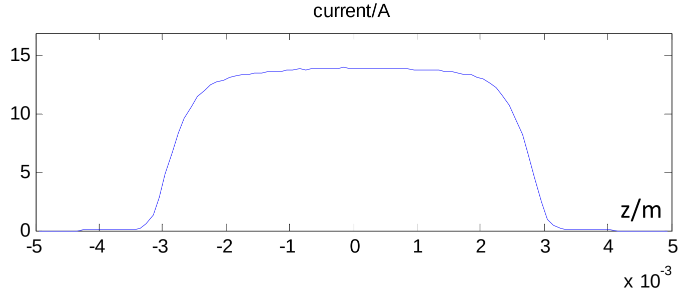
use a low order integrator with many short time steps!

example

case: XFEL from cathode to 2.6 m (after solenoid, before ACC1)

bunch (prototype): 250 pC, see http://www.desy.de/xfel-beam/s2e/xfel/Nominal/nom250pC.html

longitudinal profile (at 2.6m)

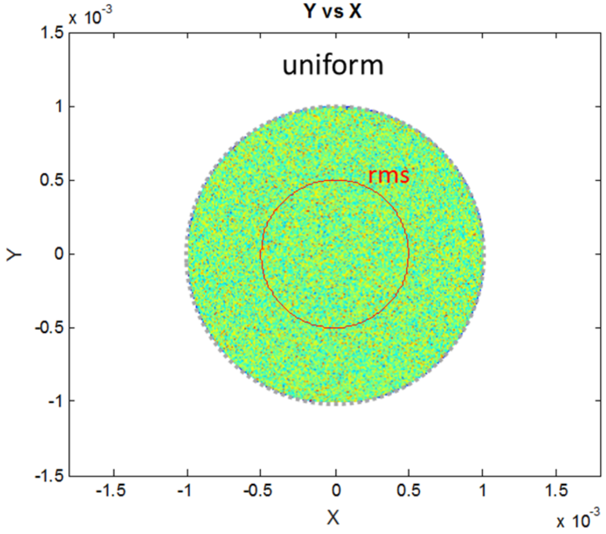


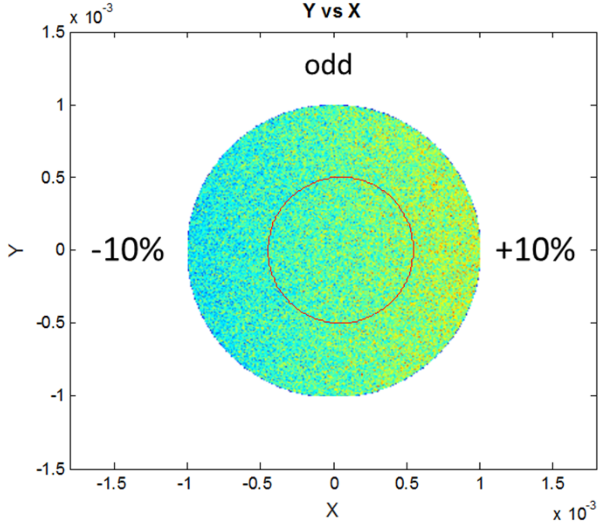
Astra generator
Lt=20psec, rt=2psec
Gun
60 MV/m, 0.2234 T

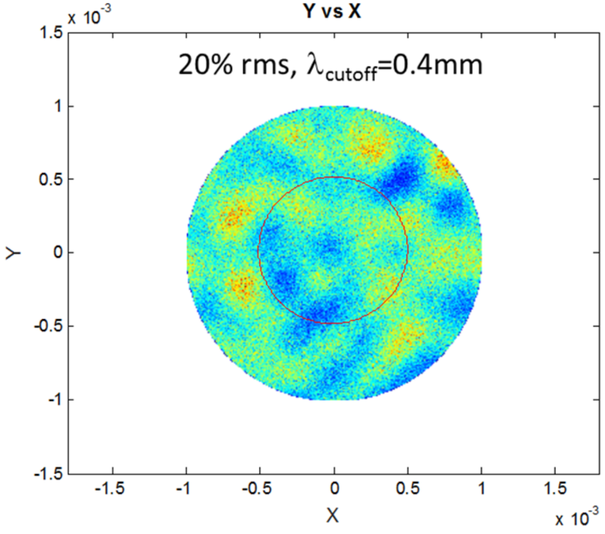
transverse distribution at cathode

uniform, R = 1 mm
(rms = 0.5 mm)

modifications







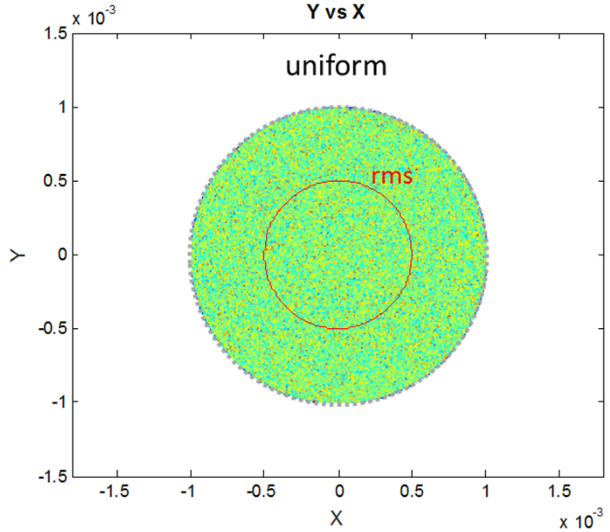
mesh properties

during injection: Δz = 1 μm $\rightarrow$ up to about 2000 meshlines
$\Delta t = T_{bunch}/500$
2^{nd} order integrator

