Modelling Thin Film Growth

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Outline

- Methodology
- Results
- Challenges
- Conclusions

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Methodology

- HTST, fixed prefactor
- Mixed MD - otf-kMC
- On-the-fly kinetic Monte Carlo Methodology
  - Defect identification
  - Saddle point search
  - Barrier Calculation
  - KMC Step
  - Repeat

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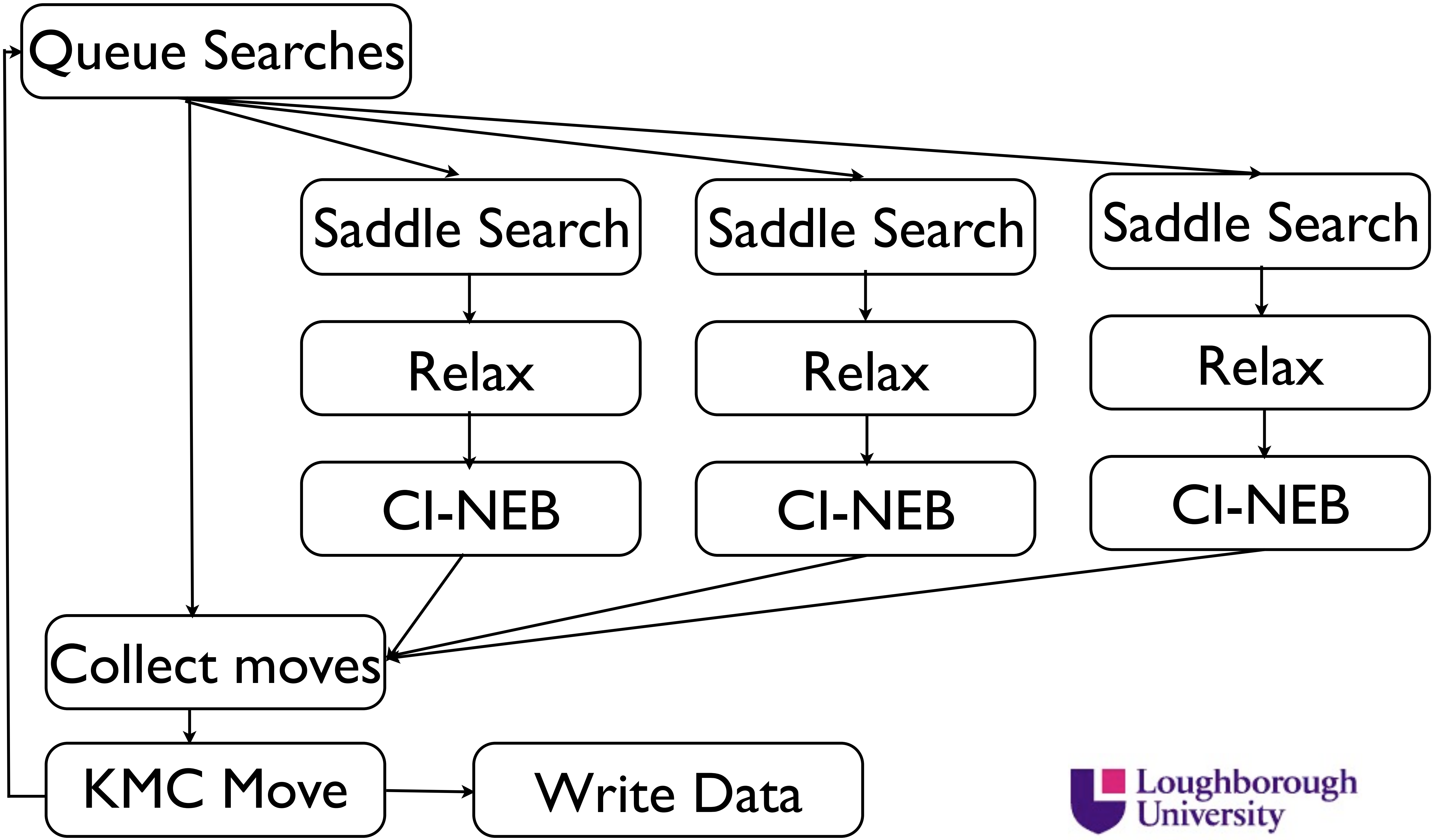
Methodology



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Methodology

- Searches are queued and executed when cores are free.
- Mixture of dimer method and RAT used for saddle searches.
- Relaxation performed to find final state.
- CI-NEB used to find barrier height.
- Duplicate saddles discarded.
- Roulette table constructed and move chosen.

Graeme Henkelman and Hannes Jónsson, J. Chem, Phys. **111** 7010 (1999)
L. Vernon PhD Thesis
G. Henkelman, B. P. Uberuaga, and H. Jónsson, J. Chem. Phys. **113**, 9901 (2000)

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Results

- Simulations of growth of thin films of interest for PV applications.
- Growth of Al and Ag (100) and (111) films - contacts and concentrators.
- Growth of ZnO - TCO.
- Growth of TiO_2 - AR coating.

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Growth of Al and Ag

- EAM type potentials.
- 6 initial layers of metal.
- 4 new layers grown.
- 10 ML/s growth rate - 350K temperature.
- Growth energies of 1 eV and 40 eV.
- Optional co-deposition of Ar.

