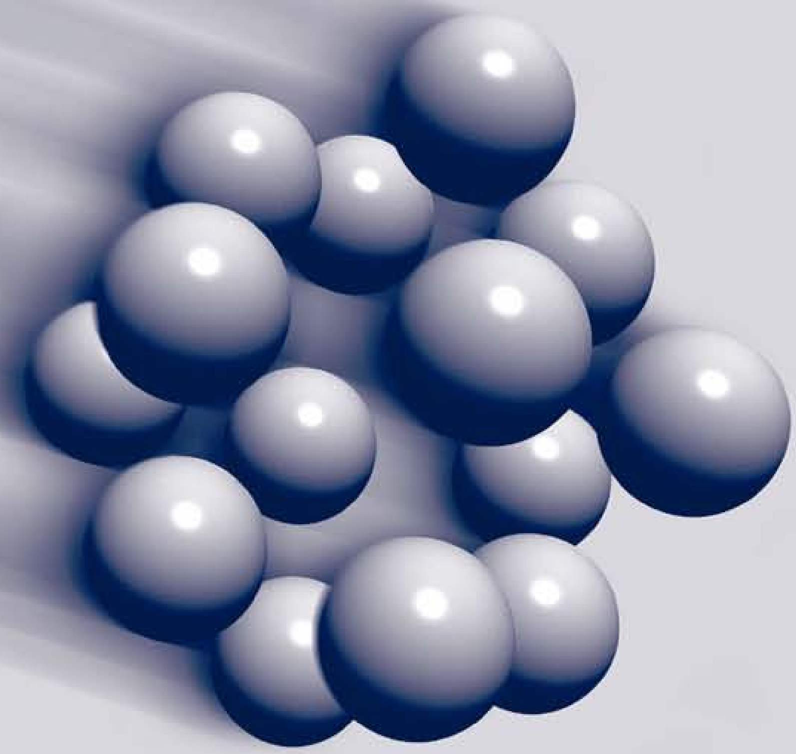
Simulation challenges for laser-cooled electron sources

Simulation challenges for laser-cooled electron sources



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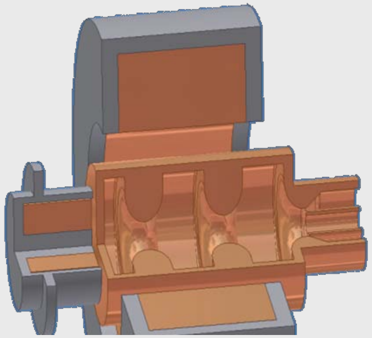
Eindhoven University of Technology
The Netherlands

There are two kinds of simulation codes:

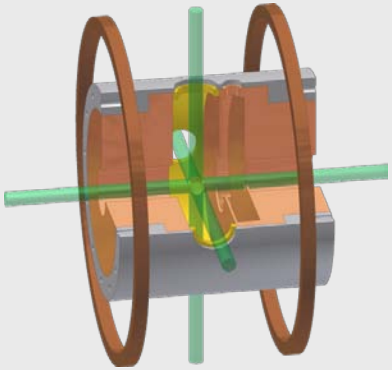
- Codes that everyone always complains about
- Codes that nobody ever uses

Brighter sources, better simulations



Photogun: for example DESY / LCLS:

- Initial emittance ~ 1 μm (eV energy spread)
- Emittance ~ preserved in entire device
- Required simulation accuracy: <1 μm



Laser-cooled sources:

- Initial emittance: < 1 nm (meV energy spread)
- Emittance?
- Desired simulation accuracy: <1 nm

Quantum degenerate sources

- …

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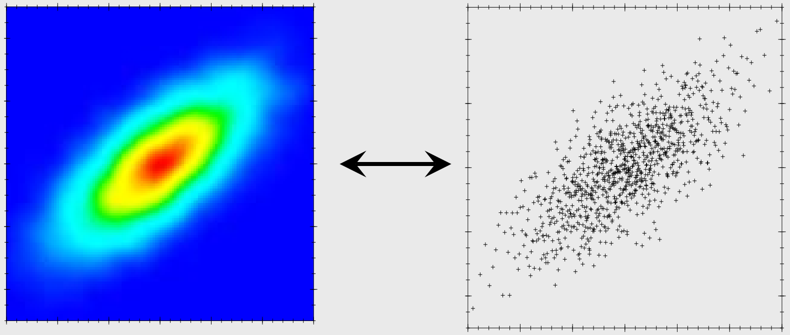
‘Typical’ simulation code: GPT

Tracks sample particles in **time-domain**

- Equations of motion

$$\frac{d\,\mathbf{p}}{dt} = q \cdot \left(\mathbf{E} + \frac{d\mathbf{r}}{dt} \times \mathbf{B} \right)$$

$$\frac{d\,\mathbf{r}}{dt} = \frac{c\,\mathbf{p}}{\sqrt{m^2 c^2 + \mathbf{p} \cdot \mathbf{p}}}$$



include all non-linear effects

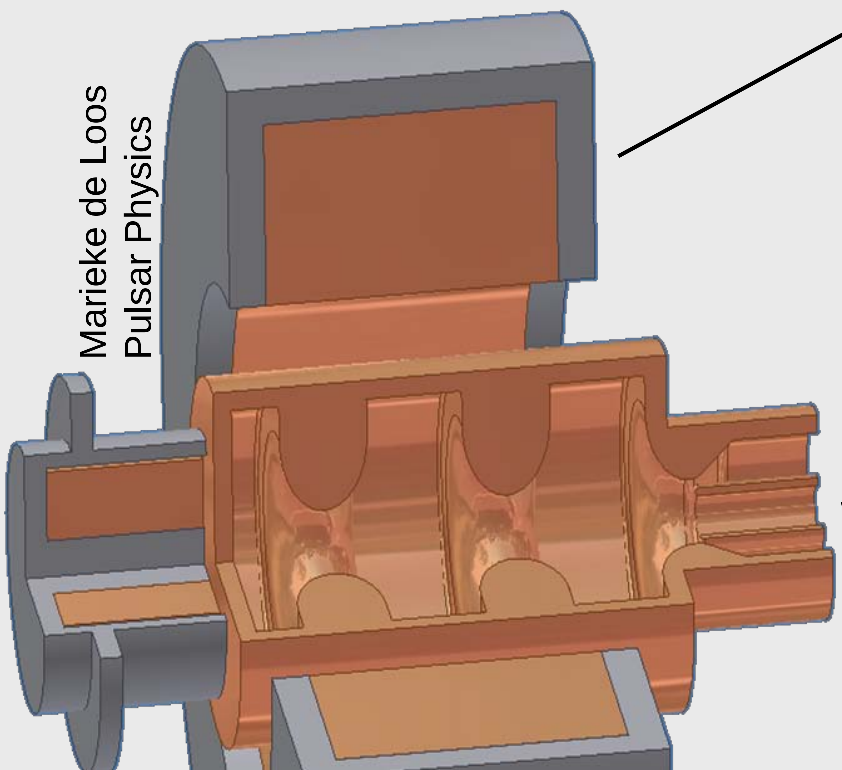
- GPT solves with 5th order embedded Runge Kutta, adaptive stepsize
- GPT can track ~10^6 particles on a PC with 1 GB memory

- Challenge: **E**(**r**,t), **B**(**r**,t), flexibility without compromising accuracy

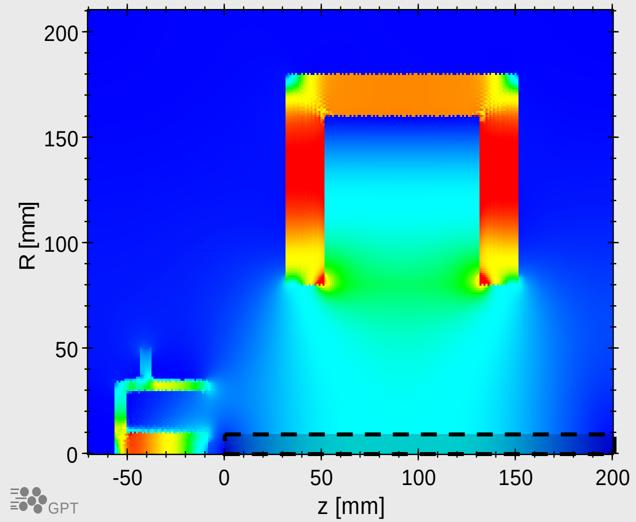
Field-maps

- 1D, 2D, 3D
- Rely on external solvers
- Fields are summed
- 3D positioning, 3D orientation