after injection: $\Delta z = Z_{bunch}$ / 100
$c\Delta t$ = 1 mm … 1 cm
5^{th} order integrator

some longitudinal profiles

at cathode



after 2.6 m

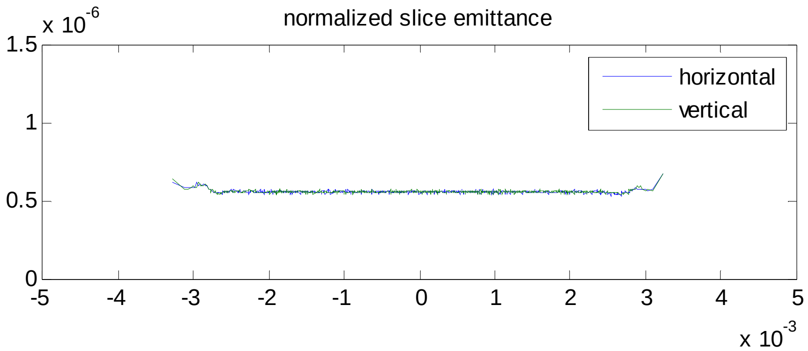
uniform

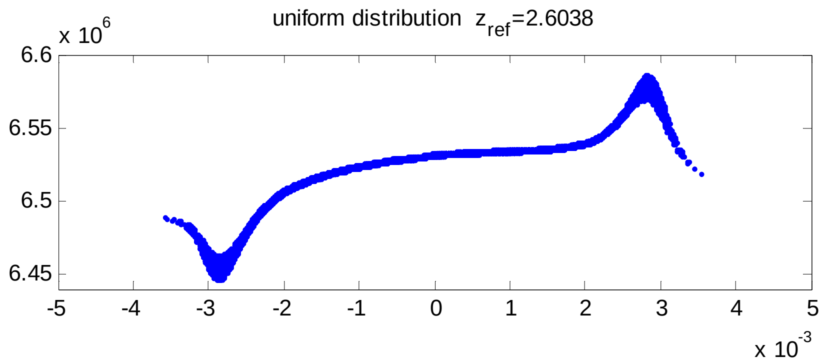
$\varepsilon\gamma\beta/\mu m$ = 0.949, 0.949 — projected

