Granularity effects

in high brightness electron bunches

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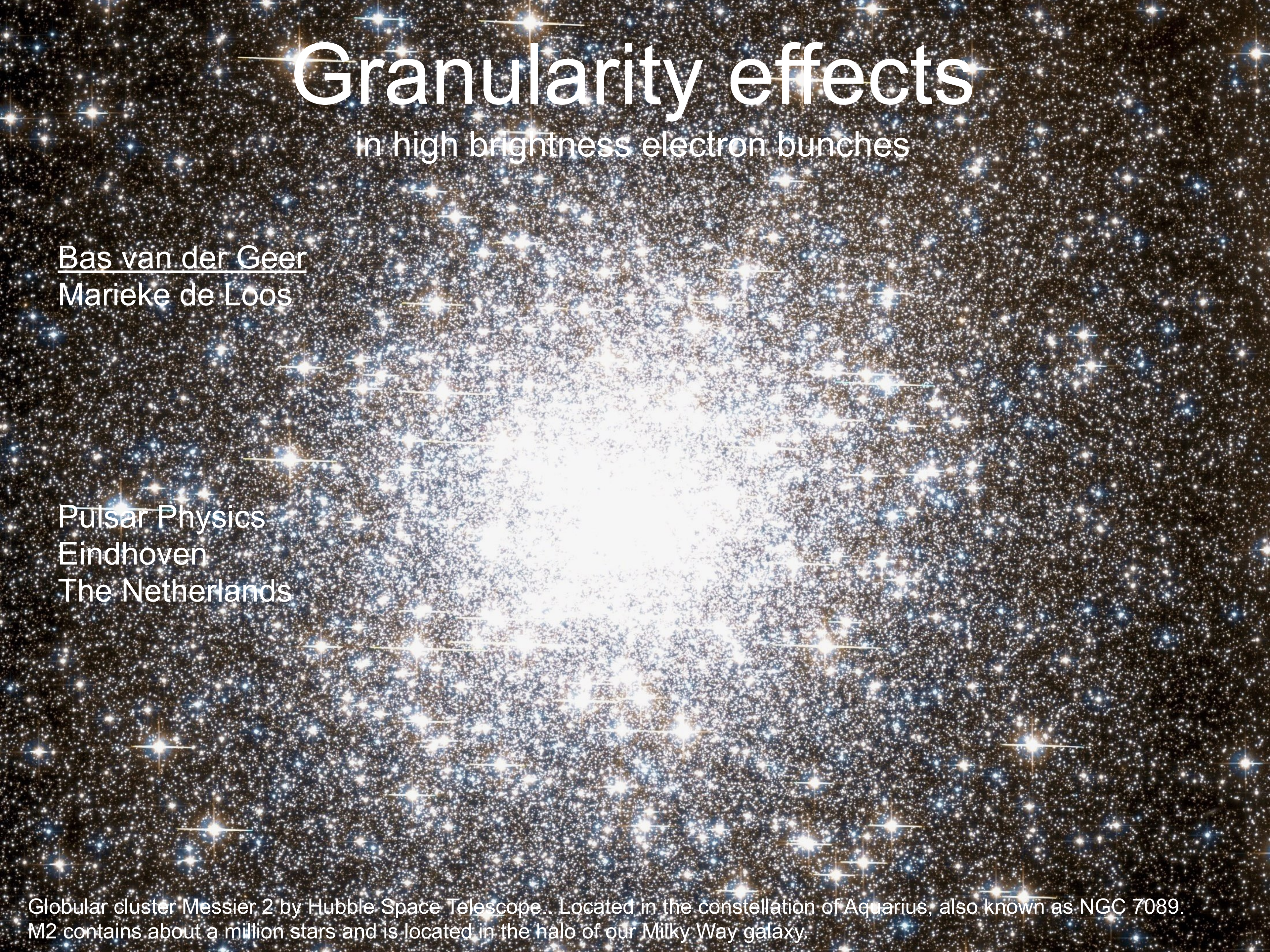
Marieke de Loos

Pulsar Physics
Eindhoven
The Netherlands



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.

Coulomb interactions

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Macroscopic:

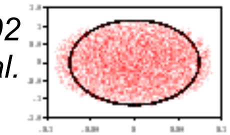
- Space-charge
- Average repulsion force
- Bunch expands
- Deformations in phase-space
- Governed by Poisson's equation

Microscopic:

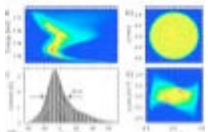
- Disorder induced heating
- Neighbouring particles 'see' each other
- Potential energy → momentum spread
- Stochastic effect
- Governed by point-to-point interactions

Example GPT simulations

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

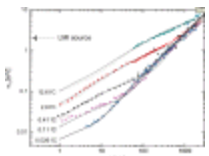


JAP 102, 093501
T. van Oudheusden et. al.

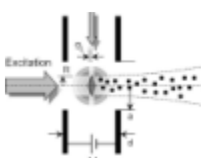


PRST-AB *9, 044203*
S.B. van der Geer et. al.

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

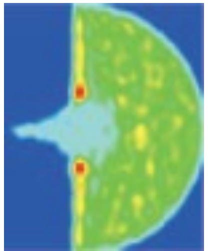


JAP *102, 094312*
S.B. van der Geer et. al.



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

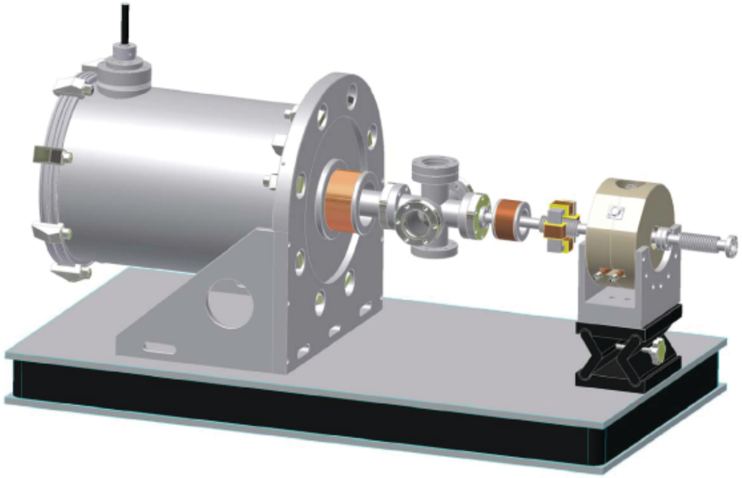
And many others…

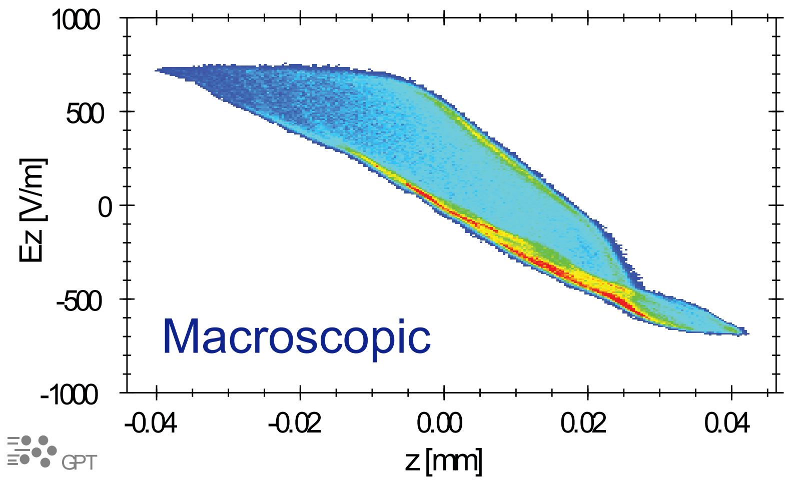


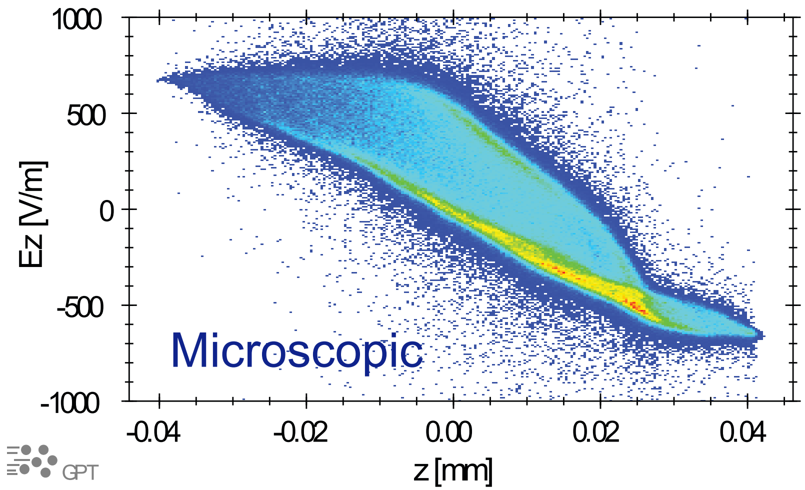
Ultrafast Electron Diffraction example (UED)

