New Feature: Local Bond Order Parameter q_6

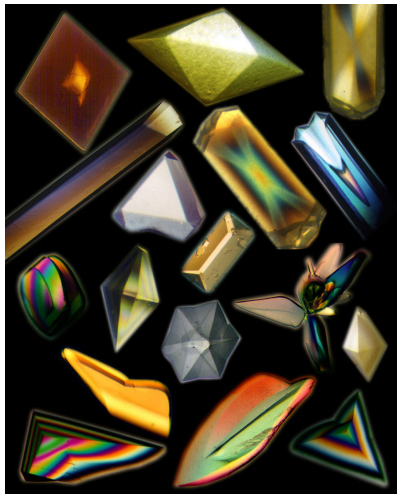
Dominic Röhm

ICP

19.04.2012

Motivation

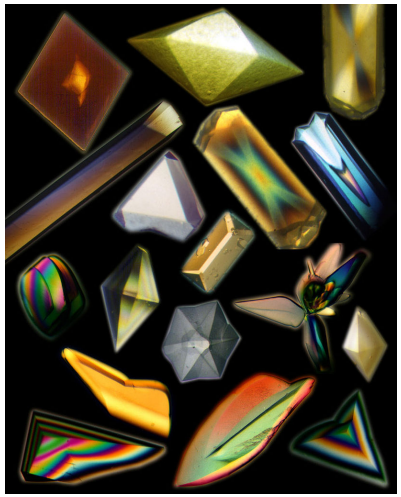
- Crystallization and Nucleation in Soft Matter Systems
- Colloidal Suspensions in polar/ionic solvents



Protein crystals

Motivation

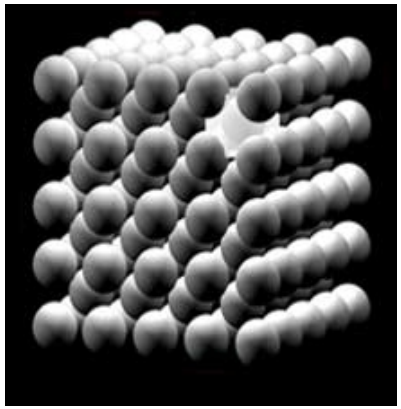
- Crystallization and Nucleation in Soft Matter Systems
- Colloidal Suspensions in polar/ionic solvents
- Dynamic and mesh–free parameters



Protein crystals

Motivation

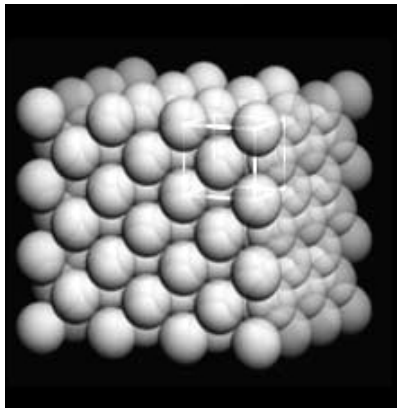
- Crystallization and Nucleation in Soft Matter Systems
- Colloidal Suspensions in polar/ionic solvents
- Dynamic and mesh–free parameters
- Detection of crystal structures or fluid/solid assignment of particles



BCC structure

Motivation

- Crystallization and Nucleation in Soft Matter Systems
- Colloidal Suspensions in polar/ionic solvents
- Dynamic and mesh–free parameters
- Detection of crystal structures or fluid/solid assignment of particles



FCC structure

Steinhardt Order Parameter

- Based on spherical harmonics, defined as:

$$q_l(i) = \sqrt{\frac{4\pi}{2l+1} \sum_{m=-l}^{l} |q_{lm}(i)|^2}, \tag{1}$$

with

$$q_{lm}(i) = \frac{1}{\widetilde{N}_b(i)} \sum_{k=0}^{\widetilde{N}_b(i)} Y_{lm}(k). \tag{2}$$

- Various enhanced methods like $q_l q_l$ (pair correlations) or average $\overline{q}_l(i)$

