Freie Universität Berlin

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

Particle	x	y	z	mass	charge
1	0.0	0.0	0.0	1.0	
2	1.0	2.0	0.0		
3	8.0	3.6	-1.3		
4	…	…	…		

Step 2

Code?!

Step 3

$$\mathbf{r}_n(t_k) = \begin{pmatrix} x_n(t_k) \\ y_n(t_k) \\ z_n(t_k) \end{pmatrix}$$

(profit)

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