Long Time Scale Simulations of Radiation Effects in Metals

Tomas Lazauskas and Zainab Al-Tooq

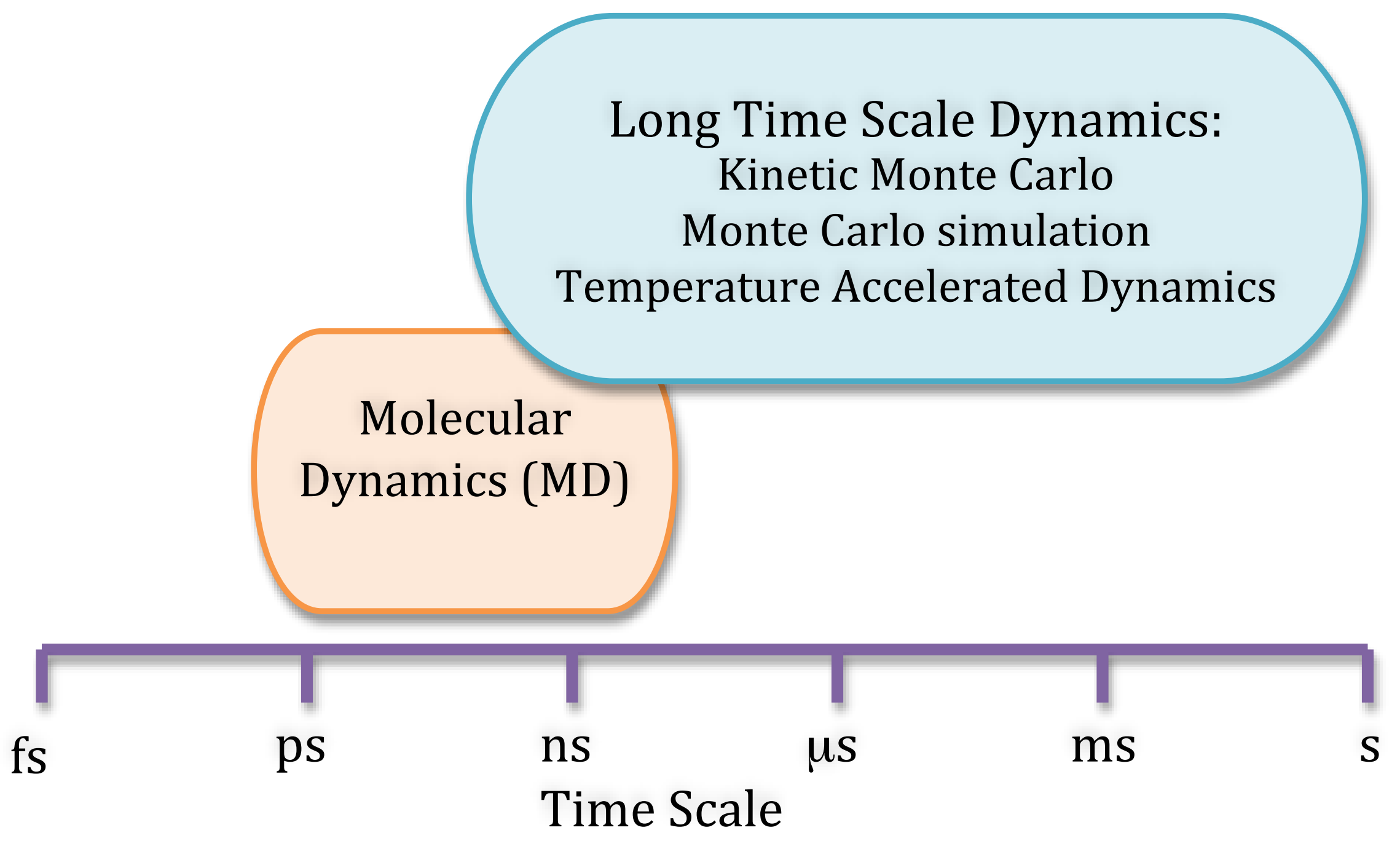
Department of Mathematical Sciences, Loughborough University
Loughborough, LE11 3TU

Introduction

Fission reactor pressure vessels experience extreme conditions during service, such as high temperature, corrosive and radiation environments. During a radiation event a particle collides with an atom (a collision cascade),which produces defects, i.e. vacancies and interstitials. These diffuse over a time scale much longer that accessible by Molecular Dynamics[1].

