UNIVERSITY OF HELSINKI

TARTU ÜLIKOOL · UNIVERSITAS TARTUENSIS · 1632

ARCHIMEDES

Haridus- ja Teadusministeerium
Estonian Ministry of Education and Research

HELSINKI INSTITUTE OF PHYSICS

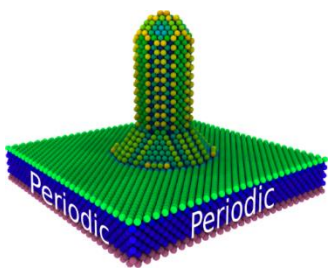
COUPLING OF ELECTROSTATIC EFFECTS TO THE ATOMISTIC SIMULATIONS

M. Veske, A. Kyritsakis, K. Eimre, V. Zadin, F. Djurabekova

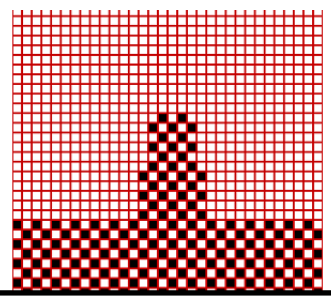
Helmod

HELMOD* – Hybrid Electrodynamics – Molecular Dynamics

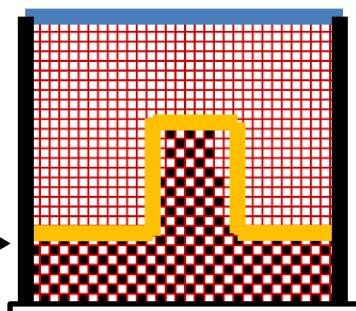
FDM Laplace equation solver to get electrostatic effects to nanostructures under high electric field



Import atom coordinates



Force atoms into grid



Apply boundary conditions

$$\Delta\phi = 0$$
$$\boldsymbol{E} = -\boldsymbol{\nabla}\phi$$

Calculate electric field

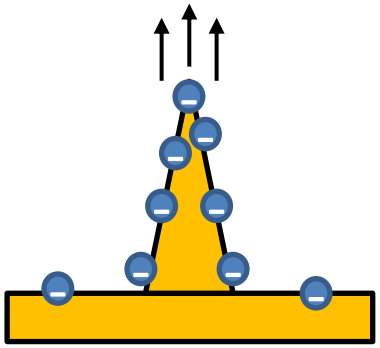
*Djurabekova *et al, Phys. Rev. E 83, 026704, 2011*

Helmod

HELMOD – Hybrid Electrodynamics – Molecular Dynamics

FDM Laplace equation solver to get electrostatic effects to nanostructures under high electric field

$\boldsymbol{E}$ →

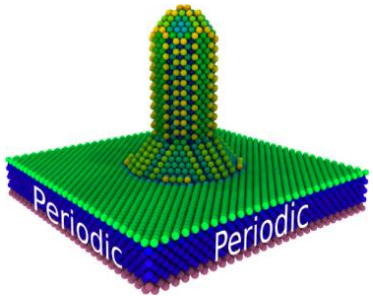


surface polarization,
field emission,
finite size effects

→

charge q
force $\boldsymbol{F}$
FE current $\boldsymbol{J}$
current density $\boldsymbol{\sigma}$
temperature T

→



Update velocities
and forces in MD
or barriers in KMC

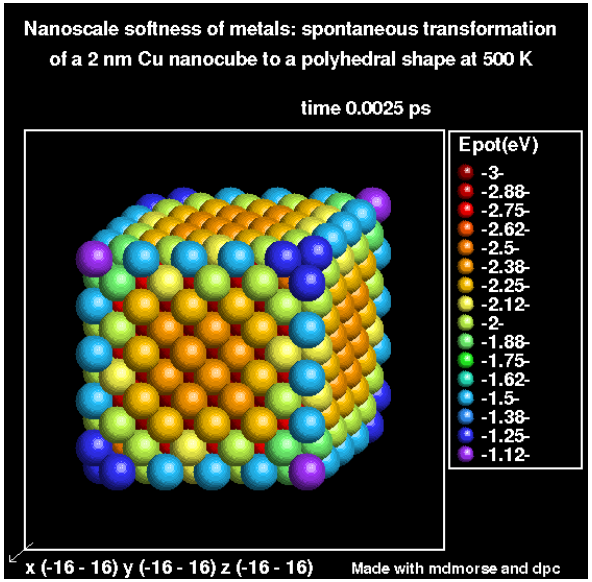
MD *vs* KMC

Molecular dynamics: solving Newton's equations of motion by using the interaction potential

$$\boldsymbol{v}_i = \boldsymbol{v}_{i-1} + \frac{\boldsymbol{F}_{i-1}}{m} \cdot dt$$
$$\boldsymbol{x}_i = \boldsymbol{x}_{i-1} + \boldsymbol{v}_{i-1} \cdot dt$$

Kinetic Monte Carlo: atom jumps from site to vacancy governed by the thermodynamics

$$P \propto e^{-E_b/k_B T}$$



Credit: Kai Nordlund

Helmod

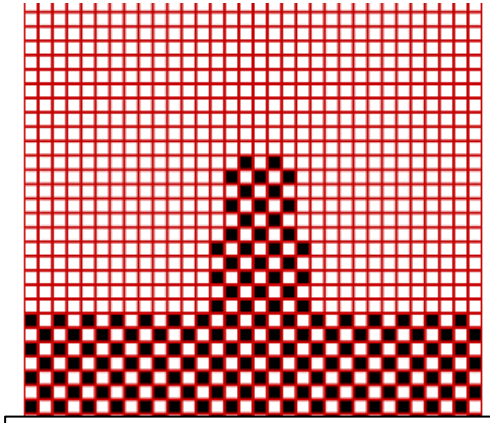
- Success in many projects
  - Veske *et al*, Shape memory effect in Cu nanotips
  - Parviainen *et al*, Electonic processes in Cu nanotips
  - Pohjonen *et al*, Dislocation nucleation on Cu nanovoid
  - etc

- Only materials with cubic symmetry
- <100> and <110> orientations
- Up to 10^5 atoms

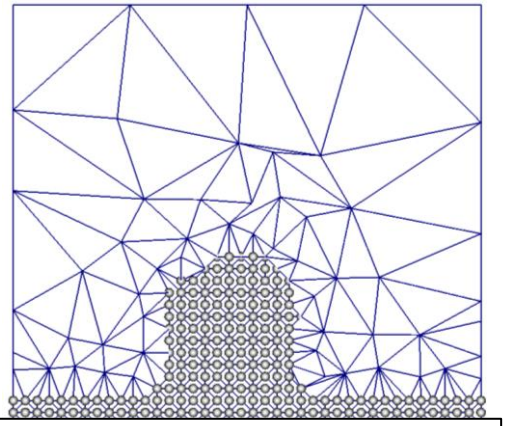
Femocs

FEMOCS - Finite Elements on Crystal Surfaces

FEM Laplace equation solver to get electrostatic effects to nanostructures under high electric field



