

## Simulation challenges for laser-cooled electron sources

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# Simulation challenges for laser-cooled electron sources

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Marieke de Loos

Pulsar Physics

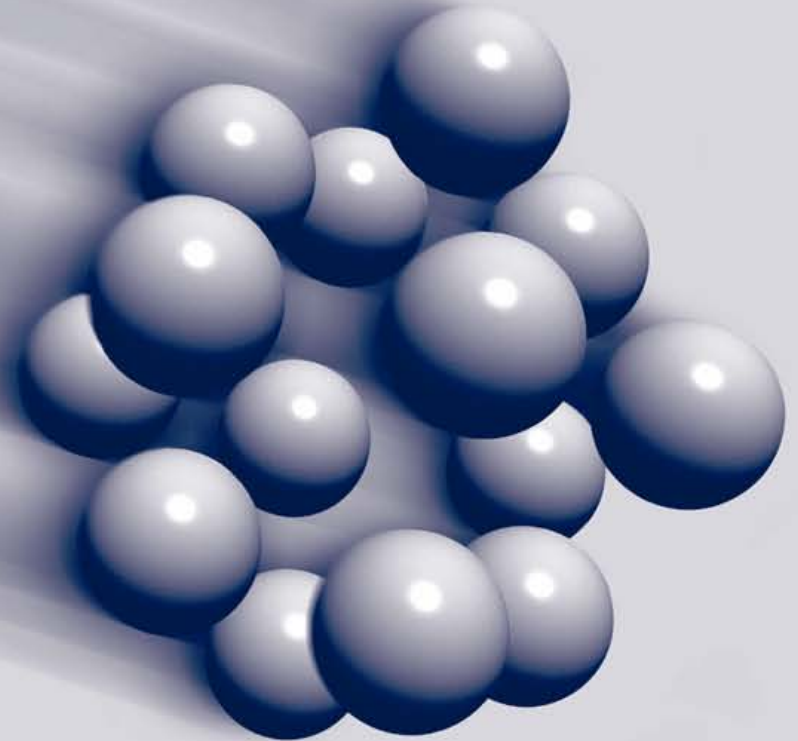
The Netherlands

Jom Luiten

Edgar Vredenburg

Eindhoven University of Technology

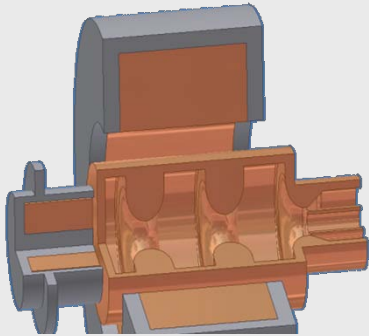
The Netherlands



There are two kinds of simulation codes:

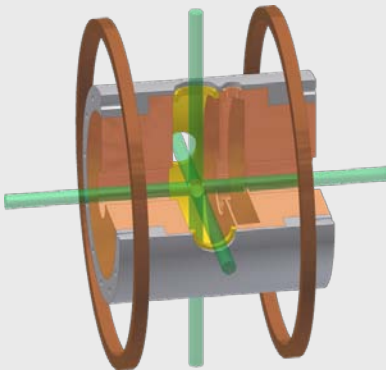
- Codes that everyone always complains about
- Codes that nobody ever uses

# Brighter sources, better simulations



Photogun: for example DESY / LCLS:

- Initial emittance  $\sim 1 \mu\text{m}$  (eV energy spread)
- Emittance  $\sim$  preserved in entire device
- Required simulation accuracy:  $<1 \mu\text{m}$



Laser-cooled sources:

- Initial emittance:  $< 1 \text{ nm}$  (meV energy spread)
- Emittance?
- Desired simulation accuracy:  $<1 \text{ nm}$

Quantum degenerate sources

- ...

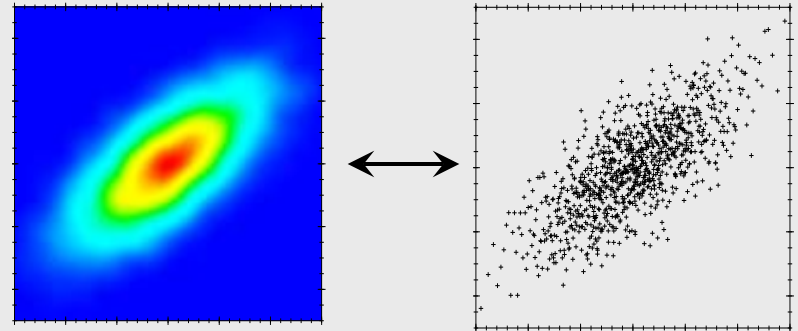
# 'Typical' simulation code: GPT

Tracks sample particles in **time-domain**

- Equations of motion

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

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



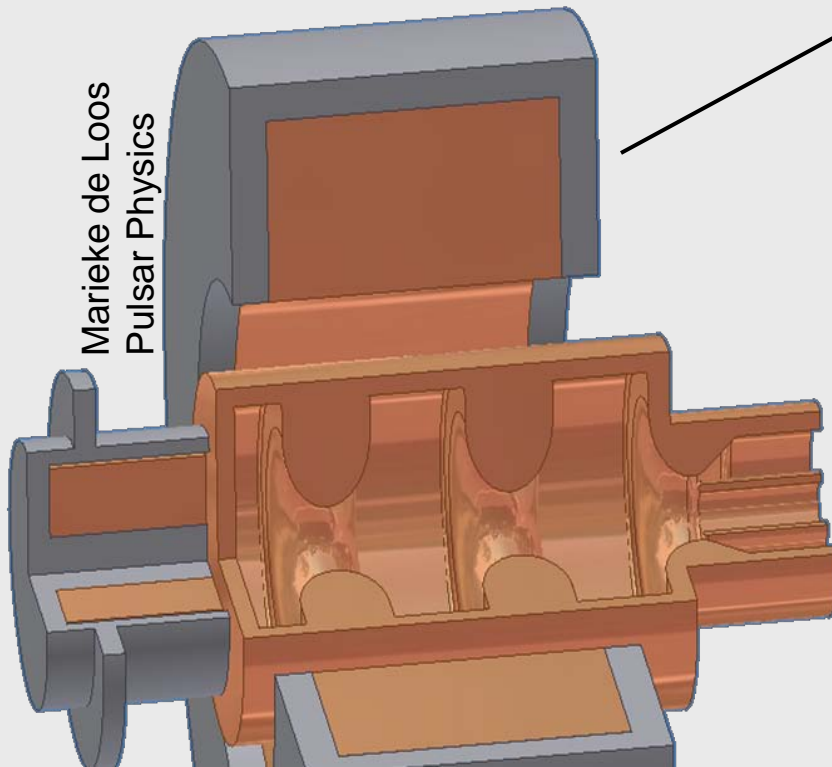
include all non-linear effects

- GPT solves with 5<sup>th</sup> order embedded Runge Kutta, adaptive stepsize
- GPT can track  $\sim 10^6$  particles on a PC with 1 GB memory
- Challenge:  $\mathbf{E}(\mathbf{r},t)$ ,  $\mathbf{B}(\mathbf{r},t)$ , flexibility without compromising accuracy