UED 100 fC

- 625000 particles
- GPT treecode (2011)







UED example: All interactions (right), versus PIC (left)

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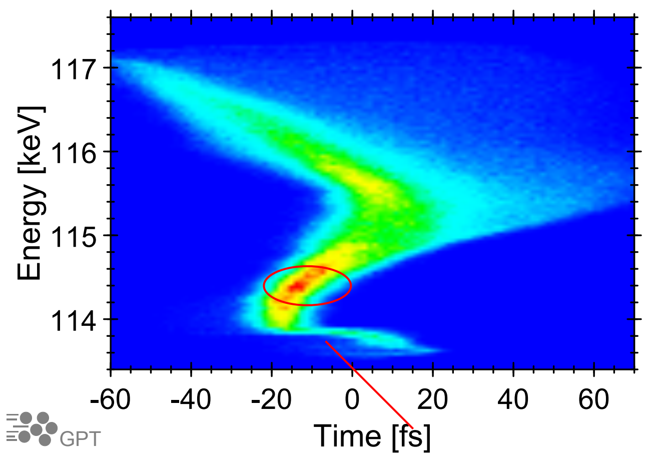
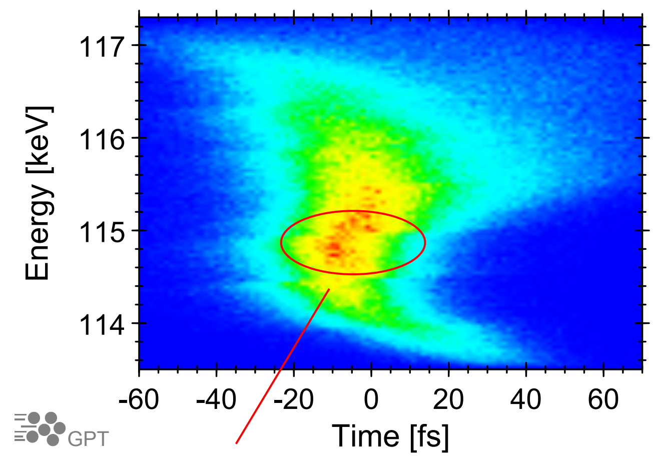
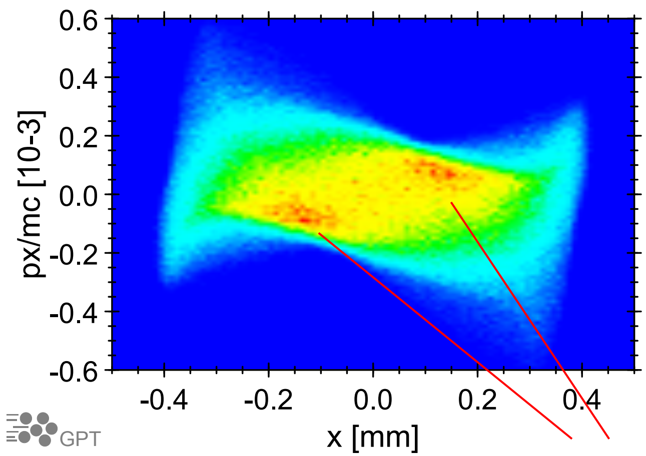
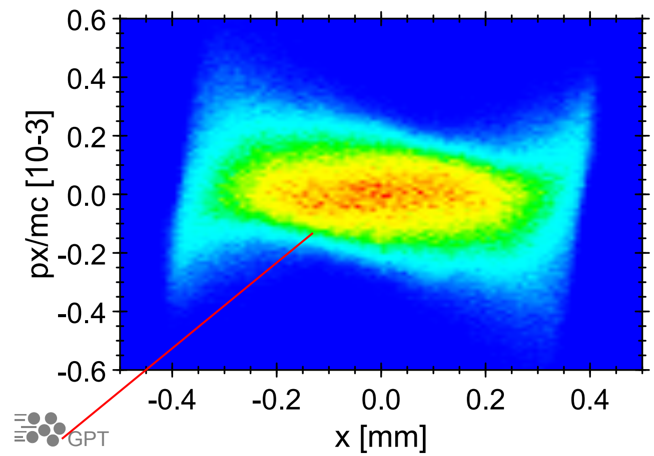
Particle-in-Cell	**Barnes-Hut**