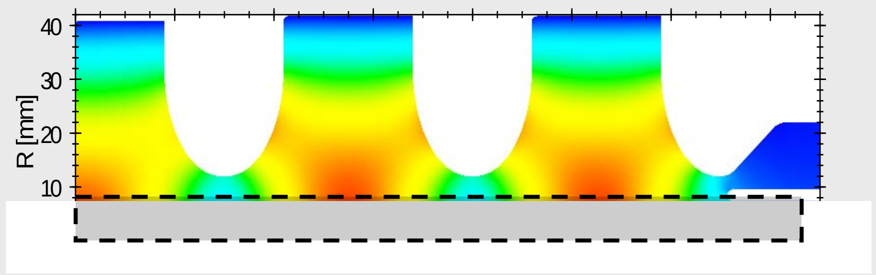
Marieke de Loos
Pulsar Physics



Magnet



Cavity



Only this part is needed for tracking

Coulomb interactions

Macroscopic:

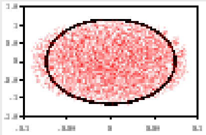
- **Space-charge**
- Average repulsion force
- Bunch expands
- Deformations in phase-space
- Governed by Poisson's equation

Microscopic:

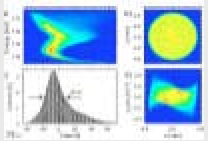
- **Disorder induced heating**
- Neighbouring particles 'see' each other
- Potential energy → momentum spread
- Stochastic effect
- Governed by point-to-point interactions

GPT simulations

PRL *93, 094802*
O.J. Luiten et. al.

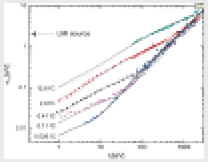


JAP 102, 093501
T. van Oudheusden et. al.

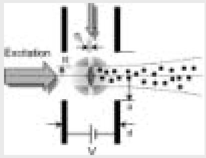


PRST-AB *9, 044203*
S.B. van der Geer et. al.

PRL *102, 034802*
M. P. Reijnders et. al.

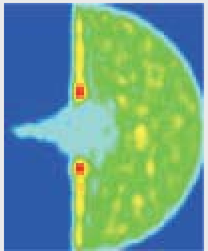


JAP *102, 094312*
S.B. van der Geer et. al.



Nature *Photonics*
Vol 2, May 2008
M. Centurion et. al.

And many others…



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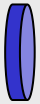
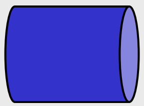
Particle-Mesh (in-Cell)



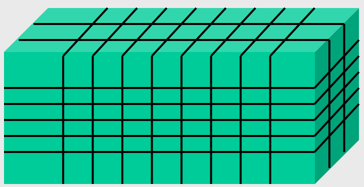
Bunch in laboratory frame

- <u>Mesh-based electrostatic solver in rest-frame</u>



Bunch in rest frame

- Bunch is tracked in laboratory frame
- Calculations in rest-frame $z' \approx \gamma z, \gamma = 1 \Big/ \sqrt{1 - v^2 / c^2}$



Meshlines

- Mesh
  - Density follows beam density
  - Trilinear interpolation to obtain charge density

ρ'

Charge density

$-\nabla^2 V' = \rho' / \varepsilon_0$

Poisson equation

- Solve Poisson equation

$\mathbf{E}' = -\nabla V' \quad \mathbf{B}' = 0$

Interpolation

- 2nd order interpolation for the electrostatic field **E**'

$\{\mathbf{E}, \mathbf{B}\} = \mathcal{L}(\mathbf{E}')$

Lorentz transformation to laboratory frame

- Transform **E**' to **E** and **B** in laboratory frame

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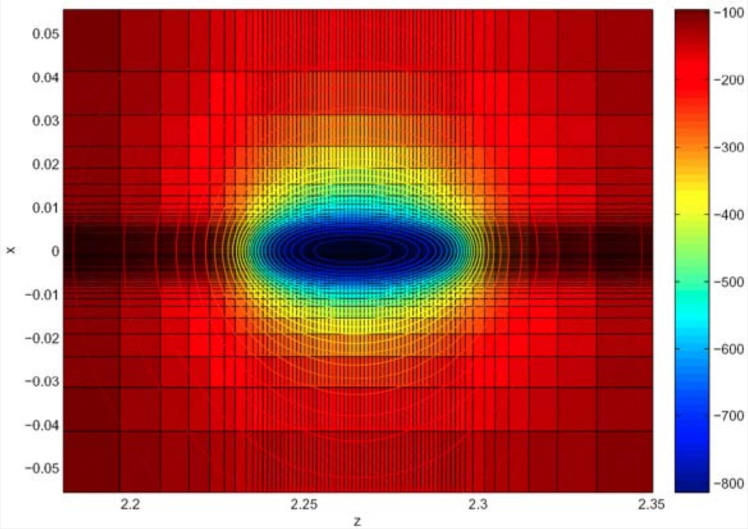
Multi-grid Poisson solver

- Key feature:
  - Anisotropic meshing to reduce number of empty nodes

- Main challenge
  - Stability

- Multi-grid solver
  - Developed by Dr. G. Pöplau Rostock University, Germany
  - Scales ~O(N^1) in CPU time
  - Select stability vs. speed

DESY TTF gun at z=0.25 m, 200k particles.



Gisela Pöplau, Ursula van Rienen, **Bas van der Geer**, and Marieke de Loos, *Multigrid algorithms for the fast calculation of space-charge effects in accelerator design*, IEEE Transactions on magnetics, Vol **40**, No. 2, (2004), p. 714.

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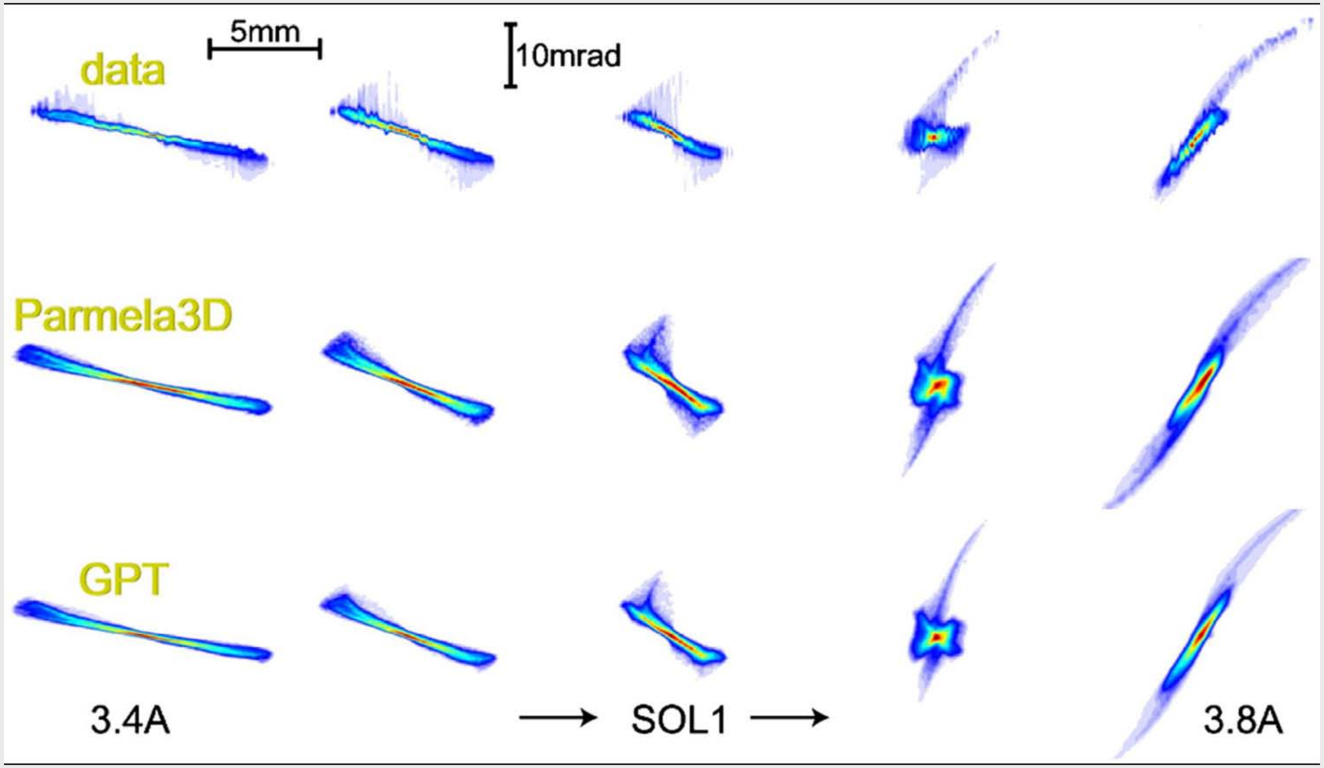
3D Space-charge simulations

Simulations codes seem to be up-to-the-job:

- GPT http://www.pulsar.nl/gpt
- Parmela3D LANL



Benchmarking of 3D space charge codes using direct phase space measurements from photoemission high voltage dc gun

Ivan V. Bazarov, et.al. PRST-AB 11, 100703 (2008).