Methodology

We use Molecular Dynamics (MD) to carry out simulations through the ballistic phase of radiation damage. The longer time scales requires the use of other techniques.



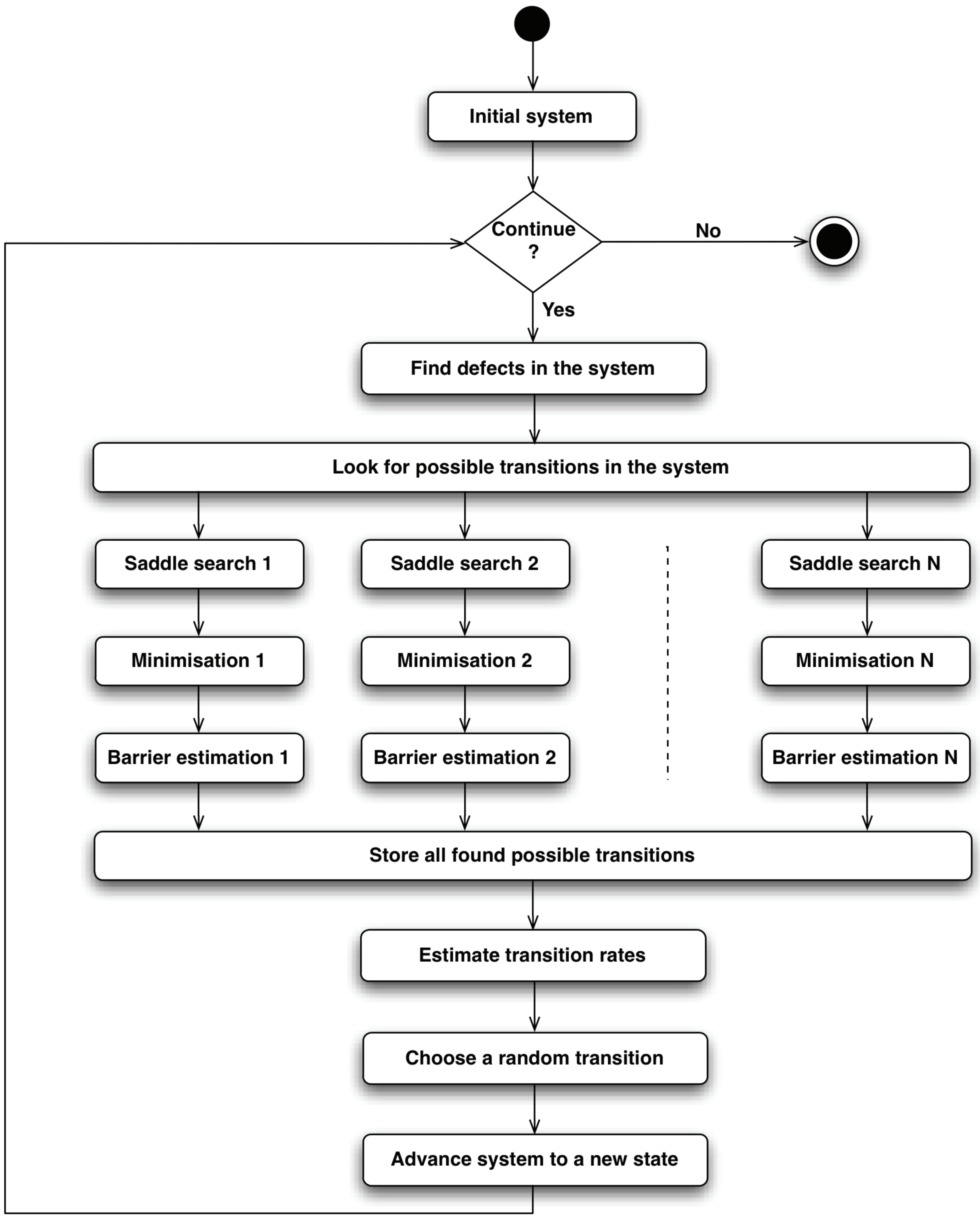
Long Time Scale Dynamics:
Kinetic Monte Carlo
Monte Carlo simulation
Temperature Accelerated Dynamics

Molecular Dynamics (MD)

fs ps ns µs ms s
Time Scale

For our long time scale simulations we use a hybrid Molecular Dynamics/on-the-fly kinetic Monte Carlo technique, which allows us to access time-scales several orders of magnitude longer than the collision cascade time.