Helmod
Finite Differences



Femocs
Finite Elements

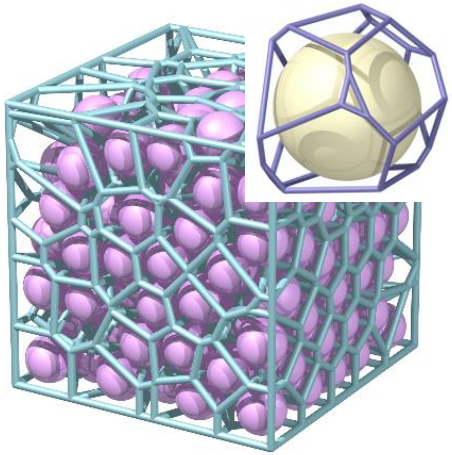
- Less nodes
  lower comput. cost
  bigger systems
- Flexible grid
  any crystal structure
  incl. amorphous

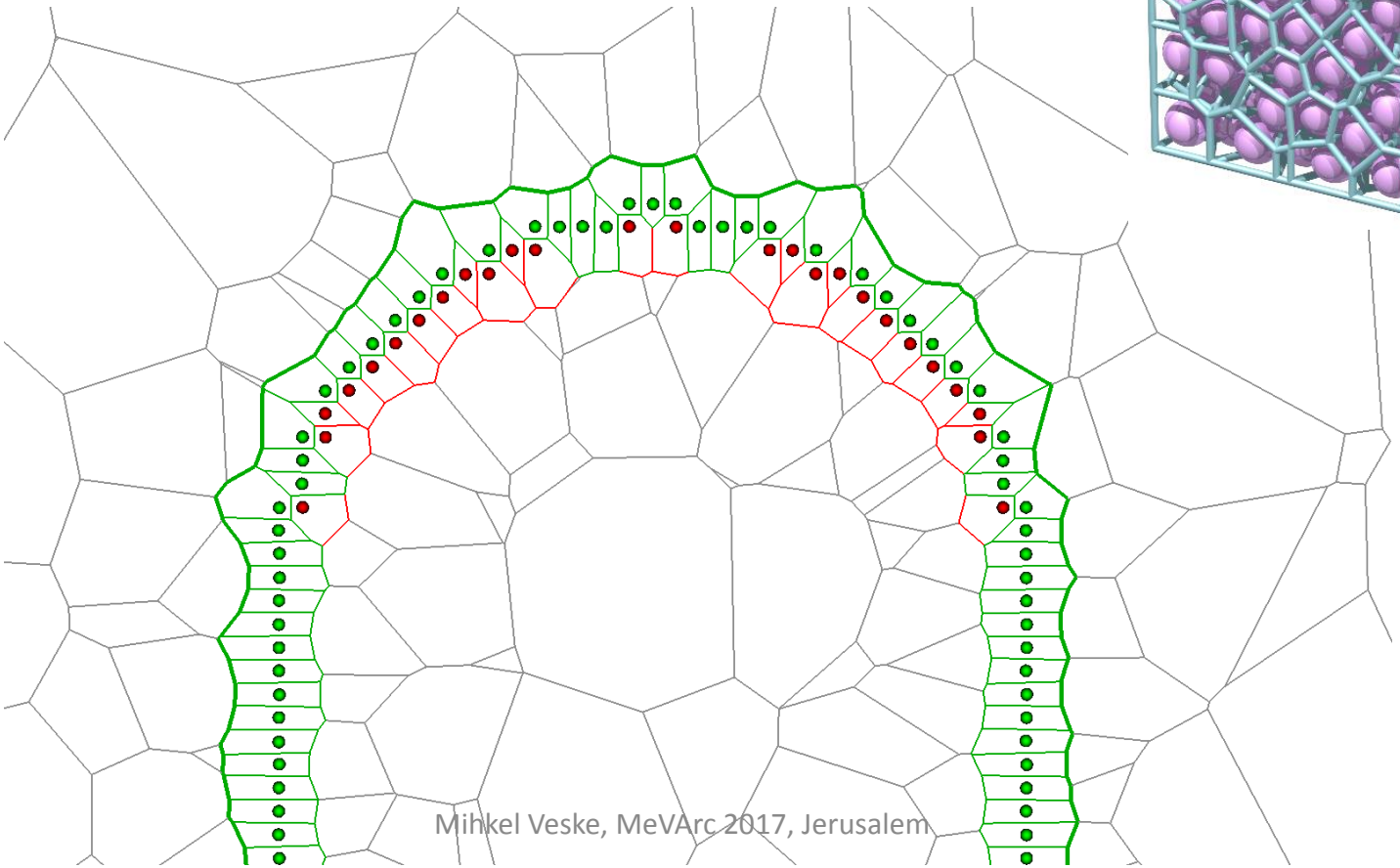
Generating mesh

Extracting surface

Coordination < nnn → rough surface →

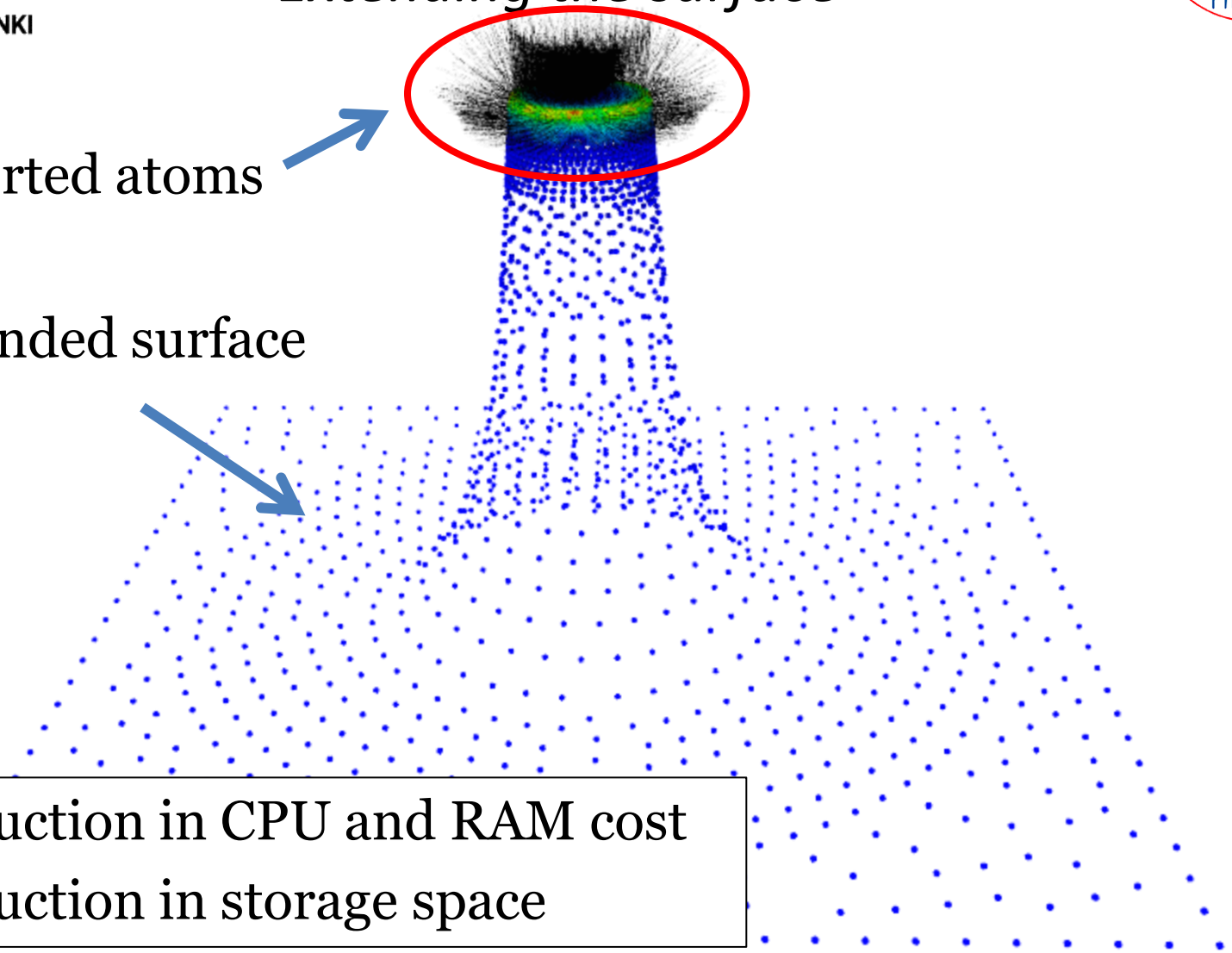
Voronoi cells → surface





Generating mesh

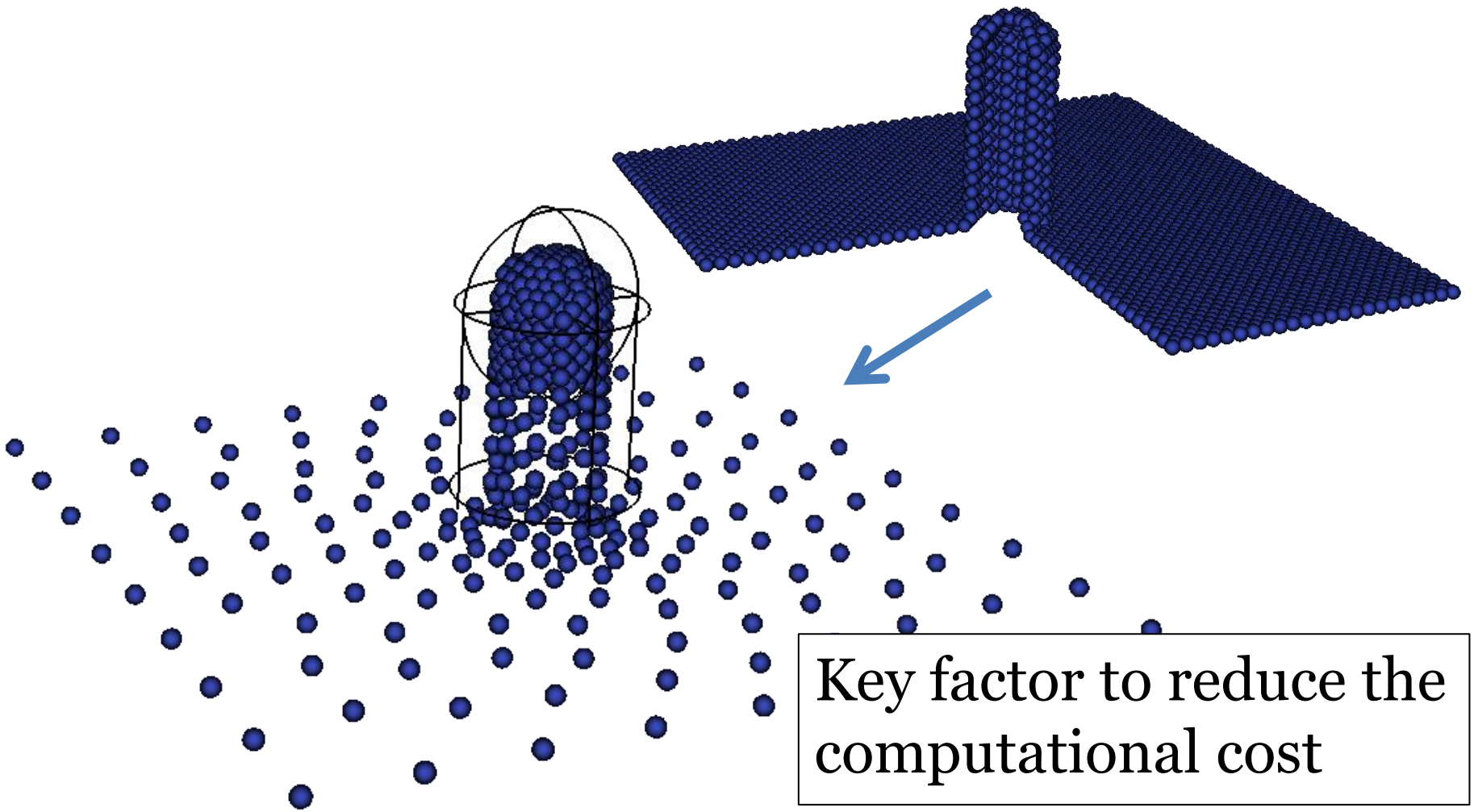