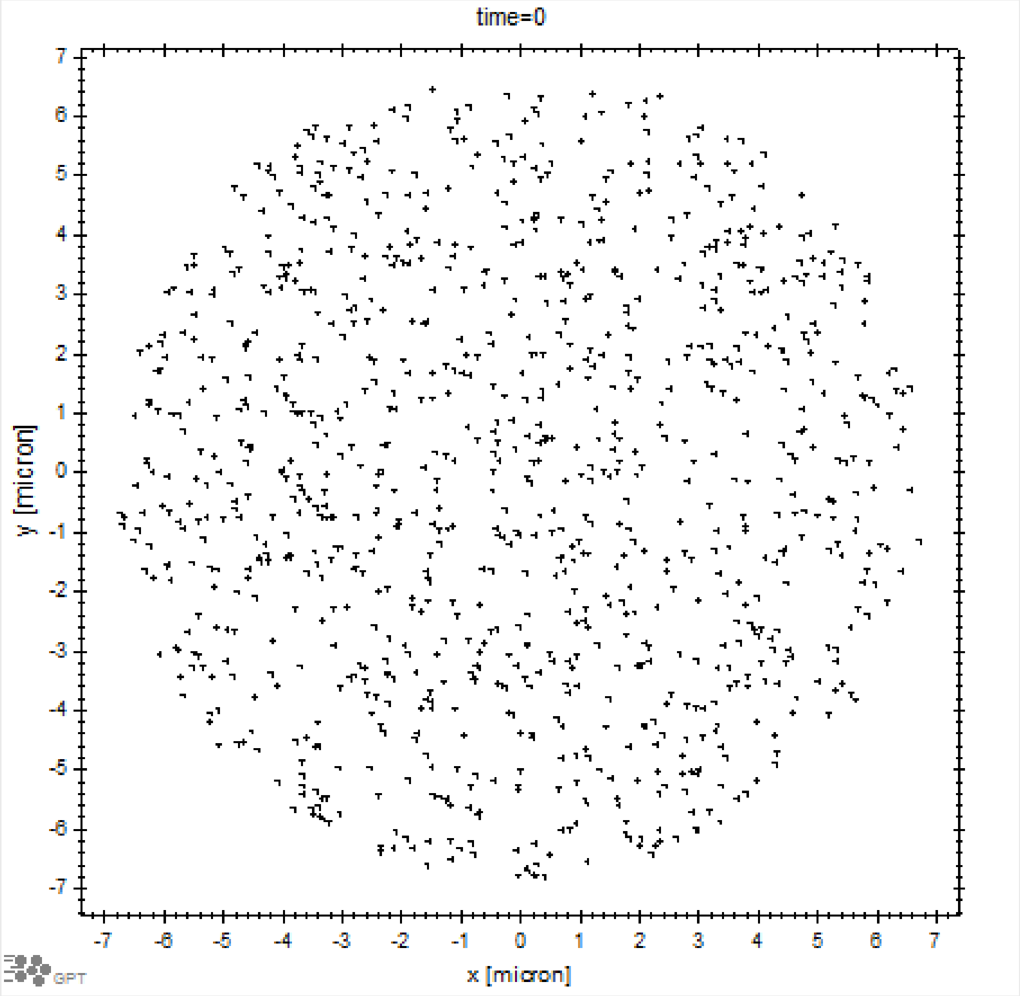
www.pulsar.nl

Laser-cooled sources

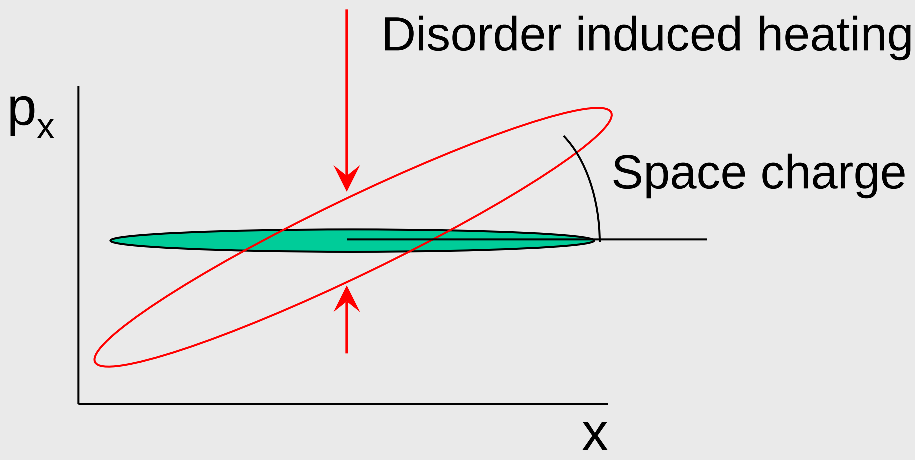
Simple test case:

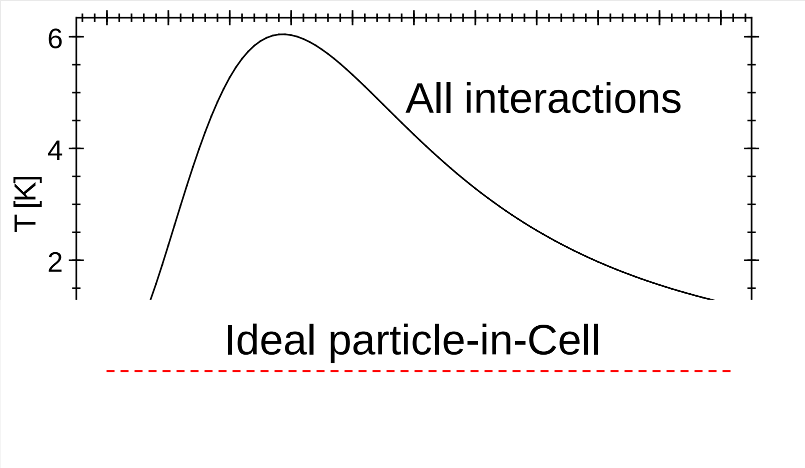
- Uniformly filled sphere
- Density $10^{18}/m^3$
- No initial temperature
- *All* pair-wise interactions