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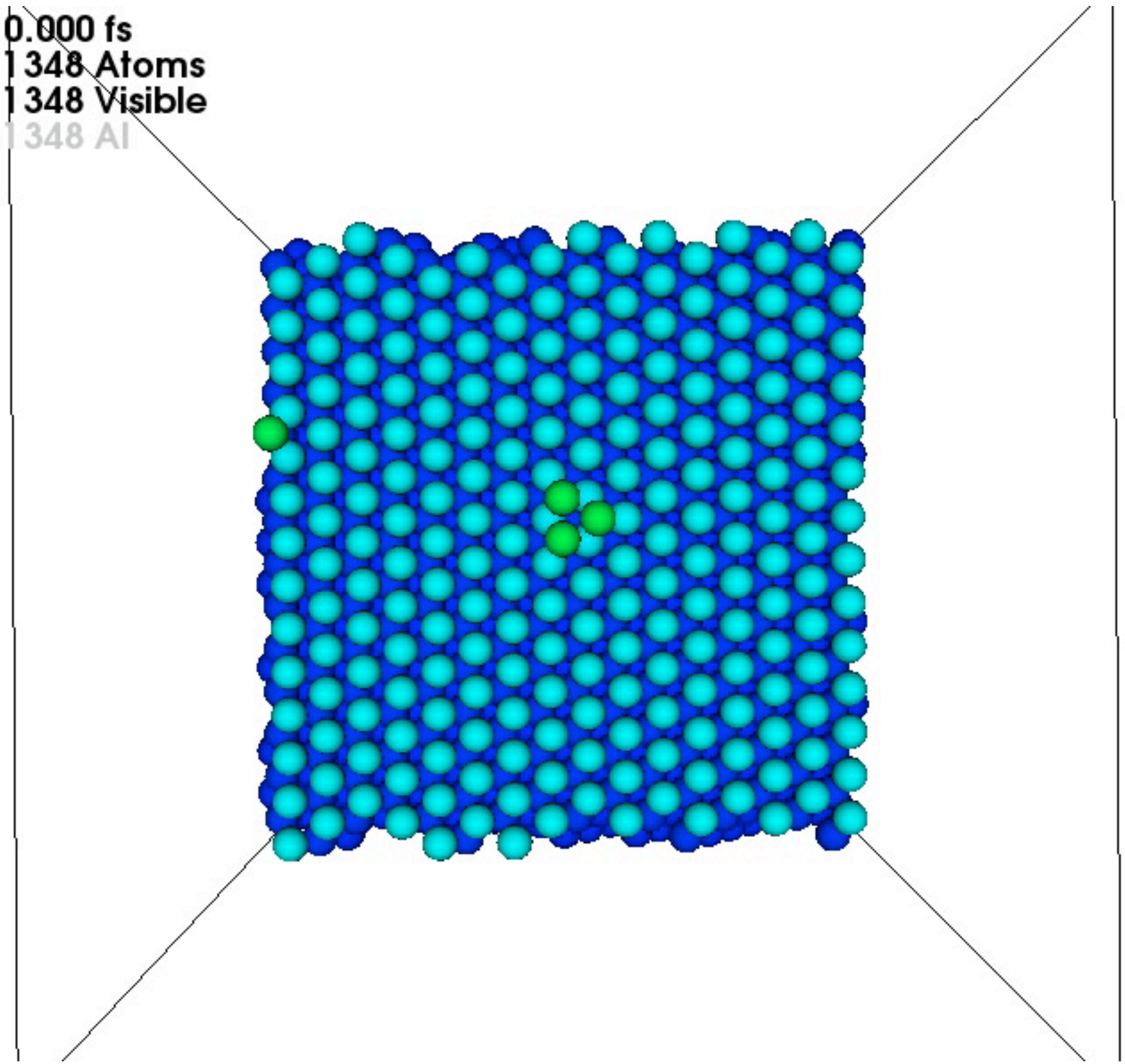
Al (111) Growth



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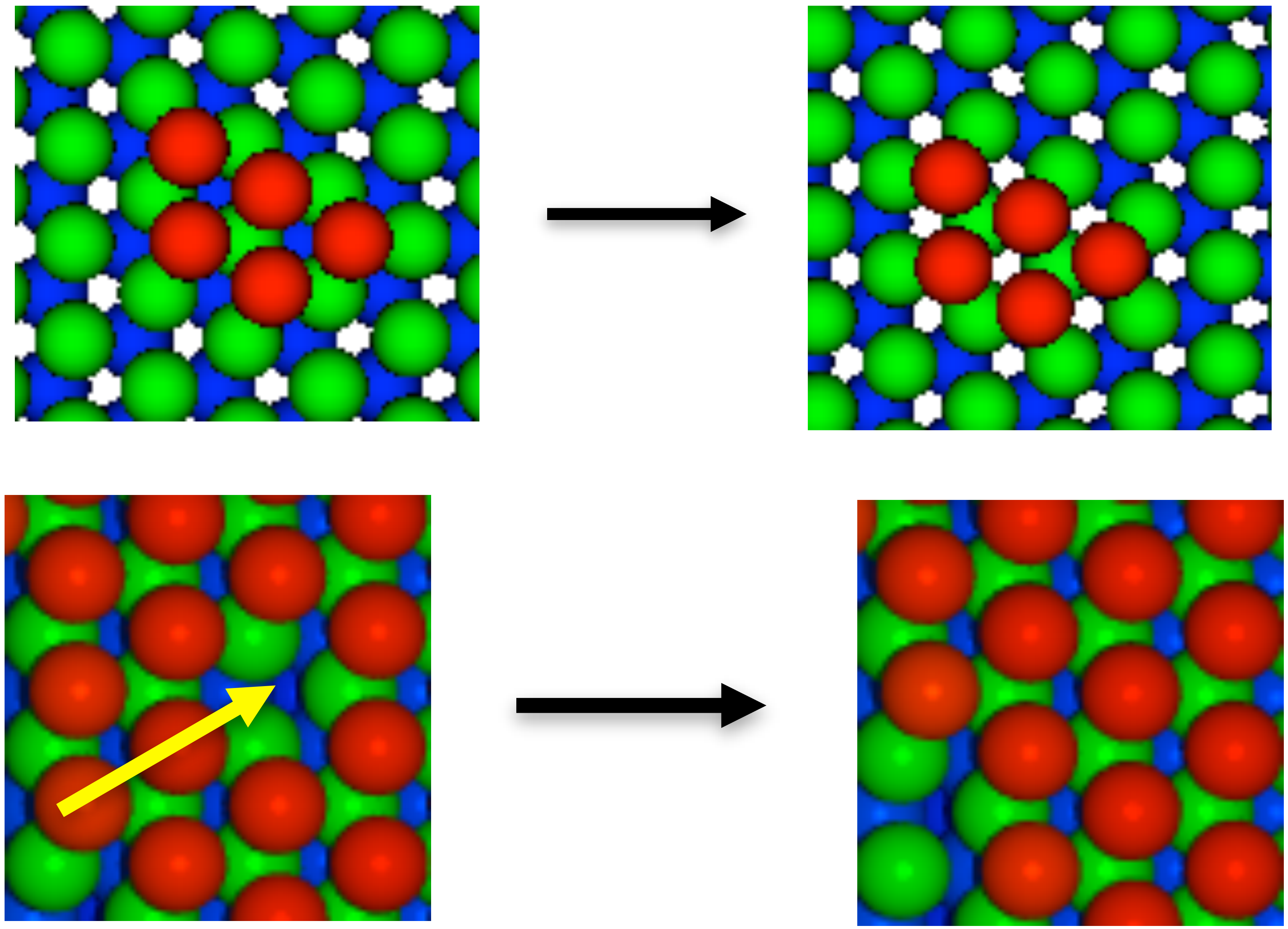
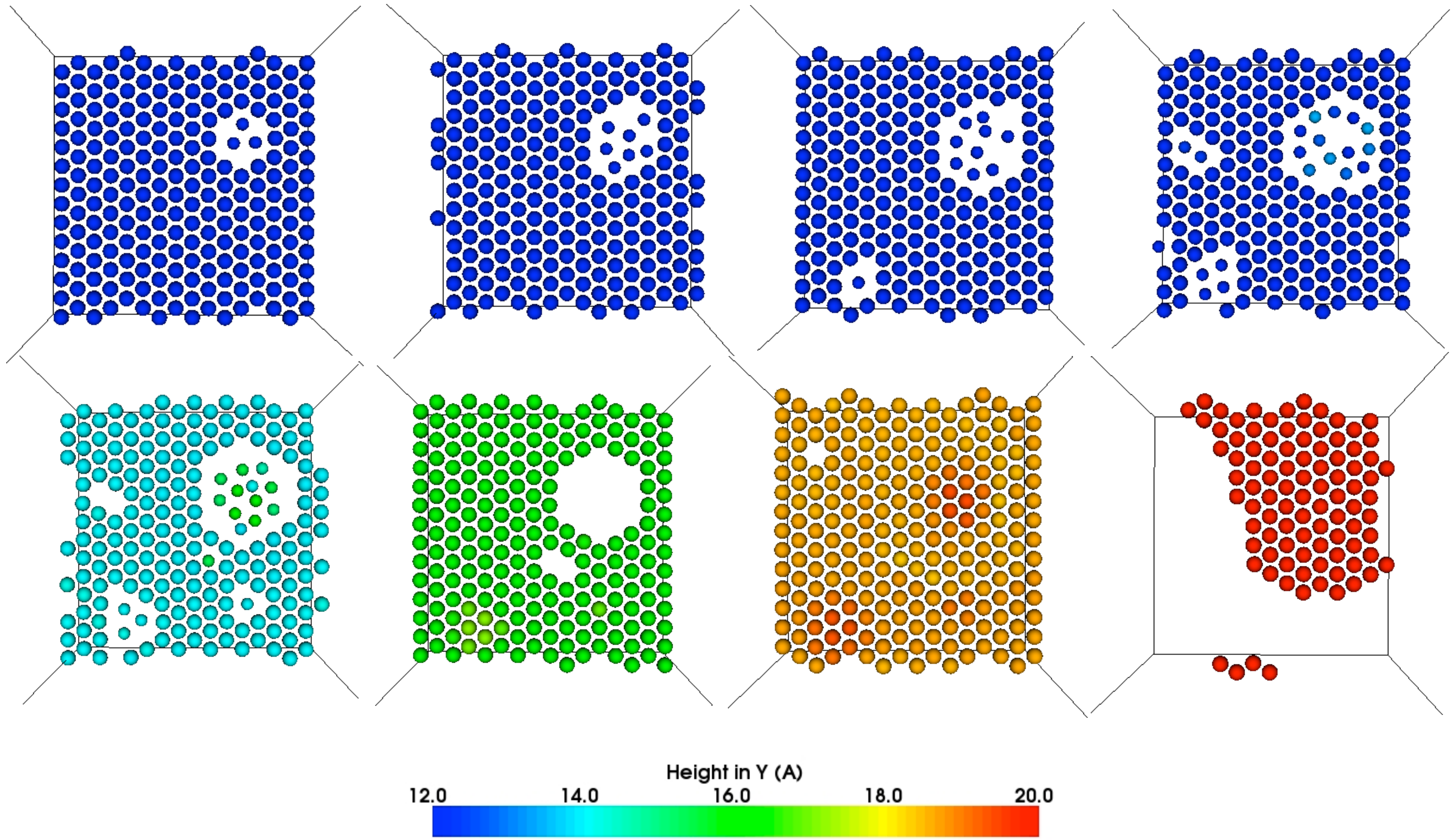
Concerted Motions