Extending the surface



- Reduction in CPU and RAM cost
- Reduction in storage space

Generating mesh

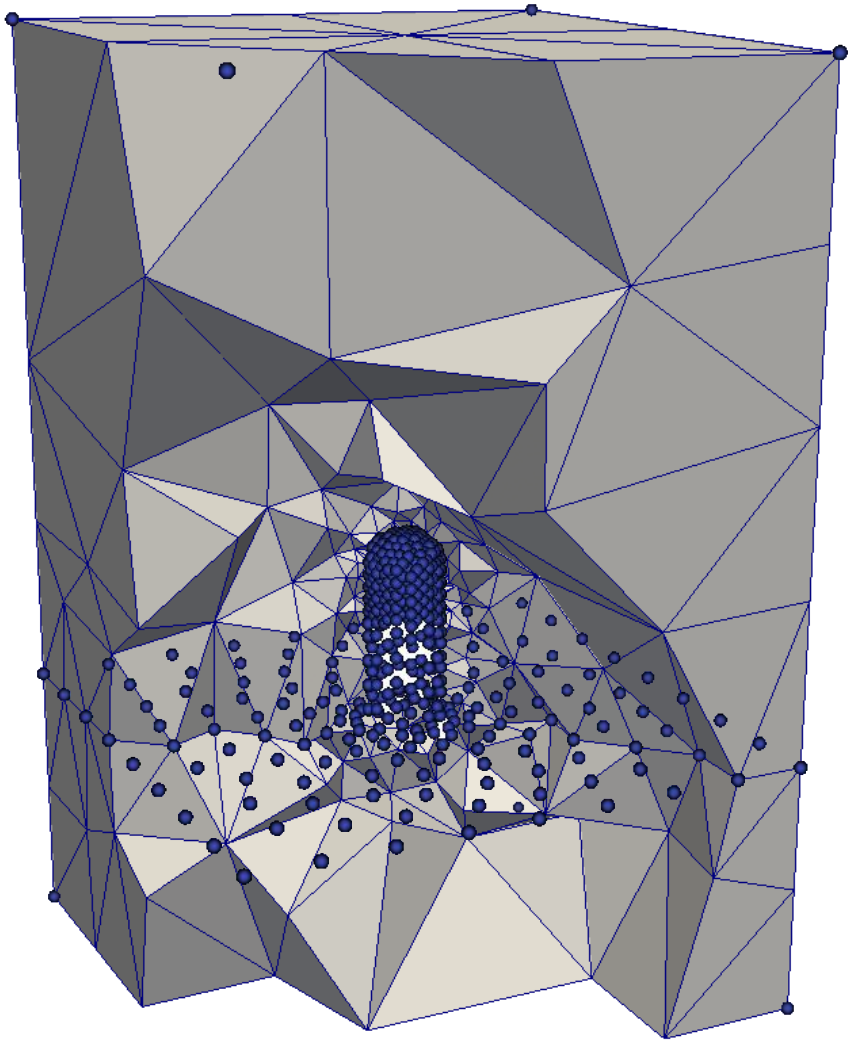
Coarsening the surface



Key factor to reduce the computational cost

Workflow

Generating elements



Tetrahedra and Voronoi cells are generated with Tetgen* that handles their size and quality

Quality = *max* (radius/edge)

*http://wias-berlin.de/software/tetgen/