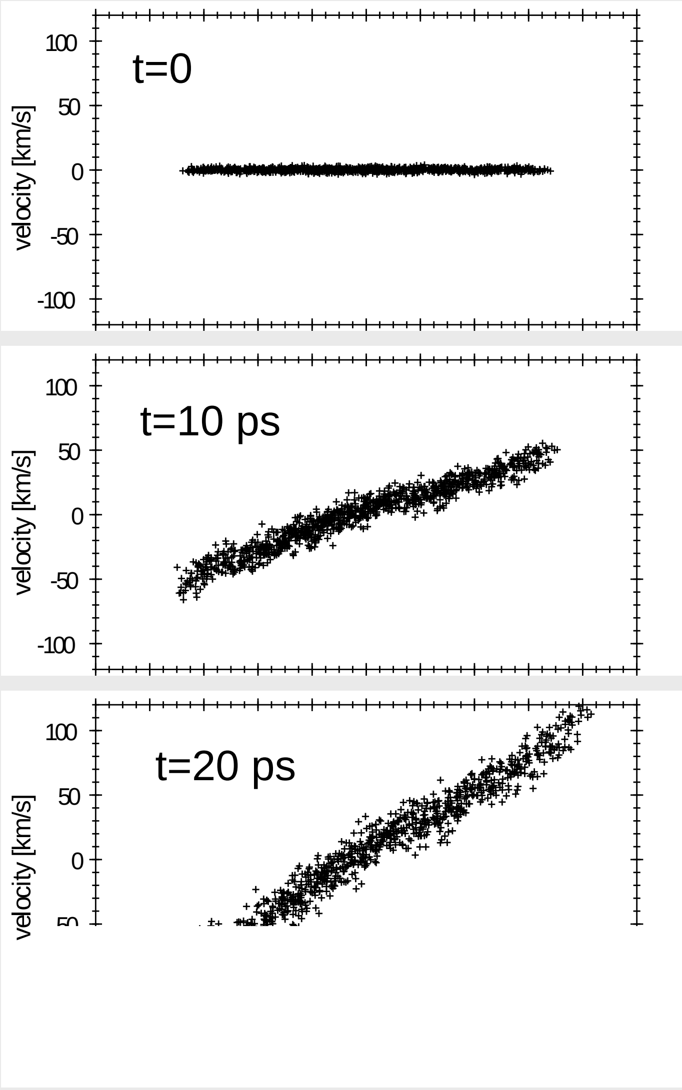
- Wait and see...



Coulomb interactions







GPT simulations: n=10^{18} m^{-3}

Disorder induced heating

Random processes

↓

Excess potential energy *U*

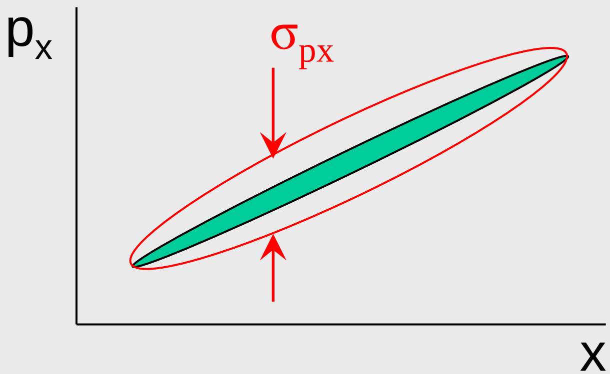
↓ Coulomb interactions

Momentum spread

↓

Temperature ↑
Brightness ↓

High *U* Low *U*



$$\left.\begin{aligned}\sigma_{p_x} &= \sqrt{m\,k\,T_x}\\ &= mc\frac{\varepsilon_x}{\sigma_x}\end{aligned}\right\}\Rightarrow T_x = \frac{mc^2}{k}\frac{\varepsilon_x^2}{\sigma_x^2}$$

$$B_\perp = \frac{J}{\pi\,k\,T}$$

Paradigm shift

RF-photoguns

Space-charge
- ‘Shaping’ the beam
- Ellipsoidal bunches

Particle-in-Cell
- Macro-particles
- One species
- Fluid assumption
- Liouville holds
- Convergent rms values

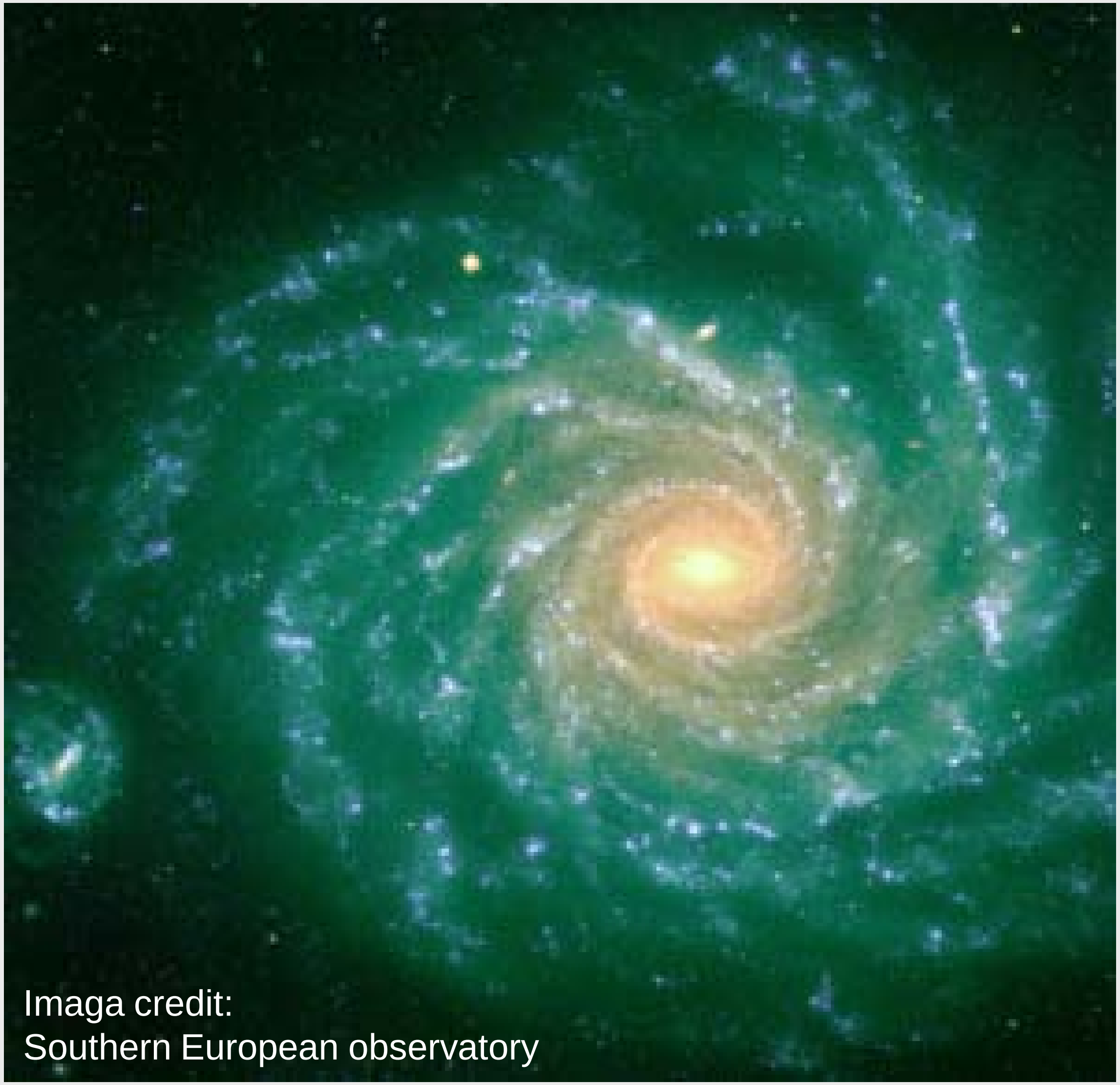
Laser cooled sources

Disorder induced heating
- Fast acceleration
- Breaking randomness

Tree-codes (B&H, FMM, P^3M)
- Every particle matters
- Ions and electrons
- Ab initio
- No Liouville to the rescue
- Divergent rms values

$$k\,T_{\text{photogun}} \gg 0.02\, n^{1/3} q^2 / \varepsilon_0 \gg k\,T_{\text{laser-cooled}}$$

Algorithms...