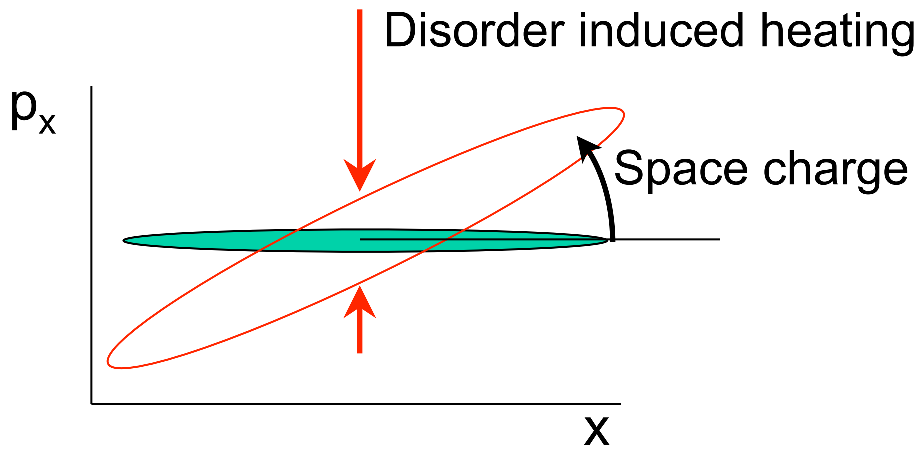
Broadening due to stochastic effects

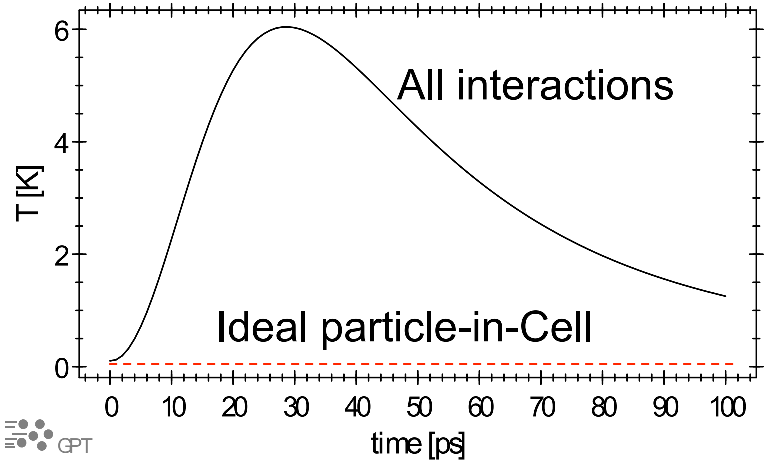


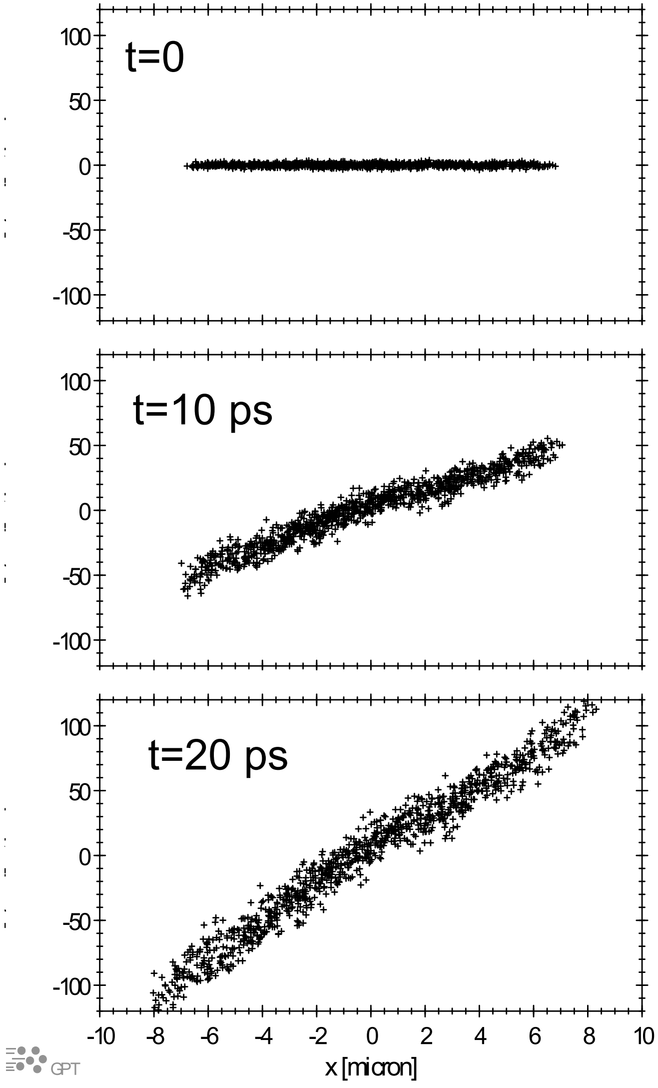


Local differences

Coulomb interactions







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

Law of distribution of the nearest neighbor

Chandrasekhar, Stochastic problems in Physics and astronomy, Reviews of Modern Physics 15, 1943.

VII. THE LAW OF DISTRIBUTION OF THE NEAREST NEIGHBOR IN A RANDOM DISTRIBUTION OF PARTICLES

This problem was first considered by Hertz (see reference 71 in the Bibliographical Notes for Chapter IV).

Let $w(r)dr$ denote the probability that the nearest neighbor to a particle occurs between r and $r+dr$. This probability must be clearly equal to the probability that no particles exist interior to r times the probability that a particle does exist in the spherical shell between r and $r+dr$. Accordingly, the function $w(r)$ must satisfy the relation

$$w(r)=\left[1-\int_0^r w(r)dr\right]4\pi r^2 n, \tag{669}$$

where n denotes the average number of particles per unit volume. From Eq. (669) we derive:

$$\frac{d}{dr}\left[\frac{w(r)}{4\pi r^2 n}\right]=-4\pi r^2 n\frac{w(r)}{4\pi r^2 n}. \tag{670}$$

Hence

$$w(r)=\exp\left(-4\pi r^3 n/3\right)4\pi r^2 n, \tag{671}$$

since, according to Eq. (669)

$$w(r)\rightarrow 4\pi r^2 n \quad \text{as} \quad r\rightarrow 0. \tag{672}$$

Equation (671) gives then the required law of distribution of the nearest neighbor.

Law of distribution of the nearest neighbor: *w*(*r*)

w(r) dr

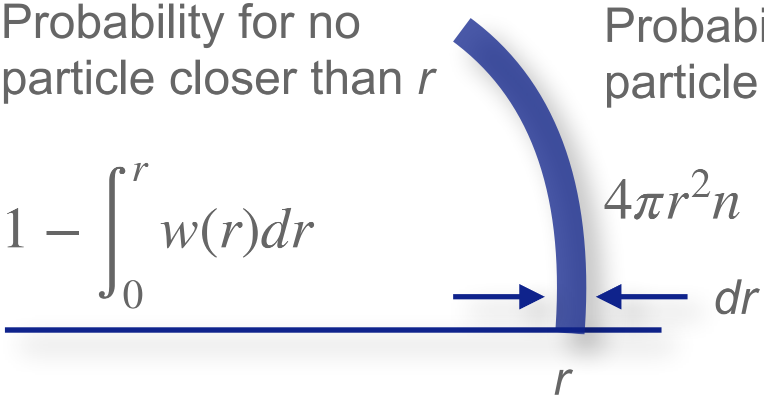
- Probability that neareast neighbor is between r and $r + dr$
- Assuming infinite random distribution with number density *n*.

Probability for no particle closer than *r*

$$1 - \int_0^r w(r)dr$$

Probability for particle between *r* and *r* + *dr*

$$4\pi r^2 n \ dr$$



$$w(r) = \left(1 - \int_0^r w(r)dr\right) 4\pi r^2 n$$

Chandrasekhar, Stochastic problems in Physics and astronomy, Reviews of Modern Physics 15, 1943.

r

Law of distribution of the nearest neighbor: *w*(*r*)

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$$w(r) = \left(1 - \int_0^r w(r)dr\right) 4\pi r^2 n$$

Yields:

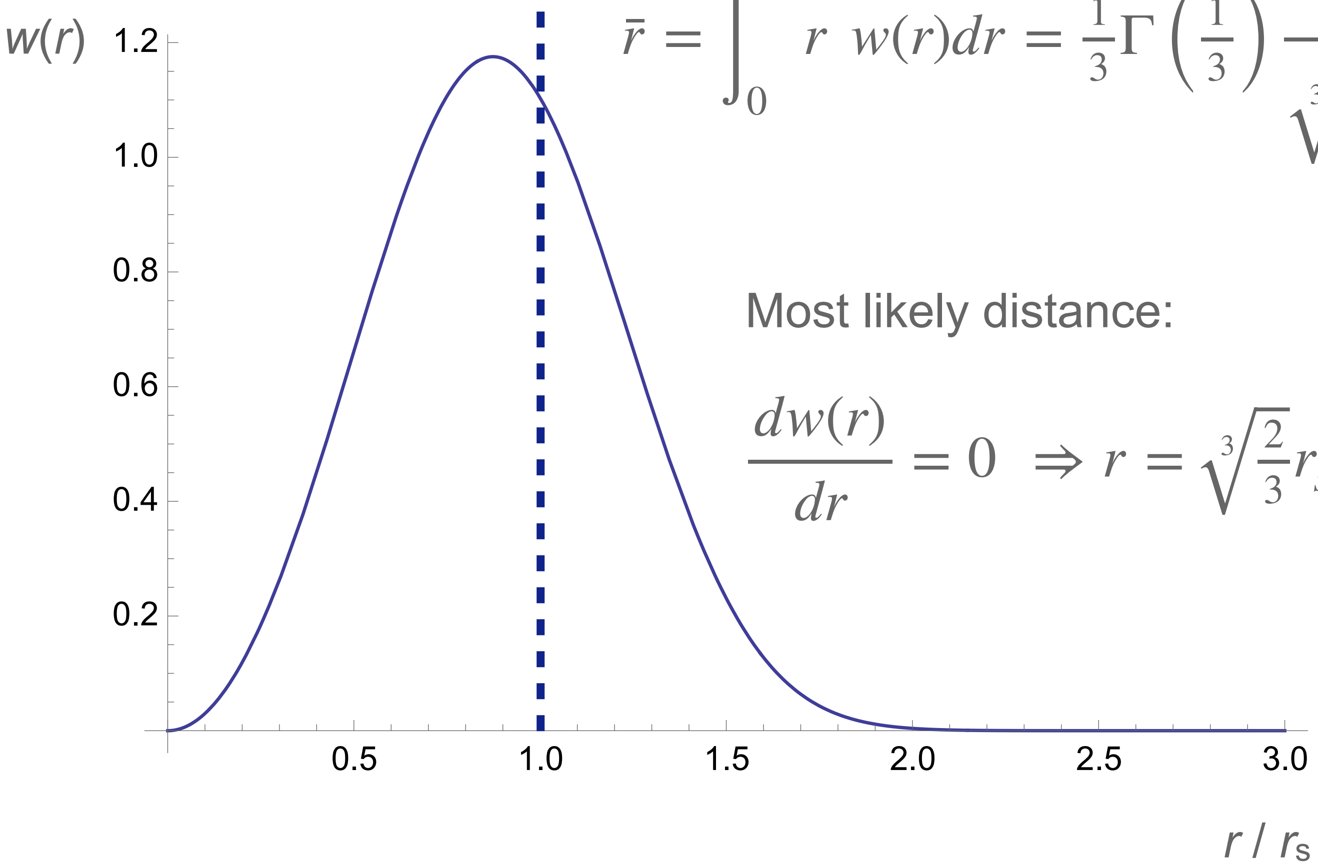
$$w(r) = \frac{4\pi r^2}{e^{\frac{4}{3}\pi r^3 n}}$$

