Granularity effects
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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.
Ultracold Electron/Ion Source

Trap & Cool
Magneto-optical trap
Density $\approx 10^{16}/m^3$
RMS size $\approx 1$ mm
$T = 100 \mu$K

Ionize
Ultracold plasma
Ionization radius $\approx 50 \mu$m

Killian et al.,
PRL 83, 4776 (1999)

Ionize
Ultracold plasma
Ionization radius $\approx 50 \mu$m

Luiten et al.,
PRL 95, 164801 (2005)
McCulloch et al.,
Nat. Phys. 7, 785 (2011)
Application: Ultrafast electron diffraction

- **Structural dynamics**
- Resolve atomic **length** and **time scales**: ~1 Å, ~100 fs
Application: Focused ion beams (FIB)

- Cross Section Imaging
- TEM sample preparation
- Machining, sputtering/milling
- Beam-induced deposition
- Channeling contrast for crystalline grain analysis
- (Logo) engraving

http://www.s3.infm.it/fib.html
Laser-cooled ion source

Ionization

Excitation

Ultra-cold ion beam

MOT parameters
Temperature: 200 \( \mu \text{K} \)
\( v_{\text{th}} \) 0.22 m/s
\( n \) 10^{18} \text{ m}^{-3}

Typical current: 10 pA
\( R \) 13 \( \mu \text{m} \)
\( \sigma_L \) 1.4 \( \mu \text{m} \)

Geometry
\( V \) 2 kV
\( d \) 20 mm
\( a \) 1 mm

Simple theory predicts total collapse of brightness
But that is without acceleration…

Coulomb interactions
Laser-cooled ion source

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Coulomb interactions

Disorder induced heating

Space charge

$p_x$

Disorder induced heating

$t=0$

$t=10$ ps

$t=20$ ps

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

Ideal particle-in-Cell

All interactions

$t=0$

$t=10$ ps

$t=20$ ps

GPT simulations: $n=10^{18}$ m$^{-3}$
Analogy of a cold beam

Rhône Glacier 2012: Bas van der Geer
We need to go inside
Coulomb interactions

Macroscopic (mean field):
- 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

And many others…
Disorder induced heating

Random processes

Excess potential energy $U$

Coulomb interactions

Momentum spread

Temperature $\uparrow$

Brightness $\downarrow$

High $U$

Low $U$

\[ \sigma_{px} = \sqrt{m k T_x} \]

\[ = mc \frac{\epsilon_x}{\sigma_x} \]

\[ \Rightarrow T_x = \frac{mc^2 \epsilon_x^2}{k \sigma_x^2} \]

\[ B_\perp = \frac{J}{\pi k T} \]
Nearest neighbor

\[ w(r) \, dr: \text{Probability that the nearest neighbor is between } r \text{ and } r+dr. \]

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

assuming a uniform random distribution with number density \( n \).

Hence: \[
w(r) = \frac{4\pi r^2 n}{e^{4\pi r^3 n}}
\]

Stochastic problems in Physics and astronomy,
Reviews of Modern Physics 15
Chandrasekhar, 1943.
Where are my neighbors?

Average distance:
\[
\bar{r} = \int_0^\infty r \cdot w(r) dr = \frac{1}{3} \Gamma\left(\frac{1}{3}\right) \frac{1}{\frac{4}{3} \pi n} \\
\approx 0.89 r_s
\]

Most likely position:
\[
\frac{d}{dr} w(r) = 0 \Rightarrow r = \frac{2}{3} r_s \approx 0.87 r_s
\]

Wigner-Seitz radius:
\[
r_s = \frac{1}{\sqrt[3]{\frac{4}{3} \pi n}}
\]
\[
\frac{1}{n} = \frac{4}{3} \pi r_s^3
\]
Average potential energy:
\[
\bar{V} = \int_{0}^{\infty} V(r)w(r)dr = \frac{1}{2} (6\pi^2)^{-1/3} \Gamma\left(\frac{2}{3}\right) \frac{n^{1/3} q^2}{\varepsilon_0}
\]

Potential energy at average position:
\[
V(\bar{r}) = \frac{1}{2 (6\pi^2)^{1/3} \Gamma\left(\frac{4}{3}\right)} \frac{n^{1/3} q^2}{\varepsilon_0}
\]

It’s the difference that matters:
\[
\frac{3}{2} kT = \bar{V} - V(\bar{r}) \approx 0.03 \frac{n^{1/3} q^2}{\varepsilon_0}
\]
Paradigm shift

**Photo/thermionic emission**

- 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, P³M)
  - Every particle matters
  - Ions and electrons
  - Ab initio
  - No Liouville to the rescue
  - Divergent rms values

\[ k T_{\text{photogun}} \gg 0.02 n^{1/3} \frac{q^2}{\varepsilon_0} \gg k T_{\text{laser-cooled}} \]
Application: Focused ion beam

- **Aim:** Lots of current at nm spotsizes
- **Design disaster:** Beams heats up during acceleration
‘Typical’ simulation code: GPT

Tracks sample particles in **time-domain**
- Relativistic equations of motion
- Fully 3D, including all non-linear effects

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

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External fields

Analytical expressions

Field-maps

Coulomb interactions

Particle in Cell

All interactions

$\{E,B\}=f(x,y,z,t)$
Algorithms...

All interactions $O(N^2)$:
- PP Particle-Particle $\rightarrow$ slow
- $P^3M$ Particle-Particle Particle-Mesh

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

Imaga credit: Southern European observatory
Barnes-Hut

Hierarchical tree algorithm:
- Includes all Coulomb interactions
- O(N log N) in CPU time
- User-selectable accuracy

GPT hardware requirements

GPT kernel:
- Programming language: C and C++
- Multi-core functionality: openMP
- Distributed scans: MPI

If you can run Microsoft Office, you can track ~1M particles

HP blade server: 16 servers, 128 cores, 1.2 kW of GPT power!
Application: Focused ion beam

- **Aim:** Lots of current at nm spotsizes
- **Design disaster:** Beams heats up during acceleration
- **Multi-objective global optimization**

Further slides are intentionally removed.
Laser-cooled e\textsuperscript{-} source

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

**Particles:**
- Charge: 0.1 pC (625k e\textsuperscript{-})
- Initial density: \(10^{18} / \text{m}^3\)
- Ionization time: 10 ps
- Initial Temp: 1 K

**GPT tracking:**
- All particles
- Realistic fields
- All interactions
Laser cooled e\textsuperscript{−} diffraction

GPT results:

\( \varepsilon_x \) 20 nm (rms)

10% slice \(~1\) nm

Energy 120 keV

Spread 1%

\( \varepsilon_z \) 60 keV fs

Charge 0.1 \( \text{pC} \)

(625,000 e\textsuperscript{−})

S.B. van der Geer, M.J. de Loos, E.J.D. Vredenbregt, and O.J. Luiten
Granularity effects are becoming increasingly relevant
• Physics: Nearest neighbor interaction

Design simulations need:
• Sub-nm precision
• Lots of particles for good statistics
• All pair-wise Coulomb interactions
• Start-to-end in 3D in complicated fields
• Multi-objective optimizations

TODO
! Break randomness in either space or time