

Step-by-step to phase-transition of anisotropic particles

Nima H. Siboni*

May 9, 2019

"The universe is random. It's not inevitable. It's simple chaos."

Heisenberg, Breaking Bad, Season 3, Episode 10.

In this project you build your first molecular dynamics code, check some (cool) properties of the algorithm, build liquid crystals, and observe one of the most delicate phase transitions of Nature. Your first step is to develop a MD-code for simulation of isotropic point particles and then use this code to simulate anisotropic particles.

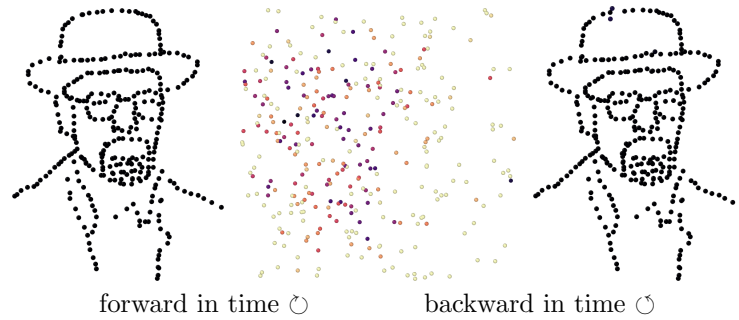
isotropic particles

Depending on how much you want to get involved in code development, you can start writing your own MD-code from scratch or you can start by completing the partially written MD-code that you receive in this course. After having the full version of the code you should check:

- a.1: momentum conservation of the algorithm,
- a.2: energy conservation of the algorithm, and
- a.3: time-reversibility of the implemented scheme.

Continued in the next page.

*email: hamidisiboni@tu-berlin.de, Büro: EW 267 .



From Heisenberg to chaos, from chaos to Heisenberg.

anisotropic particles

Now you can use the code you have developed/tested for isotropic particles and build molecules (anisotropic particles, or polymers, however you like to call them) by connecting isotropic particles with simple harmonic springs:

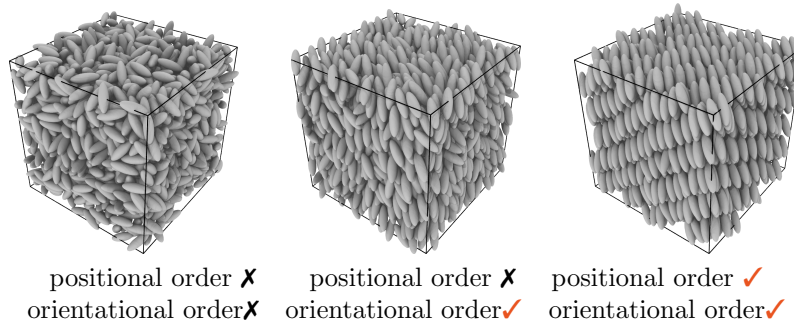


Figure 1: Three different phases of anisotropic particles.

- b.1: make dumbbells via connecting each separate pair of particles with a spring,
- b.2: make the spring stiff enough such that the dumbbells become effectively rigid bodies, and
- b.3: increase the density by compressing the system and find the isotropic-to-nematic transition.