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HIP

# Case study: Data needs in computational materials physics – atom level simulations

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# Group and specific research topics

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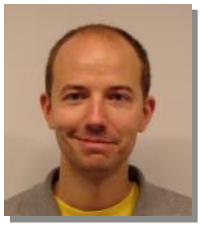

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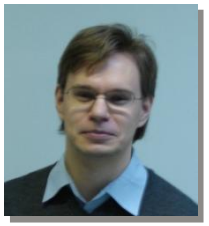

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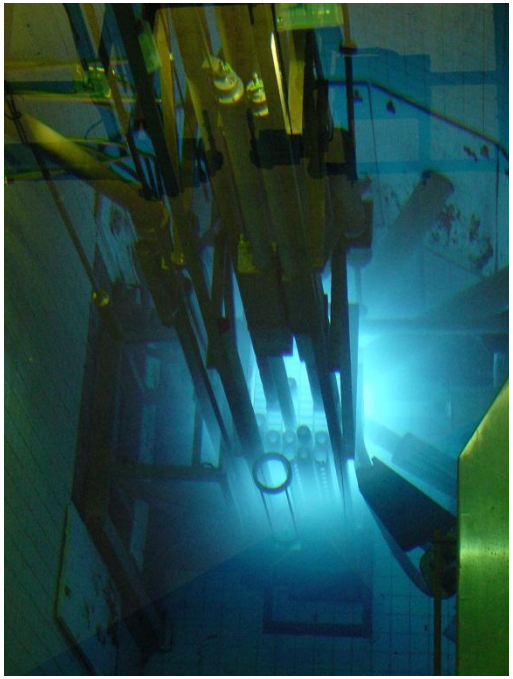
Fusion reactor mat'ls