N^2 interactions

Tough problem

Algorithms…

Many to choose from: In theory, not in practice so it seems:

All interactions $O(N^2)$:

- PP Particle-Particle
- P^3M Particle-Particle Particle-Mesh

Accuracy traded for speed:

- B&H Barnes&hut tree: $O(N \log N)$
- FMM Fast-Multipole-Method: $O(N)$
- …

Particle-Particle

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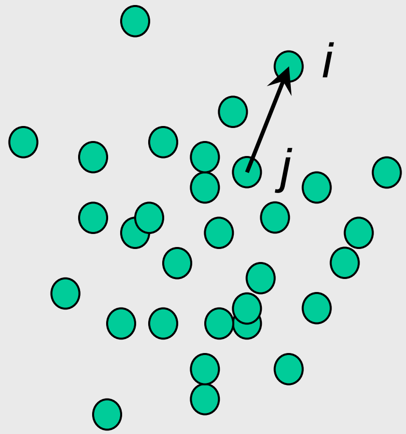
3D point-to-point:

- Uses macro-particles
- 3D
- Fully relativistic
- N^2 in CPU time



- Transform *i* to rest frame of *j*

$$\mathbf{r}_{ji} = \mathbf{r}_i - \mathbf{r}_j$$

$$\mathbf{r}'_{ji} = \mathbf{r}_{ji} + \frac{\gamma_j{}^2}{\gamma_j + 1}\left(\mathbf{r}_{ji} \cdot \boldsymbol{\beta}_j\right)\boldsymbol{\beta}_j$$

- Electrostatic field of *j*

$$\mathbf{E}'_{j\to i} = \frac{Q\mathbf{r}'_{ji}}{4\pi\varepsilon_0\left|\mathbf{r}'_{ji}\right|^3}$$

- Summation to laboratory frame

$$\mathbf{E}_i = \sum_{j\neq i}\gamma_j\left[\mathbf{E}'_{j\to i} - \frac{\gamma_j}{\gamma_j + 1}\left(\boldsymbol{\beta}_j \cdot \mathbf{E}'_{j\to i}\right)\boldsymbol{\beta}_j\right]$$

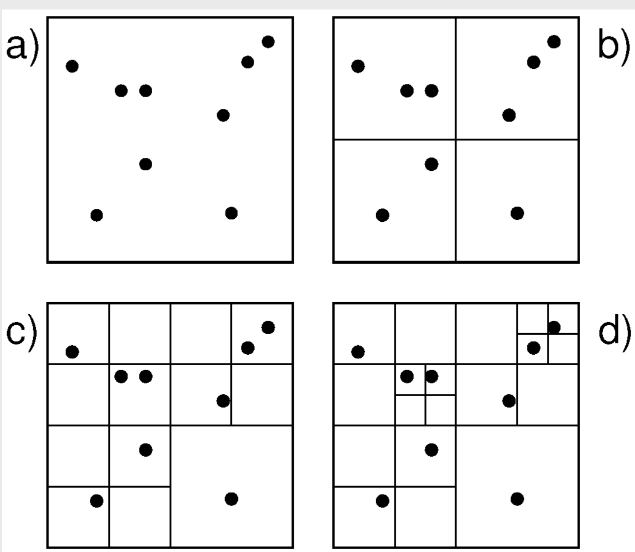
$$\mathbf{B}_i = \sum_{j\neq i}\frac{\gamma_j\boldsymbol{\beta}_j \times \mathbf{E}'_{j\to i}}{c}$$

Barnes-Hut

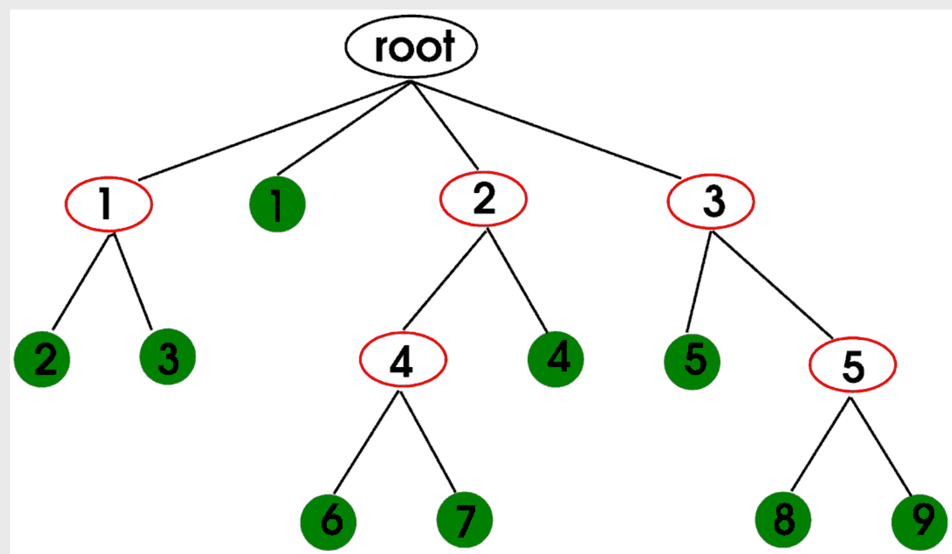
Hierarchical tree algorithm:

- Includes *all* Coulomb interactions
- O(N log N) in CPU time
- User-selectable accuracy

Division of space



Tree data structure



J. Barnes and P. Hut, Nature **324**, (1986) p. 446.

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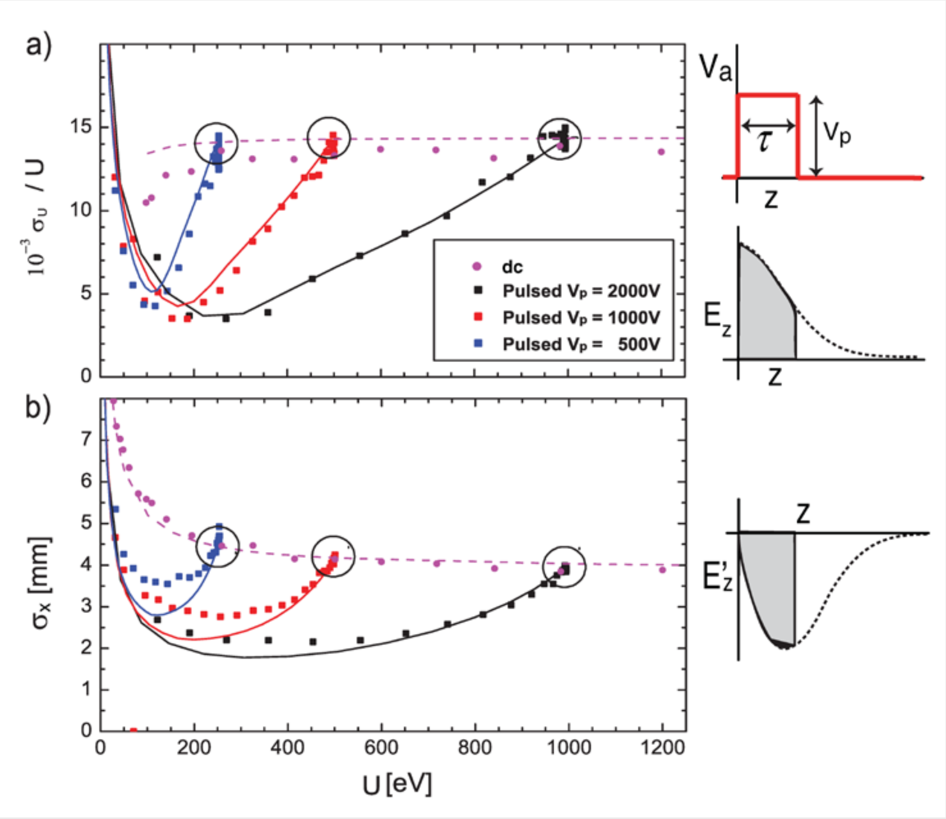
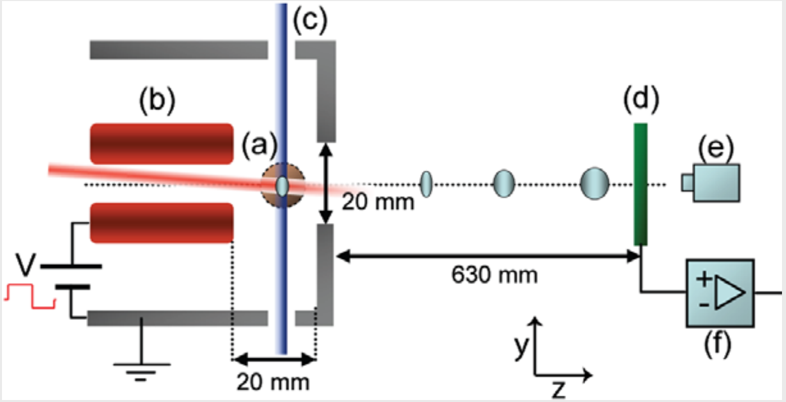
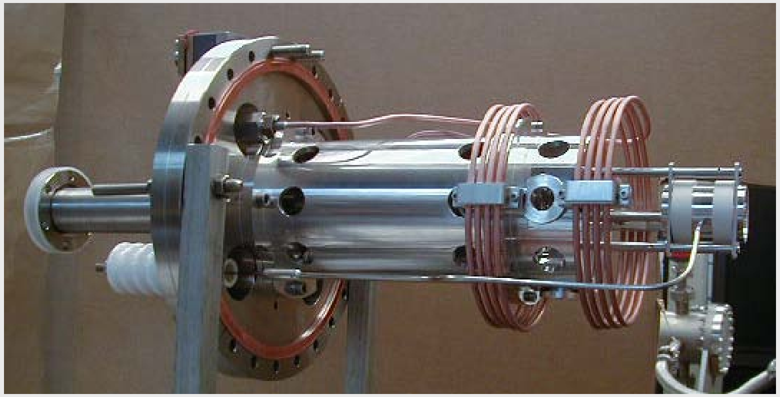
Comparison with experiments