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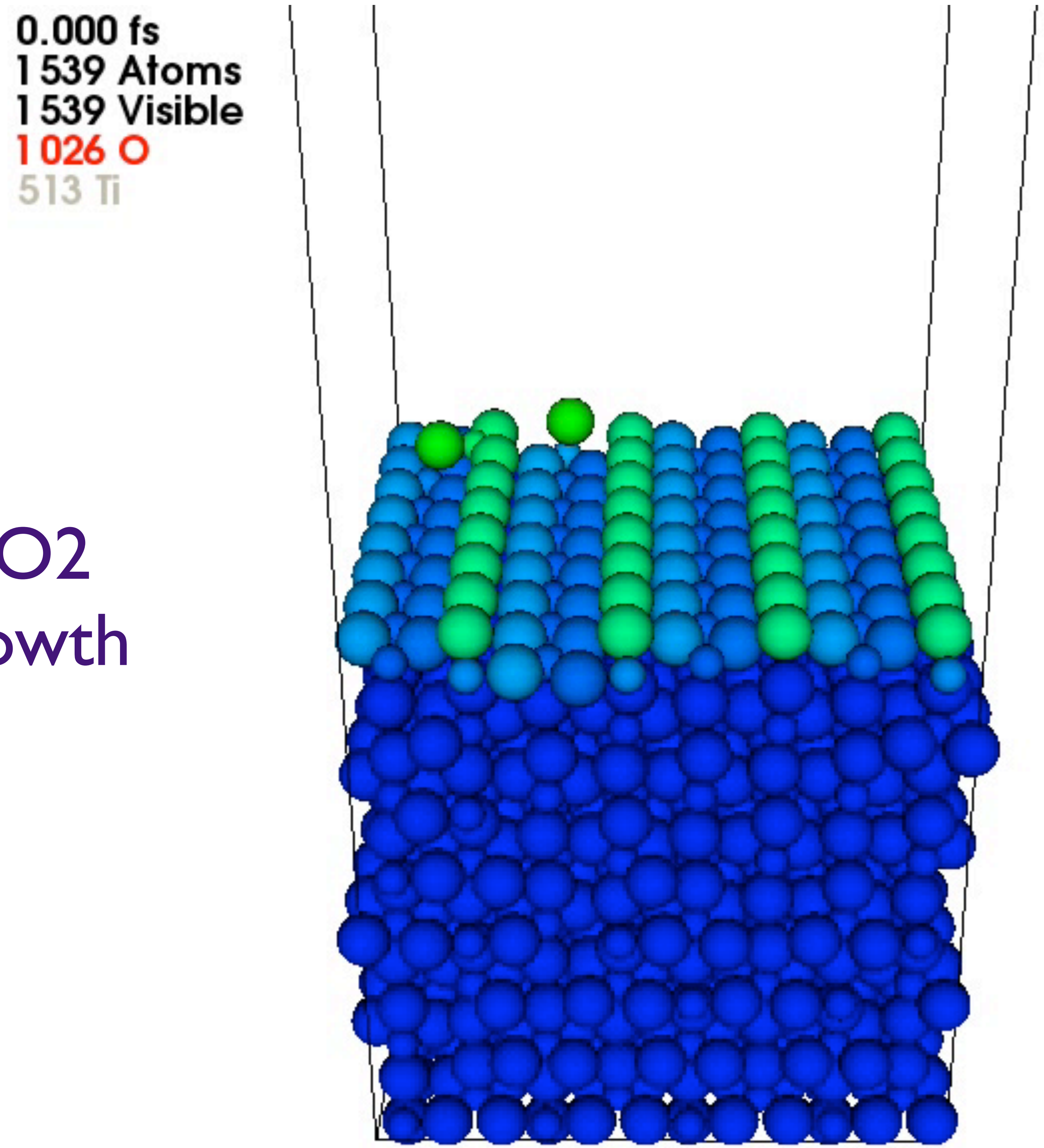
Growth of TiO_2

- Variable charge potential used.
- Modified to reproduce important transitions.
- 6 initial layers.
- 4 new layers grown.
- Deposition rate 0.5 ML/s - 350 K.