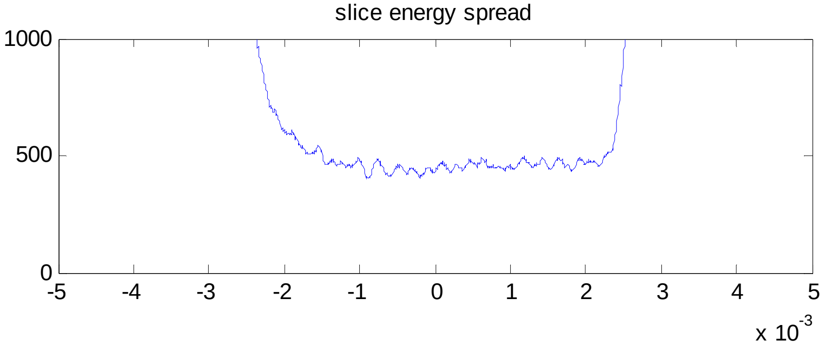
$\beta_{twiss,x,y}/m$ = 2.14, 2.14

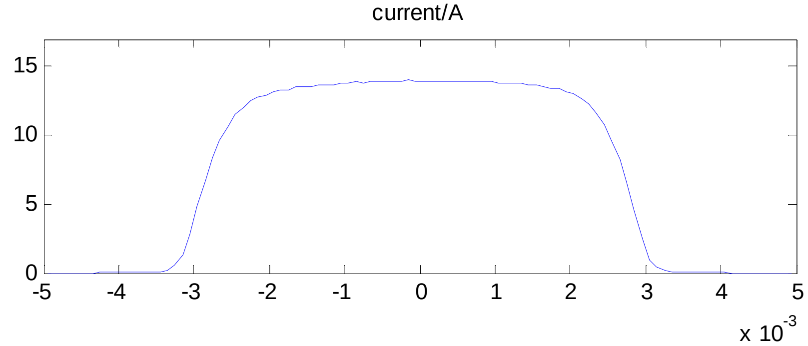
$\sigma_{E,slice}/eV$ = 443.2

} averaged for |z|<1mm

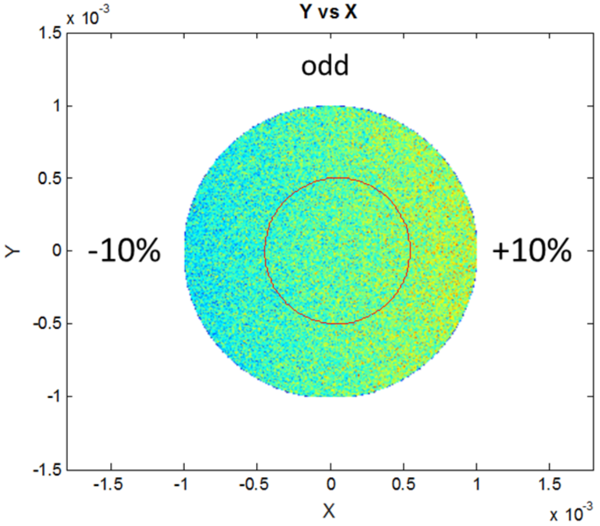








at cathode



after 2.6 m

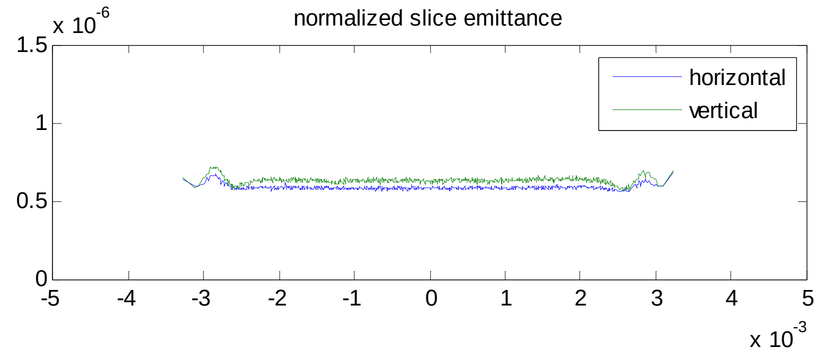
odd, 10%

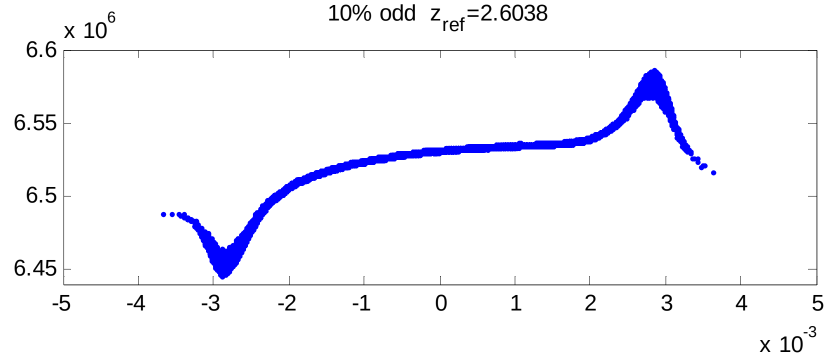
$\varepsilon\gamma\beta/\mu m$ = 0.964, 0.985 — projected