M. P. Reijnders, N. Debernardi, S. B. van der Geer, P.H.A. Mutsaers, E. J. D. Vredenbregt, and O. J. Luiten,
Phase-Space Manipulation of Ultracold Ion Bunches with Time-Dependent Fields
PRL 105, 034802 (2010).

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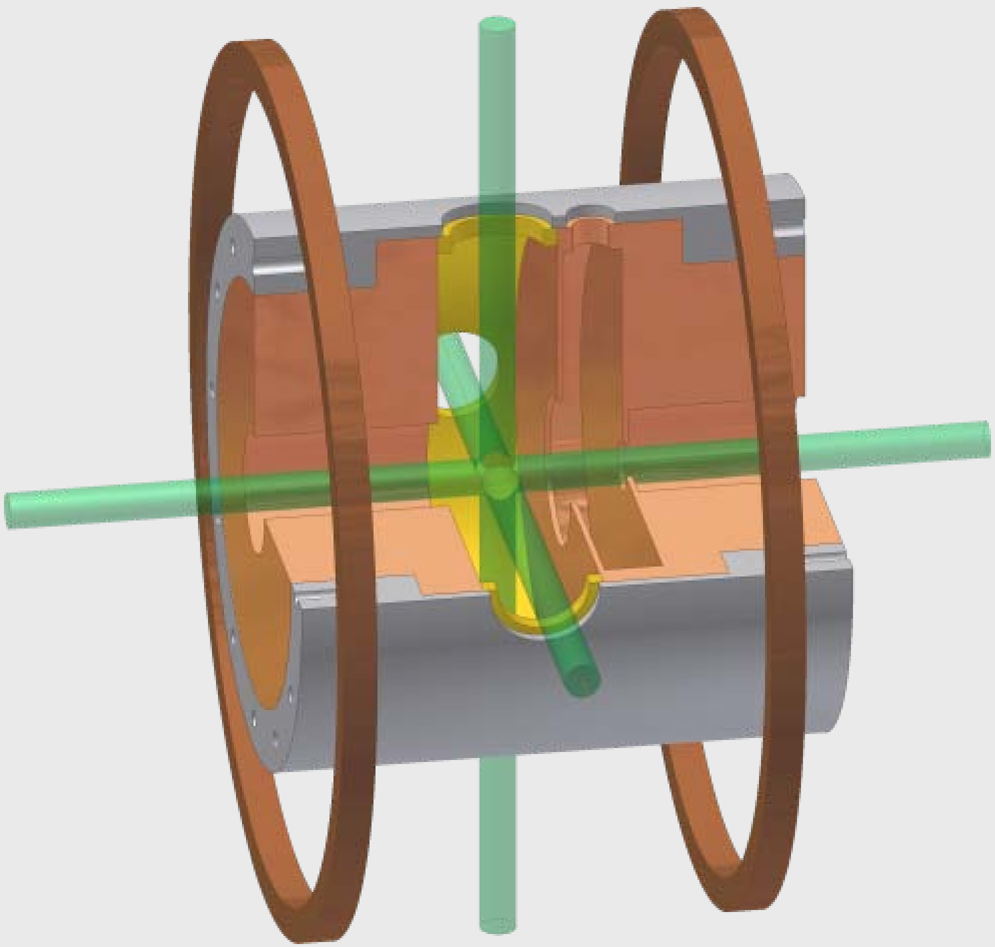
Laser-cooled e⁻ source



Fields:

Cavity field	20 MV/m rf-cavity
DC offset	3 MV/m

Particles:

Charge	0.1 pC (625k e⁻)
Initial density	10^{18} / m^3
Ionization time	10 ps
Initial Temp	1 K

GPT tracking:

All particles
Realistic fields
All interactions

Longitudinal emission dynamics

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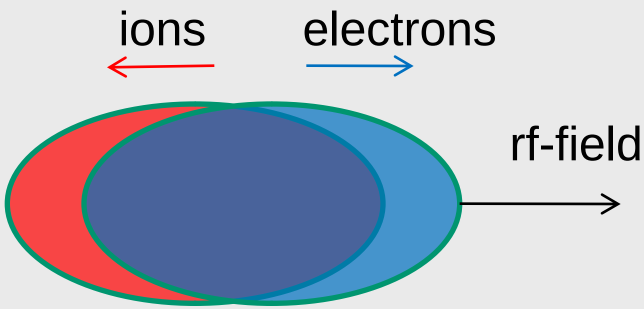
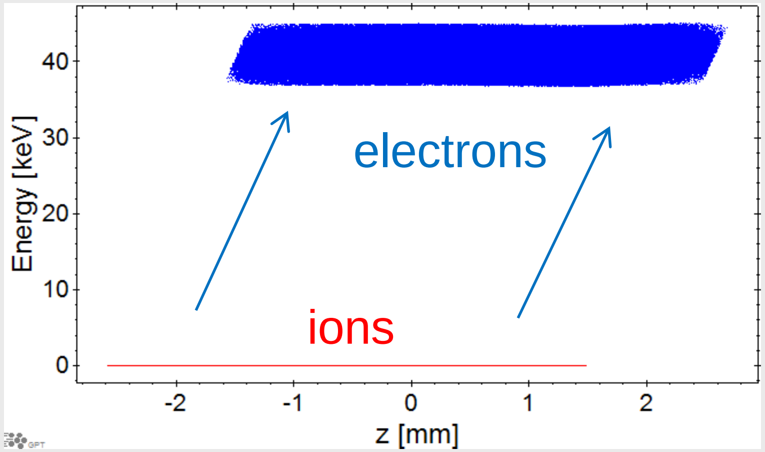
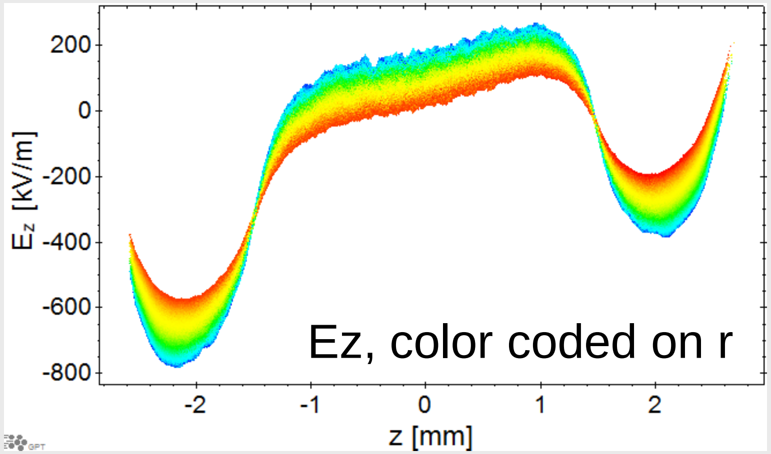
Longitudinal acceleration