TiO2 Growth



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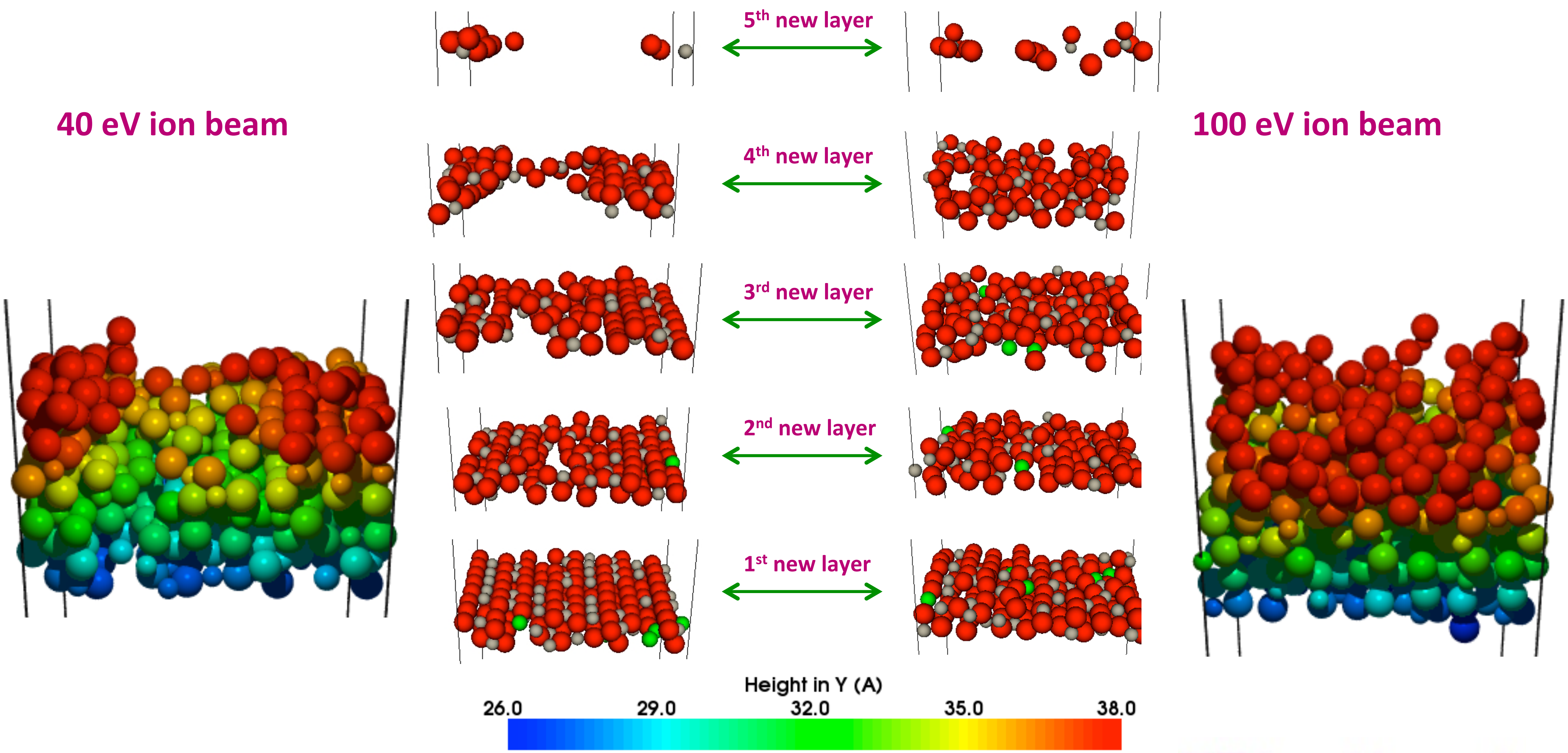
TiO_2 Growth



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Multiple Collision Cascades

- 1 keV collision cascade modelled by MD for 20 ps
- Subsequent diffusion modelled by otf-KMC
- Collision cascades performed every 0.2 s, simulates ion implantation rates
- Total of 3 collision cascades modelled

