

**PROTOMOL and its Application to  
UgelstadspHERE Dynamics  
and Coulomb Crystals**

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- Introduction
- Physical and Numerical Model
- PROTO MOL – A Molecular Dynamics Framework
- Coulomb Crystals
- UgelstadspHERE Dynamics
- Conclusions & Future Work
- Demo / Movies

- Modeling of phenomena in nature
- Study of dynamic properties of micro and macro problems
- Representation by particles
- Examples: Water molecules, sand grains, billiard, solar-system, etc.

- Particles

- Interaction between particles

- Newton's equation of motion

$$m_i \frac{d^2 \vec{x}_i(t)}{dt^2} = \vec{F}_i(t)$$

$$\vec{F}_i = -\nabla_i U(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N)$$

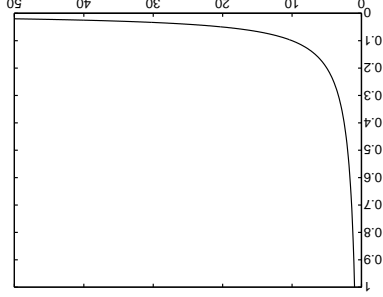
1. Compute/evaluate forces for all particles
2. Update positions & velocities

$$U = U_{\text{bonded}} + U_{\text{non-bonded}} + U_{\text{external}}$$

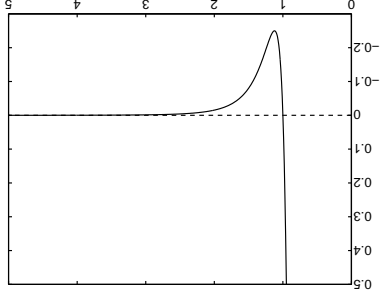
$$U_{\text{bonded}} = U_{\text{bond}} + U_{\text{angle}} + U_{\text{dihedral}} + U_{\text{improper}}$$

$$U_{\text{non-bonded}} = U_{\text{electrostatic}} + U_{\text{Lennard-Jones}}$$

$$U_{\text{electrostatic}}^{ij} = \frac{1}{4\pi\epsilon_0} \frac{q_i q_j}{\|\vec{x}_{ij}\|}$$



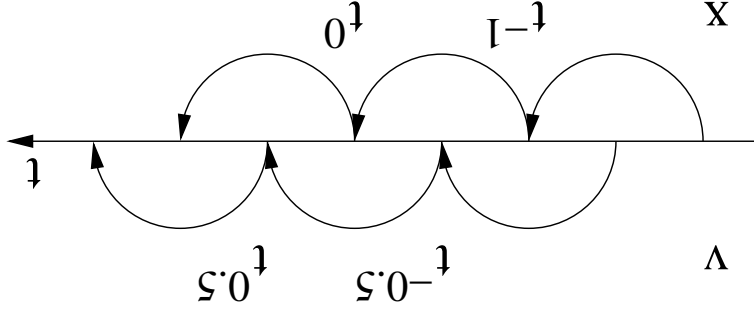
$$U_{\text{Lennard-Jones}}^{ij} = \frac{A_{ij}}{\|\vec{x}_{ij}\|^{12}} - \frac{B_{ij}}{\|\vec{x}_{ij}\|^6}$$



Often solved by Leap-Frog method:

