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MD Simulation of Coulomb Crystals

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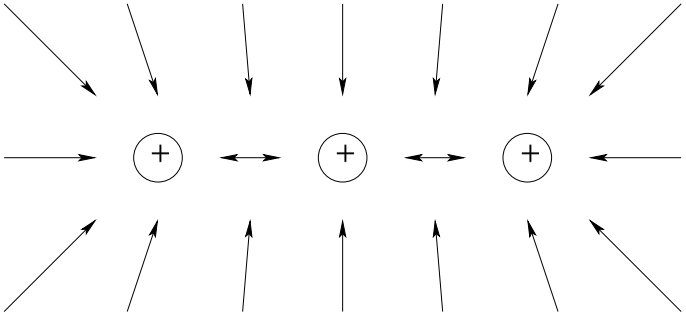
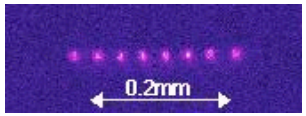
What are Coulomb crystals?

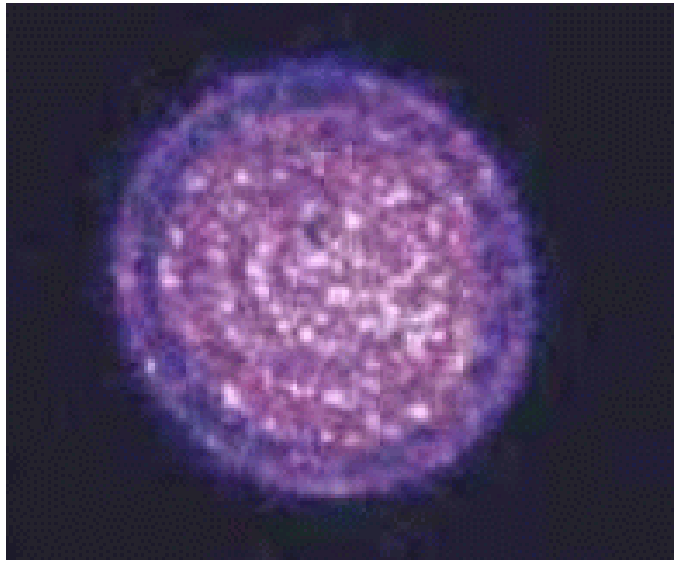
- A system of positive charged ions (1-10^6) trapped by a magnetic field.

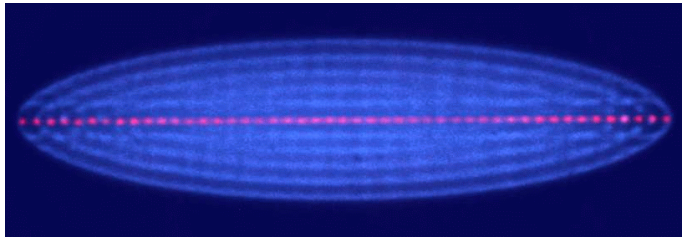




- A candidate for Quantum Processors.
- A possibility to study strongly coupled systems with only positive charges.

Experiments





Left: Monocomponent, sphere.

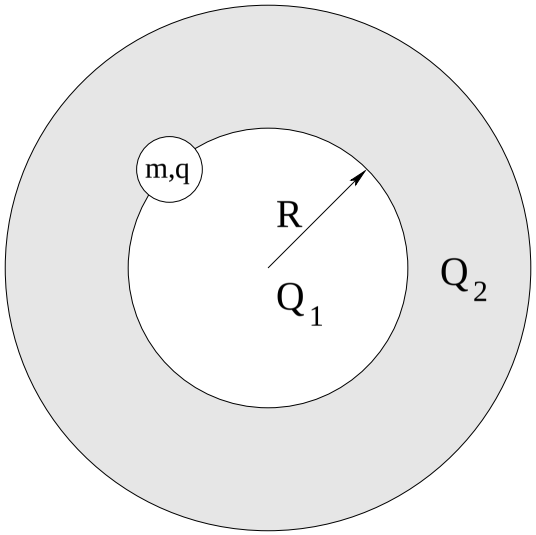
Right: Bicomponent, string, Ca^{+}_{40} (Blue), Mg^{+}_{24} (Red).

Physical model

$T = 0 \Rightarrow$ Quantum Mechanics and $\lambda = \frac{h}{mv}$ significant.