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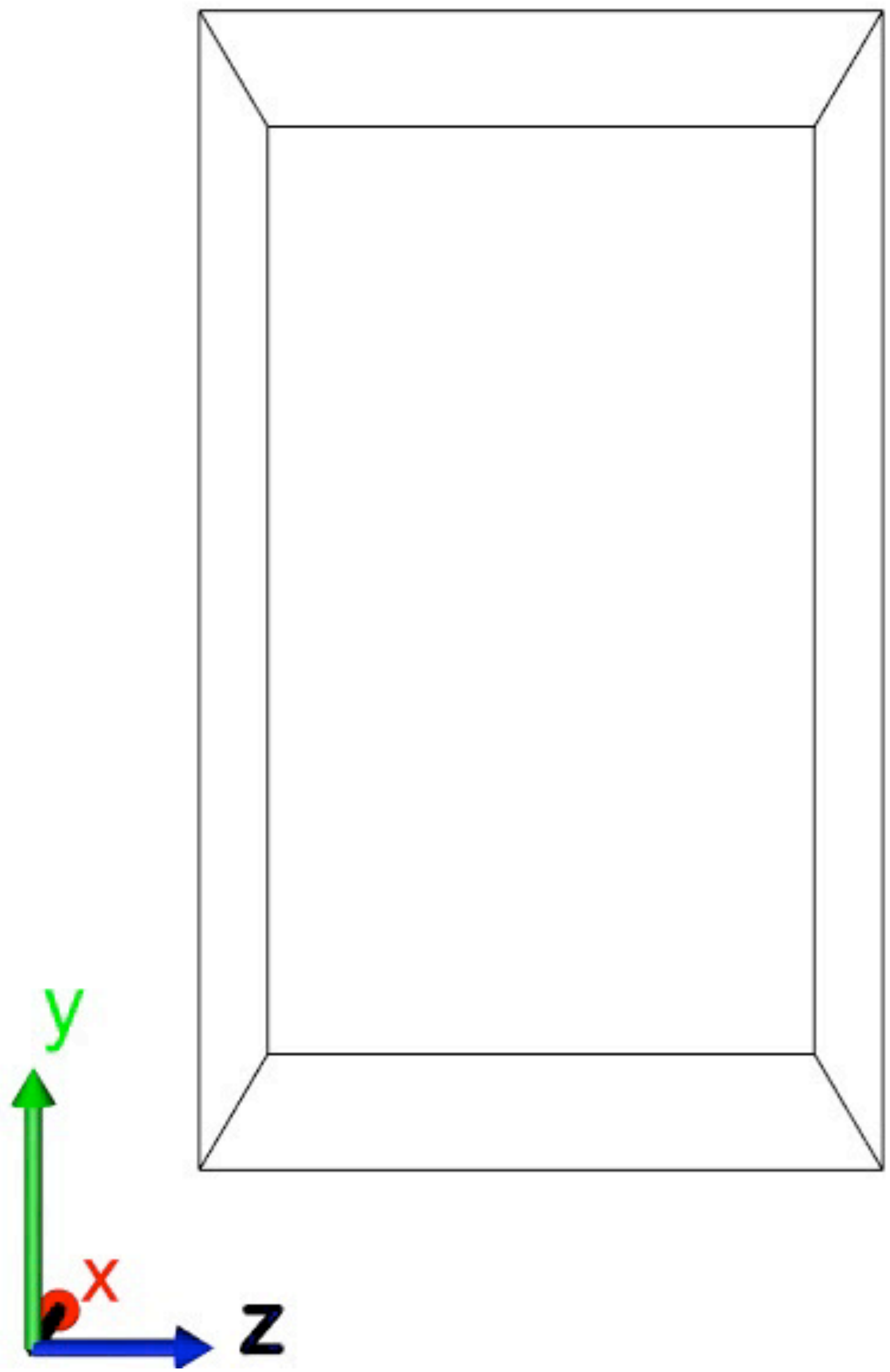
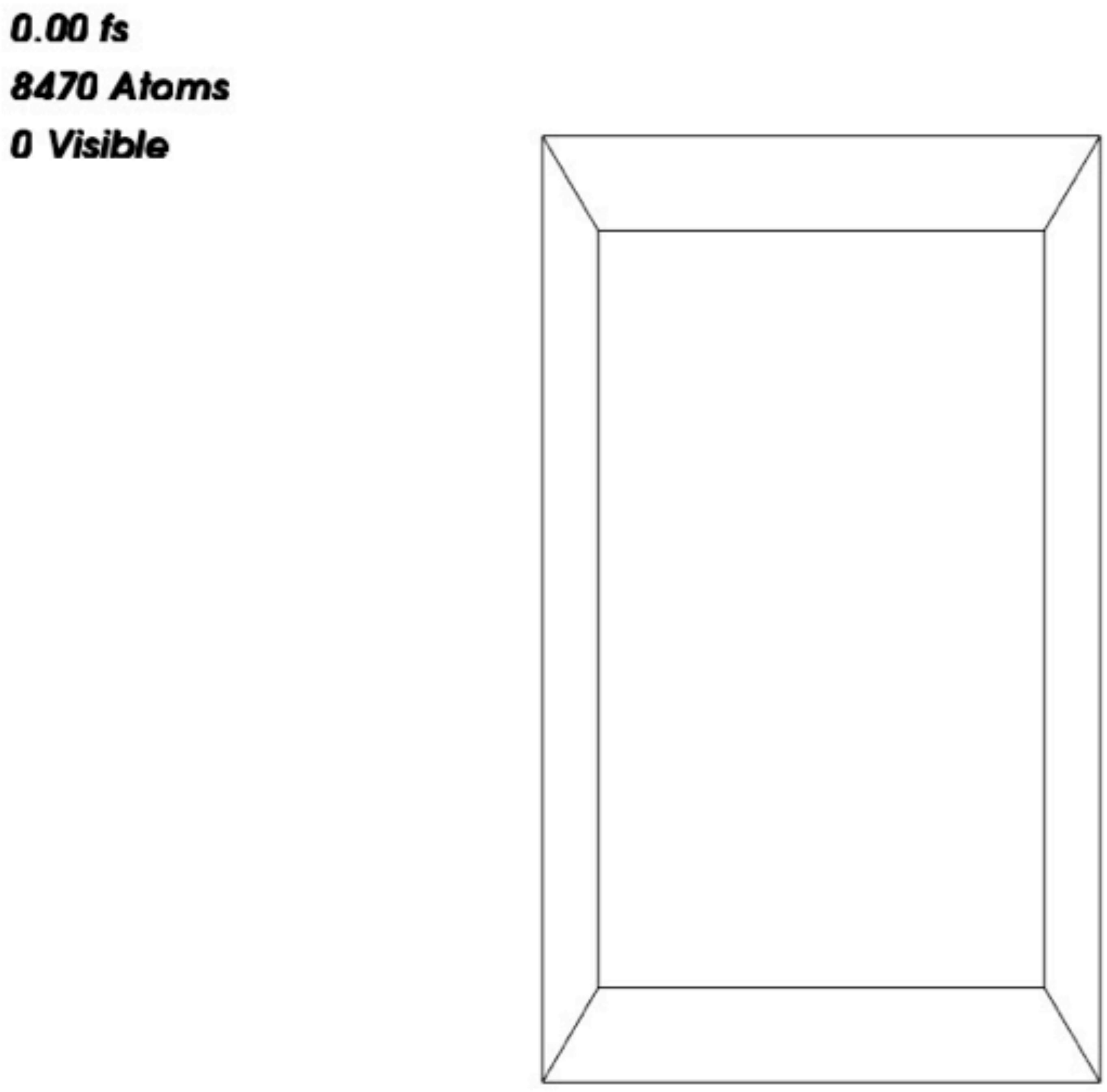
0.00 fs

8470 Atoms

0 Visible





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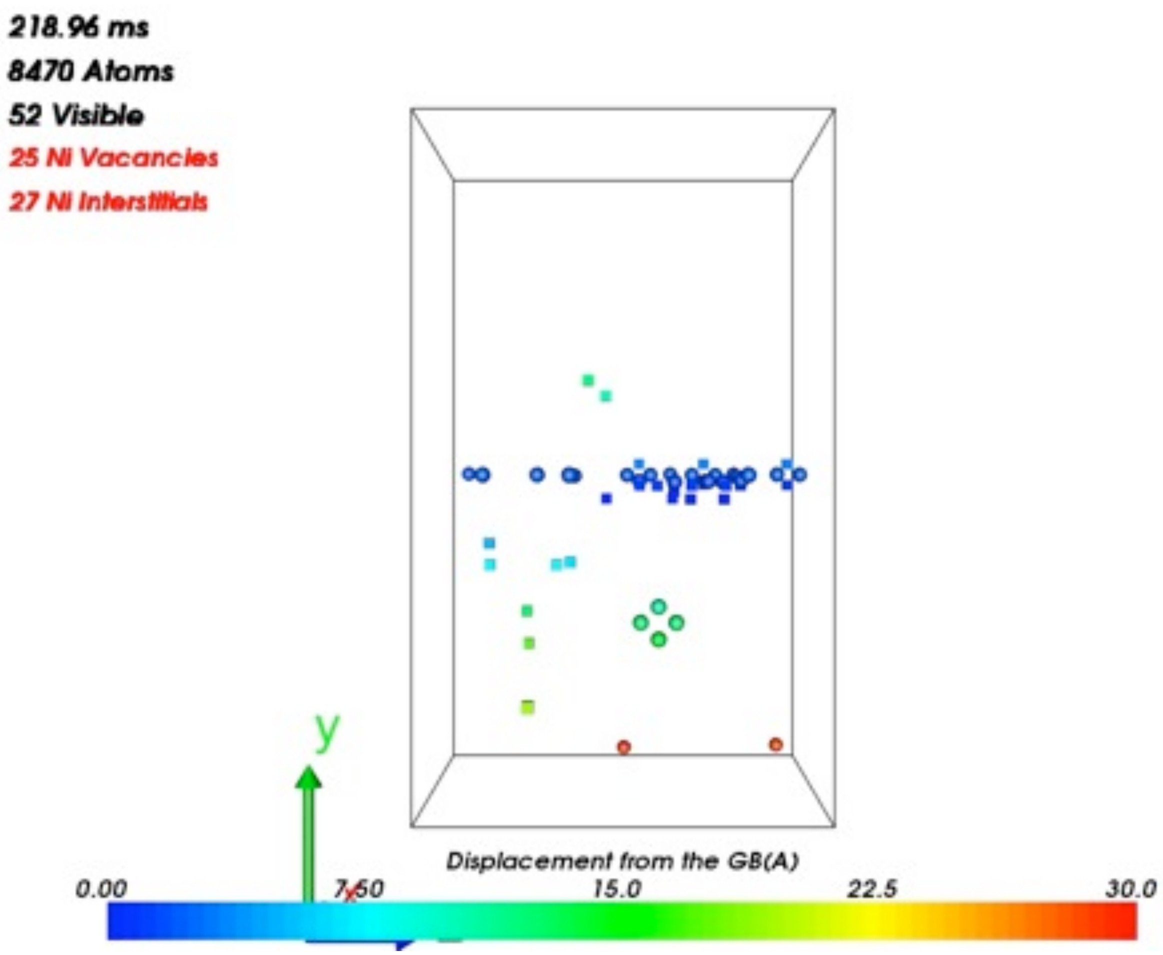