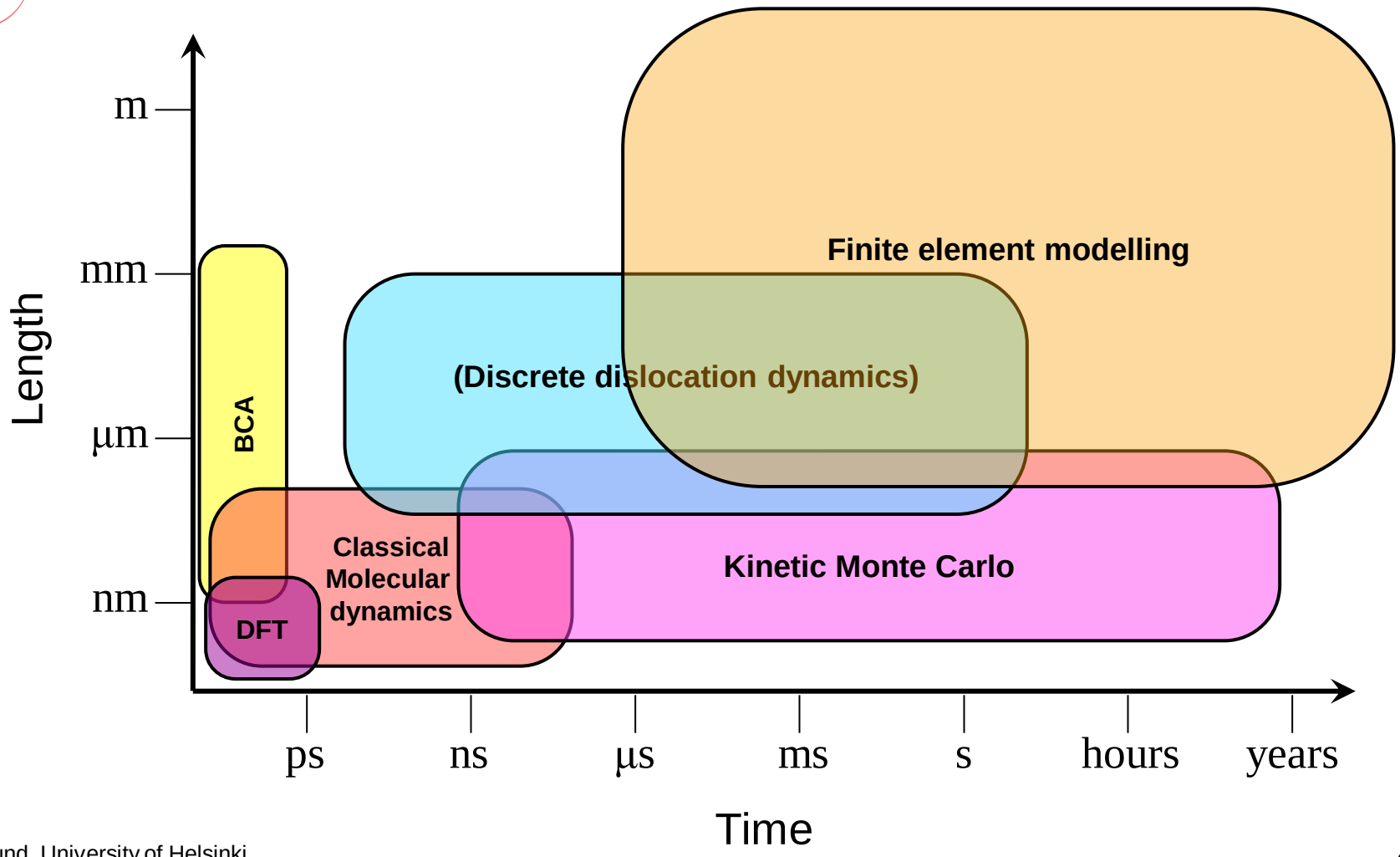
# Research theme

- Radiation effects on a material
  = what happens when an energetic particle from an accelerator or fission or fusion reactor hits a material??
- Can be harmful OR beneficial!



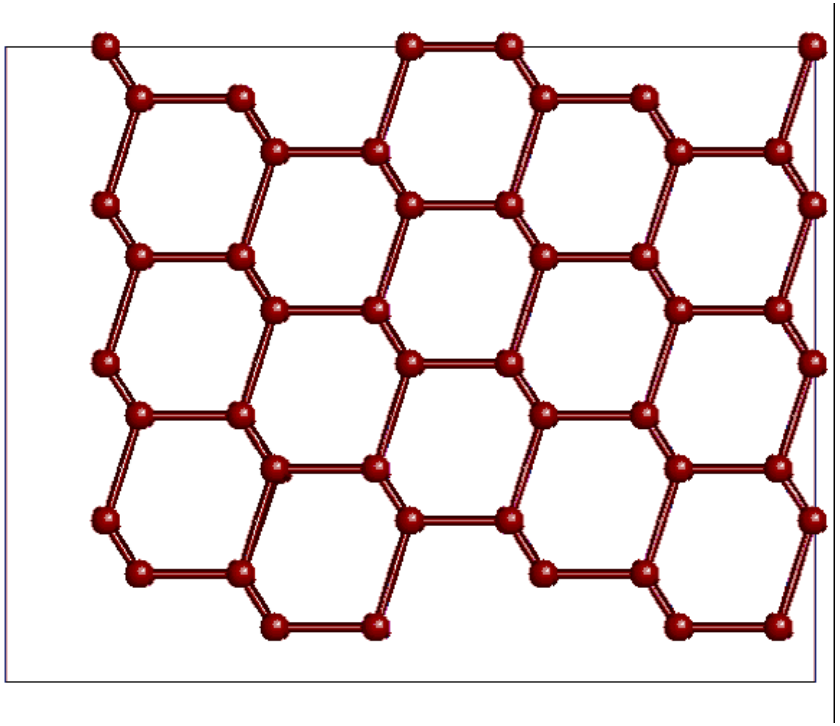
# Multiscale modelling in materials science

- The multiscale modelling framework



# Main simulation type

- The main simulation type in our group is molecular dynamics – MD
- Done on many different scales and materials
  - Quantum mechanical
  - Classical reactive bond-order potentials for organic materials
  - Classical many-body potentials for metals, semiconductors