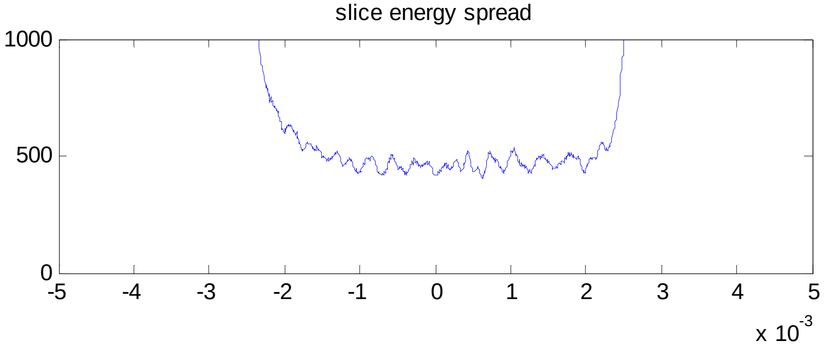
$\beta_{twiss,x,y}/m$= 2.11, 2.12

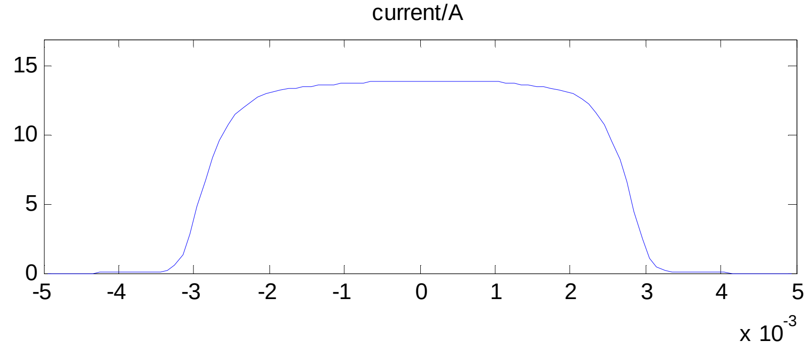
$\sigma_{E,slice}/eV$ = 463.1

} averaged for |z|<1mm

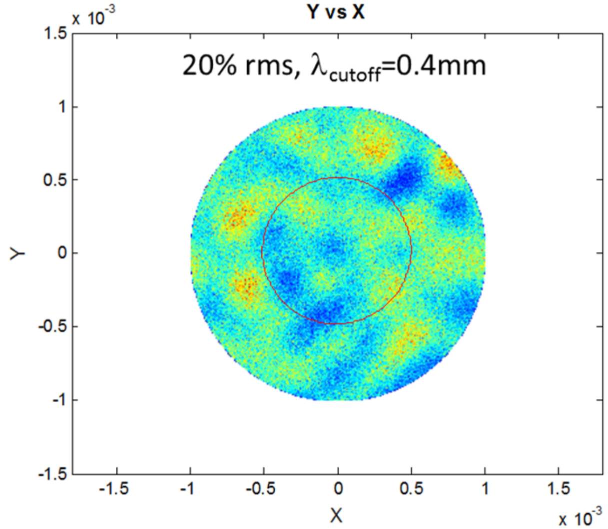








at cathode



after 2.6 m

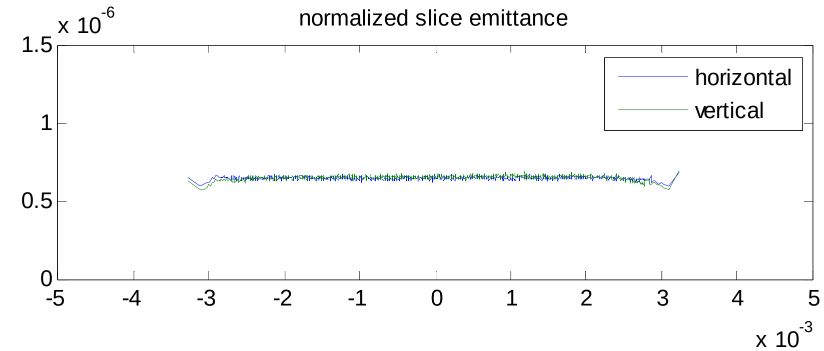
random, 20% rms, λ_{cutoff}=0.4mm

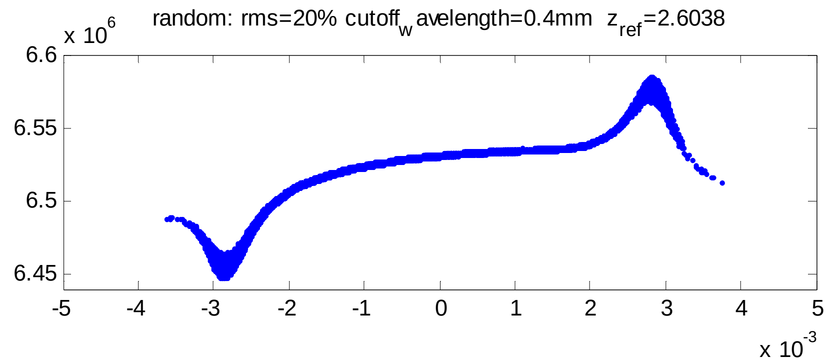
$\varepsilon\gamma\beta/\mu m$ = 1.05, 0.98 — projected