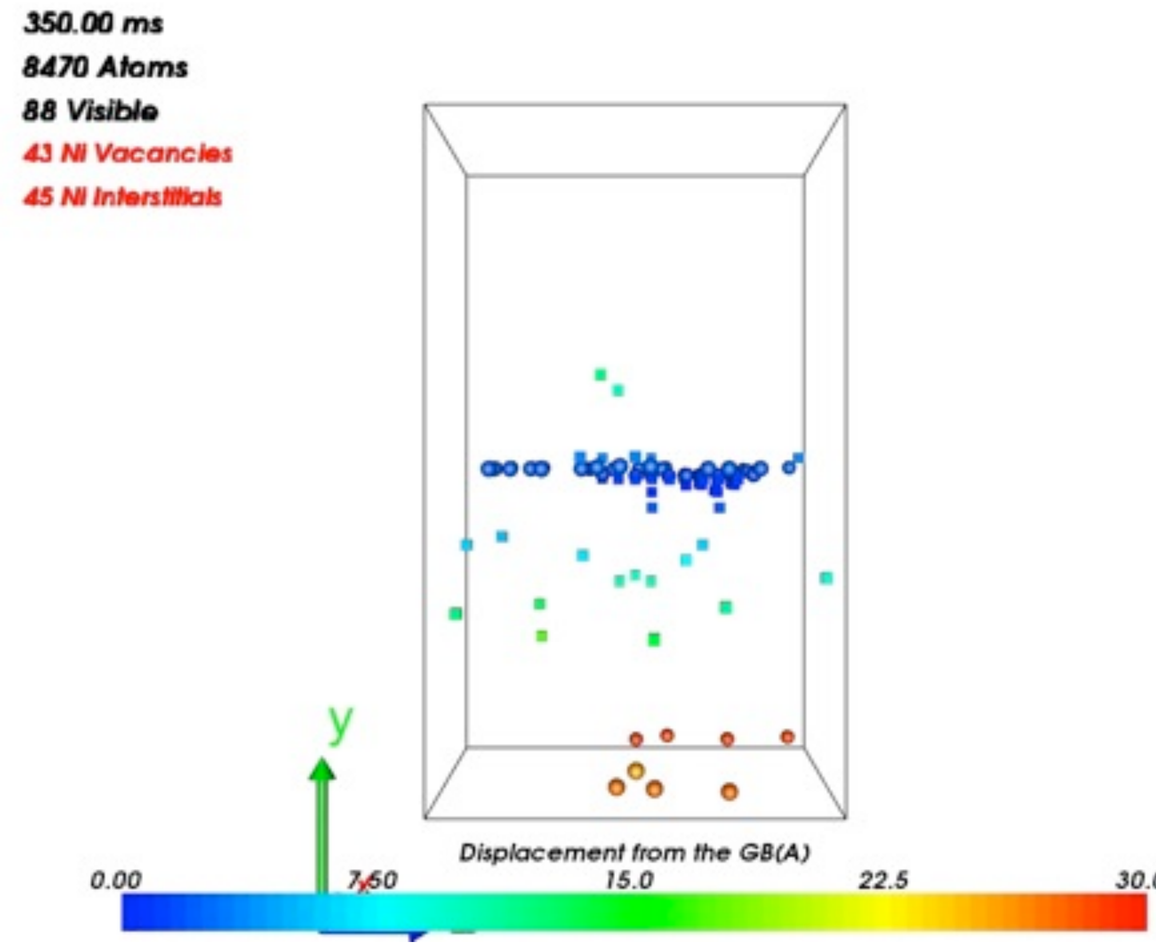

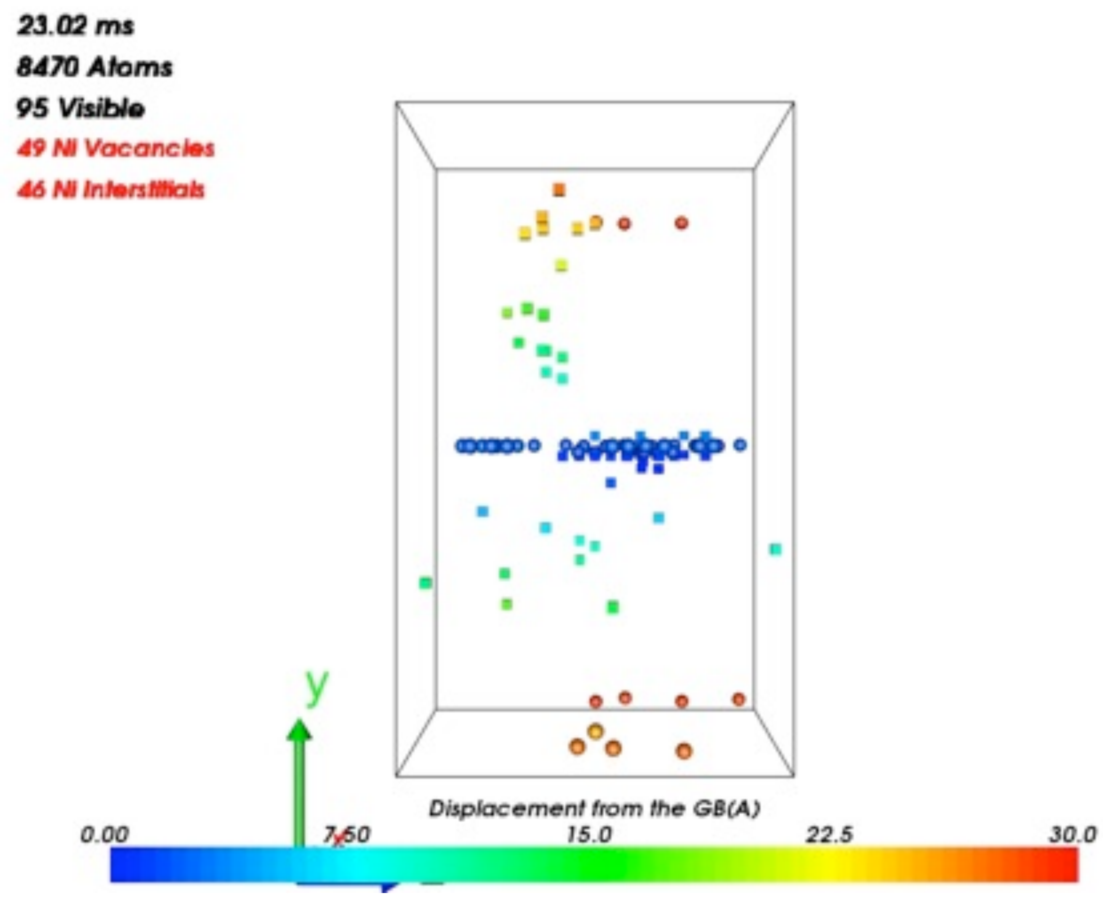

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