Long Time Scale Technique



Initial system

Continue ?

No

Yes

Find defects in the system

Look for possible transitions in the system

Saddle search 1 | Saddle search 2 | Saddle search N

Minimisation 1 | Minimisation 2 | Minimisation N

Barrier estimation 1 | Barrier estimation 2 | Barrier estimation N

Store all found possible transitions

Estimate transition rates

Choose a random transition

Advance system to a new state

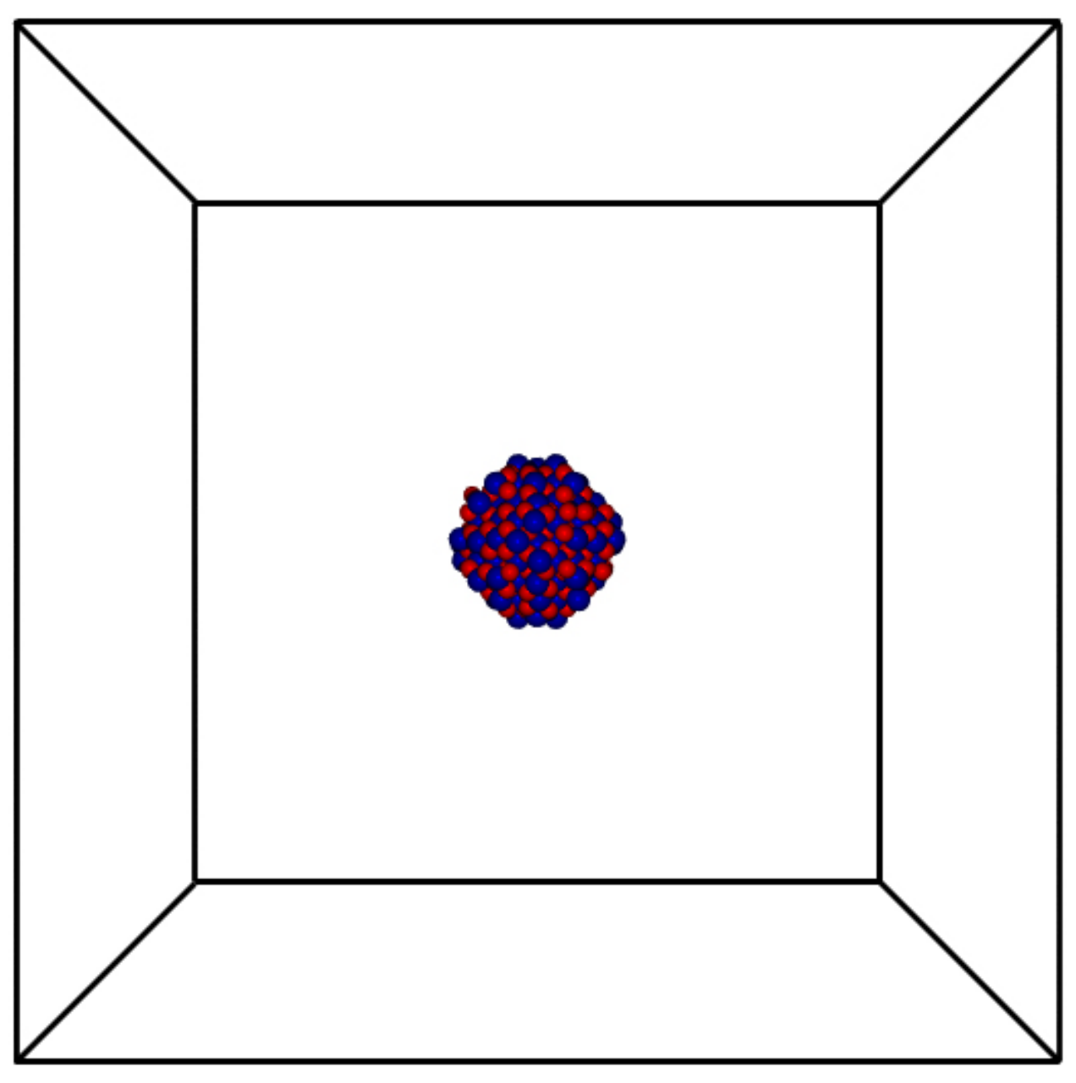
We call this technique a hybrid Molecular Dynamics/on-the-fly kinetic Monte Carlo technique.