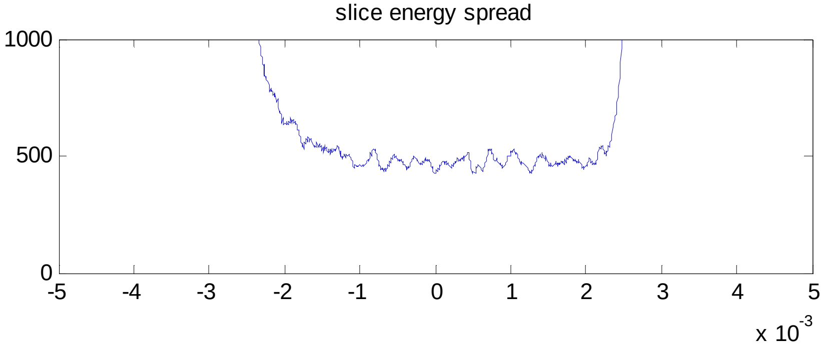
$\beta_{twiss,x,y}/m$= 2.15, 2.19

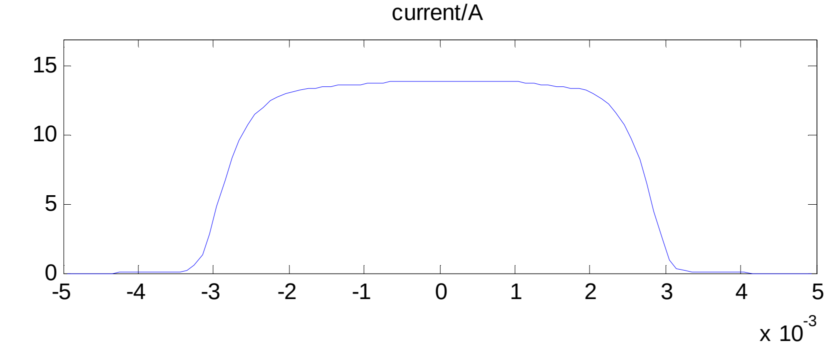
$\sigma_{E,slice}/eV$ = 478.8

} averaged for |z|<1mm







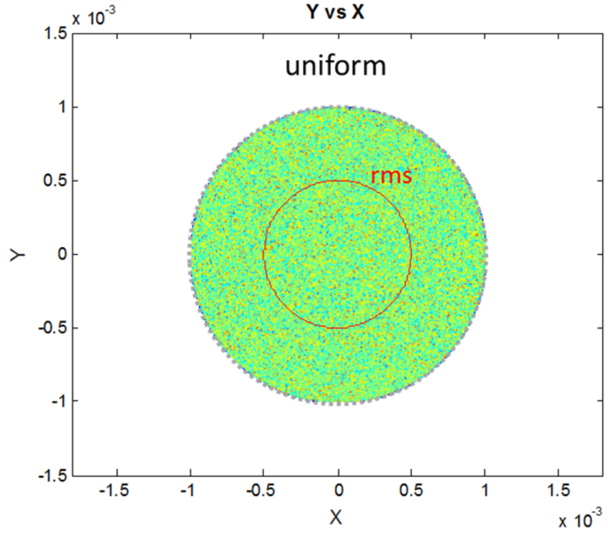


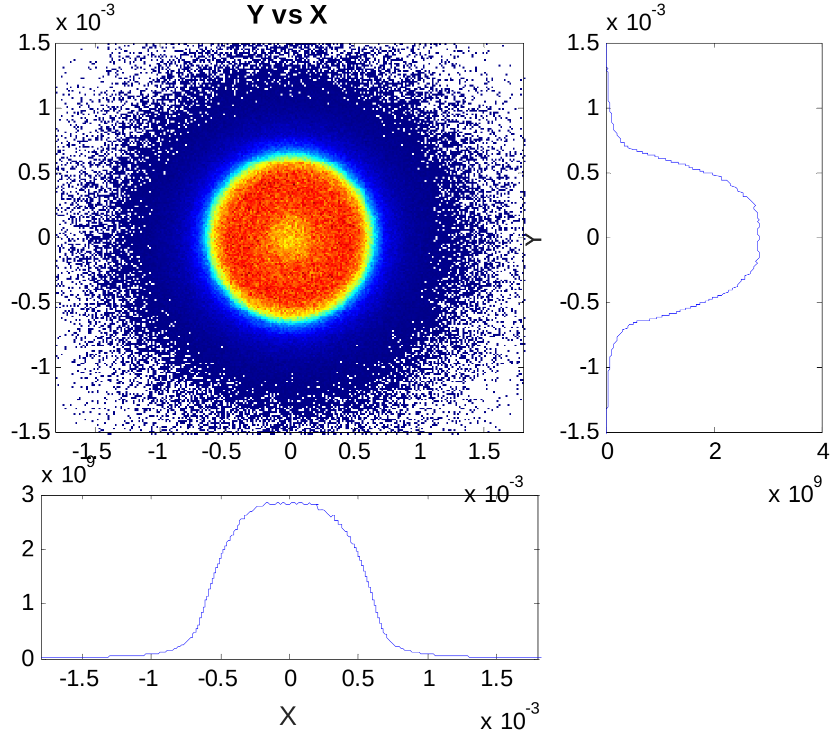
projections to

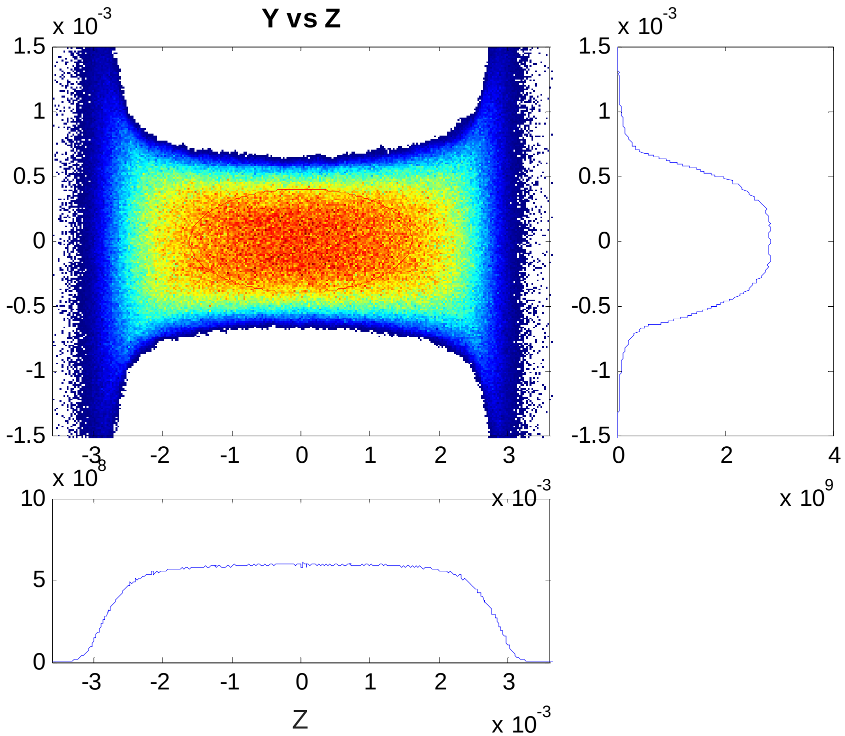
xy-plane (front view)