$$v_{t+\frac{1}{2}} = v_{t-\frac{1}{2}} + \frac{\Delta t}{m} F_t$$

$$x_{t+1} = x_t + v_{t+\frac{1}{2}} \Delta t$$



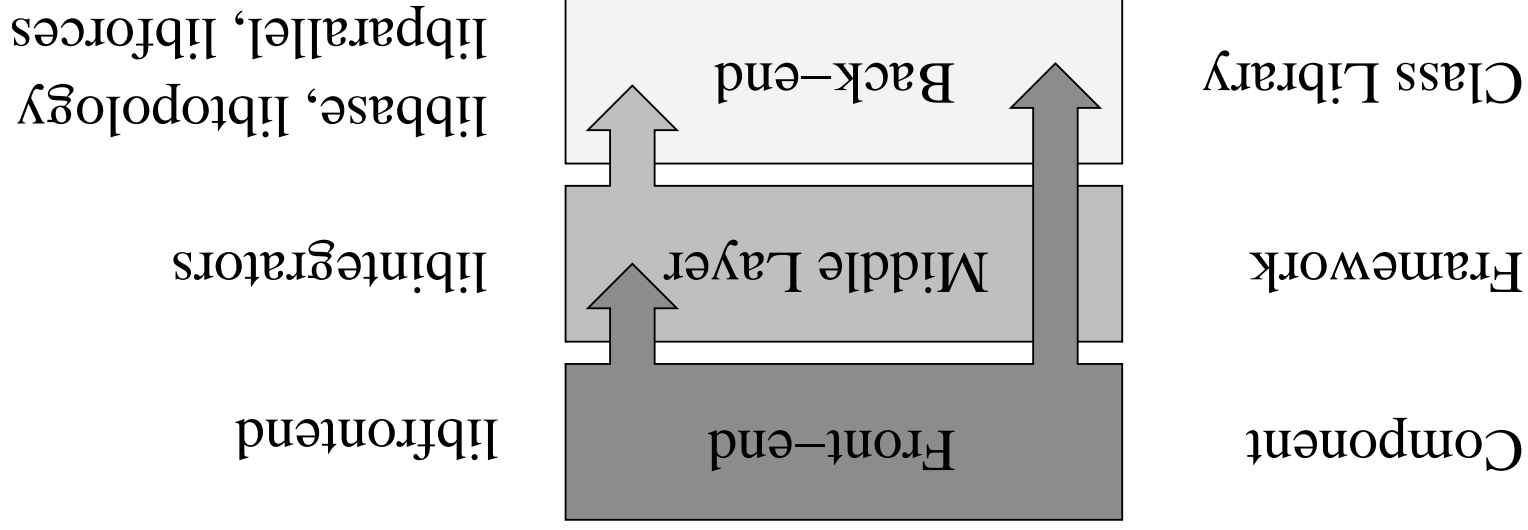
- Time step  $\Delta t$  typically 1 femtosecond ( $1 \text{ fs} = 10^{-15} \text{ s}$ )
- Multiple time-stepping to address the different time scales of forces

1. Construct initial configuration of  $x_0$ ,  $v_0$  and  $F_0$ ;
2. Loop 1 to number of steps
  - (a) Update velocities
  - (b) Evaluate forces on each particle
  - (c) Update positions
  - (d) Update velocities
3. Post-processing

- Existing (highly optimized) frameworks are not easy to extend with new algorithms
- No real encapsulation of data distribution & parallelization
- No fully customizable integrators and forces
- General purpose MD research platform
- Framework to develop and evaluate new methods – fair comparison



- An object-oriented component based framework for molecular dynamics simulations
- Designed for high flexibility, easy extensibility and maintenance, and high performance demands
- Incremental parallelization
- Support of multiple time-stepping integration
- Generic forces and fast electrostatic force evaluation algorithms like plain Ewald ( $\mathcal{O}(N^{\frac{3}{2}})$ ), Particle-Mesh-Ewald ( $\mathcal{O}(N \log N)$ ), and multi-grid ( $\mathcal{O}(N)$ )



Incremental parallelization

- Implementation sequential version of a new algorithm, for verification

- Parallel and sequential parts go hand in hand
- Benefit from already parallelized components
- Extend to parallel version

Master-slave with data replication and force decomposition

Distribute  $U = U_{\text{bond}} + U_{\text{angle}} + U_{\text{dihedral}} + U_{\text{improper}} + U_{\text{electrostatic}} + U_{\text{Lennard-Jones}}$

## Support of multiple time-stepping integration

```
Integrator {  
  level 2 Impulse { # Long-range electrostatics  
    cyclelength 4  
    force coulomb -algorithm Full -switchingFunction ComplementSWC1}  
    level 1 Impulse { # Medium varying forces  
      cyclelength 2  
      force improper, Dihedral  
      force coulomb -algorithm cutoff -switchingFunction SWC1  
      force lennardjones -algorithm cutoff -switchingFunction SWC1  
      level 0 Leapfrog { # Fast varying forces  
        timestep 1 # [fs]  
        force Bond, Angle}}
```

## Three-level Verlet/r-RESPA MTS

## Generic forces

R1 Algorithm to select an  $n$ -tuple of particles

R2 Boundary conditions

R3 Retrieve efficiently ( $\mathcal{O}(1)$ ) the spatial information of each particle