After a radiation event we identify defects (i.e. interstitials, vacancies etc) and map out a region containing the defects.

The algorithm initiates a parallel transition search where each process uses the ART, RAT or dimer technique to search for a saddle point (transition). If a search is successful, the system is relaxed to a new state by using conjugate gradient. Then the NEB or string method gives a more accurate evaluation of the barrier height between the two states. After a given number of transition search attempts have been completed, the algorithm evaluates the rates of each transition and chooses one to evolve the system.

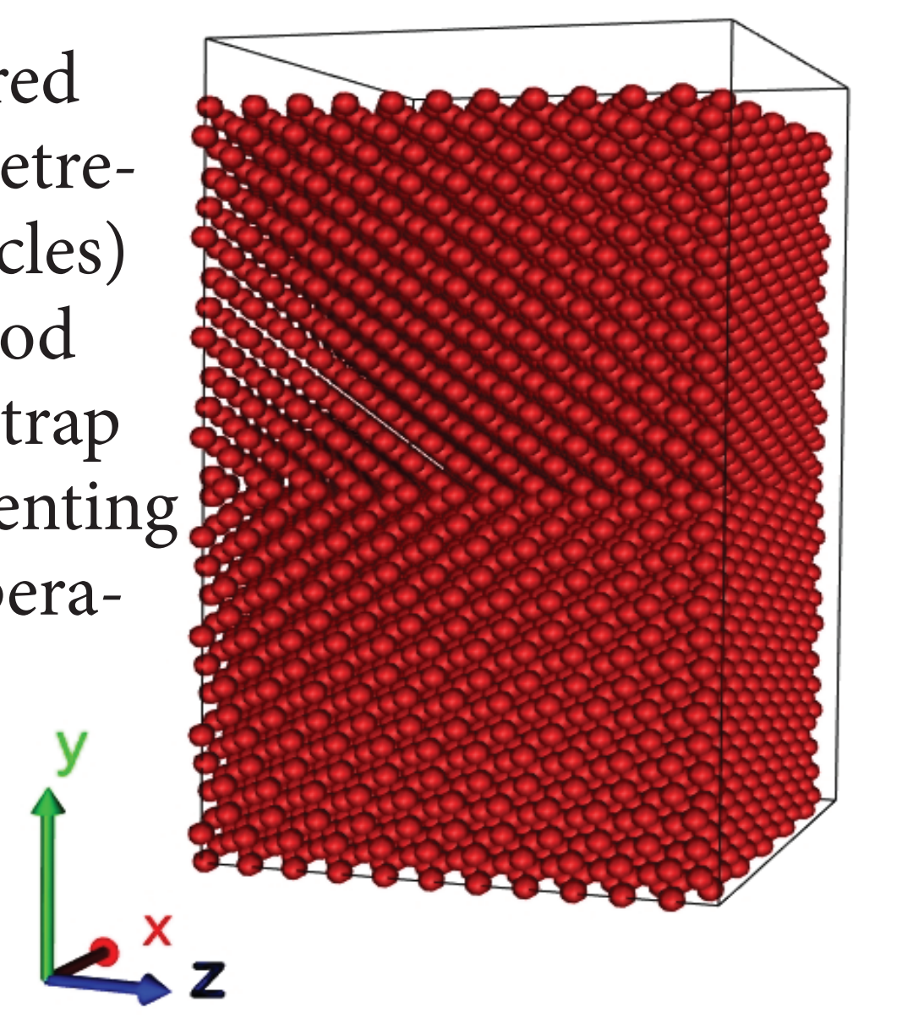
Applications

Examples are presented for potential next generation reactor materials such as oxide dispersion strengthened (ODS) steels with 0.3 at% embedded yttria nanoparticles and pure Ni.