Workflow

Separating meshes and solving diff.eq.-s

Vacuum mesh – Laplace equation

$\Delta\phi = 0$ → electric potential

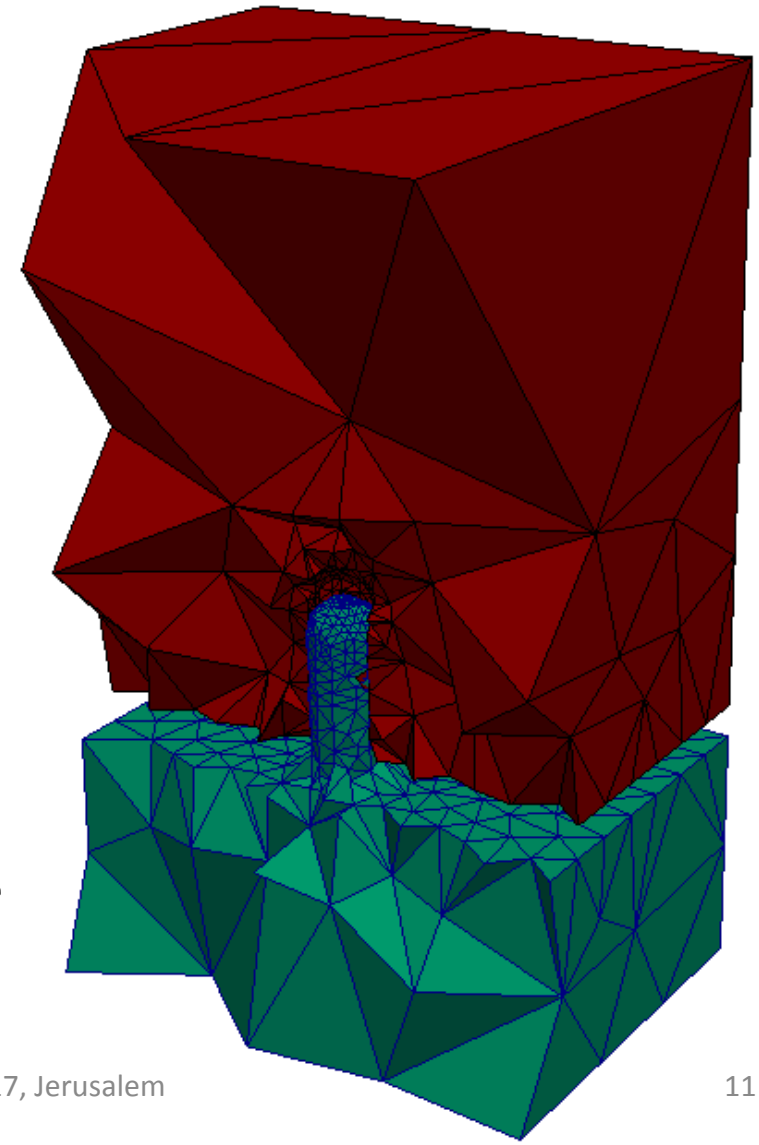
$\boldsymbol{E} = -\boldsymbol{\nabla}\phi$ → electric field

Bulk mesh – continuity & heat equation

$\boldsymbol{\nabla} \cdot (\sigma \nabla \phi) = 0$ → current density

$\boldsymbol{\nabla} \cdot (\kappa \nabla T) = -\boldsymbol{J}^2/\sigma$ → temperature