R4 Potential defining the force and energy on the  $n$ -tuple

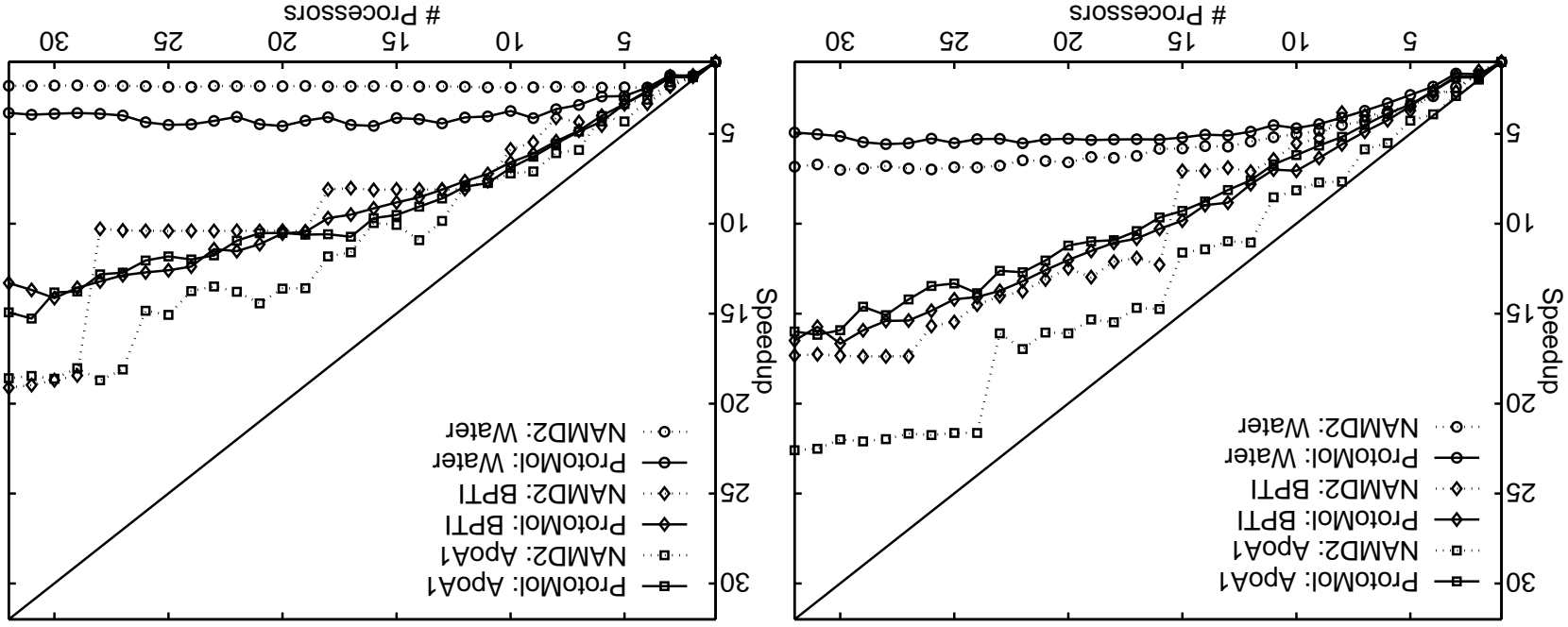
R5 Switching function to modify the potential

← Policy, Abstract Factory and Prototypes

- Object-oriented component framework, C++, 40,000 LOC, 180 classes
- Integrator hierarchy, suited for multiple time-stepping
- Generic forces and algorithms
- Switching functions to smooth/split forces/potentials
- Interface to standard I/O formats (PDB, PSF, PAR, XYZ, DCD, CHARMM 19/28, ...) and applications
- Components for parallelization & data distribution

Test case	# atoms	PROTOMOL [ $\mu$ s] / $N$	NAMD2 [ $\mu$ s] / $N$	Ratio
Water vacuum	423	25.53	28.84	0.89
periodic		36.88	35.23	1.05
BPTI vacuum	14,281	54.8	62.25	0.88
periodic		97.01	85.15	1.14
ApoA1 vacuum	92,224	60.96	70.88	0.86
periodic		100.04	109.04	0.92

Pentium III, 1.26 GHz running Linux RedHat

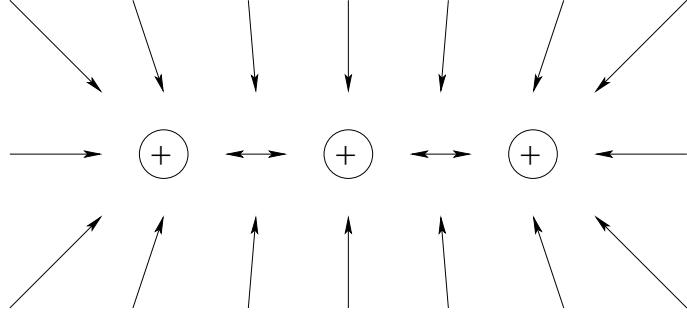


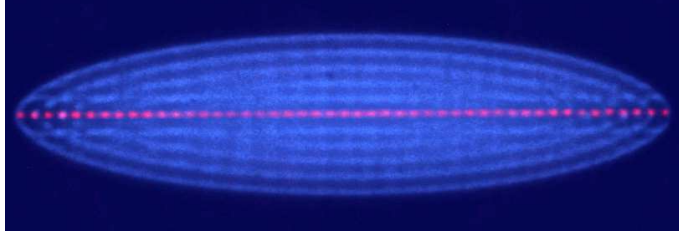
Origin2000, 195MHz R10000 processors



What are Coulomb Crystals?