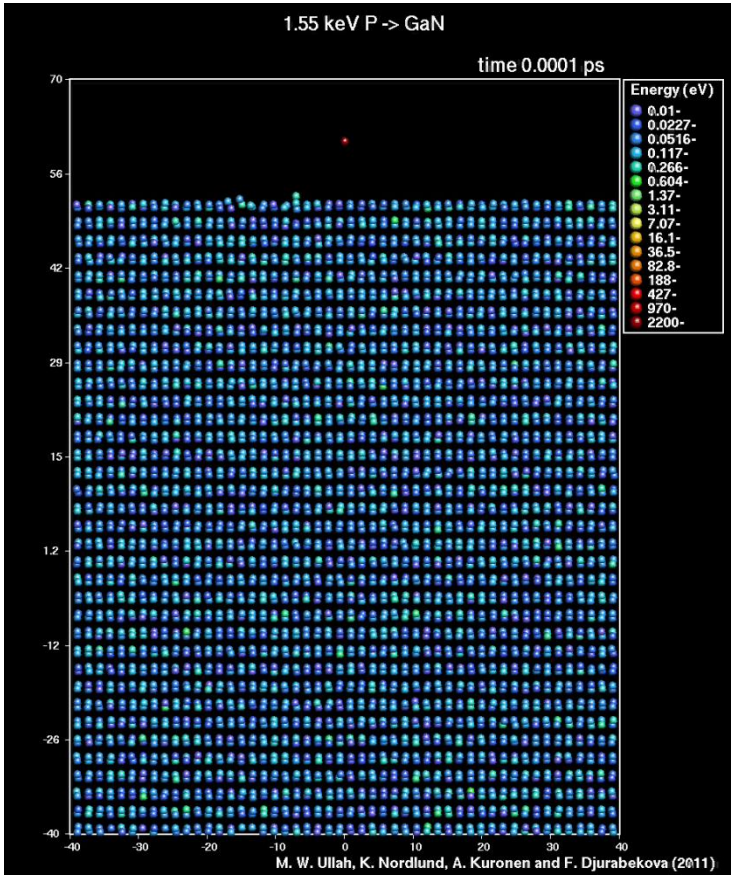


# Range of simulation sizes and data needs

- Initial input data usually trivial, 1 – 10 Mb
  - Intermediate inputs can be largish, 1 – 100 Gb
- Quantum mechanical:
  - 100 – 200 atoms, a few hundred events, < 1000 time steps
    - Output data trivial (< 1 Gb)
- Nanocluster  formation and deposition
  - 1000 – 100000 atoms, thousands of events @ 10000 time steps:
    - Output data 10 – 1000 Gb
- Damage buildup in fusion reactors:
  - 1000 – 10000 atoms, thousands of events @ 10000 time steps:
    - Output data 10  Gb – 1000 Gb
- keV cascades in solids
  - 1 – 1000 million atoms, hundreds of events:
    - Output data 1 – 100 Tb

# Example of user case

- Ion and nanocluster ion irradiation of GaN (Finnish-Russian collaboration ENIGAZ)
  - 5.5 million atoms
  - Hundreds of cascades
- Output structure: physical data + movie file
- Data need for project:
- Without movie file:
  - 1 Gb/event, 2 Tb total
- If movie files were stored:
  - 90 Gb/event, 180 Tb total