Subramanyan Chandrasekhar
1910 - 1995, Lahore, India (now Pakistan)

1983 nobel prize: "for his theoretical studies of the physical processes of importance to the structure and evolution of the stars"

Law of distribution of the nearest neighbor: $w(r)$

$$w(r) = \frac{4\pi r^2}{e^{\frac{4}{3}\pi r^3 n}}$$



Average distance:

$$\bar{r} = \int_0^\infty r\ w(r)dr = \tfrac{1}{3}\Gamma\left(\tfrac{1}{3}\right)\frac{1}{\sqrt[3]{\frac{4}{3}\pi n}} \approx 0.89 r_s$$

Most likely distance:

$$\frac{dw(r)}{dr} = 0 \ \Rightarrow r = \sqrt[3]{\frac{2}{3}} r_s \approx 0.87 r_s$$

Wigner-Seitz radius: r_s

Assumptions:

- Volume per particle: $V = 1/n$

$$\|$$

- Volume of a sphere $V = \frac{4}{3}\pi\ r_s^3$

Yields:

$$r_s = \frac{1}{\sqrt[3]{\frac{4}{3}\pi n}}$$

Fame

Wigner
Nobel prize in physics

Fortune

Seitz
Tobacco lobbyist
Climate change denier

Nearest neighbor in *k*-dimensions

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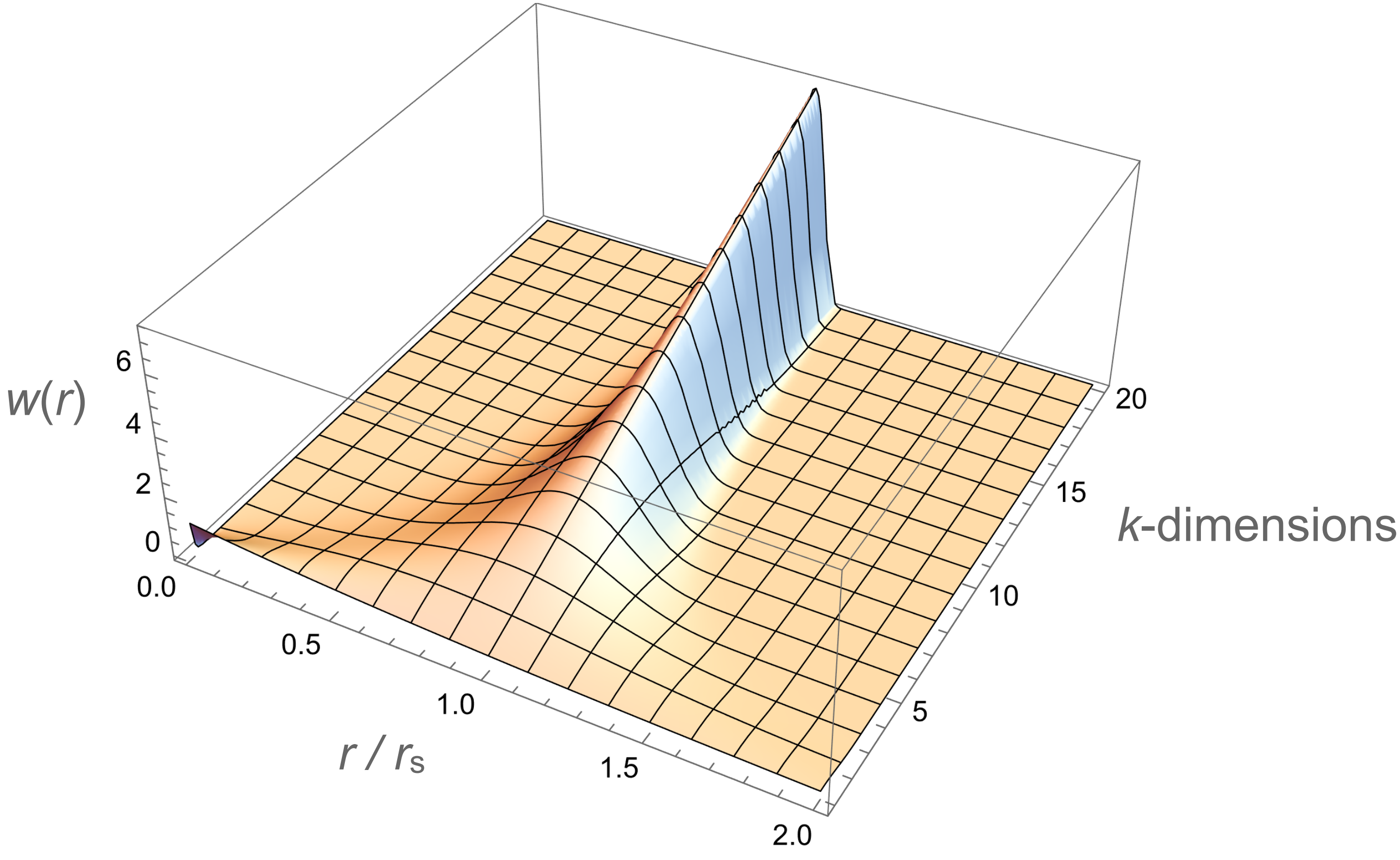
Relevant:

- 'Pencil beam' regime in electron microscopes
- 'Pancake' regime near photocathodes



Disorder induced heating

Random processes

↓

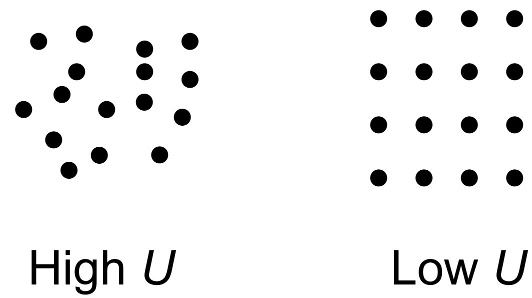
Excess potential energy *U*

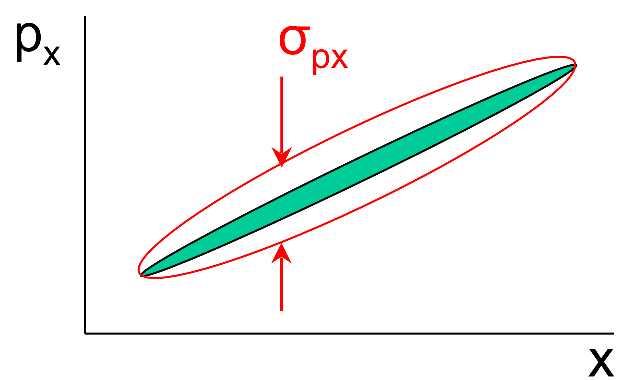
↓ Coulomb interactions

Momentum spread

↓

Temperature ↑
Brightness ↓





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

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

Nearest neighbor: Potential

Electrostatic potential:

- $$V(r) = \frac{q^2}{4\pi\epsilon_0 r}$$

Average potential energy:

- $$\bar{V} = \int_0^\infty V(r)w(r)dr = \frac{1}{2\sqrt[3]{6\pi^2}}\Gamma\left(\frac{2}{3}\right)\frac{n^{1/3}q^2}{\epsilon_0}$$

Potential energy at average position:

- $$V(\bar{r}) = \frac{1}{2\sqrt[3]{6\pi^2}}\frac{1}{\Gamma\left(\frac{4}{3}\right)}\frac{n^{1/3}q^2}{\epsilon_0}$$