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



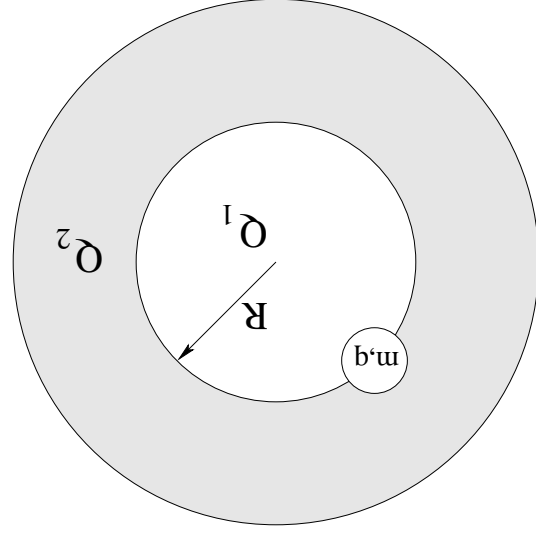


Left: Monocomponent, sphere.

Right: Bicomponent, string,  $\text{Ca}^+$  (●),  $\text{Mg}^+$  (●).

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

$T \approx 1\mu\text{K} \Leftrightarrow$  Classical Approximation  $\Leftrightarrow$  Classical Molecular Dynamics (Newton's equation of motion)



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

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

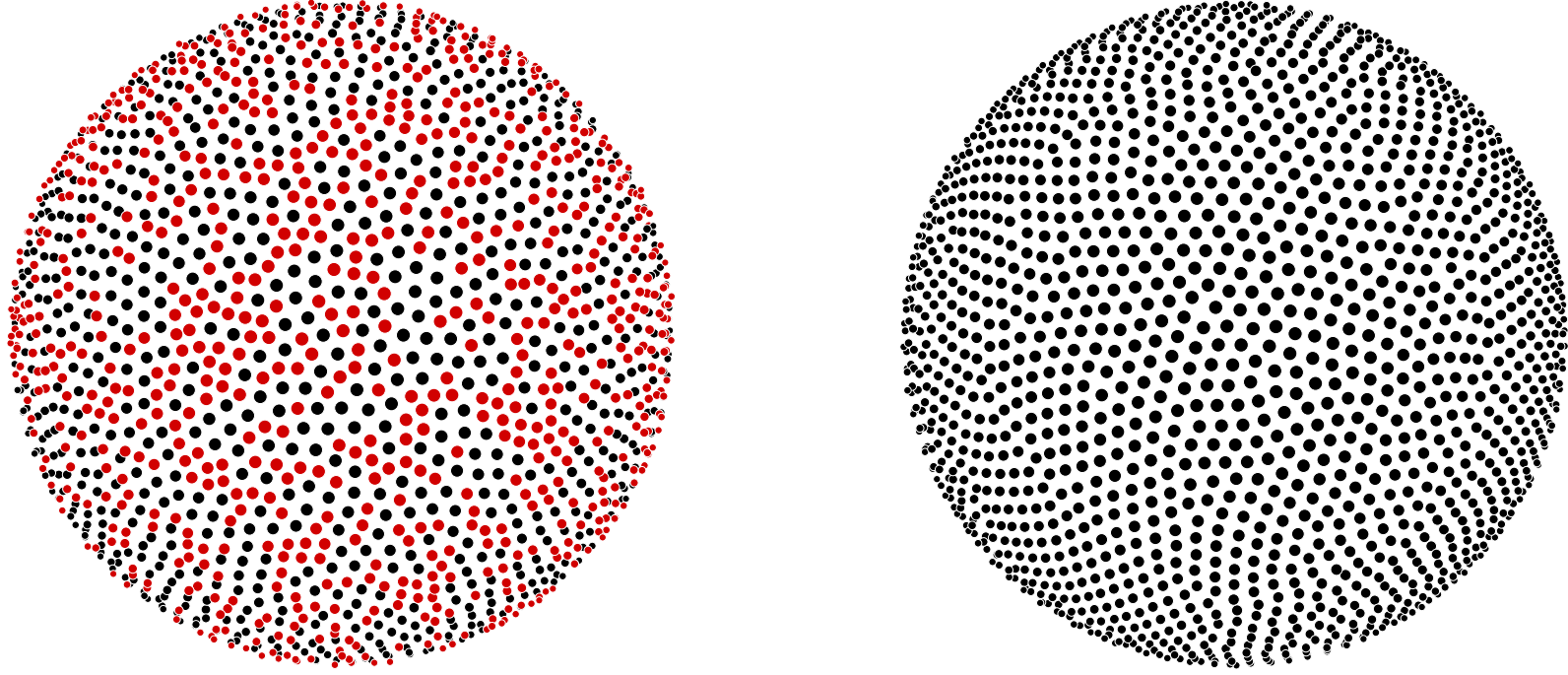
NB: Independent of  $m$ .