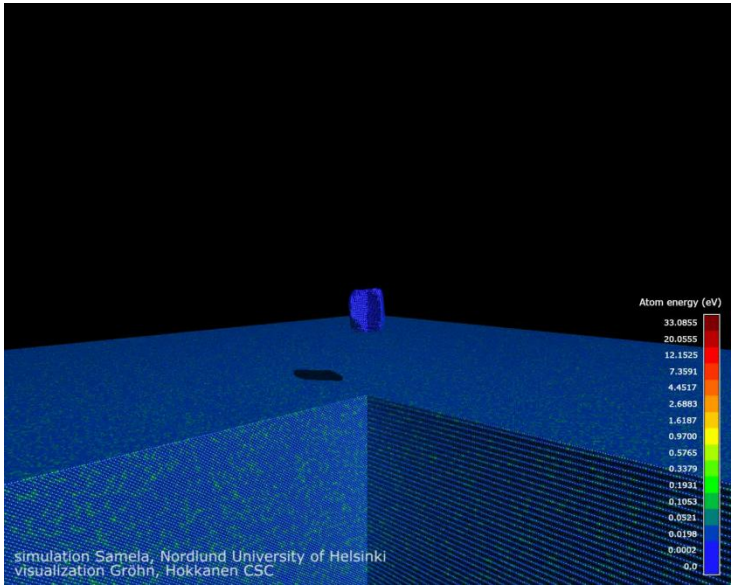


# A high-end user case

- Cratering in Au
- 50 million – 4 billion atoms
  - Single atom output at

    4 billion atoms = 250 Gb
  - Minimal movie file with

    10 frames 2.5 Tb




- If we would do 100 events > 250 Tb…

  (If all movie frames would be output > 2.5 Eb …)
- Minimal long-term storage only physics outputs and final atom coordinates: ~ 25 Tb

# Comments: pros and cons

- Big file size handling is really tedious:
  - Slow analysis, slow moving, even slow file copy within single machine
- Good news: file sizes are easily tunable:
  - Small # atoms: often like 10000 frames output
  - Huge # atoms: ~10 frames of output
  - Physics resolution is lost, but usually we can live with that
- Bad news: we would almost always want to store all final atom coordinates
- Intermediate-term storage space often also a problem:
  - Want to store many movie files in full for 1-2 years
  - Local disk suitable, but keeps filling up

# File format

- All input, most outputs are simple ascii files
  - Human (physicist) readable

```
Neighbours per atom =  26.801300 drmin      2.4481
 elstop allocating
*** first time in elstop in proc   0,  21 data points read in
*** Elstop atom type and file 1 Cuin/elstop.Cu.Cu.in                       , v=
  24644.
Total and last FDe =       0.247      0.247 eV for       1 atoms.
rec    -9.9889   -9.9950  -20.9007       0.0    4001     200.0000  0
t       0.0 ECM pos.      -7.96     -7.95    -16.59 Eksum      252.05
Nliq     0 at time       0.0
 Saving positions to md.movie at t=       0.41
  ... Done !
bpc P   -5.1780   -5.4358   14.2262 sz   36.150   36.150   36.150    47241.63
     Step     Time     Atoms     Temp          Epot_ave   Total En      Change
ec      1       0.41    4001   487.3960      -3.4842      -3.4212     0.0000
ec      2       0.81    4001   487.2544      -3.4842      -3.4212     0.0000
ec      3       1.22    4001   486.2748      -3.4842      -3.4213    -0.0002
```

```
        4001
 Frame number       1    0.20839     fs boxsize  36.150000   36.150000   36.150000
Cu   -17.171275   -17.171398   -17.170782  1         1
Cu   -17.171154   -15.363929   -15.363820  1         2
Cu   -15.363557   -17.171259   -15.363895  1         3
Cu   -15.363913   -15.363804   -17.171200  1         4
Cu   -17.171249   -17.171156   -13.556300  1         5
Cu   -17.171004   -15.363441   -11.748477  1         6
Cu   -15.363760   -17.170994   -11.749114  1         7
Cu   -15.363263   -15.363691   -13.555793  1         8
Cu   -17.171185   -17.171452    -9.941247  1         9
```

- Movie file can also be binary

# Sharing?

- Before publication, we do not want to share anything with outsiders

- After publication:
  - Some of the raw data is not really of interest to anybody else, only the final analyzed data which fits in a publication
  - Some data (atom coordinates in movie file and defect coordinates extracted from them) is of interest to ~ 3-30 other research groups in the world and a sharing system could be useful after publication
    - On the other hand just request by email works fine as well and likely is less effort