$T \approx 1\mu$K $\Rightarrow$ Classical Approximation $\Rightarrow$ Classical Molecular Dynamics (Newton's equation of motion)

Physical model (cont.)



$$F_{\text{Coul}} = \frac{1}{4\pi\epsilon_0}\frac{Q_1 q}{R^2}, F_{\text{Trap}} = m\omega^2 R.$$

$$F_{\text{Coul}} = F_{\text{Trap}} \Rightarrow R = \left(\frac{Q_1}{4\pi\epsilon_0\omega^2}\frac{q}{m}\right)^{\frac{1}{3}}.$$

NB: Independent of $\frac{q}{m}$.

- Investigation of the structure and dynamics of so-called ions trapped in a electric and magnetic field (Paul Trap) with 1 - 10^6 ions.
- Radial distribution and shell structure (or not) of mono- and bicomponent (Ca^{+}_{40} and A^{2+}_{80}) crystals.
- Dynamical features of finite temperature (1μK).
- Future work: Full treatment of quantal effects.

$$m_i \frac{\partial^2}{\partial t^2} \vec{x}_i(t) = \vec{F}_i(t) - \xi \frac{\partial}{\partial t} \vec{x}_i(t) \qquad (1)$$

$$\frac{\partial}{\partial t} \xi = \alpha \left(T - T_{\text{equlibrium}} \right) \qquad (2)$$

$$\vec{F}_i = -\nabla_i U \qquad (3)$$

$$U = \frac{1}{4\pi\epsilon_0} \sum_{i=1, j>i}^{N} \frac{q_i q_j}{\left\| \vec{x}_{ij} \right\|} + \frac{1}{2} \sum_{i=1}^{N} m_i \omega^2 \vec{x}_i^2 \qquad (4)$$

Molecular Dynamics (MD) (cont.)

Newton's equation of motion solved by the numerical Leap-Frog method with Nosé-Hoover thermostat:

$$v^{t+\frac{1}{2}} = v^{t-\frac{1}{2}} - \frac{\Delta t}{m}\left(F^t - \xi^t v^{t-\frac{1}{2}}\right) \tag{5}$$

$$\frac{\partial \xi^{t+\frac{1}{2}}}{\partial t} = Q\left(\sum_{i=1}^{N} m_i (v_i^{t+\frac{1}{2}})^2 - \frac{3N}{2k_b}T\right) \tag{6}$$

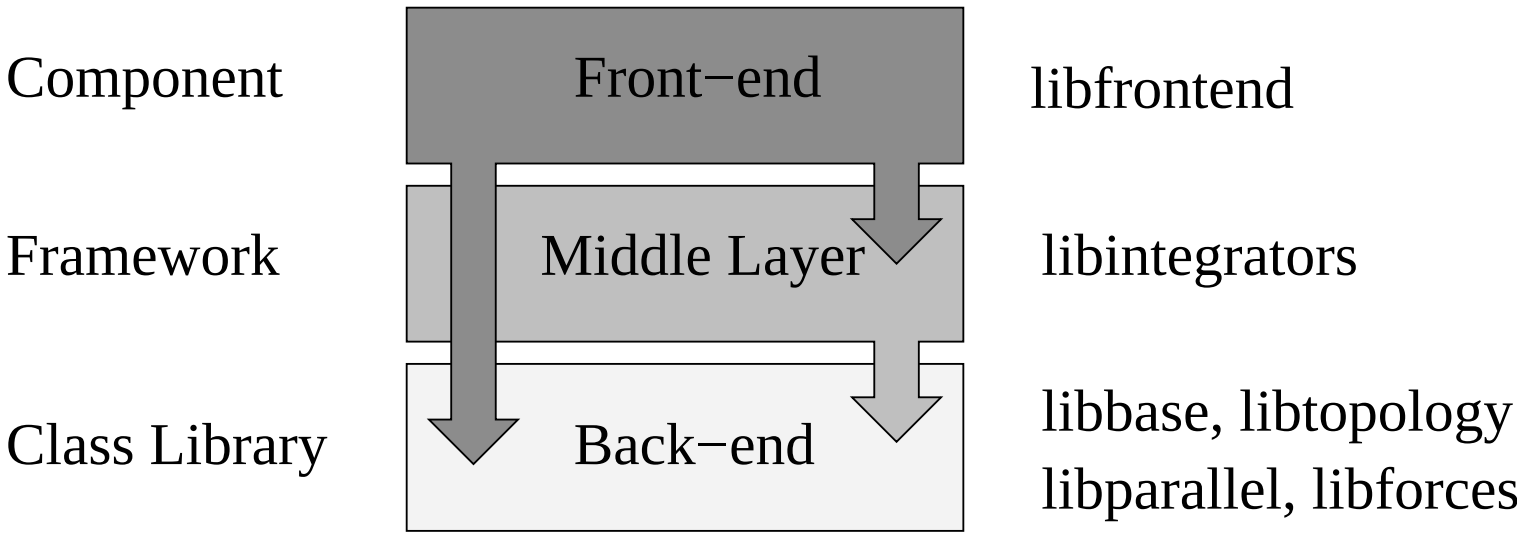
$$x^{t+1} = x^t + \Delta t v^{t+\frac{1}{2}} \tag{7}$$