## Molecular Dynamics simulations

$$U = \frac{1}{4\pi\epsilon_0} \sum_{i=1, j>i}^N \frac{q_i q_j}{\|\vec{x}_{ij}\|} + \frac{1}{2} \sum_{i=1}^N m_i \omega_i^2 x_i^2 \quad (3)$$

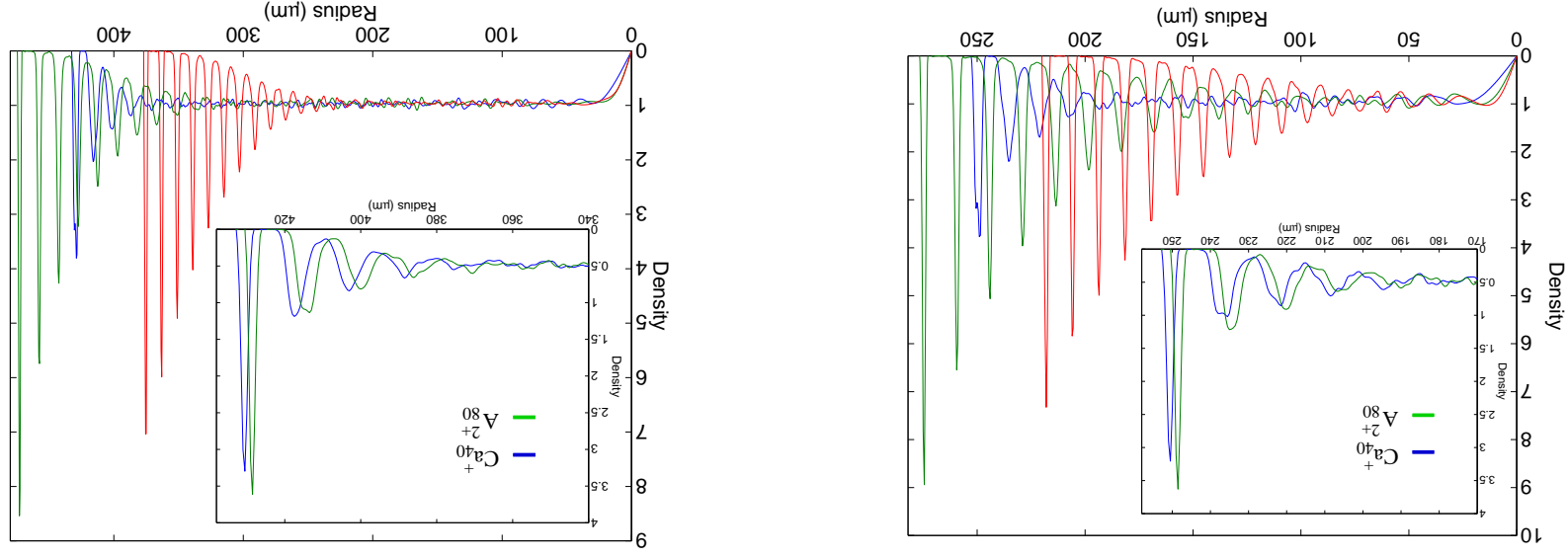
- Newton's equation of motion solved by the numerical Leap-Frog method with Nosé-Hoover thermostat

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



Left: Front hemisphere of the outer shell, 20,288  $\text{Ca}^{40}_+$ .

Right: Front hemisphere of the outer shell, 10,144  $\text{Ca}^{40}_+$  (●) and 10,144  $\text{A}^{80}_{2+}$  (●).