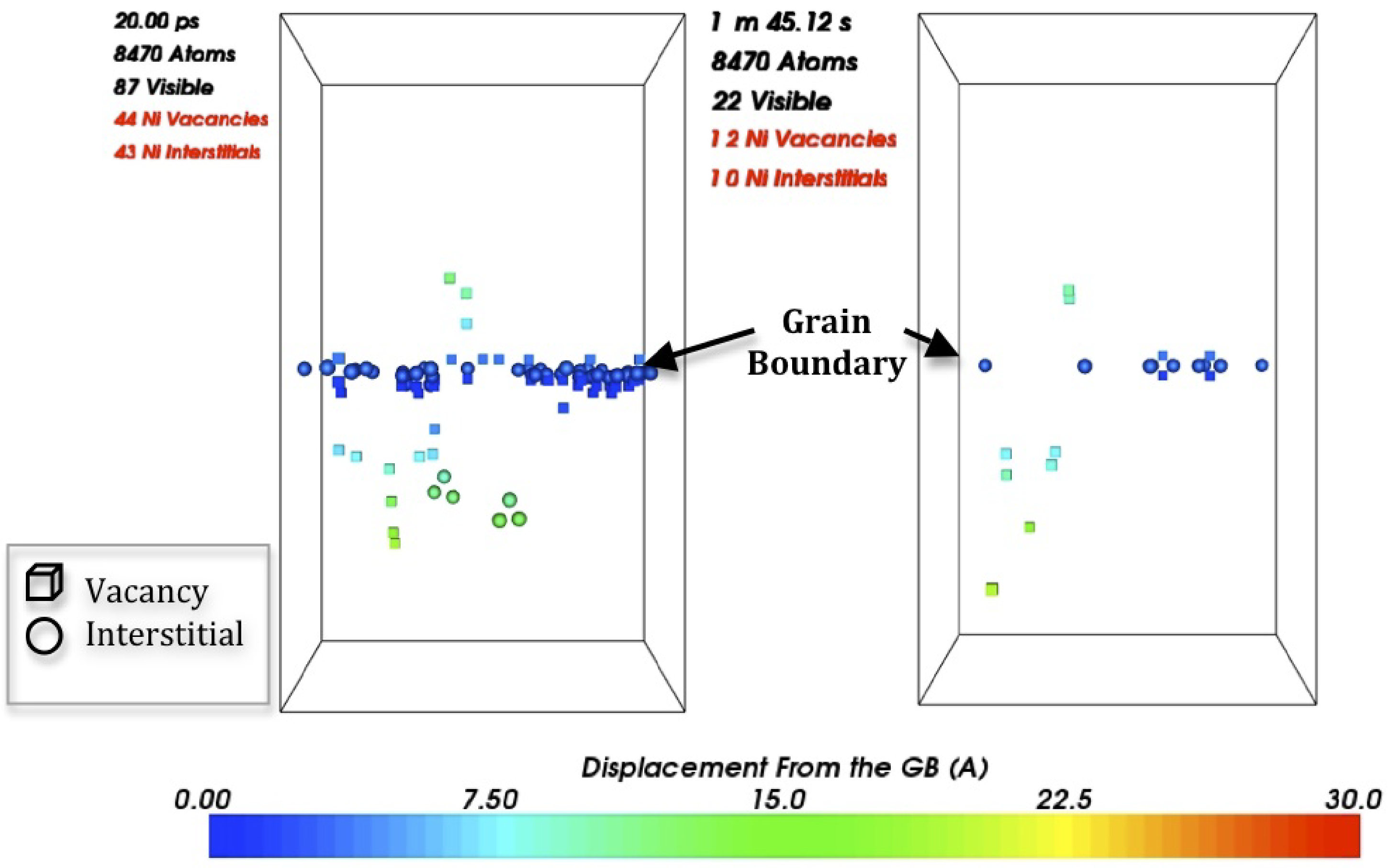


→ ODS steels are nano-structured ferritic alloys (NFAs) with nanometre-scale precipitates (e.g. yttria particles) within them. They have shown good radiation resistance, the ability to trap He in fine scale bubbles,thus preventing swelling and providing high-temperature strength.