$$\xi^{t+1} = \xi^t + \Delta t \frac{\partial \xi^{t+\frac{1}{2}}}{\partial t}. \tag{8}$$

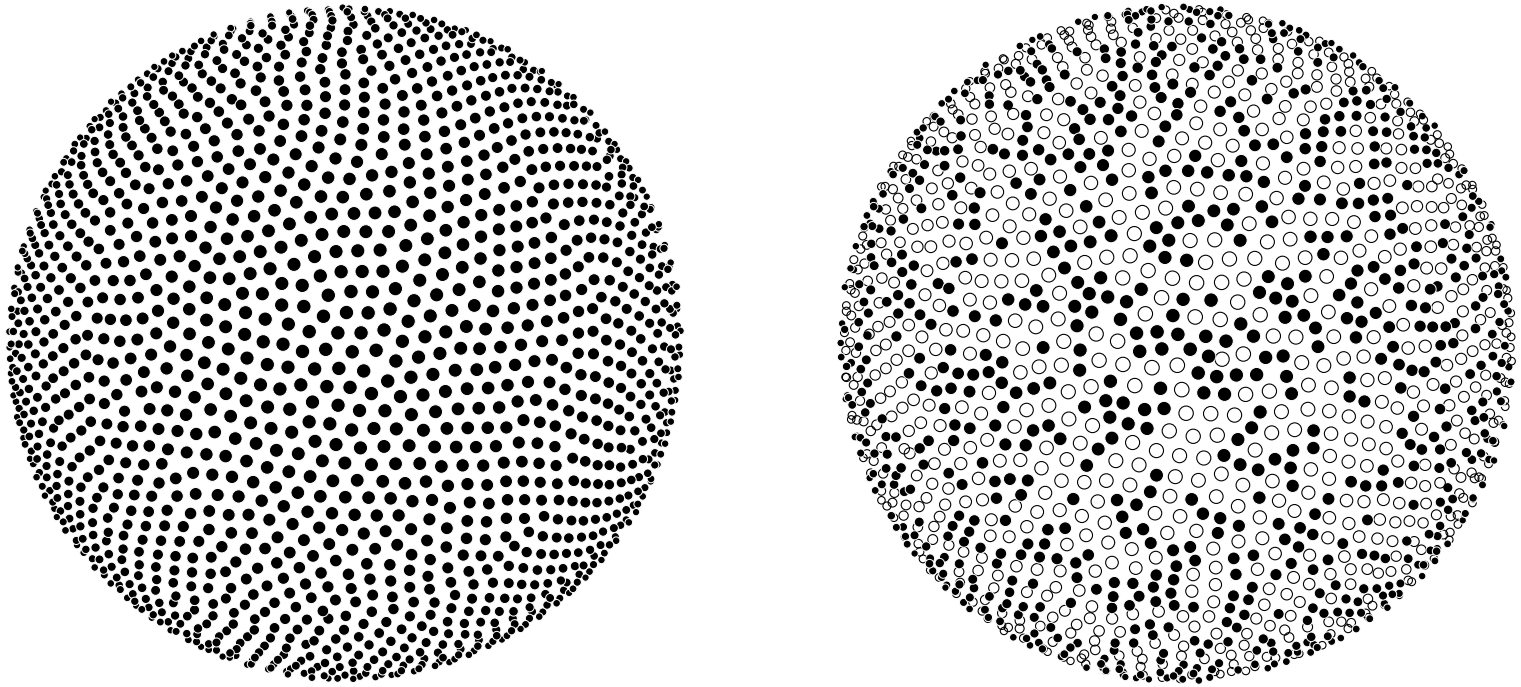
PROTOMOL – a molecular dynamics framework

- An object-oriented component based framework for molecular dynamics simulations.
- Designed for high flexibility, easy extendibility and maintenance, and high performance demands, including parallelization.
- Support of multiple time-stepping integration.
- Fast electrostatic force evaluation algorithms like plain Ewald ($O(N^{\frac{3}{2}})$), Particle-Mesh-Ewald ($O(N \log N)$), and Multigrid summation ($O(N)$).