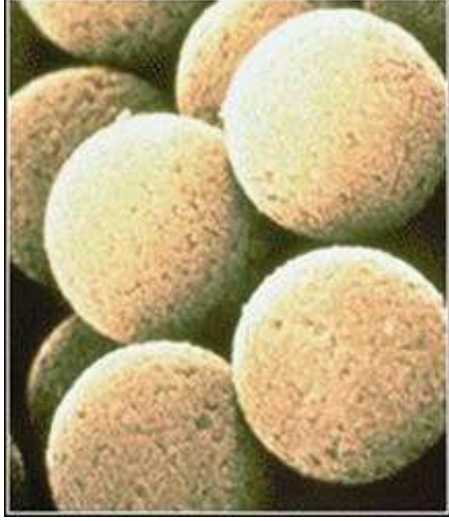


Left: 20,288  $A_{80}^{2+}$  (-), and 10,144  $Ca_{40}^{40+}$  (-), and 20,288  $Ca_{40}^{40+}$  (-) ions. Right: 100,000  $A_{80}^{2+}$  (-), and 50,000  $Ca_{40}^{40+}$  (-), and 100,000  $Ca_{40}^{40+}$  (-) ions. The inner part has been smoothed.



- Simulations result in clear outer shell structure in large bicomponent ion crystals with identical  $q/m$  ratio
- Each component have slightly different shell radii resulting in an interesting “double structure” of each shell
- The inner part – no-structured – is of fluid nature

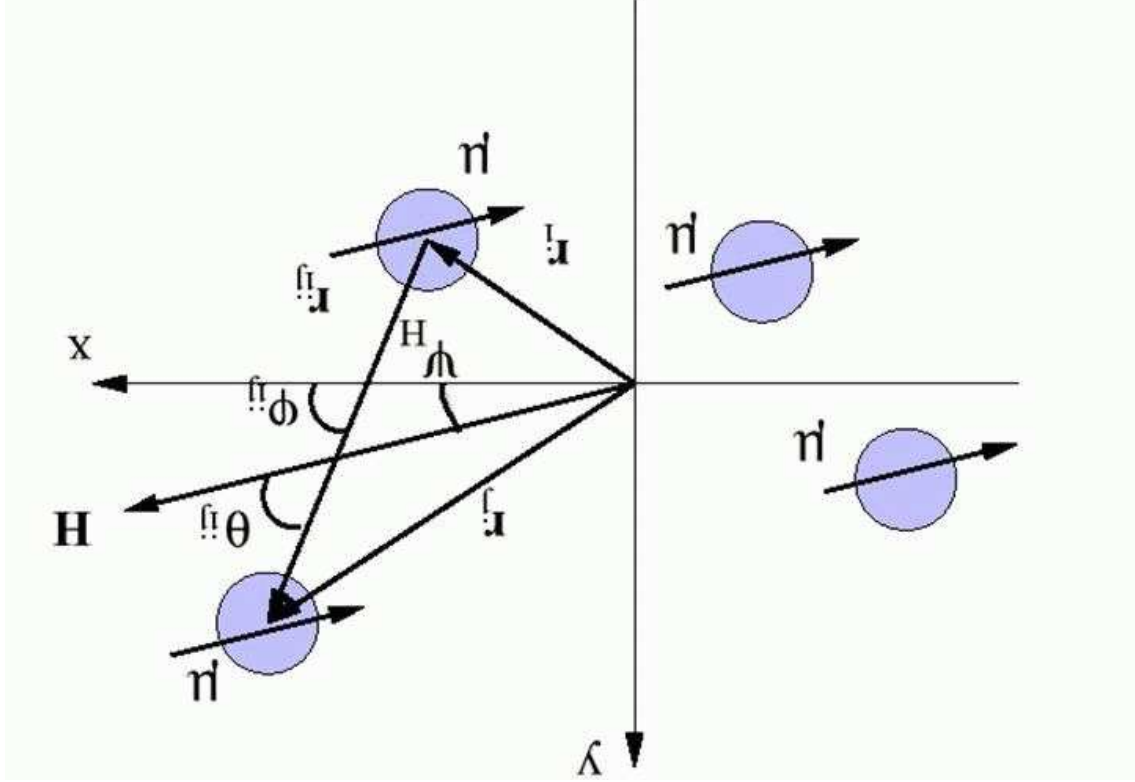
- Size range of 1-100  $\mu\text{m}$
- Uniform to 1% of the size
- Syntheses: polyethylene
- Can be magnetized