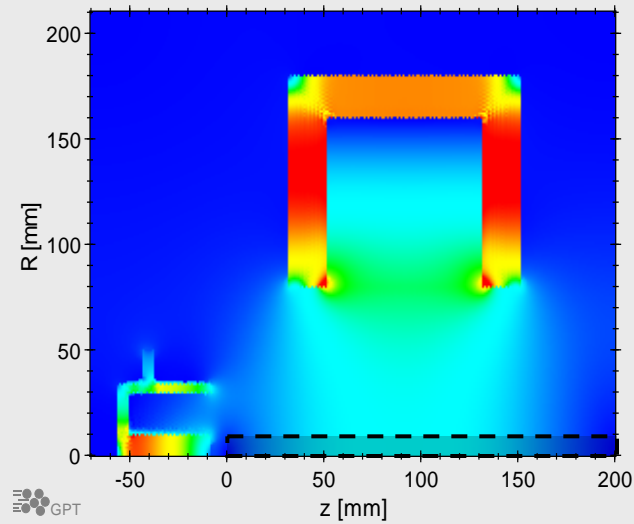


# Field-maps

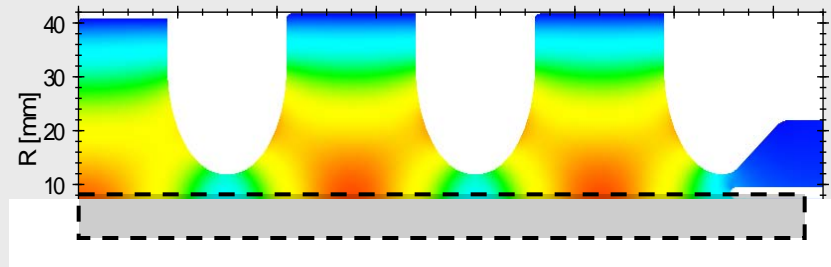
- 1D, 2D, 3D
- Rely on external solvers
- Fields are summed
- 3D positioning, 3D orientation



### Magnet



### Cavity



Only this part is needed for tracking



# Coulomb interactions

## Macroscopic:

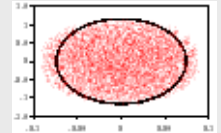
- **Space-charge**
- Average repulsion force
- Bunch expands
- Deformations in phase-space
- Governed by Poisson's equation

## Microscopic:

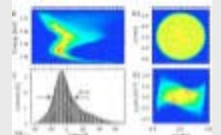
- **Disorder induced heating**
- Neighbouring particles 'see' each other
- Potential energy → momentum spread
- Stochastic effect
- Governed by point-to-point interactions

## GPT simulations

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



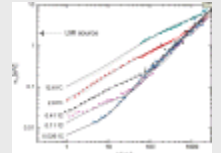
**JAP 102, 093501**  
T. van Oudheusden et. al.



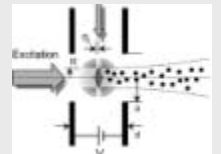
**PRST-AB 9, 044203**  
S.B. van der Geer et. al.



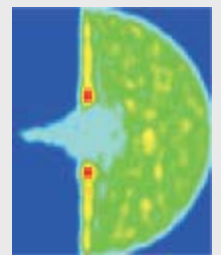
**PRL 102, 034802**  
M. P. Reijnders et. al.



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



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



And many others...



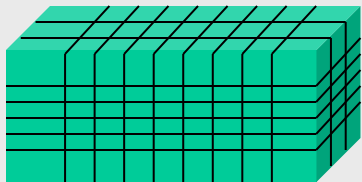
# Particle-Mesh (in-Cell)



Bunch in laboratory frame



Bunch in rest frame



Meshlines

$\rho'$

Charge density

- Mesh-based electrostatic solver in rest-frame

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

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

$$-\nabla^2 V' = \rho' / \epsilon_0$$

Poisson equation

- Solve Poisson equation

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

Interpolation

- 2<sup>nd</sup> order interpolation for the electrostatic field  $\mathbf{E}'$

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

Lorentz transformation to laboratory frame

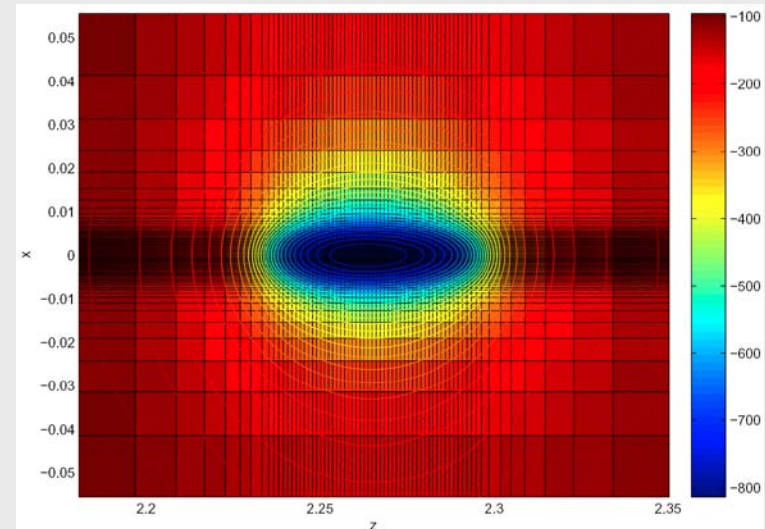
- Transform  $\mathbf{E}'$  to  $\mathbf{E}$  and  $\mathbf{B}$  in laboratory frame



# 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  $\sim O(N^1)$  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.

