

Type

Computational.

Requirements

- Programming skills (c++)
- Statistics and data analysis



QR code
zum pdf der Ausschreibung

For further information please contact:

Marco Klement
Institute for Multiscale Simulation
(MSS)
Department of Chemical and
Biological Engineering (CBI)
Cauerstrasse 3, IZNF,
91058 Erlangen,
Room 00.139
email: marco.klement@fau.de
web: www.mss.cbi.fau.de

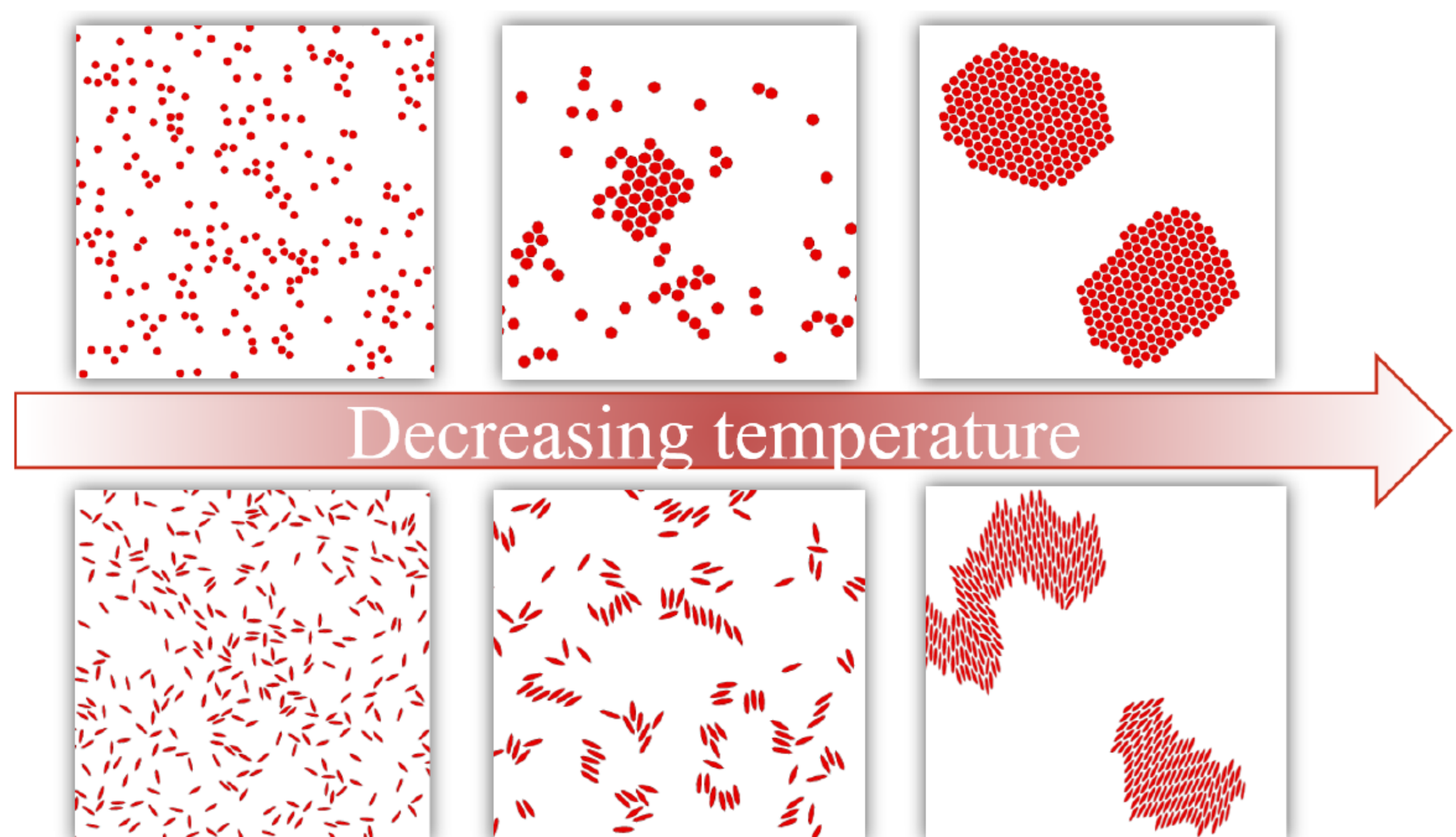
Machine-Learning assisted simulation of colloids

Background

A patterned surface has useful optical properties. For example light is scattered in different directions depending on its wavelength. Spherical colloids are useful to create patterns in a plane. Deposited on a substrate the pattern can be processed further and be exploited.

Machine-learning is treated like a solution to everything. Image and speech recognition are well known examples. Examples of scientific application are learned potentials or learned system propagation.

In this project we want use TensorFlow framework to model attractive elliptic particles. With simulations we will investigate the patterns obtained with these particles.



Aim

- Use a molecular dynamics simulation to study attractive ellipsoidal colloids.
- Investigate the relation between temperature, shape, and order.
- To describe the particle interaction create a neural network model using TensorFlow and train it using numerical force computations.