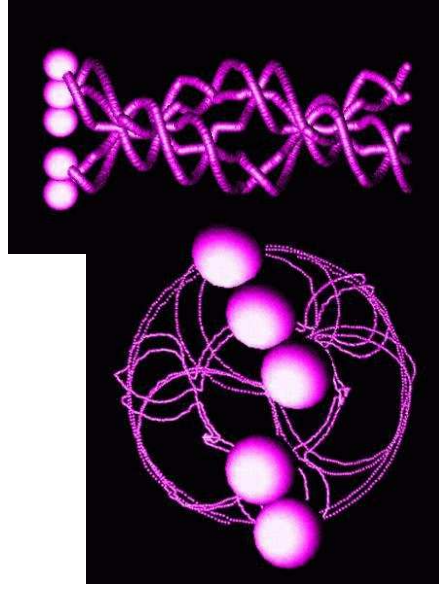


- Medicine
- Paint technology
- Computers
- Phase transition simulations

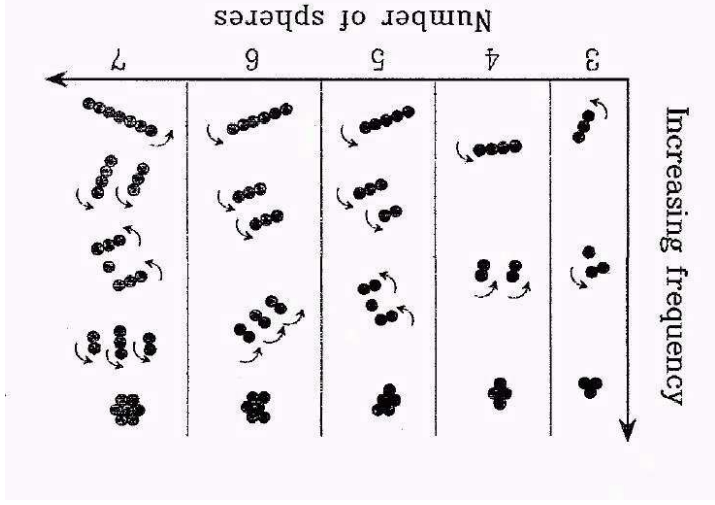


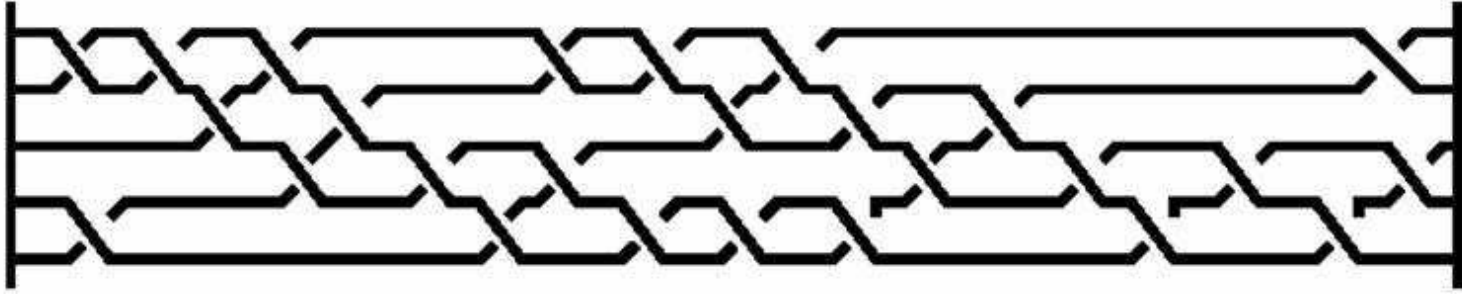
- Magnetic nano-size particles suspended in a fluid
- Dilute ferrofluid:  $> 10$  vol % ferro-particles
- No hysteresis (superparamagnetic)
- Based on kerosene ferrofluid





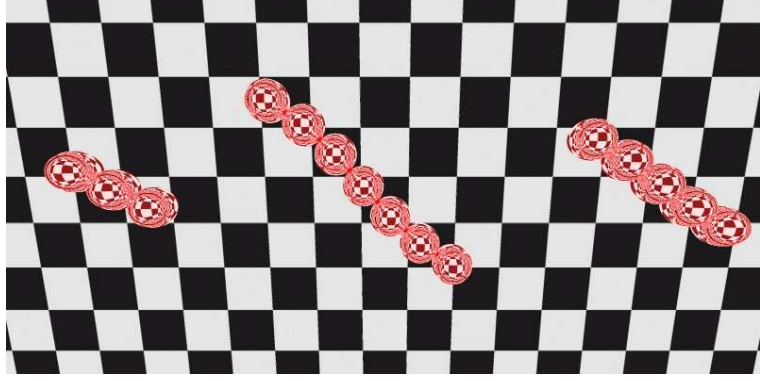
With a rotating field stretched out in time