Steinhardt Order Parameter

- Based on spherical harmonics, defined as:

$$q_l(i) = \sqrt{\frac{4\pi}{2l+1} \sum_{m=-l}^{l} |q_{lm}(i)|^2}, \tag{1}$$

with

$$q_{lm}(i) = \frac{1}{\widetilde{N}_b(i)} \sum_{k=0}^{\widetilde{N}_b(i)} Y_{lm}(k). \tag{2}$$

- Various enhanced methods like $q_l q_l$ (pair correlations) or average $\overline{q}_l(i)$
- $q_l q_l$ defines if two particles are connected (threshold)
- If the particle is connected e.g. to 4, 6, 8, ... or more particles

Steinhardt Order Parameter

- Based on spherical harmonics, defined as:

$$q_l(i) = \sqrt{\frac{4\pi}{2l+1} \sum_{m=-l}^{l} |q_{lm}(i)|^2}, \tag{1}$$

with

$$q_{lm}(i) = \frac{1}{\widetilde{N}_b(i)} \sum_{k=0}^{\widetilde{N}_b(i)} Y_{lm}(k). \tag{2}$$

- Various enhanced methods like $q_l q_l$ (pair correlations) or average $\overline{q}_l(i)$
- $q_l q_l$ defines if two particles are connected (threshold)
- If the particle is connected e.g. to 4, 6, 8, ... or more particles
- Average $\overline{q}_l(i)$:

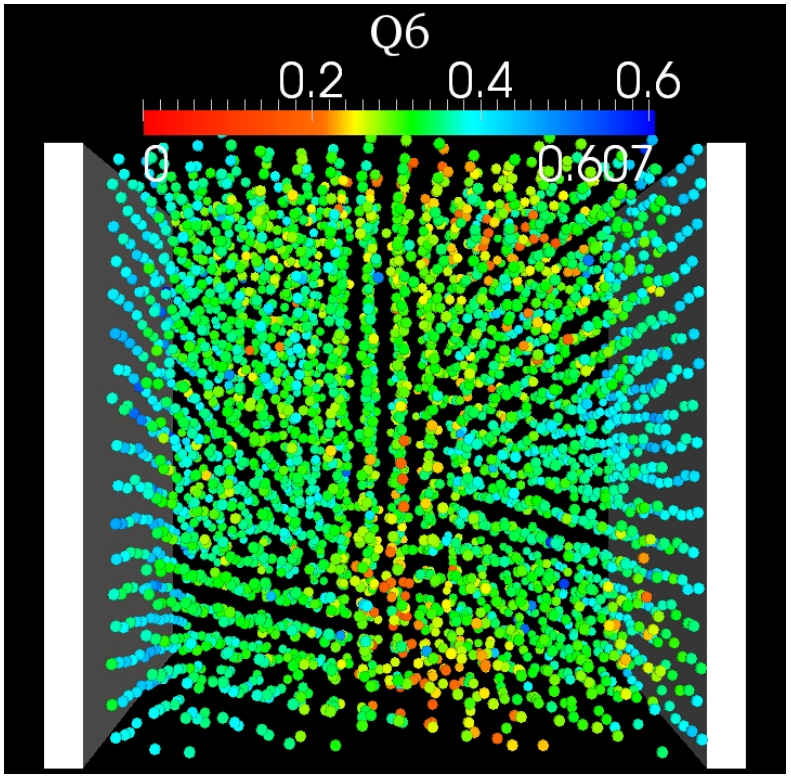
$$\overline{q}_l(i) = \sqrt{\frac{4\pi}{2l+1} \sum_{m=-l}^{l} |\overline{q}_{lm}(i)|^2}. \tag{3}$$

Visualization of $\overline{q}_l(i)$

movie

Outlook

- MPI version of different bond order calculations based on plain q_6
- Documented Python/TCL interface
- Included in ESPResSo 3.2



$\overline{q}_l(i)$ Parameter of a Colloidal Crystal

Thanks