PROTOMOL – a molecular dynamics framework (cont.)



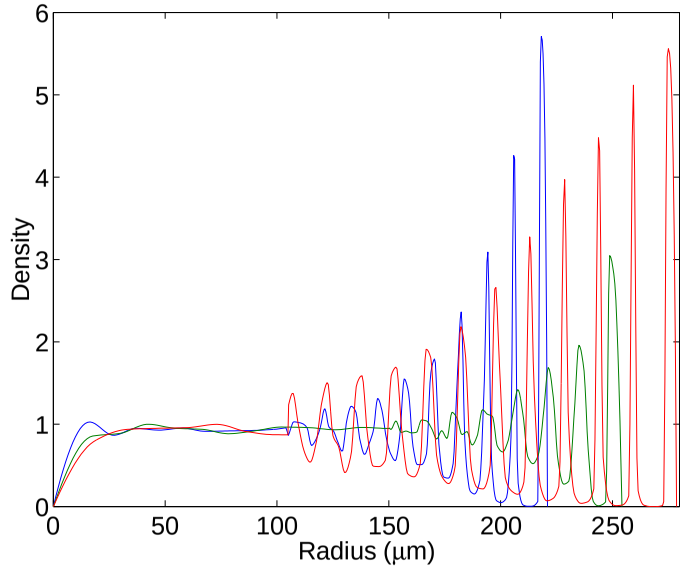
Front hemisphere of the outer shell

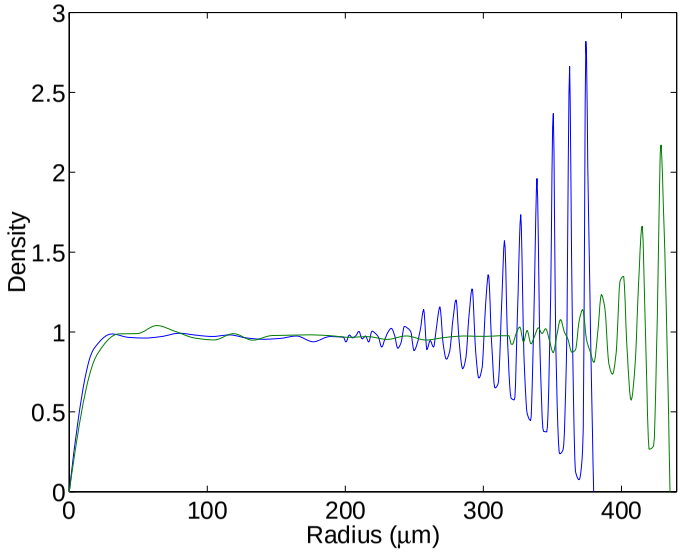


Left: System of a 20,288 Ca^{+}_{40}.

Right: System of a 10,144 $Ca^{+}_{40}(\circ)$ and 10,144 $A^{2+}_{80}(\bullet)$ system.

Radial distribution of mono- and bicomponent crystals





Left: 20,288 Ca^{+}_{40} (Blue), and 10,144 Ca^{+}_{40} and 10,144 A^{2+}_{80} (Green), and 20,288 A^{2+}_{80} (Red) ions. **Right**: 100,000 Ca^{+}_{40} (Blue), and 50,000 Ca^{+}_{40} and 50,000 A^{2+}_{80} (Green) ions. The inner part has been smoothed.

Conclusions

- Simulations result in clear outer shell structure in large bicomponent ion crystals with identical q/m ration.
- Each component have slightly different shell radii resulting in an interesting “double structure” of each shell.

Partners

- Jan Petter Hansen, University of Bergen.
- Michael Drewsen, The ion Trap group, Institute of Physics and Astronomy, University of Aarhus.
- PROTOMOL is a collaboration work with Jesús A. Izaguirre, CSE, University of Notre Dame, USA.