Disorder induced heating

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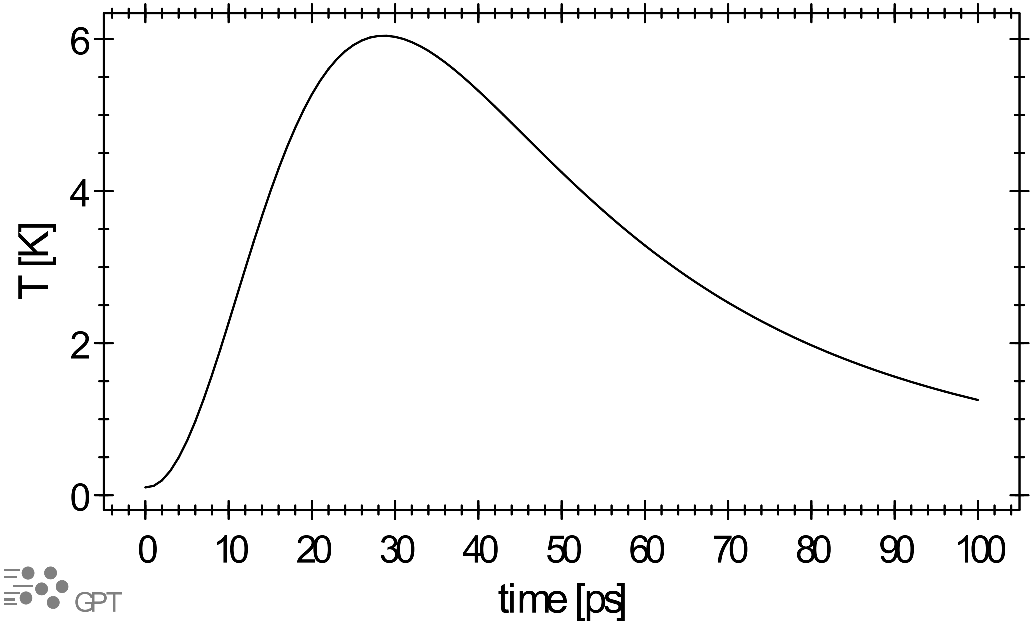
Initial random distribution

- Gives excess electrostatic energy
- Will be released over time
- $\frac{3}{2}kT = \boxed{\bar{V} - V(\bar{r})} \approx 0.03\frac{n^{1/3}q^2}{\epsilon_0}$

Example:

- $n=10^{18}$ / m^3
- T=4 K
- $1/\omega_p$=17 ps



Nearest neighbor: Electrostatic field

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Electrostatic field:

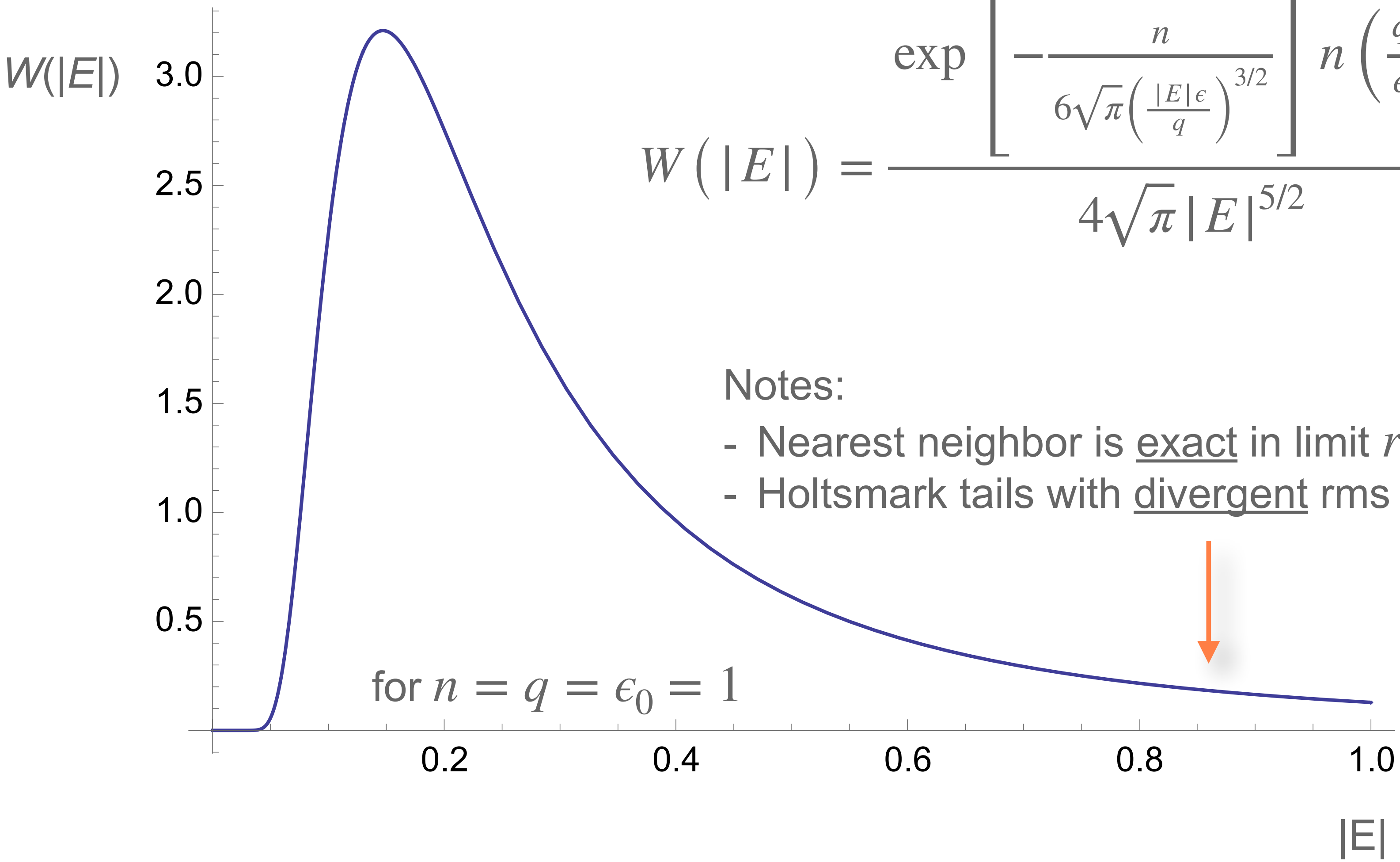
- $|E| = \frac{q}{4\pi r^2}$ therefore $r(|E|) = \sqrt{\frac{q}{4\pi\epsilon_0 |E|}}$

Probability *W*(|*E*|)

- $W(|E|) = w(r|E|)\left|\frac{d\,r(|E|)}{d|E|}\right|$
- $= \frac{\exp\left[-\frac{n}{6\sqrt{\pi}\left(\frac{|E|\epsilon}{q}\right)^{3/2}}\right] n\left(\frac{q}{\epsilon}\right)^{3/2}}{4\sqrt{\pi}|E|^{5/2}}$

Nearest neighbor: Electrostatic field

$$W(|E|) = \frac{\exp\left[-\frac{n}{6\sqrt{\pi}\left(\frac{|E|\epsilon}{q}\right)^{3/2}}\right] n \left(\frac{q}{\epsilon}\right)^{3/2}}{4\sqrt{\pi}\,|E|^{5/2}}$$



Notes:

- Nearest neighbor is exact in limit $r \to \infty$
- Holtsmark tails with divergent rms value

Ultrafast Electron Diffraction example (UED)

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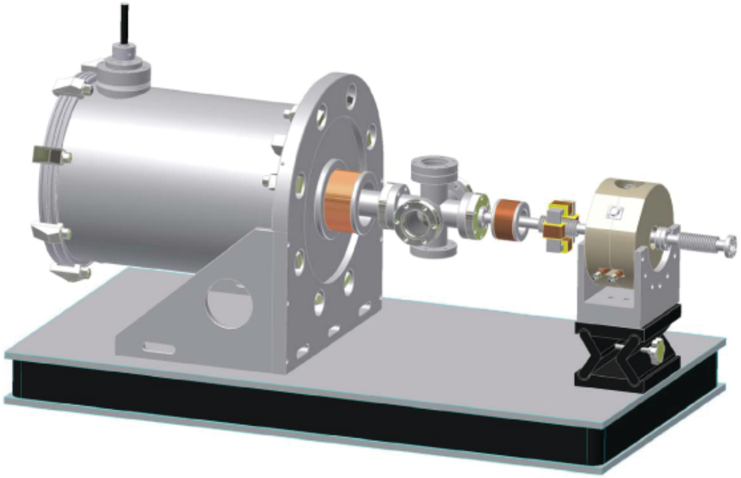
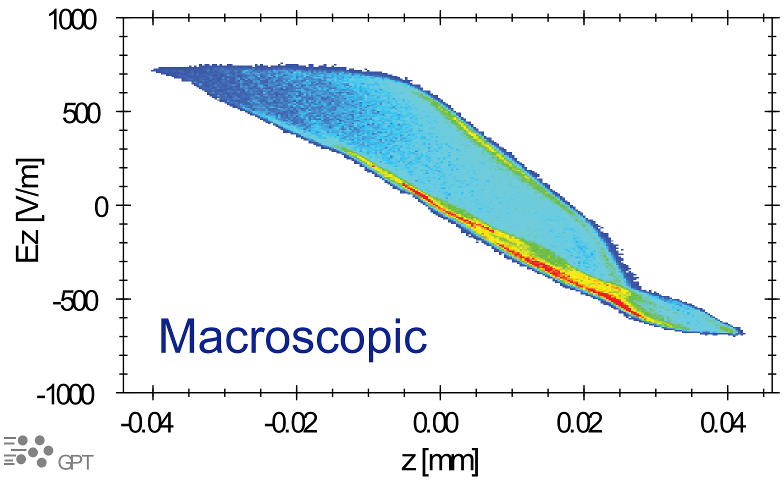
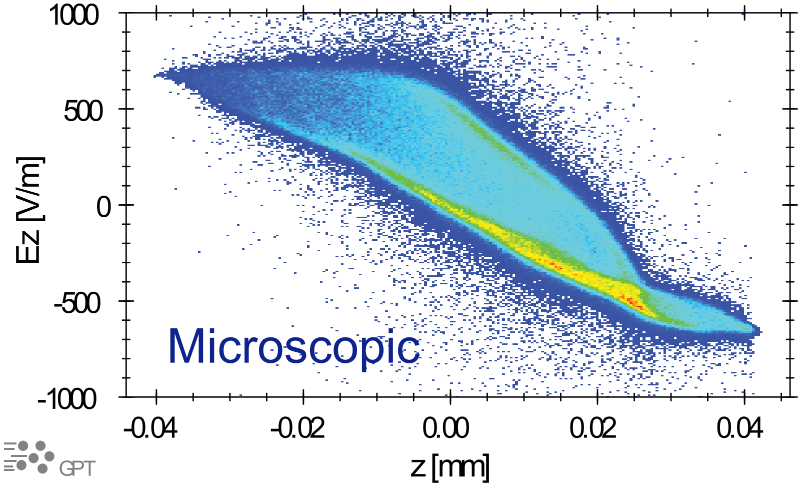
UED 100 fC