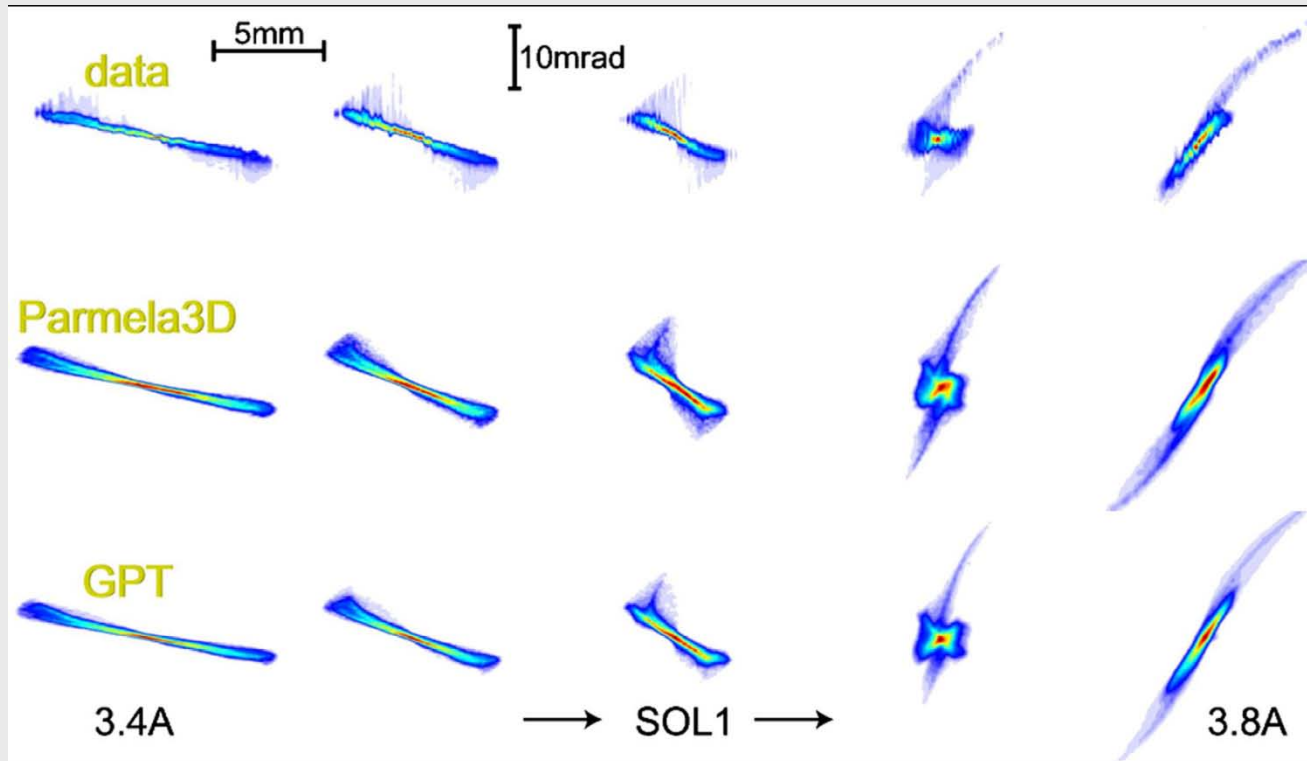




# 3D Space-charge simulations

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**

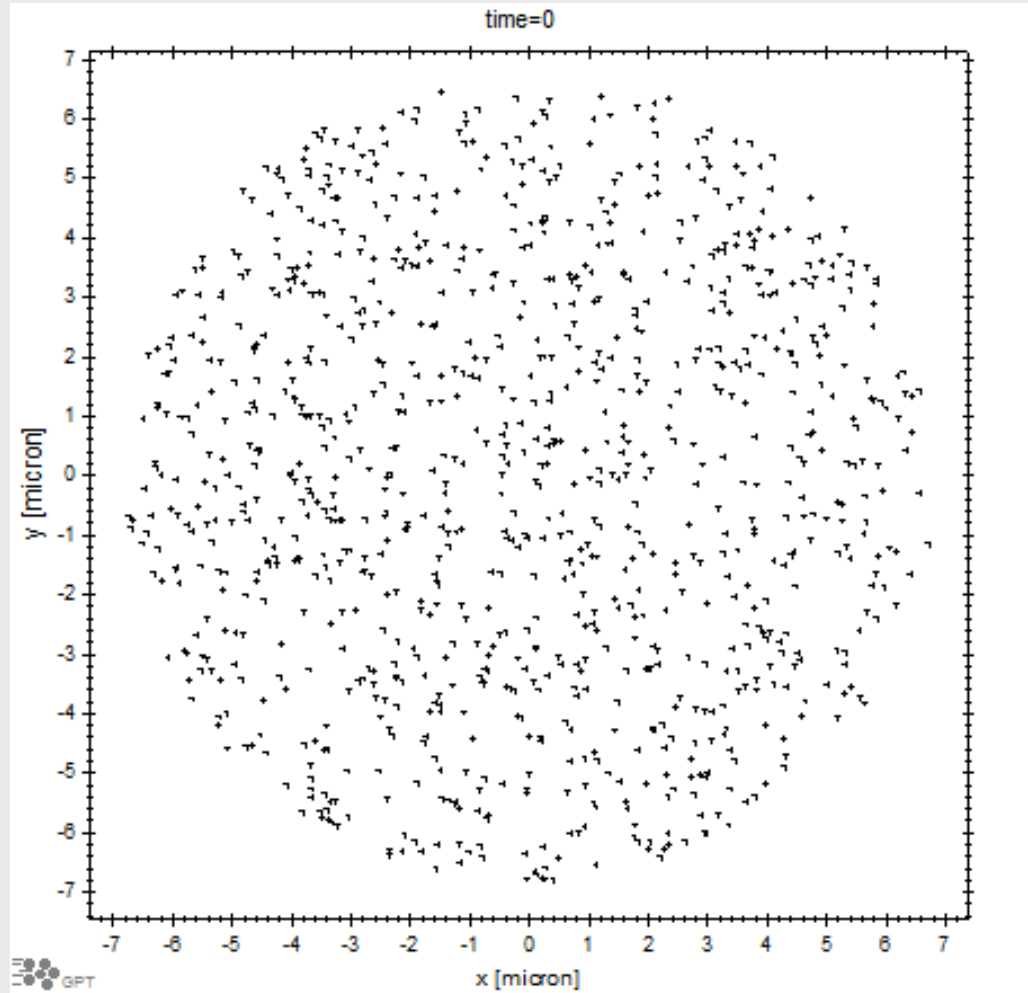
Ivan V. Bazarov, et.al.  
PRST-AB 11, 100703  
(2008).



# Laser-cooled sources

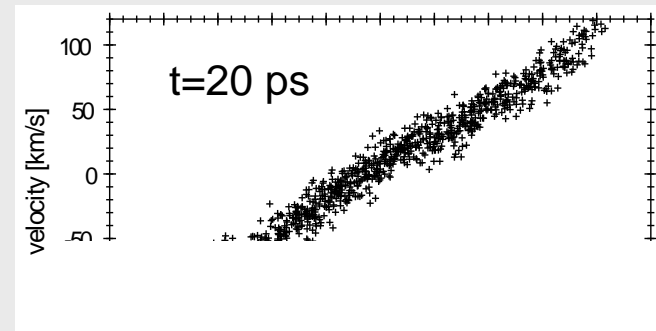
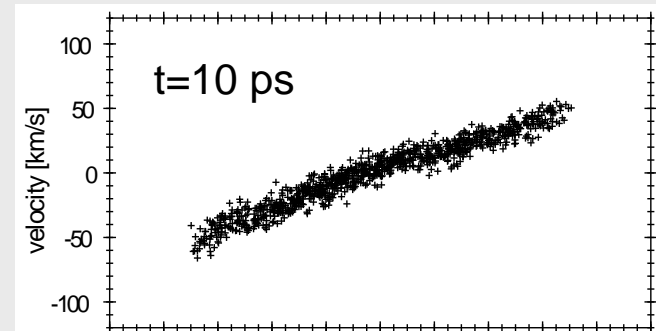
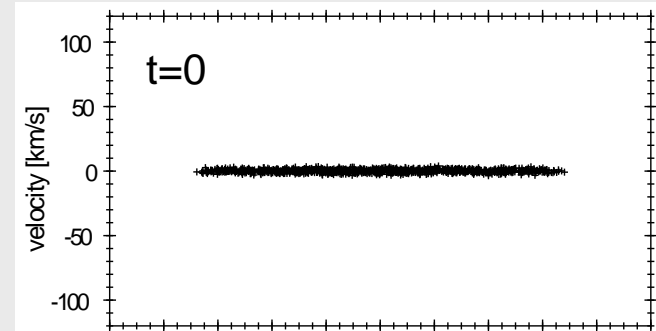
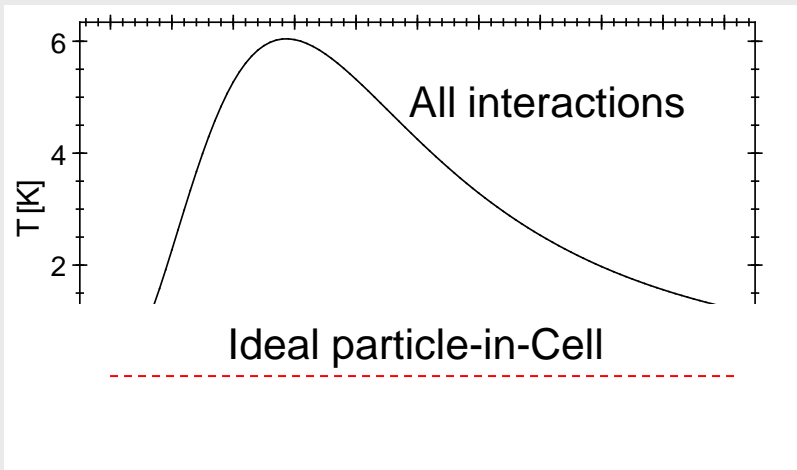
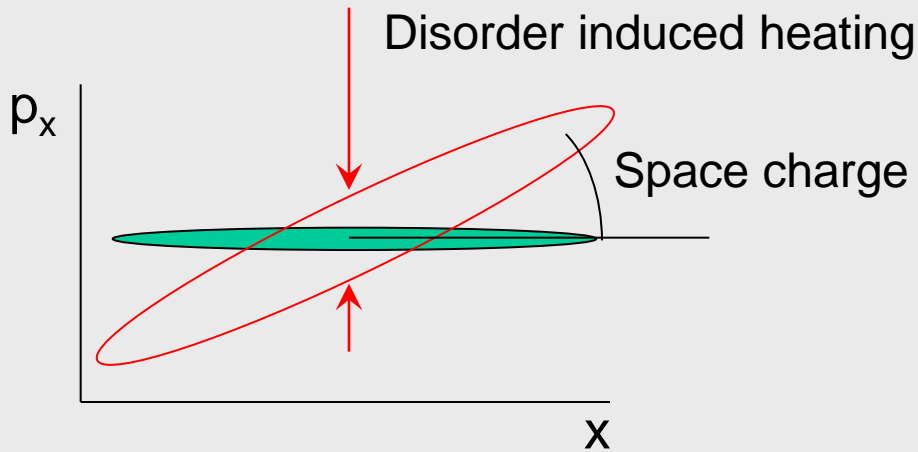
Simple test case:

- Uniformly filled sphere
- Density  $10^{18}/\text{m}^3$
- No initial temperature
- *All* pair-wise interactions
- Wait and see...





# Coulomb interactions





# Disorder induced heating

Random processes



Excess potential energy  $U$



Coulomb interactions

Momentum spread



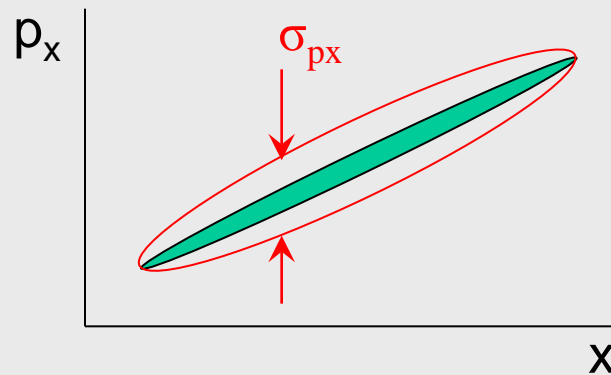
Temperature  $\uparrow$   
Brightness  $\downarrow$



High  $U$



Low  $U$



$$\left. \begin{aligned} \sigma_{p_x} &= \sqrt{m k T_x} \\ &= mc \frac{\epsilon_x}{\sigma_x} \end{aligned} \right\} \Rightarrow T_x = \frac{mc^2}{k} \frac{\epsilon_x^2}{\sigma_x^2} \quad B_{\perp} = \frac{J}{\pi k T}$$



# 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

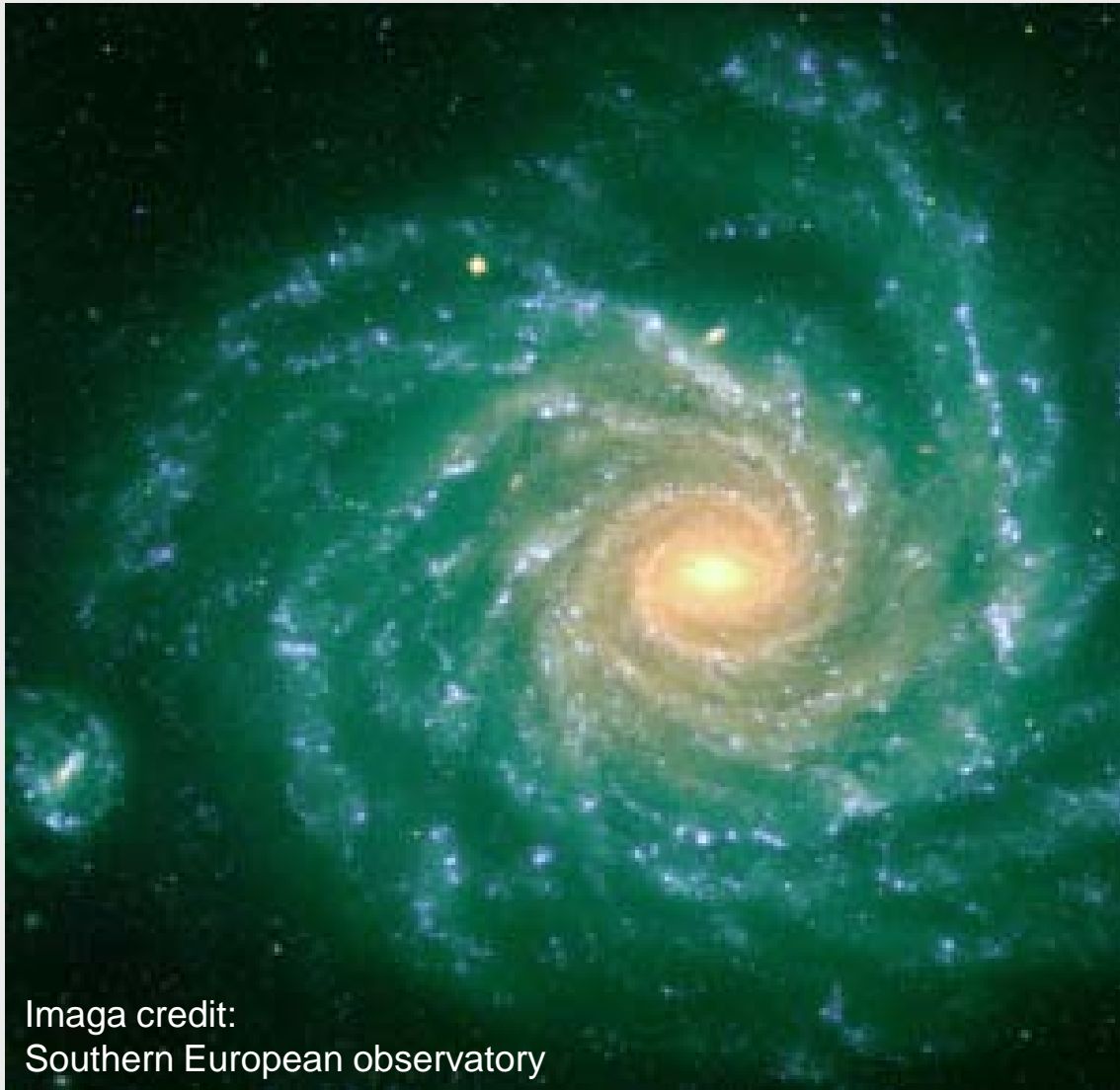
Tree-codes (B&H, FMM, P<sup>3</sup>M)

- Every particle matters
- Ions and electrons
- Ab initio
- No Liouville to the rescue
- Divergent rms values

$$k T_{\text{photogun}} \gg 0.02 n^{1/3} q^2 / \epsilon_0 \gg k T_{\text{laser-cooled}}$$



