Group Assignment 2

Computational Techniques for Molecular Modeling 2020-2021

CdF - 03/2021

Reading Assignment

- *Michael Griebel, Stephan Knapek, Gerhard Zumbusch, Numerical Simulation in Molecular Dynamics, Springer 2007 (downloadable from springerlink)*
  - *Chapter 3*

Groups

- *Group 1*
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- *Group 2*
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  - *S. Pertesana CHEM*
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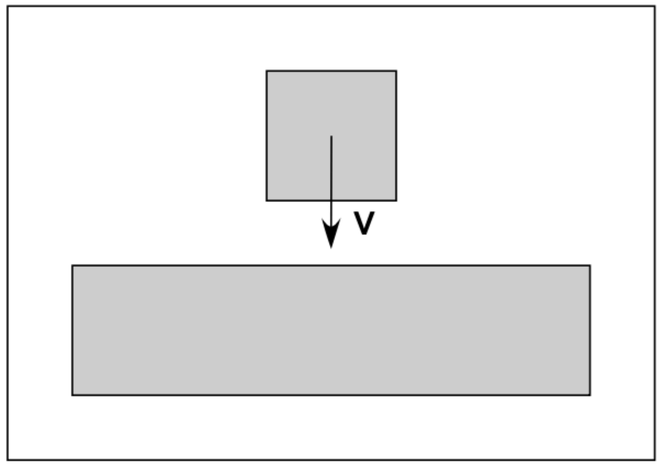
Reading Assignment Takes Away

- Cut-off distance for short range potentials
- Linked Cell Method to efficiently compute inter-particle forces

Programming Assignment 2

- *Griebel-Knapek-Zumbusch Sec. 3.6.1 pag. 66*
  - ***BUT :*** *using* ***Periodic Boundary Conditions***



- **N.B.:** There is a typo in the problem parameters $L_2 = 200$
- For initial conditions see file init_ptcl_mesh, demo 2

Programming Assignment 2

- init_ptcl_mesh, demo 2 demmonstrates :
  - efficiently dividing particles into cells
  - using cellfun to traverse cell-array
  - using linear indexing and find to only process non-empty cells