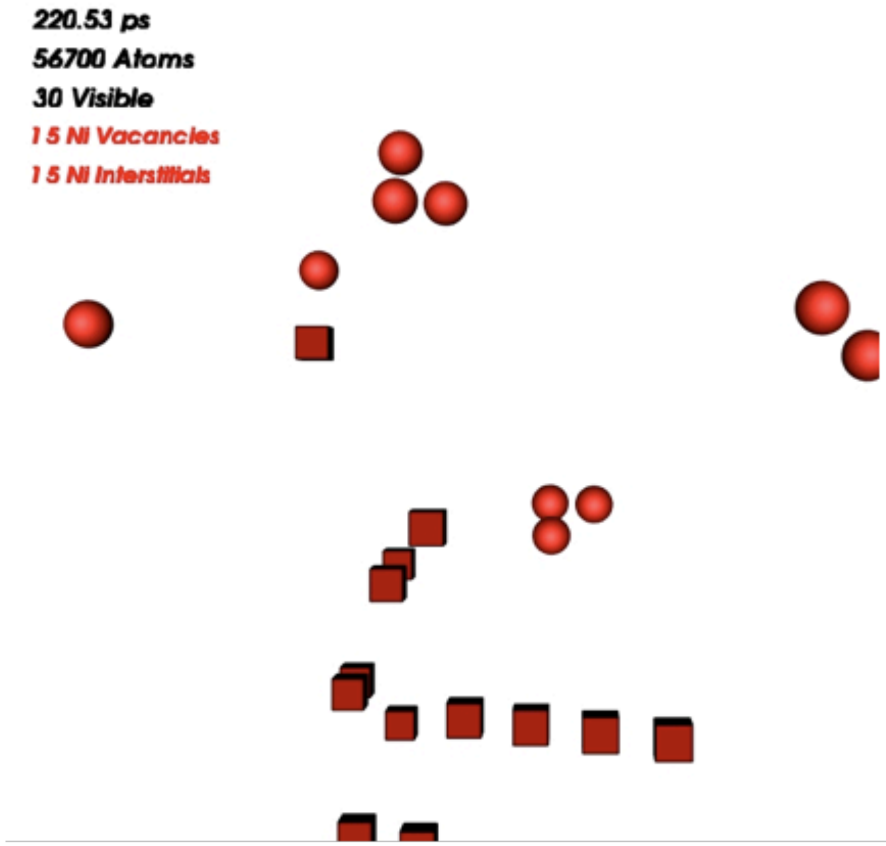
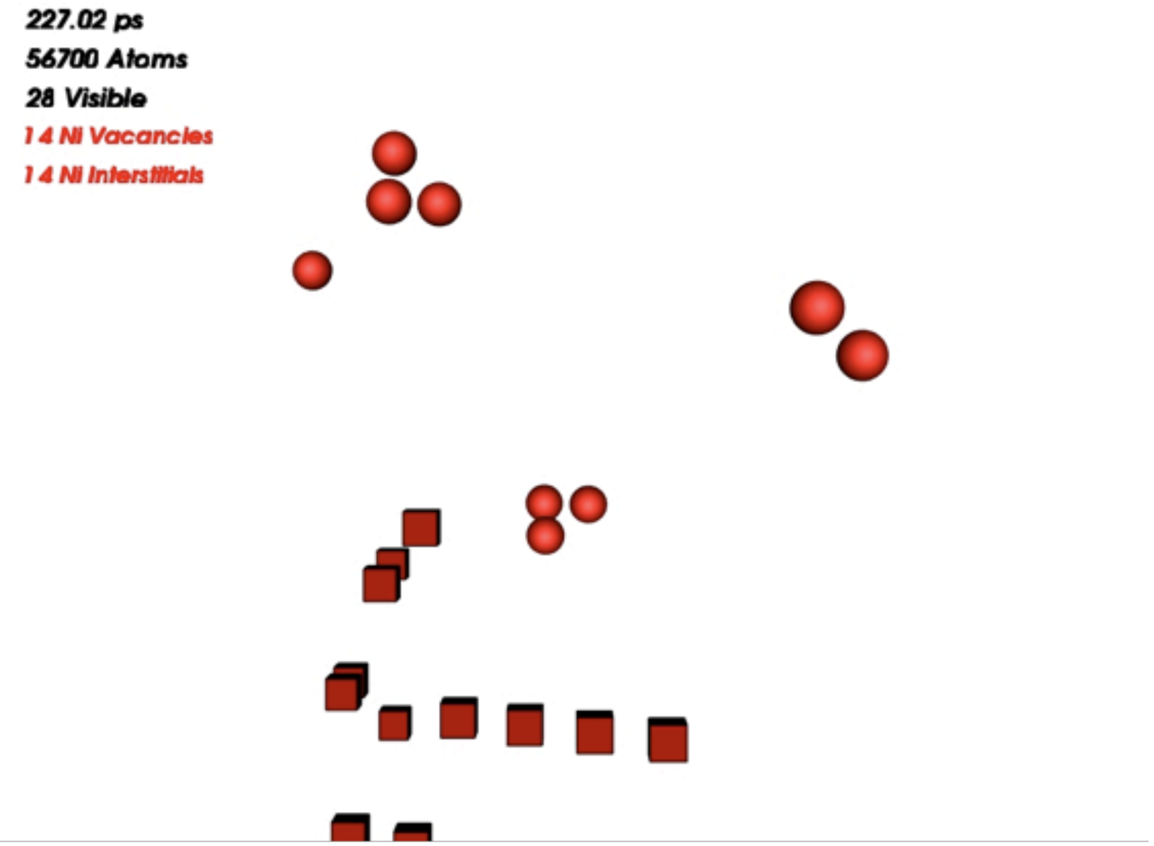
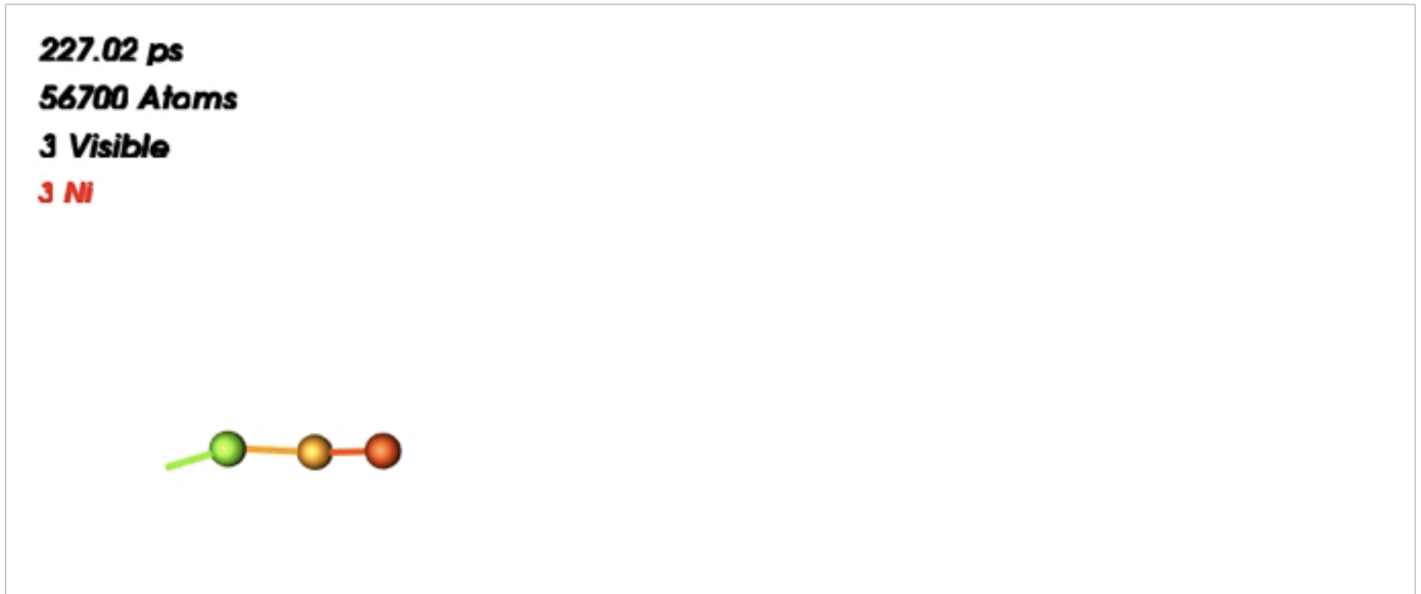
Concerted Events