# Algorithms...



Imaga credit:  
Southern European observatory

$N^2$  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<sup>3</sup>M Particle-Particle Particle-Mesh

Accuracy traded for speed:

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

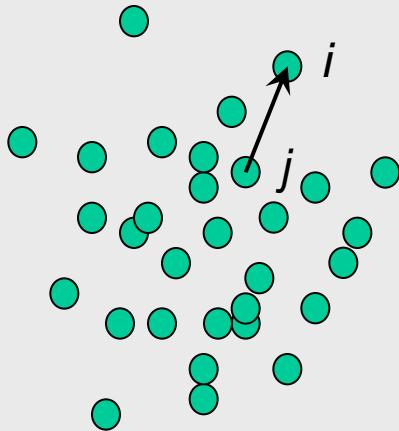




# Particle-Particle

3D point-to-point:

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



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

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

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

- Electrostatic field of  $j$

$$\mathbf{E}'_{j \rightarrow i} = \frac{Q \mathbf{r}'_{ji}}{4\pi\epsilon_0 |\mathbf{r}'_{ji}|^3}$$

- Summation to laboratory frame

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

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



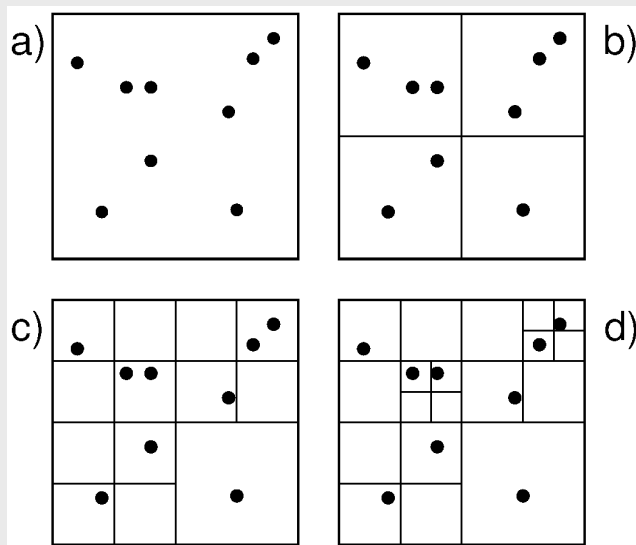


# Barnes-Hut

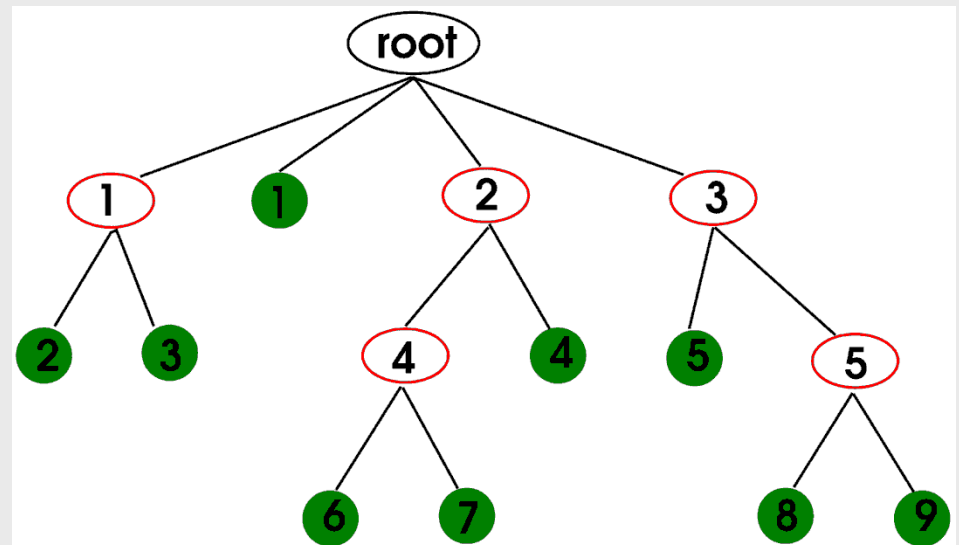
Hierarchical tree algorithm:

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

Division of space

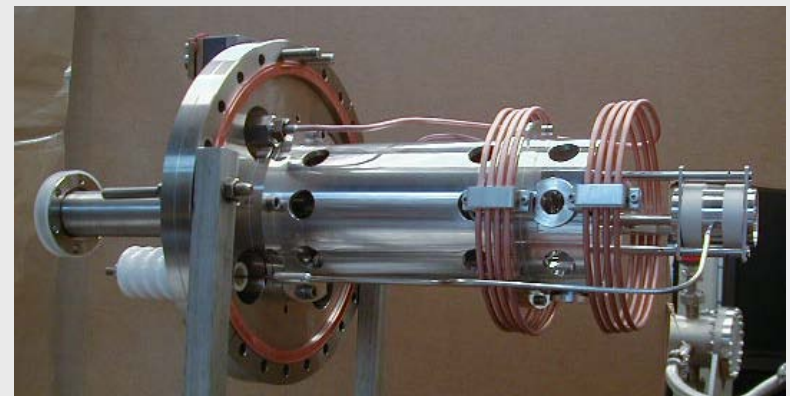
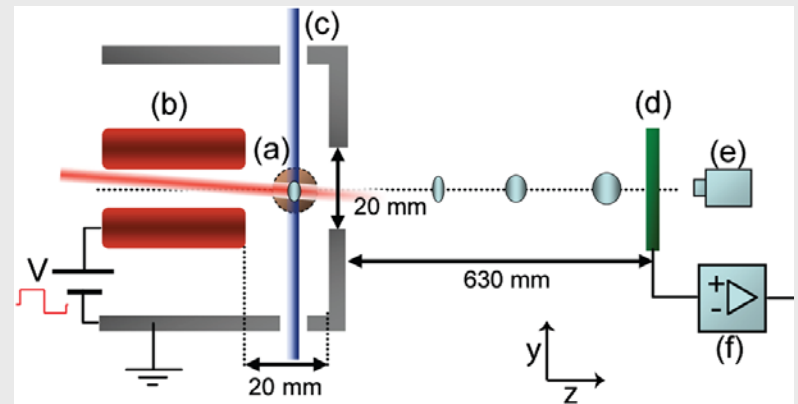
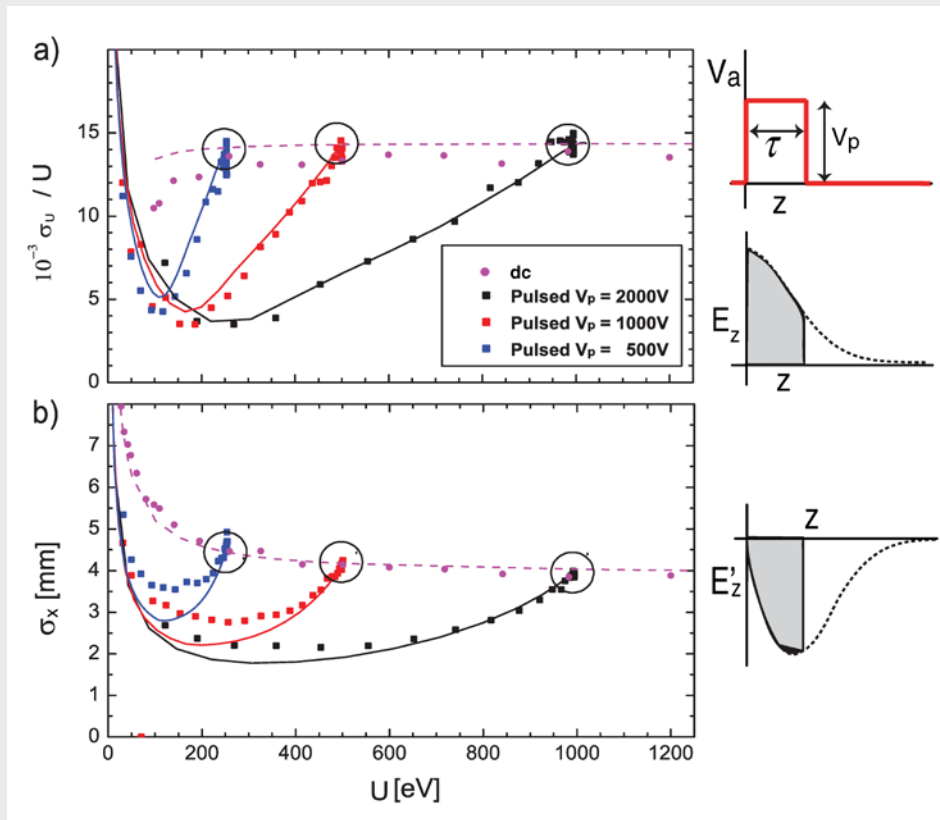