etc, e.g. mechanical stress

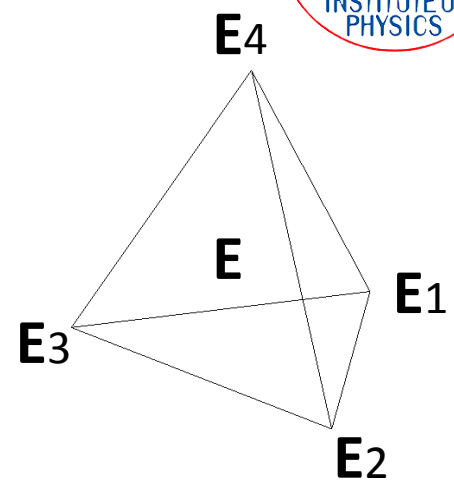


Workflow

Interpolating solution

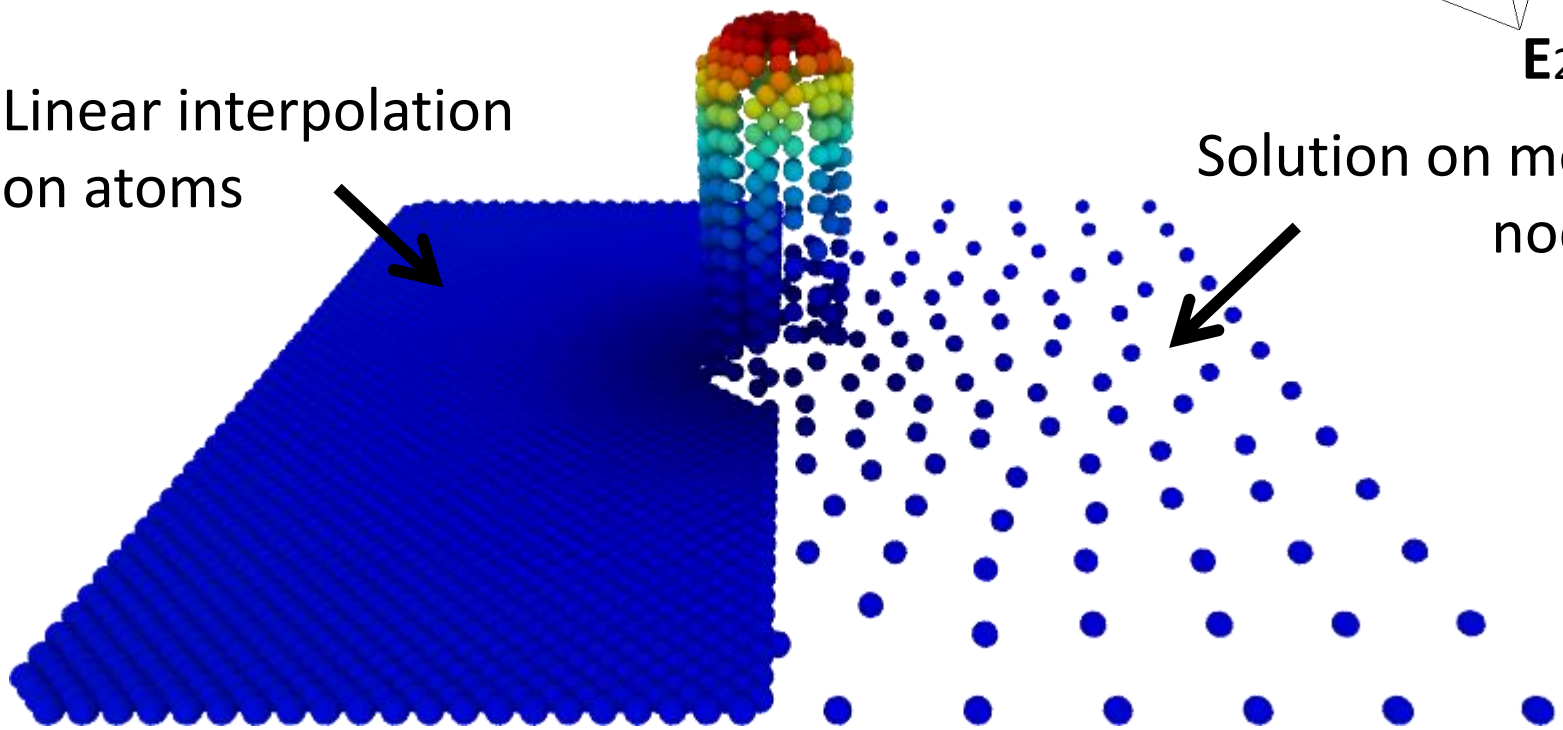
Interpolation with barycentric coordinates:

$$\boldsymbol{E}_i = \sum_j \lambda_{ij} \cdot \boldsymbol{E}_j\,, \qquad \sum_j \lambda_{ij} = 1\ \forall\ i$$