Due to their high-temperature properties Ni-based alloys represent an interesting class of materials for next generation nuclear power plants. There is a large body of work aimed at understanding the effect of radiation on Ni-based materials especially at grain boundaries. ←



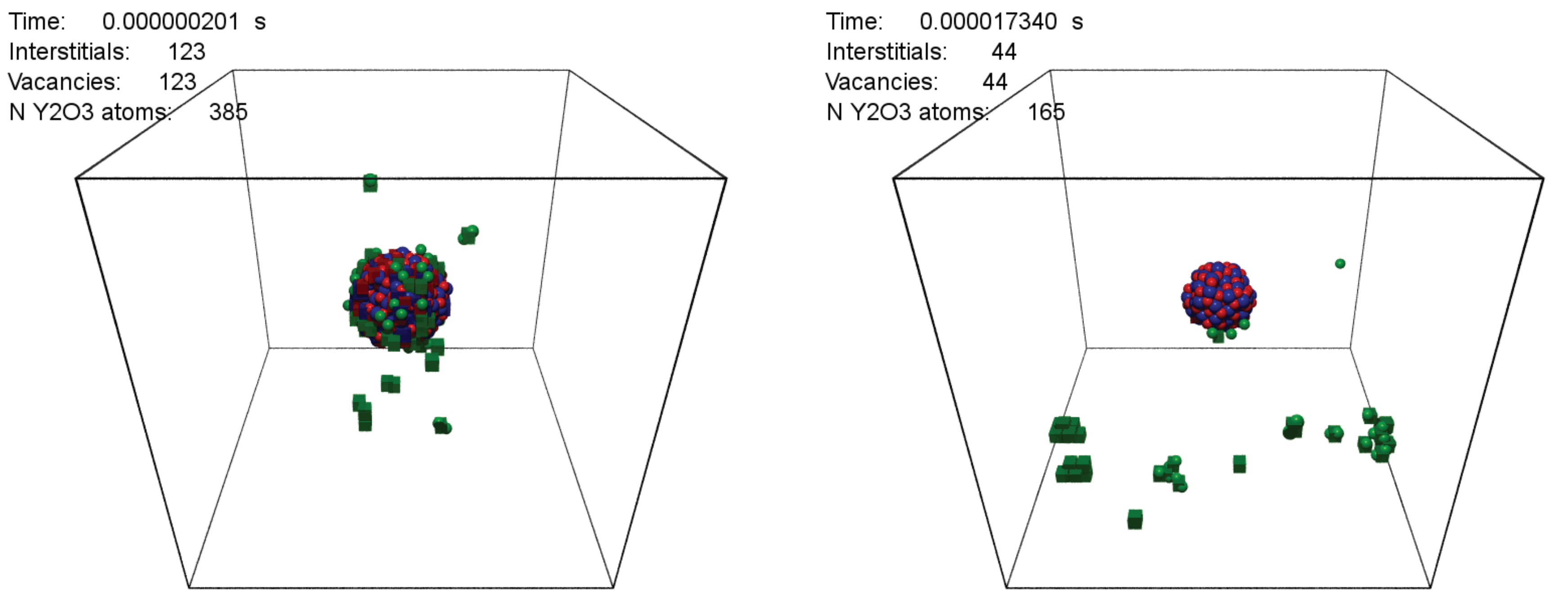
Results in Ni Systems



Simulating a 1 keV collision cascade in a Ni system containing a ∑ 5 GB for 20 ps using MD results in most defects accumulated at the GB. Otf-KMC was then used to simulate the evolution of defects in the resulting system at a temperature of 500 K. Most of the interstitials are annihilated or recombined with vacancies and the vacancies were found to form clusters or combine with interstitials. Although we saw vacancy diffusion to the GB, the vacancies diffuse over much longer timescales and are more likely to form clusters than the interstitials.

Multiple collision cascades also have been modelled. MD is run for for 20 ps followed by otf-KMC for approximately 0.2 seconds. This is repeated to model dose effects.

Results in ODS Systems



Possible processes that are responsible for better ODS steels performance in radiation environments were found. Results suggests that yttria nanoparticles are resistant to radiation, can absorb the energy from the cascades, act like obstacles by stopping collision sequences and attract and trap the defects around their boundaries.

Conclusions

The hybrid Molecular Dynamics/on-the-fly Kinetic Monte Carlo technique has proven to be a powerful tool to model complex systems and reach long time scales compared to MD simulations. Therefore MD collision cascades followed by this technique allows us to simulate radiation damage during typical reactor lifetime.

Contact details

Tomas Lazauskas
t.lazauskas@lboro.ac.uk

Acknowledgments

Supervisors: Roger Smith, Steven Kenny

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[1] A typical reactor lifetime is ~ 40 years with the maximum number of displacements per atom induced by the radiation being of the order of 0.05 in the region next to the reactor core.