Tree data structure



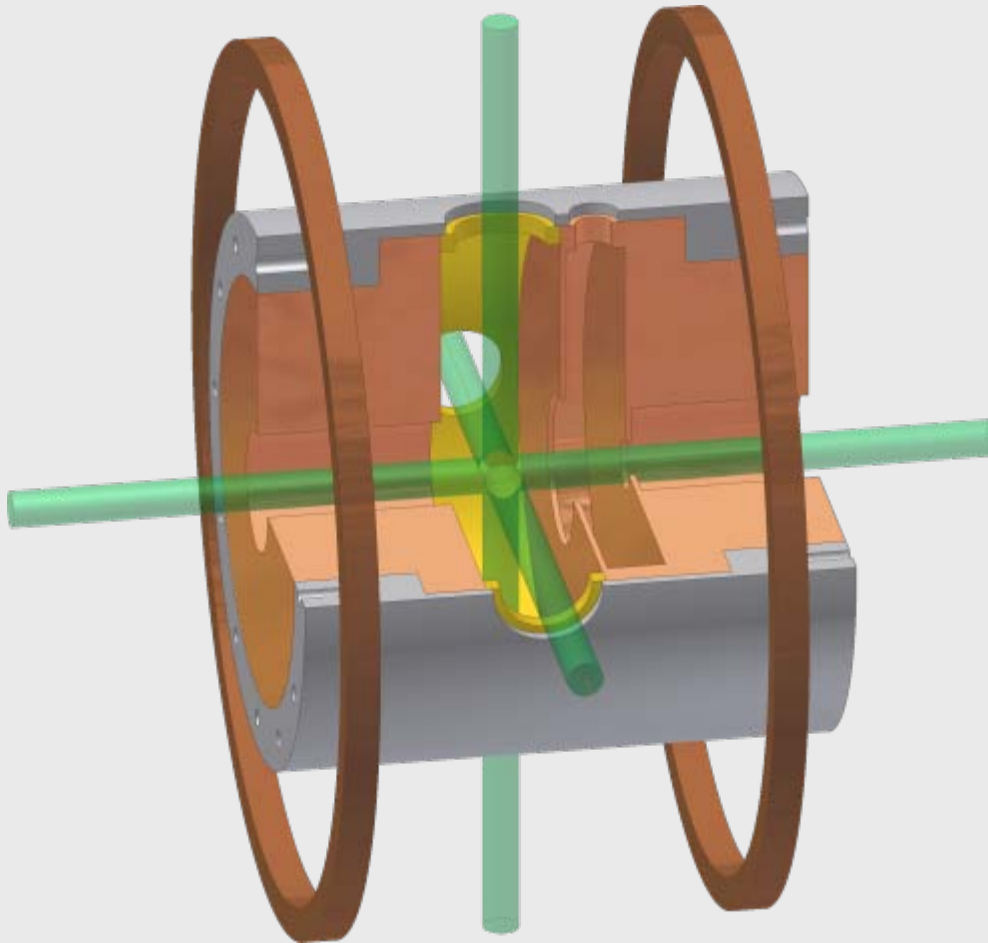


# Comparison with experiments



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

# Laser-cooled e<sup>-</sup> source



## Fields:

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

## Particles:

Charge	0.1 pC (625k e <sup>-</sup> )
Initial density	10 <sup>18</sup> / m <sup>3</sup>
Ionization time	10 ps
Initial Temp	1 K

## GPT tracking:

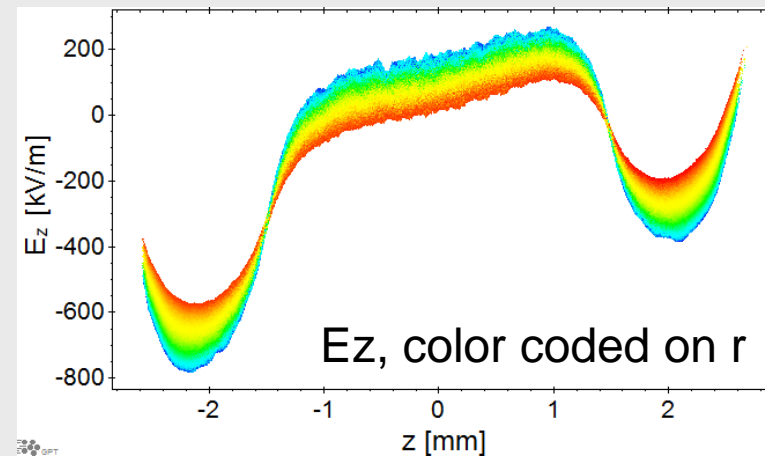
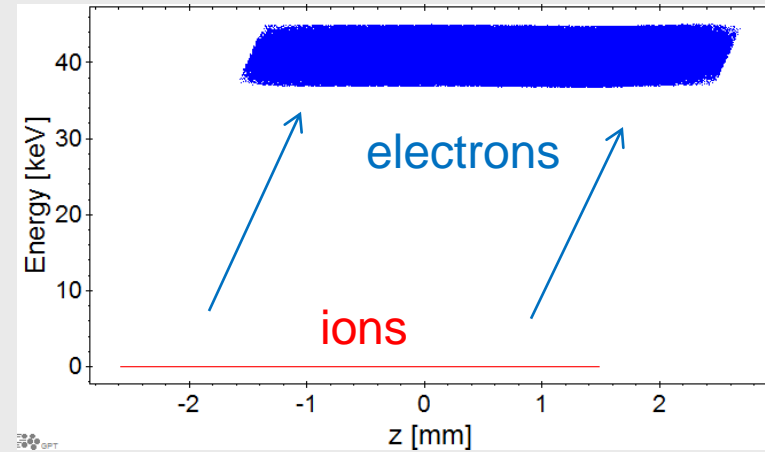
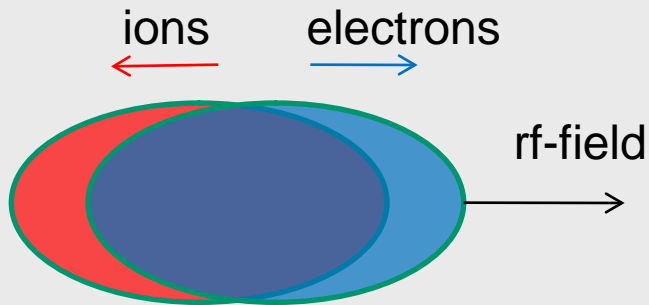
All particles  
Realistic fields  
All interactions



