

Computational Sciences Projektseminar

A Python package for non-bonded interactions in periodic systems



2nd group project: Ewald summation / PME

Design/implement a complete Python package

Develop on github

Use a test-driven approach

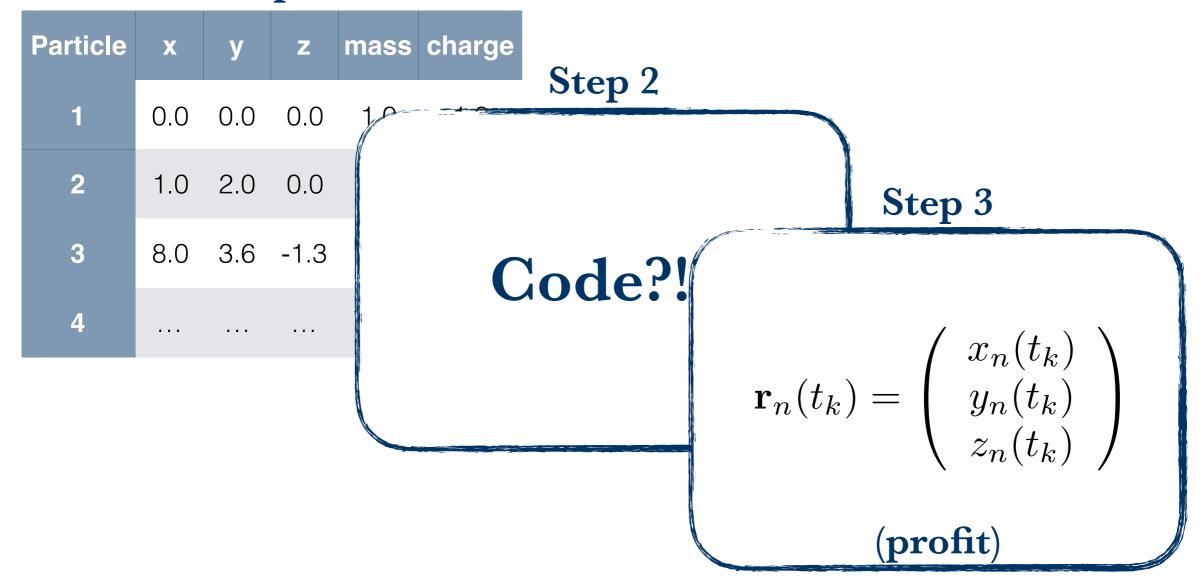
Use Ewald summation or particle mesh Ewald

Use molecular dynamics or Metropolis Monte Carlo



What we want...

Step 1





Interface example

```
from PACKAGE_NAME import optimize, simulate

parameters = dict(
    mass=...,
    charge=...,
    lj_sigma=...,
    lf_epsilon=...,
    ...)

r_opt = optimize(r_init, parameters, n_steps=100)
r sim = simulate(r opt, parameters, dt=0.001, length=1000)
```



Design brainstorming

Which components (energy, neighborlists, ...)

• Multi-species Lennard-Jones?

$$\epsilon_{ij} = \sqrt{\epsilon_i \cdot \epsilon_j}$$

$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2}$$

• Internal units?

Parameter representation?



Identify modules and dependencies