- 625000 particles
- GPT treecode (2011)







Data analytics for divergent tails

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Student

- FWHM
- Disadvantage: Bin-size affects the results

Commercial company (semiconductor)

- Use d_{50} or d_{95}

Hardcore beamline physicist

- Cut 5% of the outliers
- And keep using rms-based quantities

How NOT to simulate stochastic effects

Do NOT naively use macro particles
That is NOT a good idea
Seriously, do NOT do this
It will NOT give correct results

Why NOT:

- $\frac{3}{2}kT = \bar{V} - V(\bar{r}) \approx 0.03\frac{n^{1/3}q^2}{\epsilon_0}$
- If we have α particles per macro particle, we get for T_α:
- $\frac{3}{2}kT_\alpha \approx 0.03\frac{\left(\frac{n}{\alpha}\right)^{1/3}(\alpha q)^2}{\epsilon_0} = \alpha^{5/3}\,\frac{3}{2}kT$
- Emittance scales with $\sqrt{T/m}$, but whatever your metric, forget it.

Particle-in-cell: (Multi-grid) Poisson solver

Key features

- Anisotropic meshing to reduce number of empty nodes

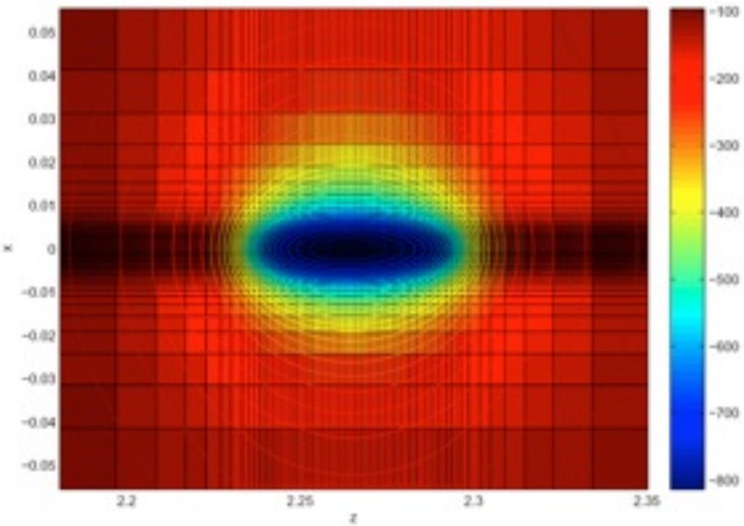
Multi-grid solver

- Developed by Dr. G. Pöplau
  Rostock University, Germany
- Scales $O(N^{\sim 1.1})$ in CPU time
- Typical use: ~10k to ~100M particles

Implementation

- MPI-usage reduces noise:
- We track more particles, on same grid

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



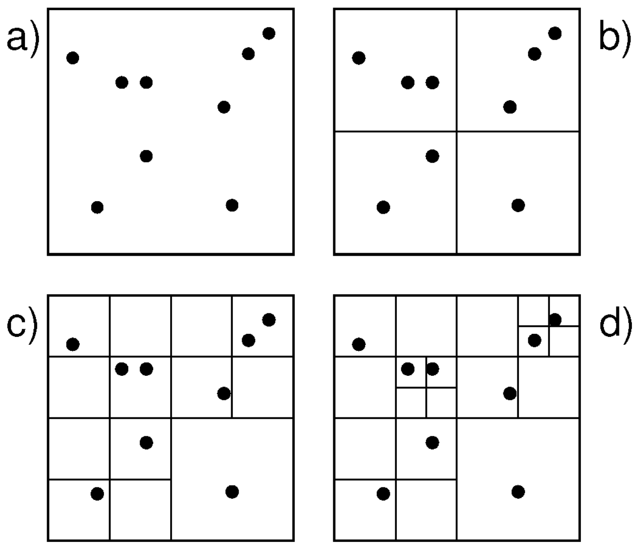
- Gisela Pöplau, Ursula van Rienen, Bas van der Geer, and Marieke de Loos, Multigrid algorithms for the fast calculation of space-charge effects in accelerator design, IEEE Transactions on magnetics, Vol 40, No. 2, (2004), p. 714.

GPT: Barnes-Hut

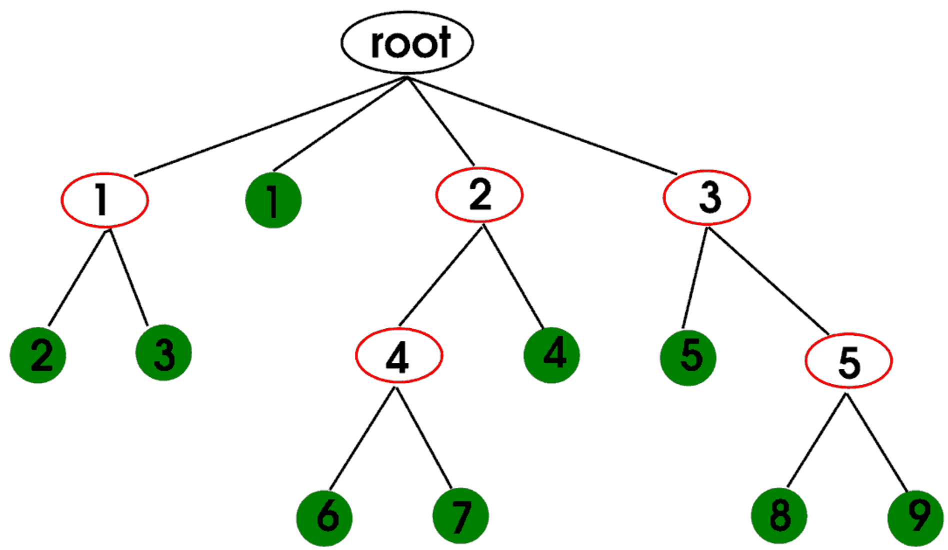
Hierarchical tree algorithm

- Includes stochastic Coulomb interactions in 3D
- *O*(*N* log *N*) in CPU time
- MPI implementation in GPT distributes same tree over all nodes