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Challenges

- Speed
- Fidelity

Speed

- Main cost is function evaluations - 98-99% of time.
- Need to minimise by choice of methodology and parameters.
- Filtering out low energy transitions that don't contribute to system evolution.
- Issue in most systems we have studied.

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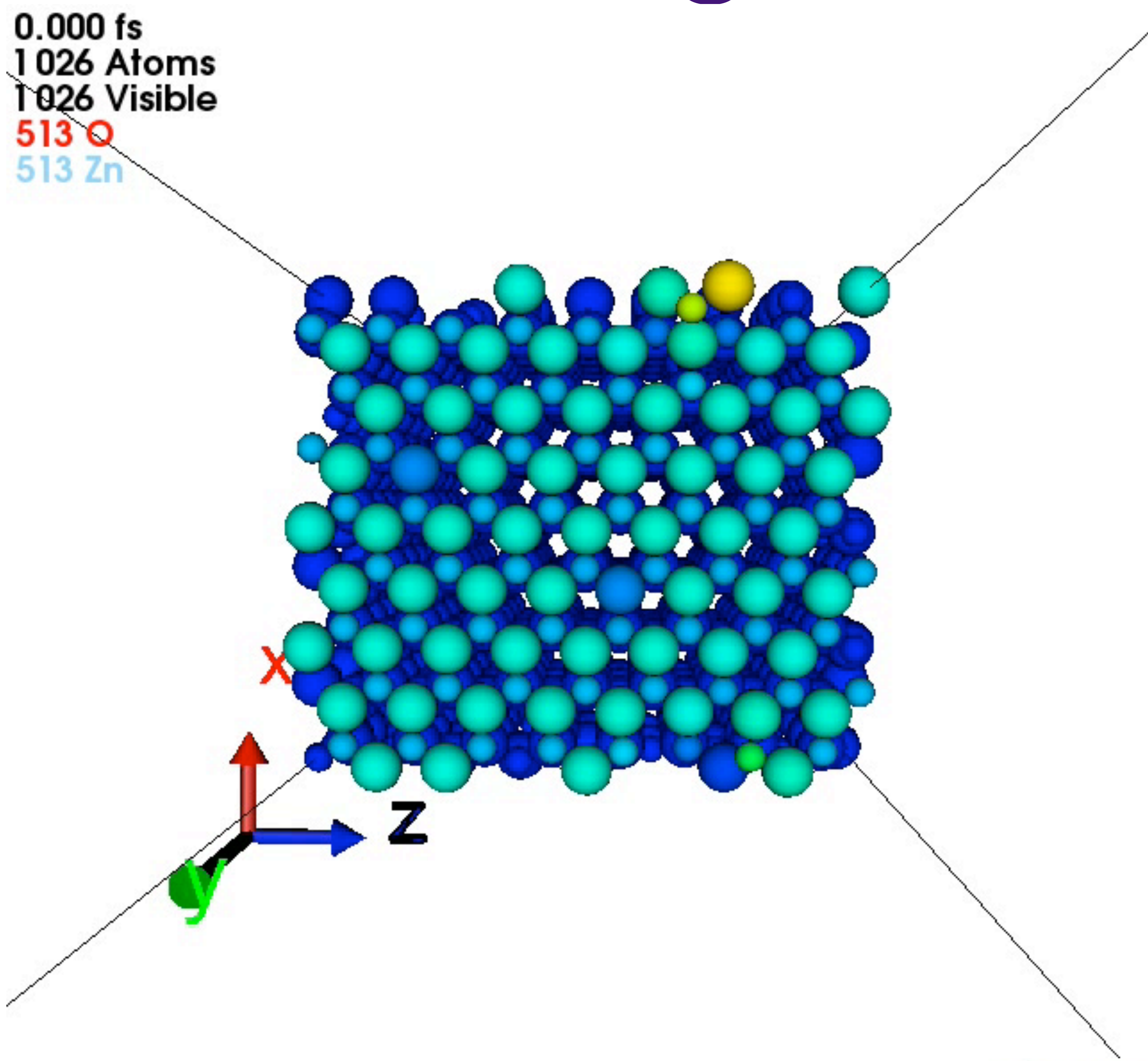
Challenges



Fidelity

- How many searches is enough?
- Fixed number of searches checked to see whether sufficient.

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Conclusions

- Very powerful tool for studying evolution of systems.
- Can already study real systems.
- Still work to be done on refining the methodology.
- Developments needed:
  - Auto-identification of events that don’t contribute to the system evolution.
  - Understanding when to stop searches.

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