yz-plane (top view)

at cathode



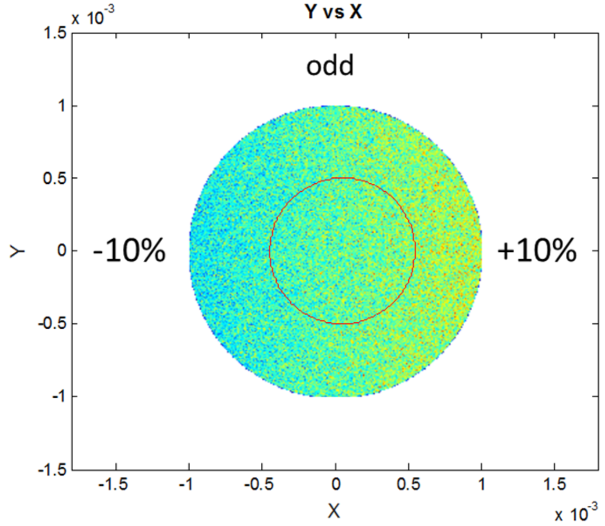


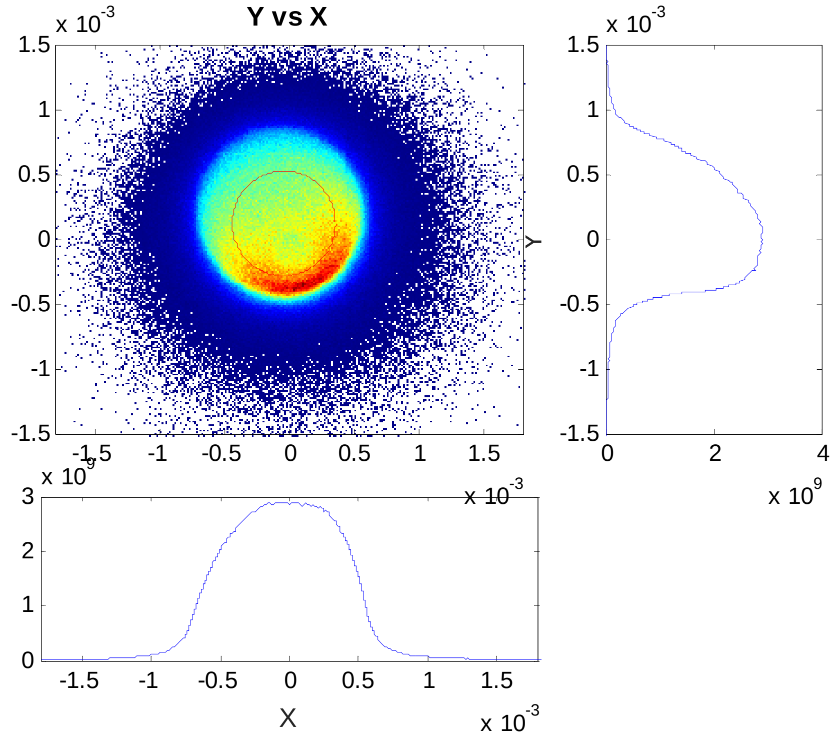


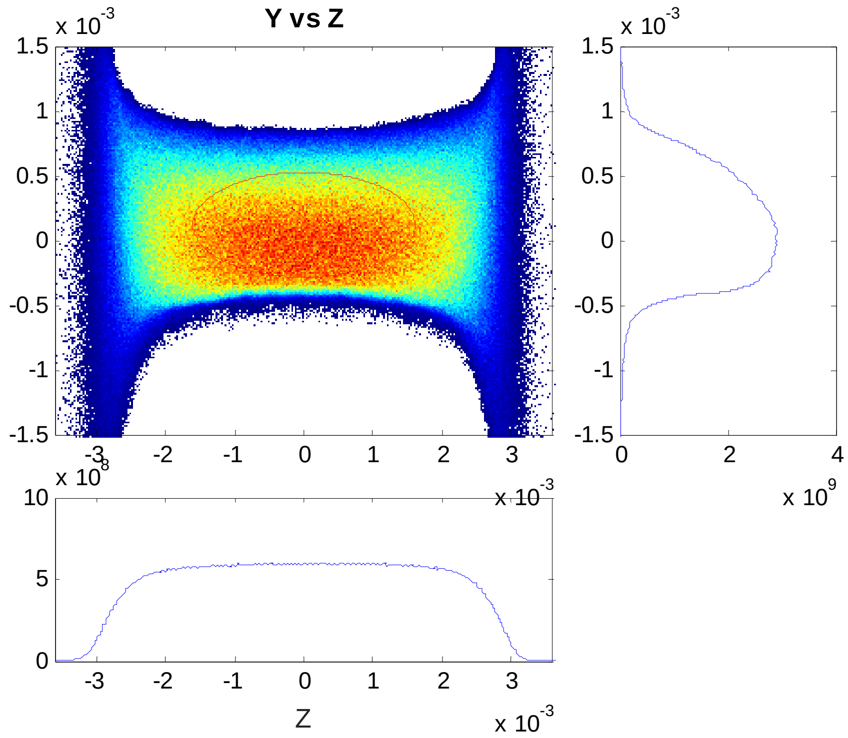
after 2.6 m

uniform

at cathode



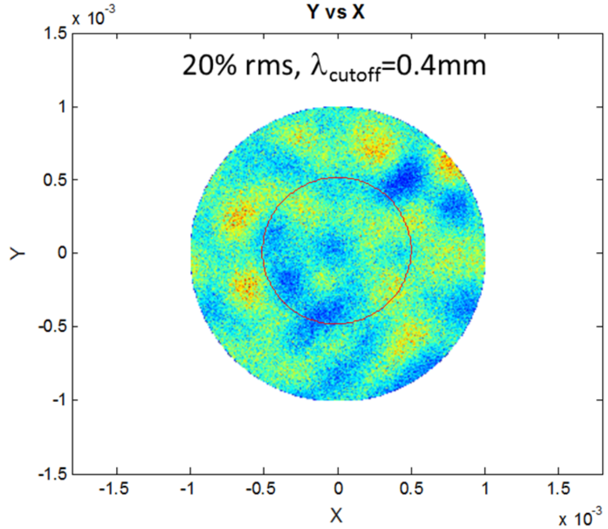


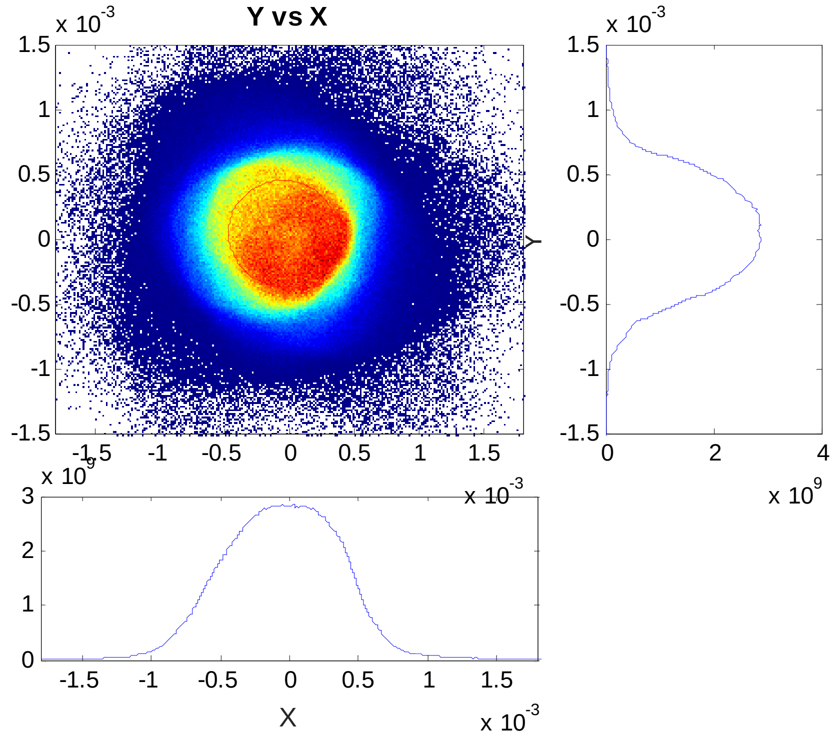


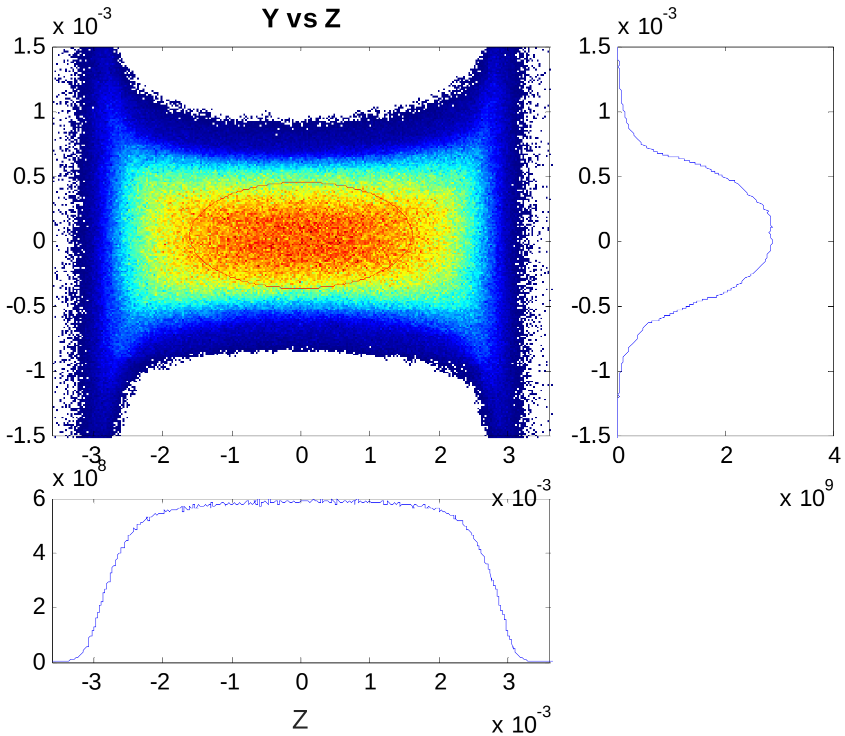
after 2.6 m

odd, 10 %

at cathode

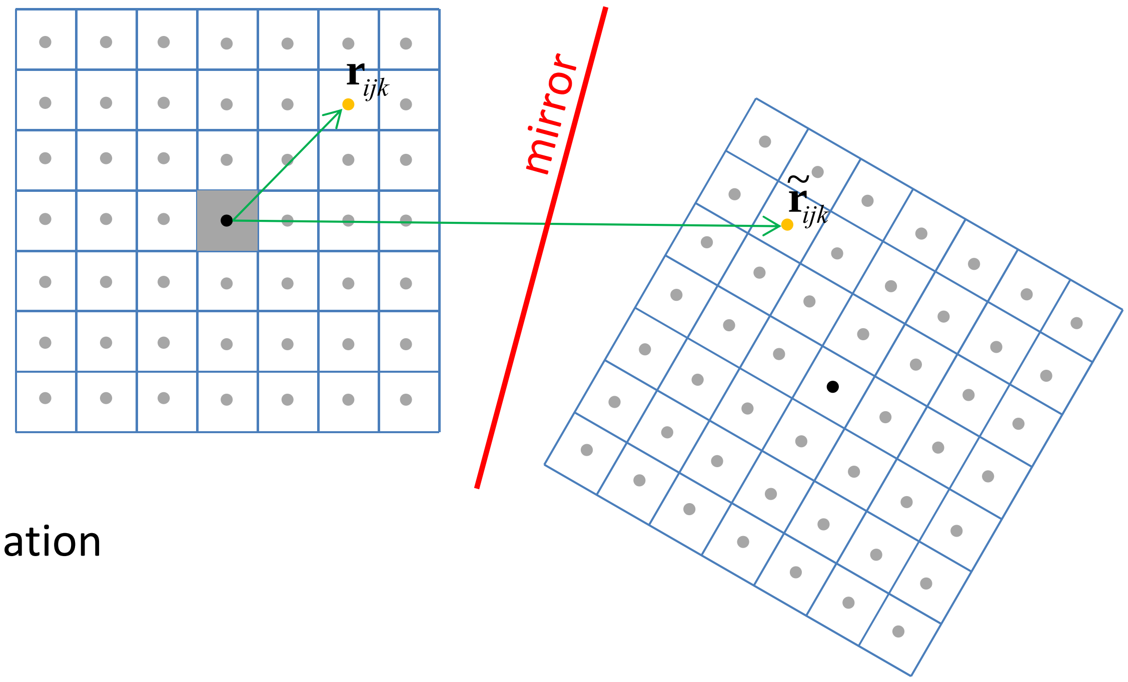






after 2.6 m