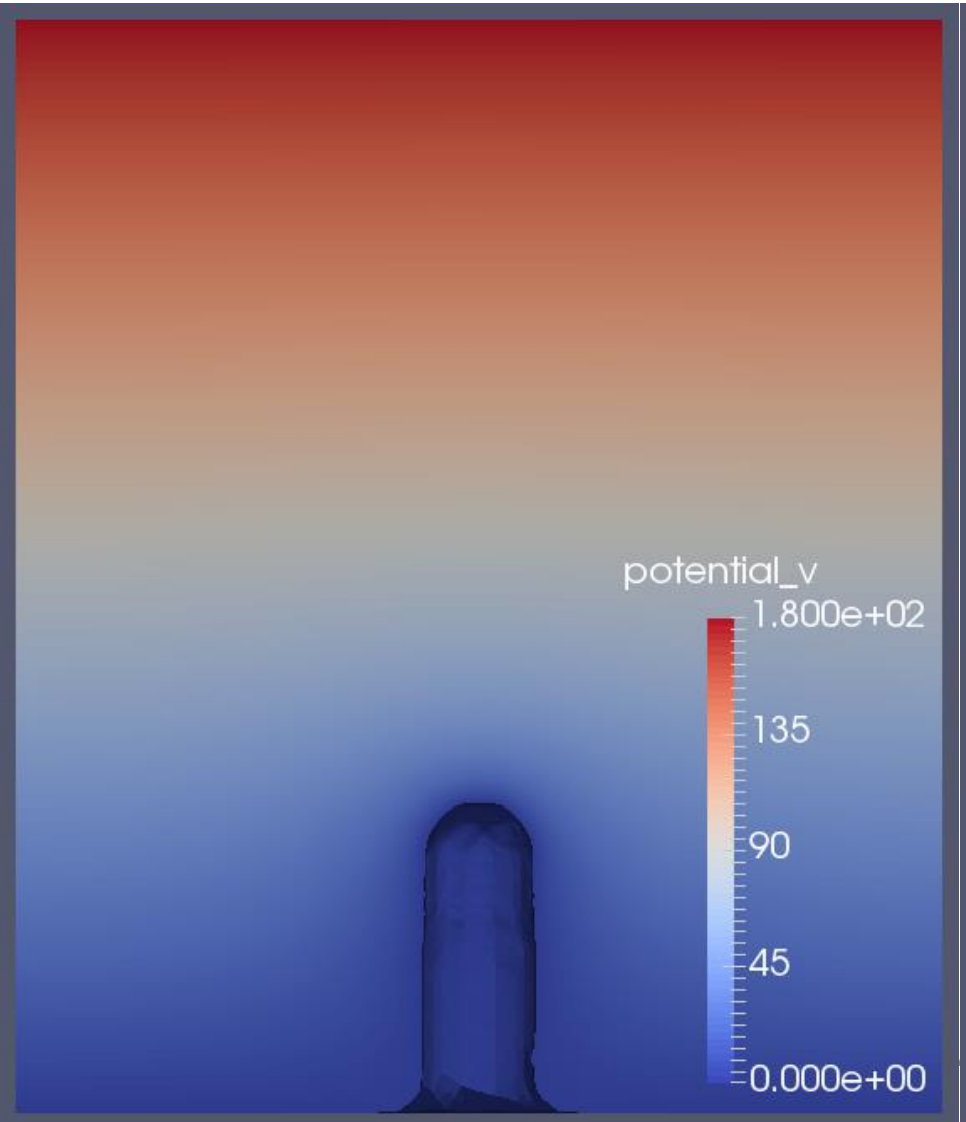
Linear interpolation on atoms

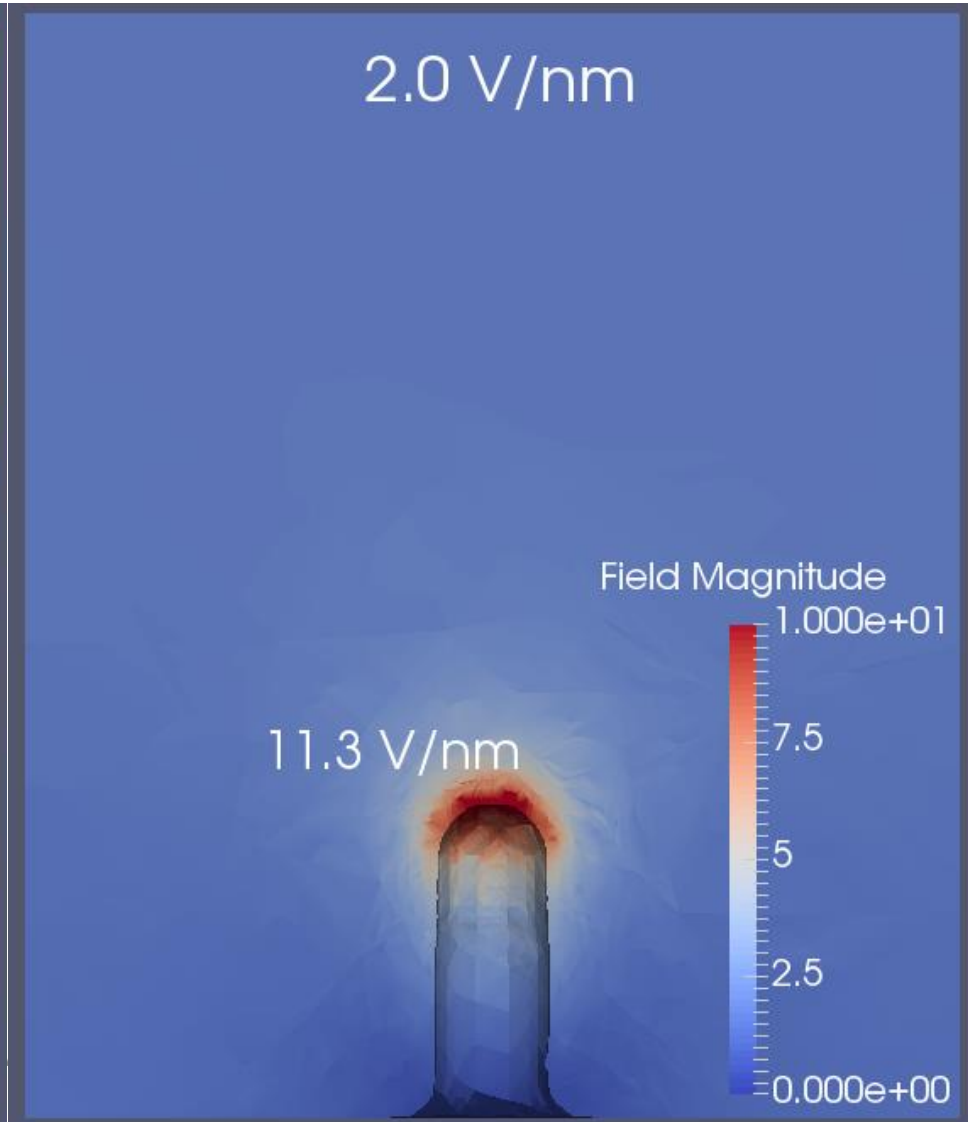
Solution on mesh nodes



Results

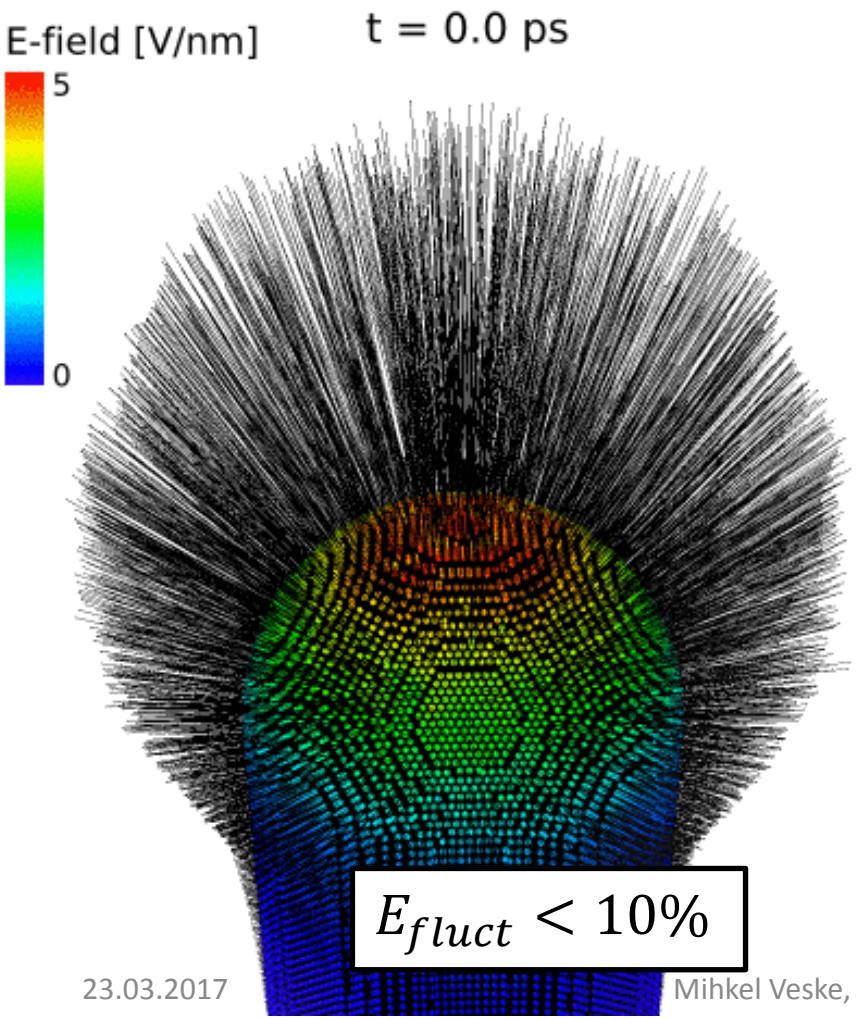
Electric potential & electric field



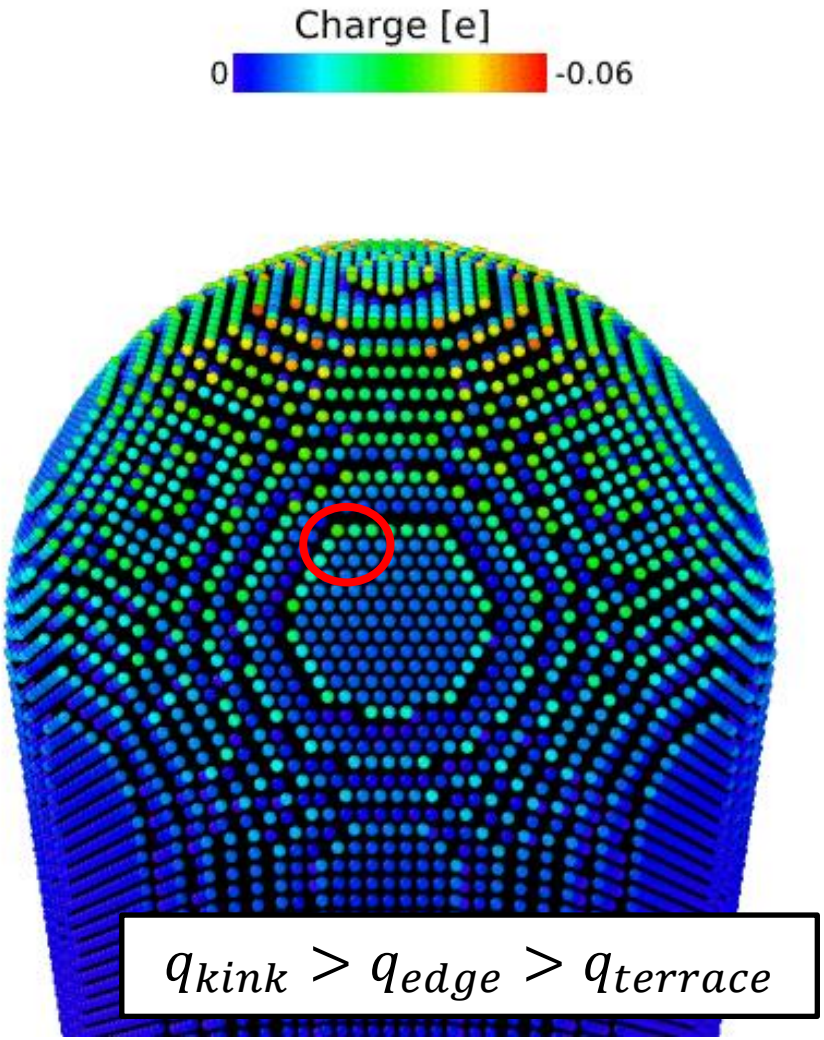


Results

Electric field & atomic charge



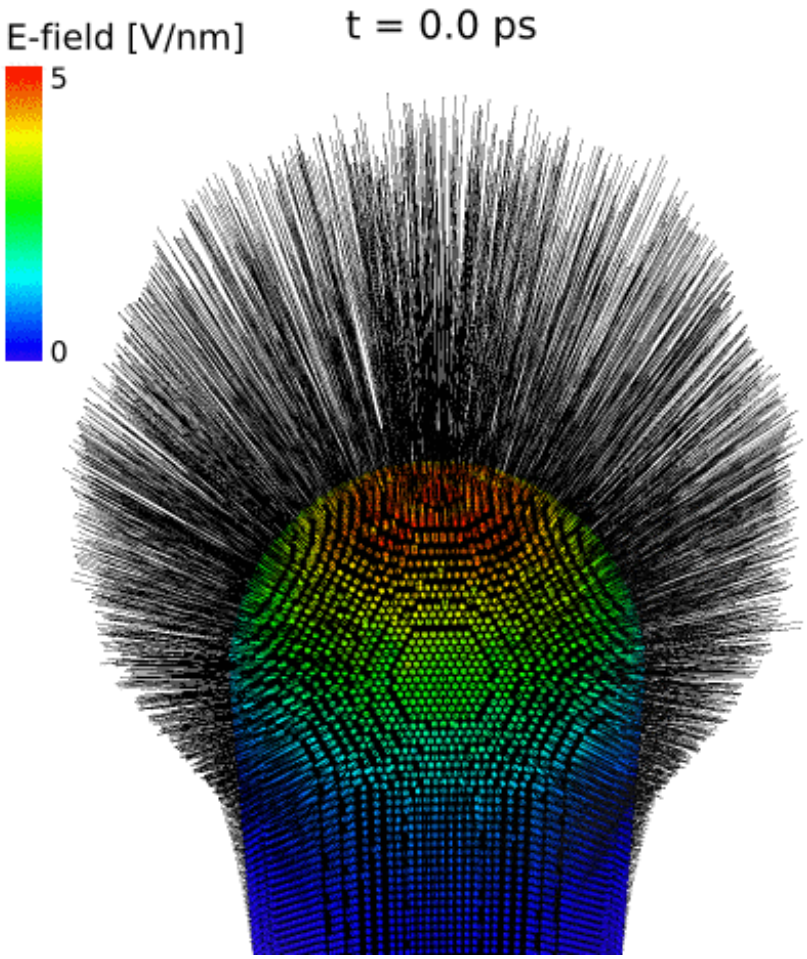