# Longitudinal emission dynamics

## Longitudinal acceleration

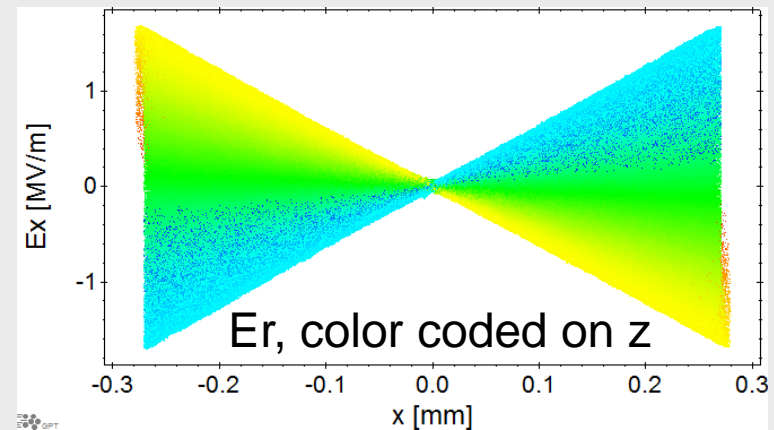
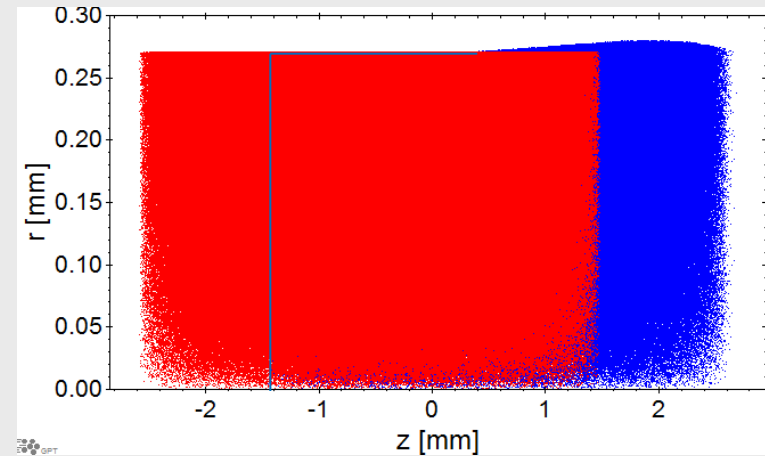
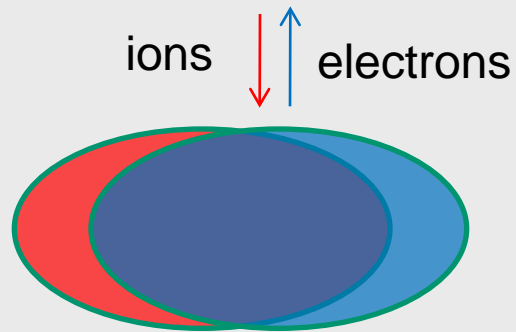
- rf field
- Combined spacecharge



# Transverse emission dynamics

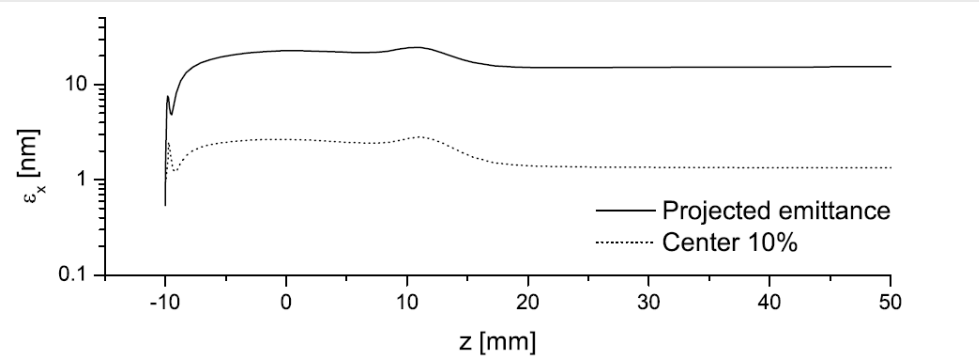
## Transverse acceleration

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

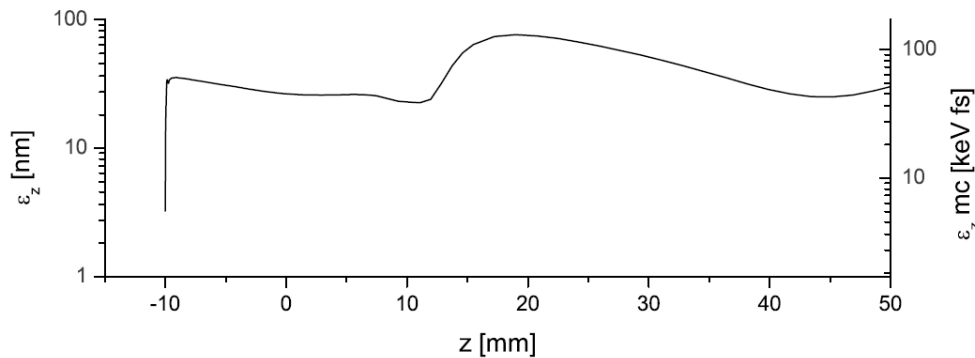




# Laser cooled e<sup>-</sup> diffraction

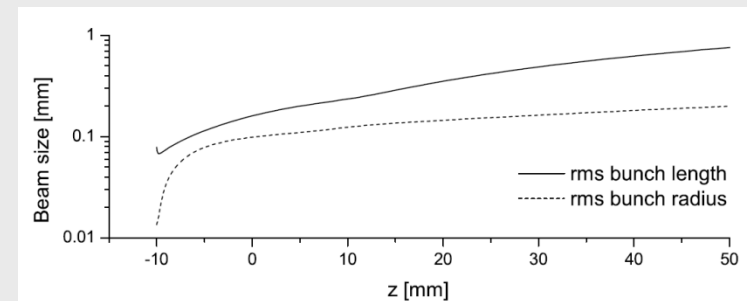
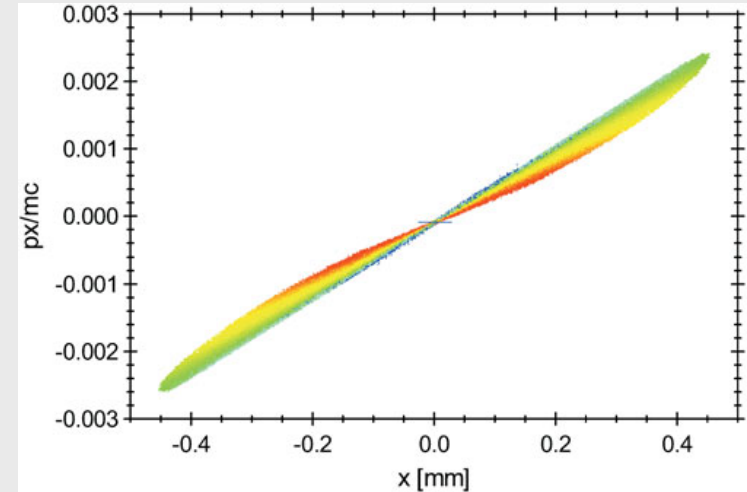


(a)