random, 20% rms, λcutoff=0.4mm



$$\tilde{\mathbf{r}}_{ijk} = \mathbf{M}\{\mathbf{r}_{ijk}\}$$ mirror transformation

$$\tilde{v}_{ijk} = \int K\left(\mathbf{M}\{\mathbf{r}_{ijk}\} - \mathbf{r}'\right)\rho(\mathbf{r}')\,dV'$$

$$= \sum_{uvw} \int_{\Delta V_{uvw}} K\left(\mathbf{M}\{\mathbf{r}_{ijk}\} - \mathbf{r}'\right)\frac{q_{uvw}}{\Delta V}\,dV'$$

$$= \sum_{uvw} q_{uvw} \int_{\Delta V} K\left(\mathbf{M}\{\mathbf{r}_{ijk}\} - \mathbf{r}' - \mathbf{r}_{uvw}\right)\frac{dV'}{\Delta V}$$

$$= \sum_{uvw} q_{uvw} G\left(\mathbf{M}\{\mathbf{r}_{ijk}\} - \mathbf{r}_{uvw}\right)$$

with $K(\mathbf{r}) = \dfrac{1}{4\pi\varepsilon_0 r}$

special case: $\mathbf{M}\{\mathbf{r}_{ijk}\} - \mathbf{r}_{uvw} = \Delta\begin{pmatrix} i-u \\ j-v \\ \alpha-k-w \end{pmatrix}$

$$G\left(\mathbf{M}\{\mathbf{r}_{ijk}\} - \mathbf{r}_{uvw}\right) = g_{(i-u)(j-v)(-k-w)}$$

$\rightarrow$ convolution