- rf field
- Combined spacecharge



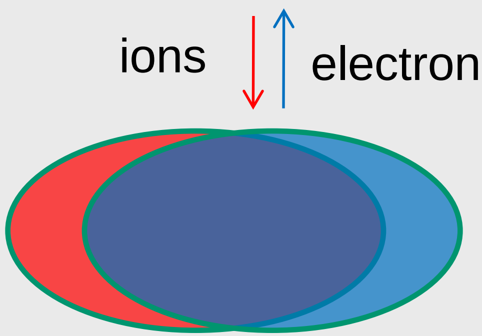


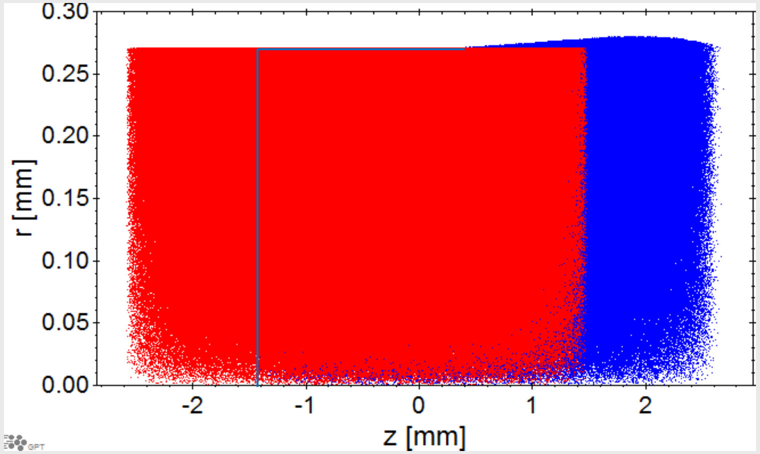


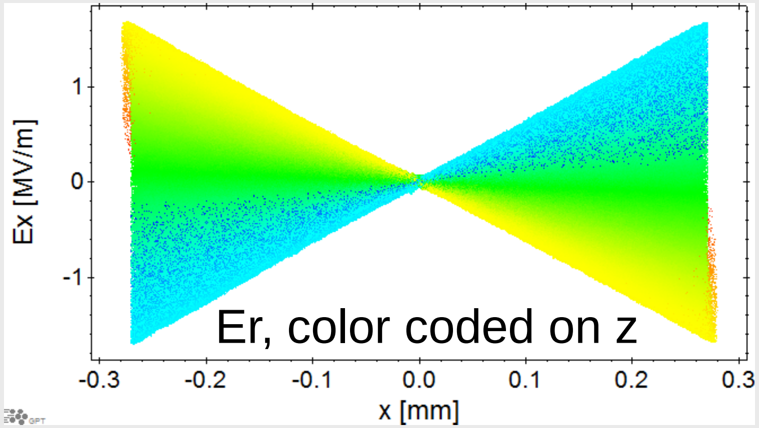
Transverse emission dynamics

Transverse acceleration

- While new ones are still being ionized
- While ions keep them together







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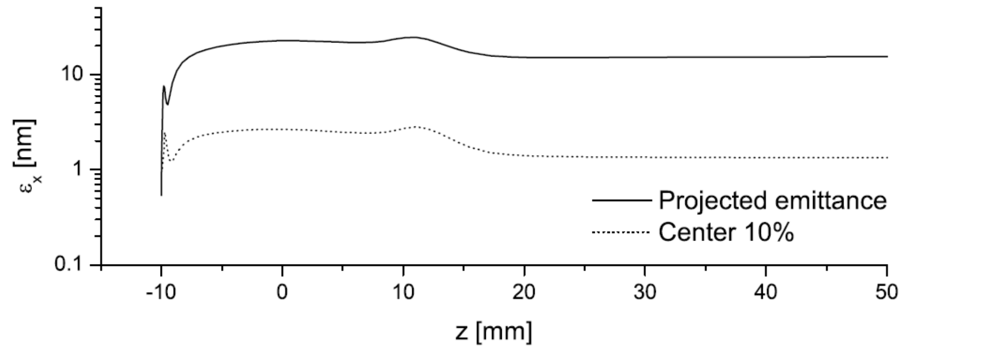
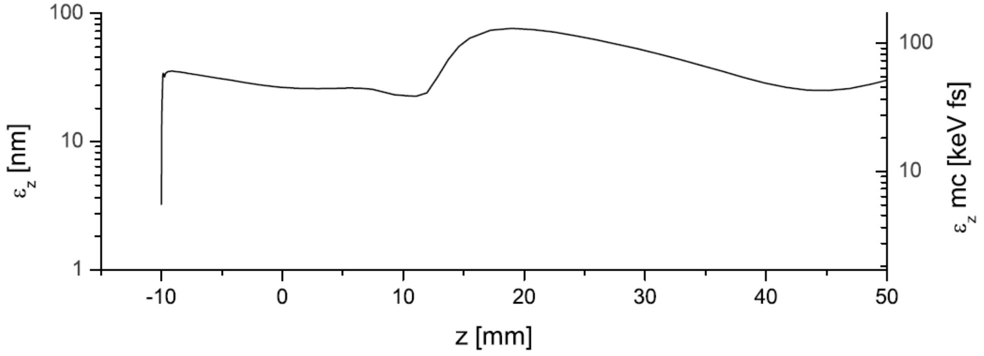
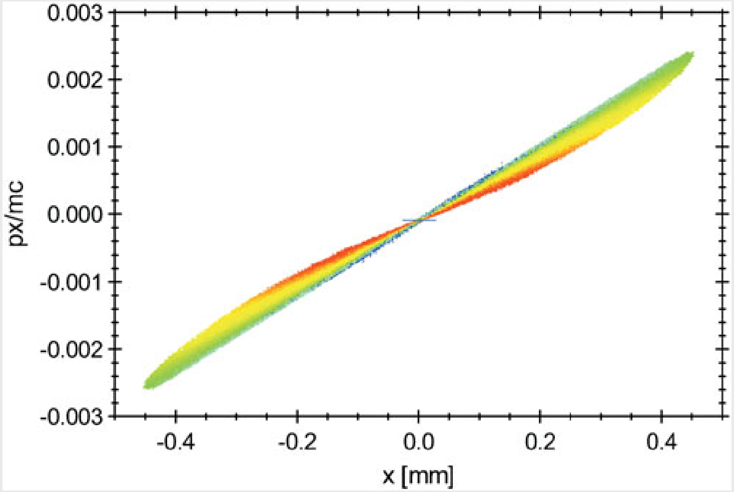
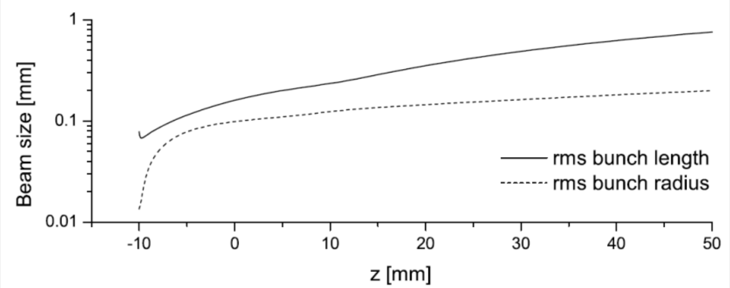
Laser cooled e⁻ diffraction



(a)