Division of space

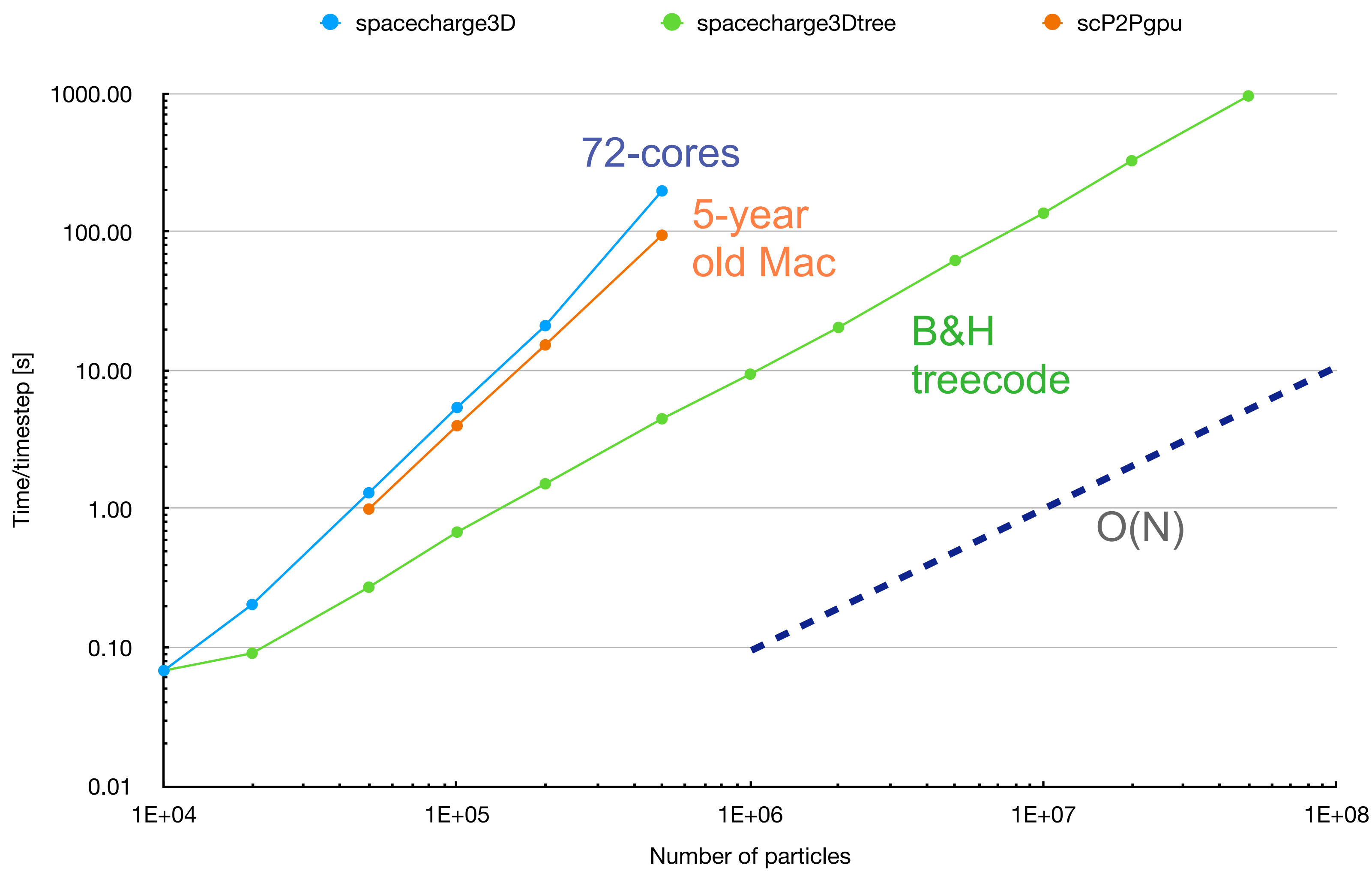


Tree data structure



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

Scaling



spacecharge3D
spacecharge3Dtree
scP2Pgpu
1000.00
100.00
10.00
1.00
0.10
0.01
Time/timestep [s]
1E+04
1E+05
1E+06
1E+07
1E+08
Number of particles
72-cores
5-year
old Mac
B&H
treecode
O(N)

Possible simulation approaches

Particle coordinates

Transform particle positions to zero momentum frame

Particles	Obtain electrostatic field:
1k	
10k	- $O(N^2)$ on a GPU
100k	
1M	- Barnes & Hut (GPT)
10M	
100M	- Particle-Particle-Particle-Mesh
1G	- Fast multipole method

Transform E-field to lab frame (gives *E* and *B*)

Track equations of motion


GPT
Bas van der Geer
The end

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.

Space-charge models in GPT

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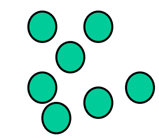
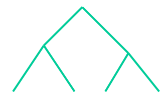
Intuitive (naïve) model

- 3D point-to-point Relativistically correct
  $O(N^2)$, N≈1000, no need for rest-frame



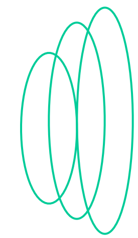
Barnes&Hut treecode

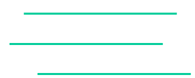
- 3D point-to-point O(N log N), N≈1M, rest-frame



Special cases

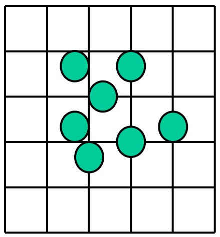
- 2D point-to-circle Cylindrically symmetric set-up
- 2D point-to-line Continuous beams
  $O(N^2)$, N≈1000, fast if applicable





PIC model

- 3D mesh-based Anisotropic multi-grid Poisson solver
  O(N), N≈1M, rest-frame
  Developed with Rostock University



GPT overview

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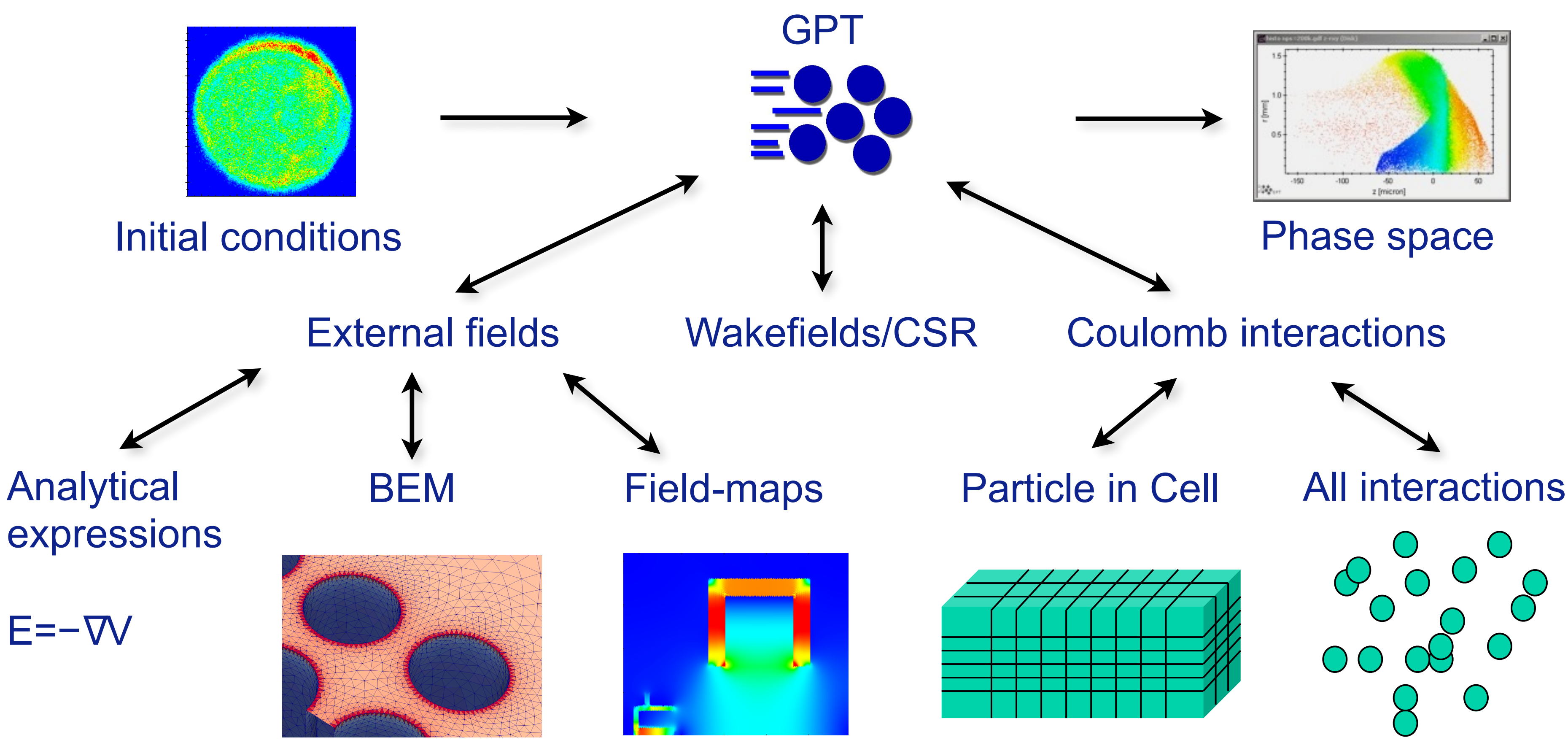
GPT tracks particles in time-domain through EM fields