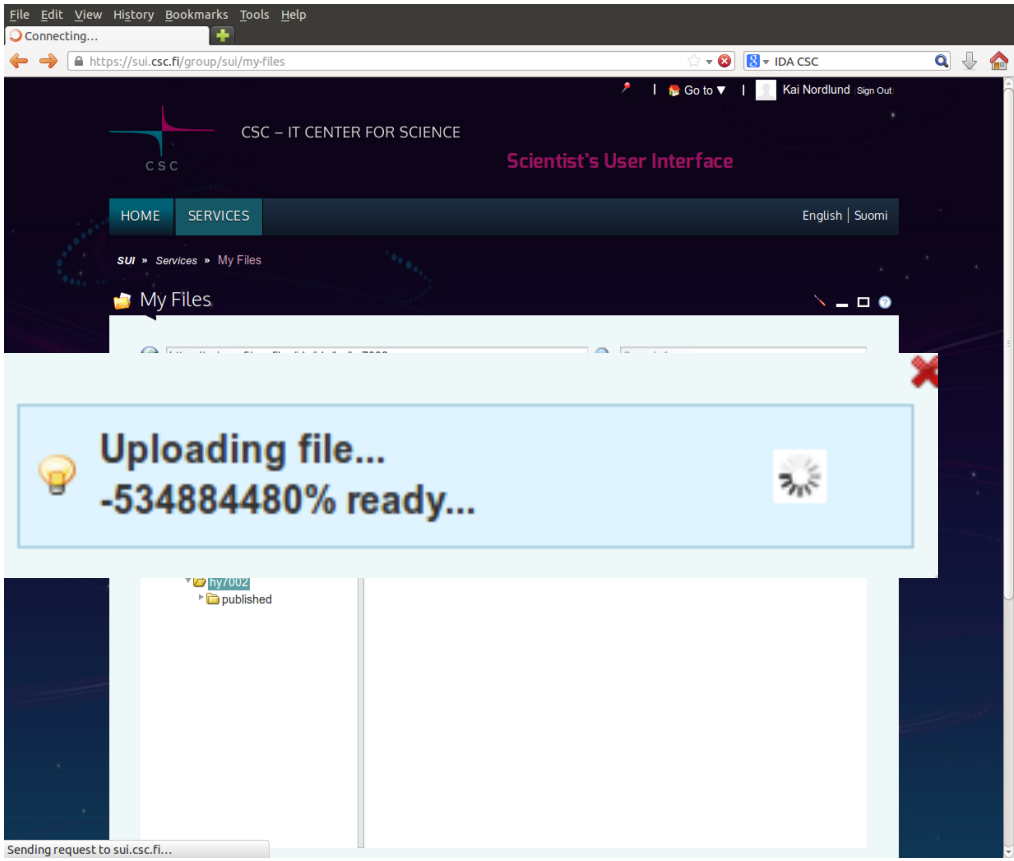
# Time scales for storage?

- Running files and all outputs:
  - ~1 PhD student lifetime (~5 years)
- Most important inputs and outputs:
  - ~ 1 Professor lifetime (~50 years)
  - For my own data storage has worked by data migration from one Unix disk to another for ~ 20 years now
  - Right now 70 Gb long-term storage (including all emails)

```
-rw-r--r-- 1 knordlun Domain Users   628 Jun 21  1995 Vofsize.ltersoff
-rw-r--r-- 1 knordlun Domain Users 16209 Jun 21  1995 coords.in
-rw-r--r-- 1 knordlun Domain Users   628 Jun 21  1995 Vofsize
-rw-r--r-- 1 knordlun Domain Users   116 Jun 21  1995 out.energyofsize
-rw-r--r-- 1 knordlun Domain Users 16209 Jun 21  1995 coords.in.bkp
-rw-r--r-- 1 knordlun Domain Users   374 Jun 21  1995 Vofsize.bkp
-rw-r--r-- 1 knordlun Domain Users  1914 Jun 21  1995 Vofsize.a
```

# First experience of IDA usage

- I tested the TTA/IDA storage recently for a set of nanocluster simulations
- Experience:
  - Graphical user interface non-intuitive, difficult to find place where to store
  - Worked fine except:



# Comments, questions?