$E_{fluct} < 10\%$

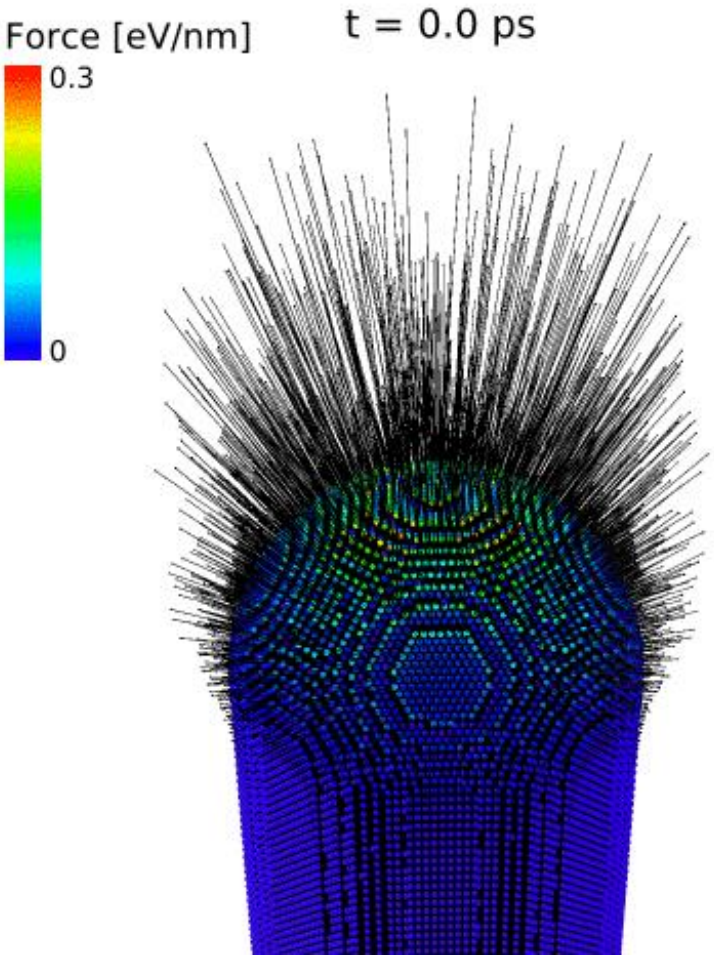


$q_{kink} > q_{edge} > q_{terrace}$

Results

Electric field & electrostatic force



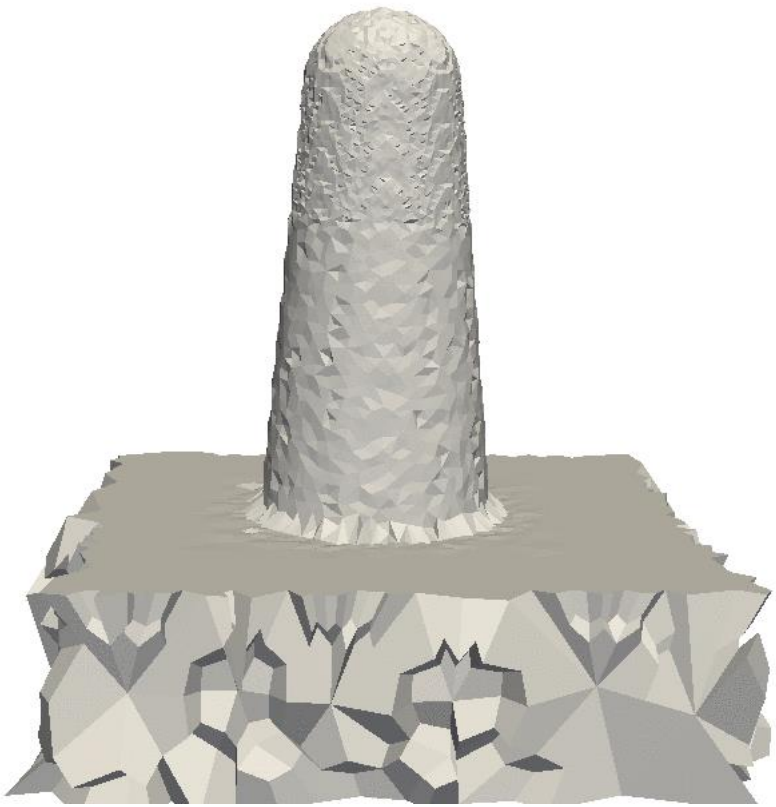


Results

Pre-breakdown

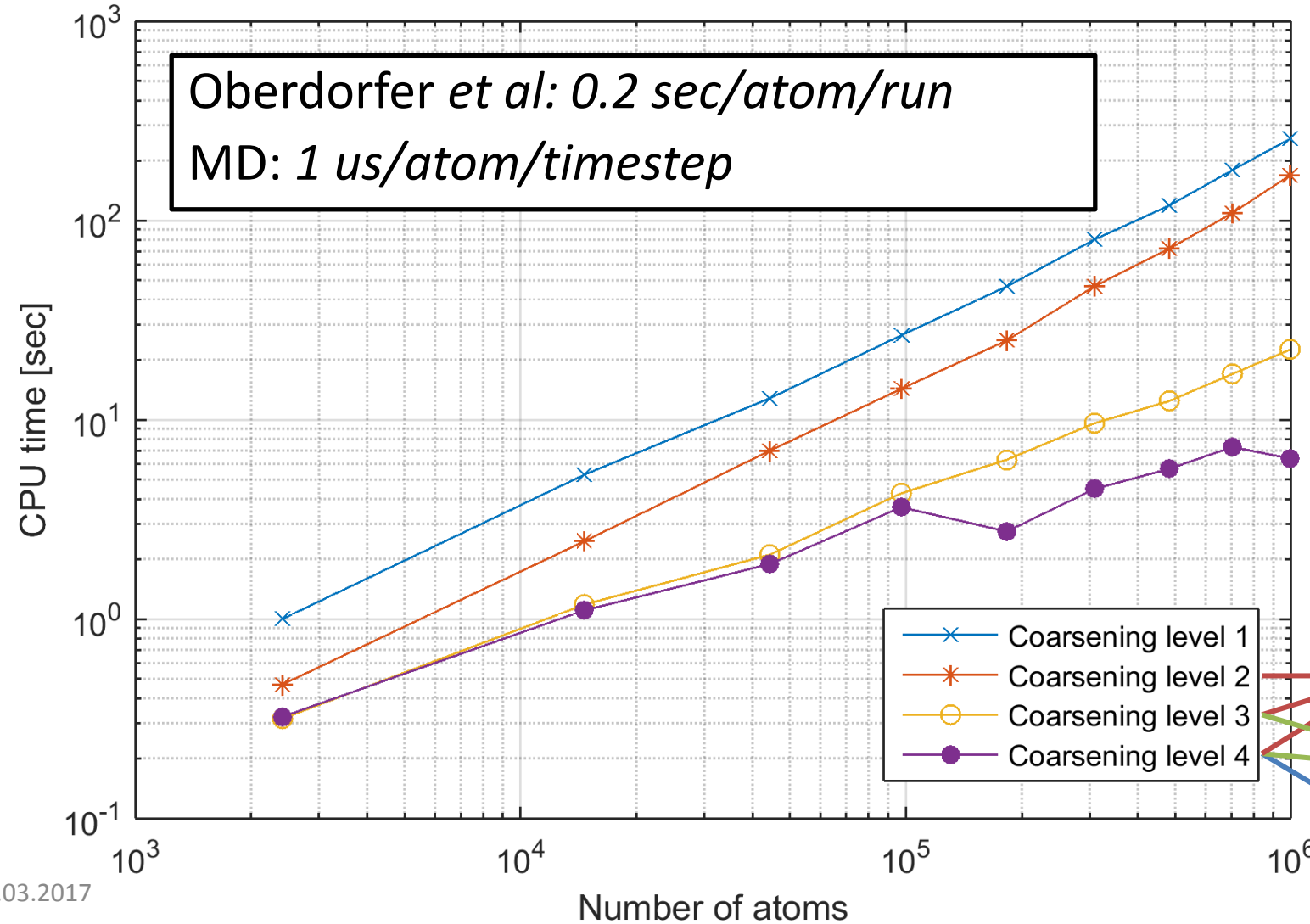
E_0 = 1.2 V/nm

T_{max} = 3000 K



Further from
A. Kyritsakis *et al*

Overall performance



Advances

- Handles two orders of magnitude more atoms than previously
- Any crystal structure and orientation, including amorphous systems
- Low cost of extending the surface
  - less atoms in MD / kMC
- (partial) support for parallel computations
- Flexible interface
  - Fortran (PARCAS), C (KIMOCS), C++ (LAMMPS)