- Relativistic equations of motion
- Fully 3D, including all non-linear effects



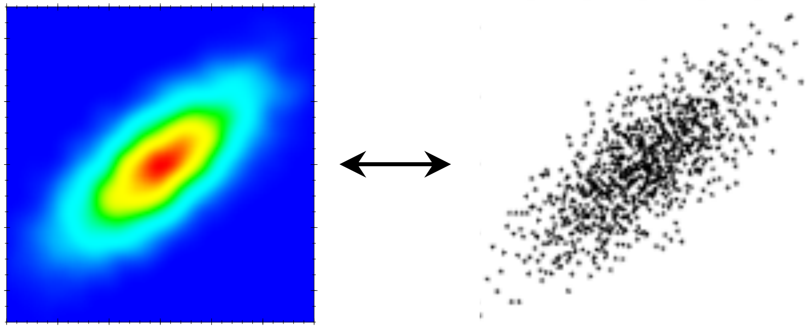
Equations of motion

GPT tracks sample particles in time-domain

- Equations of motion

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

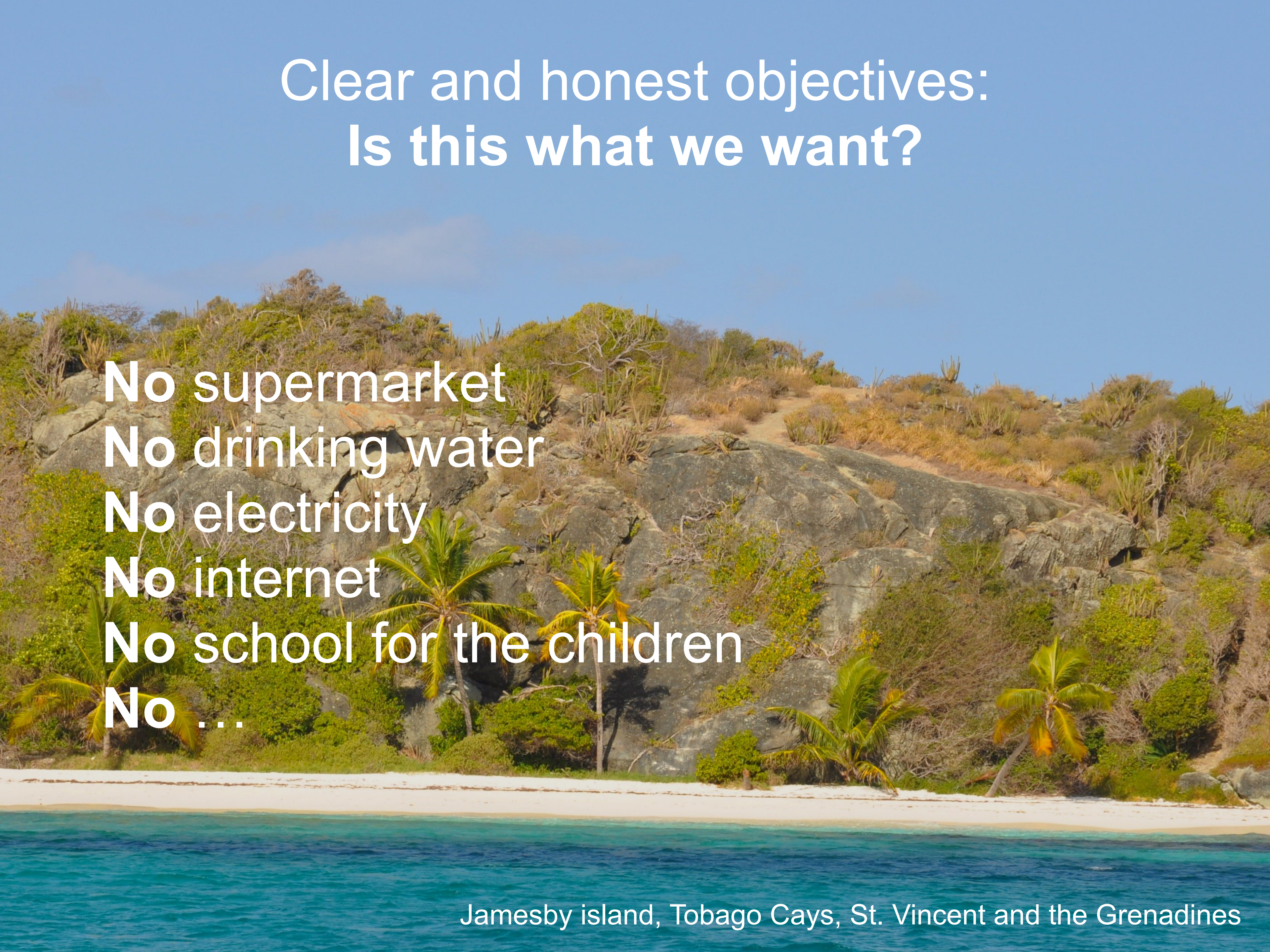
$$\frac{d\mathbf{r}}{dt} = \frac{c\,\mathbf{p}}{\sqrt{m^2c^2 + \mathbf{p}\cdot\mathbf{p}}}$$



- Include all non-linear effects

- Solved with 5th order embedded Runge Kutta, adaptive stepsize
- GPT can easily track millions of particles on a normal PC

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


Clear and honest objectives:
Is this what we want?
No supermarket
No drinking water
No electricity
No internet
No school for the children
No …
Jamesby island, Tobago Cays, St. Vincent and the Grenadines

GPT ‘paradise’ that doesn’t exist

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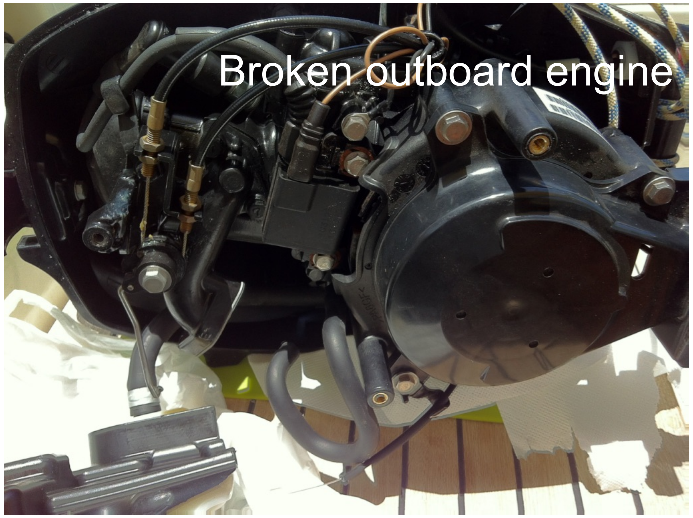
Over the years I have heard many ‘dreams’:

- Track as many particles as possible
- Use 3D field-maps for the entire set-up
- Optimise for hundreds of variables
- Fancy user interfaces
- We need the lowest rms-emittance
- …

All wrong. In fact:

- We want to design a machine that actually works
- We want to understand why an existing machine does not work (and fix it)



Equations of motion: Accuracy

ALL simulation results are wrong

The question is:

- Are the results usable?
- And that, depends on your goals!

Aim:

- Find the **lowest** accuracy that meets your goals
- **Barely good enough** is what we want

GPT algorithm:

- Tries to find the **largest stepsize**
  where all particles still meet accuracy criteria

PIC: Energy spread in rest-frame

Assumptions

- Zero momentum frame with Lorentz factor γ_v
- Relative kinetic energy spread α, measured in laboratory frame

	Kinetic energy	Lorentz factor
• Average particle:	$E_{kin}=(\gamma_v-1)\,mc^2$	1
• Fastest particle:	$(1+\alpha)\,E_{kin}$	
• Slowest particle:	$(1-\alpha)\,E_{kin}$	

$$\gamma_{u'} = 1 + \frac{1}{2}\frac{\gamma_v - 1}{\gamma_v + 1}\alpha^2 + O(\alpha^3)$$

Conclusion

- You need excessive energy spread to get relativistic velocities in the zero-momentum frame