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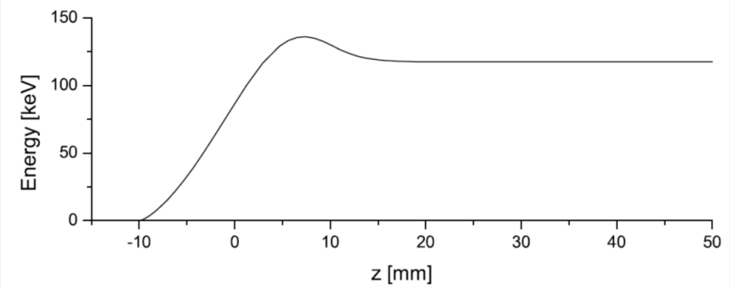
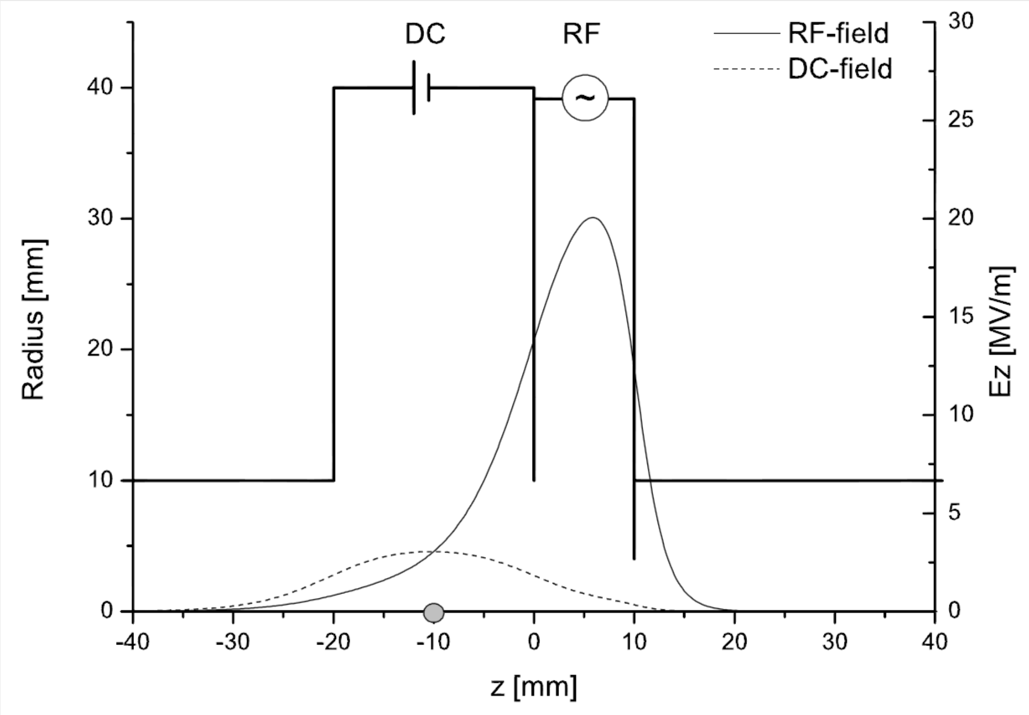


GPT Simulations include:

- Realistic external fields
- Start as function of time and postion
- Relativistic equations of motion
- All pair-wise interactions included

Laser cooled e⁻ diffraction



GPT results:

ε_x	20 nm (rms)
10% slice	**~1 nm**
Energy	120 keV
Spread	1%
ε_z	60 keV fs
Charge	**0.1 pC**
	(625,000 e⁻)

Ultracold Electron Source for Single-Shot, Ultrafast Electron Diffraction
Microscopy and Microanalysis 15, p. 282-289 (2009).
S.B. van der Geer, **M.J. de Loos**, E.J.D. Vredenbregt, and O.J. Luiten

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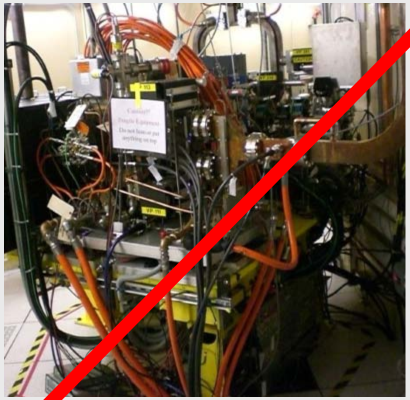
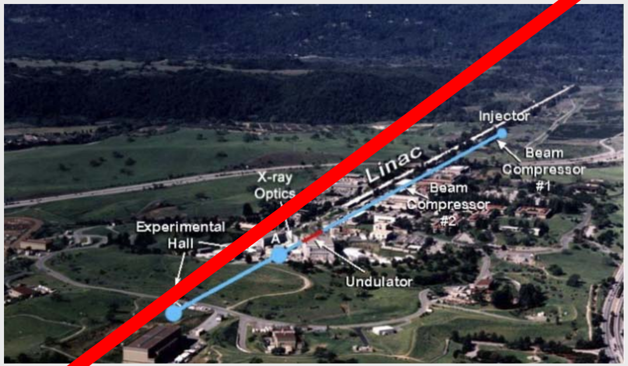
Miniaturized DESY/LCLS





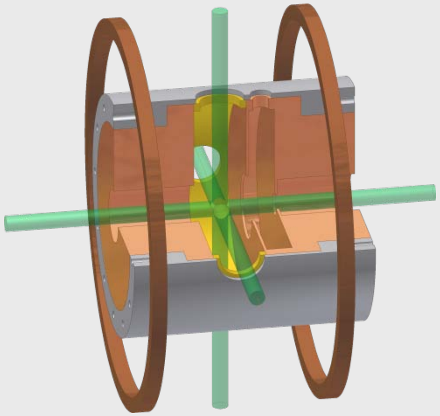
RF-photogun

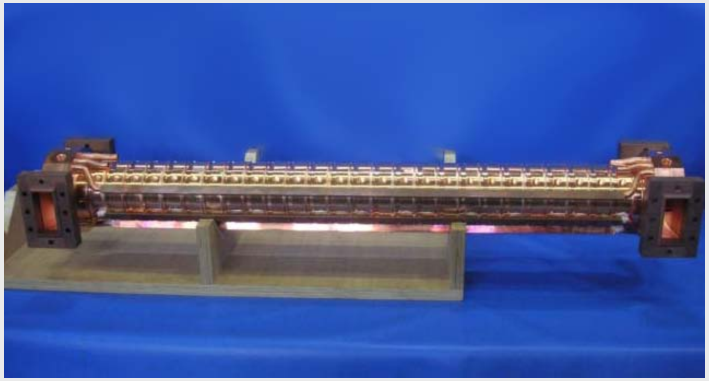
GeV Accelerator

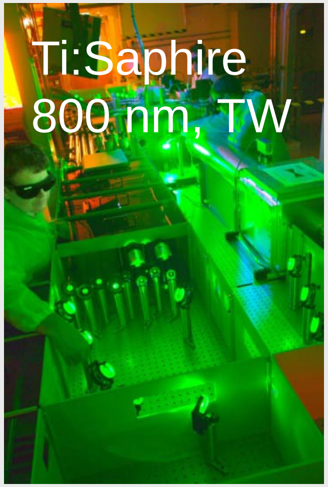
Undulator

laser-cooled source

MeV accelerator







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FEL equations

$$\frac{\varepsilon_n}{\gamma} = \frac{\lambda_{rad}}{4\pi} \qquad \lambda_{rad} = \frac{\lambda_u}{2\gamma^2}\left(1+\frac{K^2}{2}\right) \qquad \bar{\rho} = \rho\frac{mc\gamma}{\hbar k} = \frac{\sigma(p_z)}{\hbar k}$$

$$L_g = \frac{1}{\sqrt{3}}\sqrt[3]{\frac{2mc\gamma^3\sigma^2\lambda_u}{\mu e K^2 I}} = \frac{4\pi\sigma^2}{\lambda_{rad}}$$

$$\rho_{FEL} = \frac{1}{4\pi\sqrt{3}}\frac{\lambda_u}{L_g} \qquad P = \gamma\frac{mc^2}{e} I\,\rho_{FEL}$$

$$\sigma_W = \frac{\rho_{FEL}}{2}\gamma\frac{mc^2}{e} \qquad I_{\max} = \frac{Q}{\varepsilon_z/\sigma_W}$$

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FEL

Charge	1 pC	0.1 pC
Maximum field	20 MV/m	20 MV/m
Slice emittance	13 nm	1 nm
Longitudinal emittance	1 keV ps	0.1 keV ps
Peak current	100 A	1 mA
Energy	1.3 GeV	15 MeV
Undulator strength	0.1	0.5
λ_U	1.3 mm	800 nm
ρ_{FEL}	0.0002	0.00002
$\rho_{QUANTUM}$		0.1
Gain Length	0.28 m	2 mm
Wavelength	0.1 nm	0.4 nm
Power (1D)	25 MW	50 W, 60k photons

www.pulsar.nl

Conclusion

Laser-cooled sources:

- Require new simulation techniques
  for the calculation of all pair-wise Coulomb interactions
- Such as Barnes&Hut method (such as implemented in GPT)

- Produce phase-space distributions with divergent rms values

Current status:

- We can track ~10^6 particles in 3D in realistic fields

Future developments:

- Track more particles

Globular cluster Messier 2 by Hubble Space Telescope.. Located in the constellation of Aquarius, also known as NGC 7089.
M2 contains about a million stars and is located in the halo of our Milky Way galaxy.