Statistical analysis  $\Leftrightarrow$  knots theory (Writhe)

- Leapfrog
- Dipole-dipole and the dipole-mirror interactions ( $\mathcal{O}(N^2)$ )
- Mirror effects
- Friction

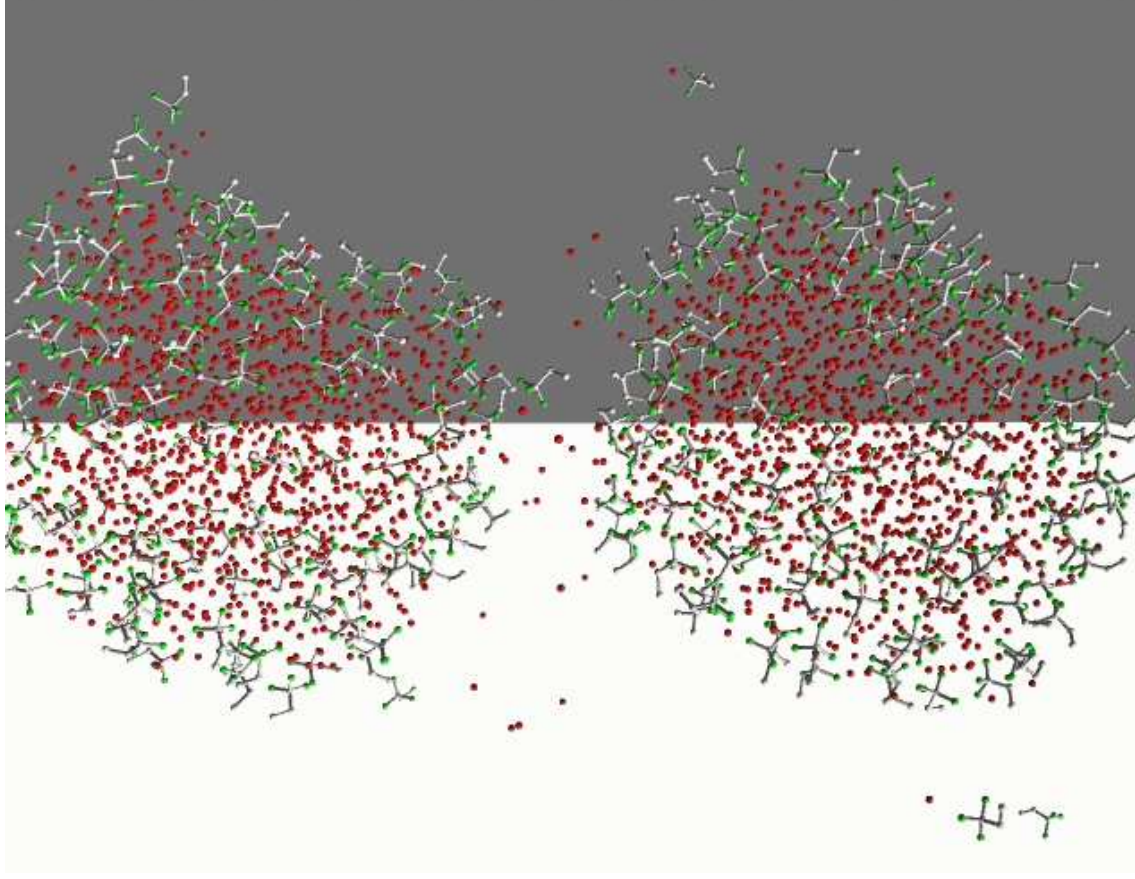


Ugelstad spheres in a magnetic fluid and an applied magnetic field.



- Dipole-dipole interaction
- Stoke's law for spheres in a viscous medium
- Runge-Kutta's fourth order
- Hydrodynamics interaction between spheres
- Acceleration
- Parallel computing & large systems
- Faster force algorithm – less than  $\mathcal{O}(N^2)$

Coalescence of two water droplets in a gas phase. Particles represent hydrophilic and hydrophobic groups.



- Well suited for non-core MD simulations
- General MD framework for research & education
- Platform to develop and evaluate novel methods & algorithms
- Good sequential and parallel scaling

- Automatic choice of optimal methods and their parameters
- Generalization of parallelization & data distribution
- I/O enhancement – to reach new user groups
- Abstraction by (scientific) design patterns
- Integrators

- Jan Petter Hansen and his students, University of Bergen.
- Michael Drewsen, The ion Trap group, Institute of Physics and Astronomy, University of Aarhus.
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