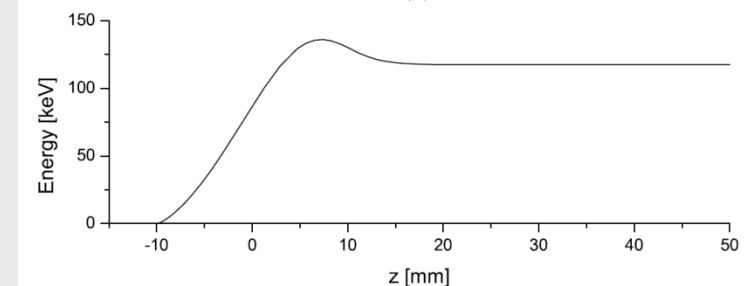


GPT Simulations include:

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

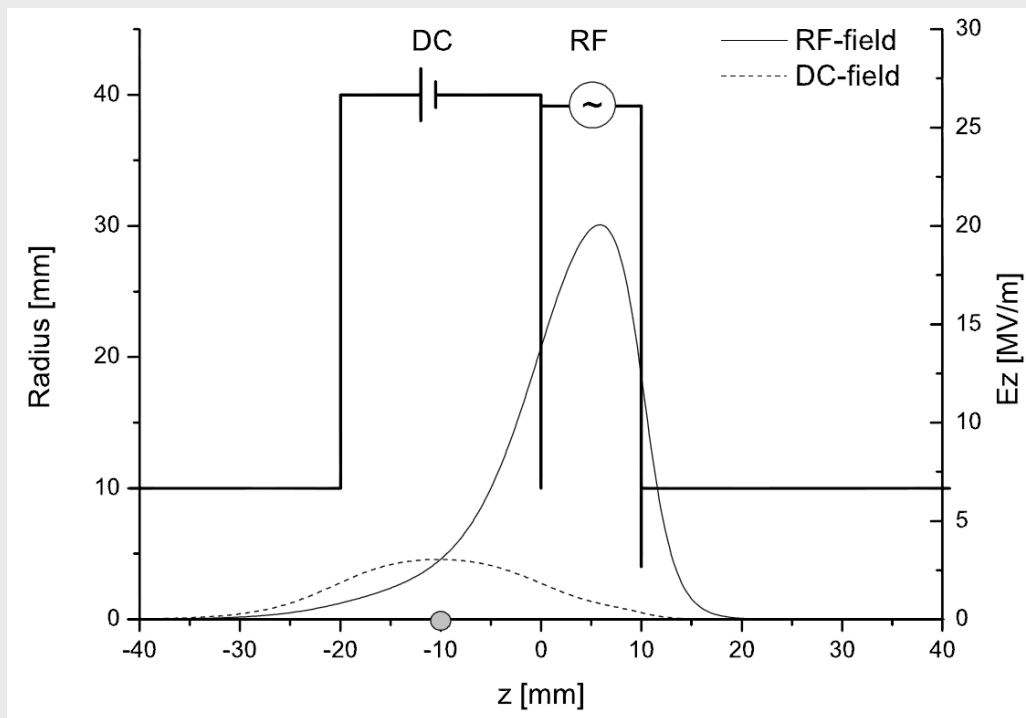


(a)





# Laser cooled e<sup>-</sup> diffraction



## GPT results:

$\epsilon_x$  20 nm (rms)  
10% slice **~1 nm**

Energy 120 keV  
Spread 1%  
 $\epsilon_z$  60 keV fs

Charge **0.1 pC**  
(625,000 e<sup>-</sup>)

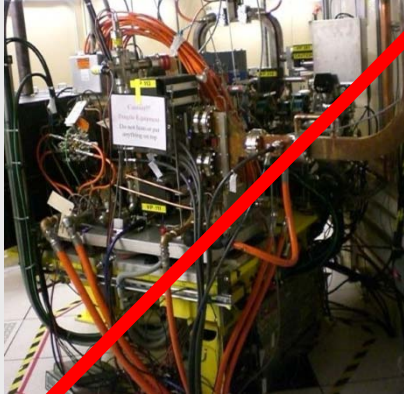
## Ultracold Electron Source for Single-Shot, Ultrafast Electron Diffraction

Microscopy and Microanalysis 15, p. 282-289 (2009).

S.B. van der Geer, **M.J. de Loos**, E.J.D. Vredenburg, and O.J. Luiten



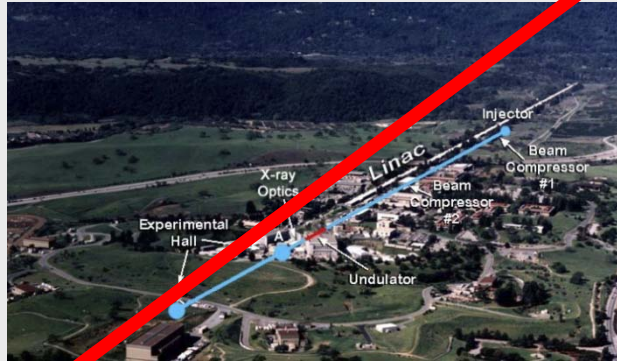
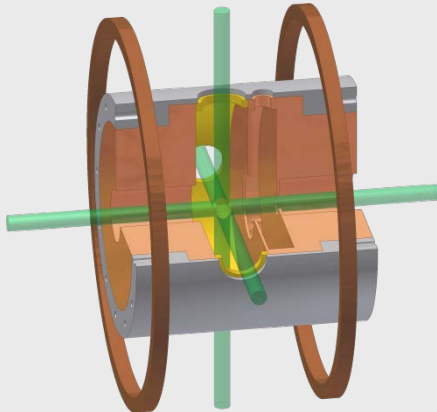
# Miniaturized DESY/LCLS



RF-photogun



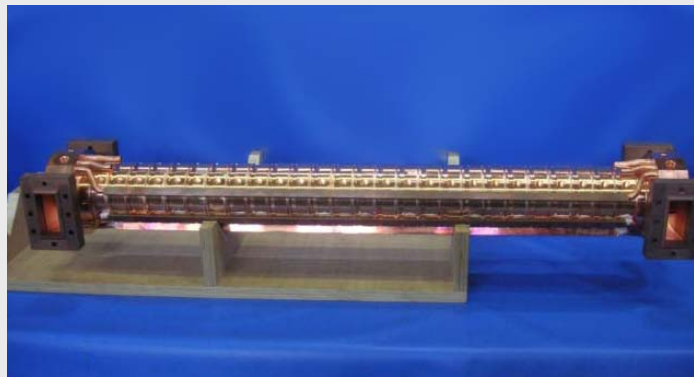
laser-cooled source



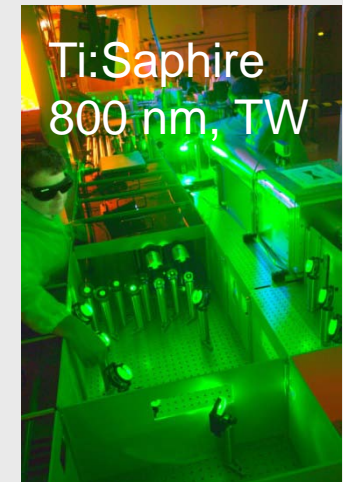
GeV Accelerator



MeV accelerator



Undulator







# FEL equations

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

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

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

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



# FEL

<u>Charge</u>	<u>1 pC</u>	<u>0.1 pC</u>
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
$\lambda_U$	1.3 mm	800 nm
$\rho_{FEL}$	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



# 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  $\sim 10^6$  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.