Non-adiabatic Tight Binding Simulations of Radiation Damage in Metals

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Young Investigators Symposium, ORNL, 13 Oct 2008

Imperial College London

EPSRC
Engineering and Physical Sciences Research Council

THE THOMAS YOUNG CENTRE
LONDON CENTRE FOR THEORY AND SIMULATION OF MATERIALS

Materials for Fusion Reactors

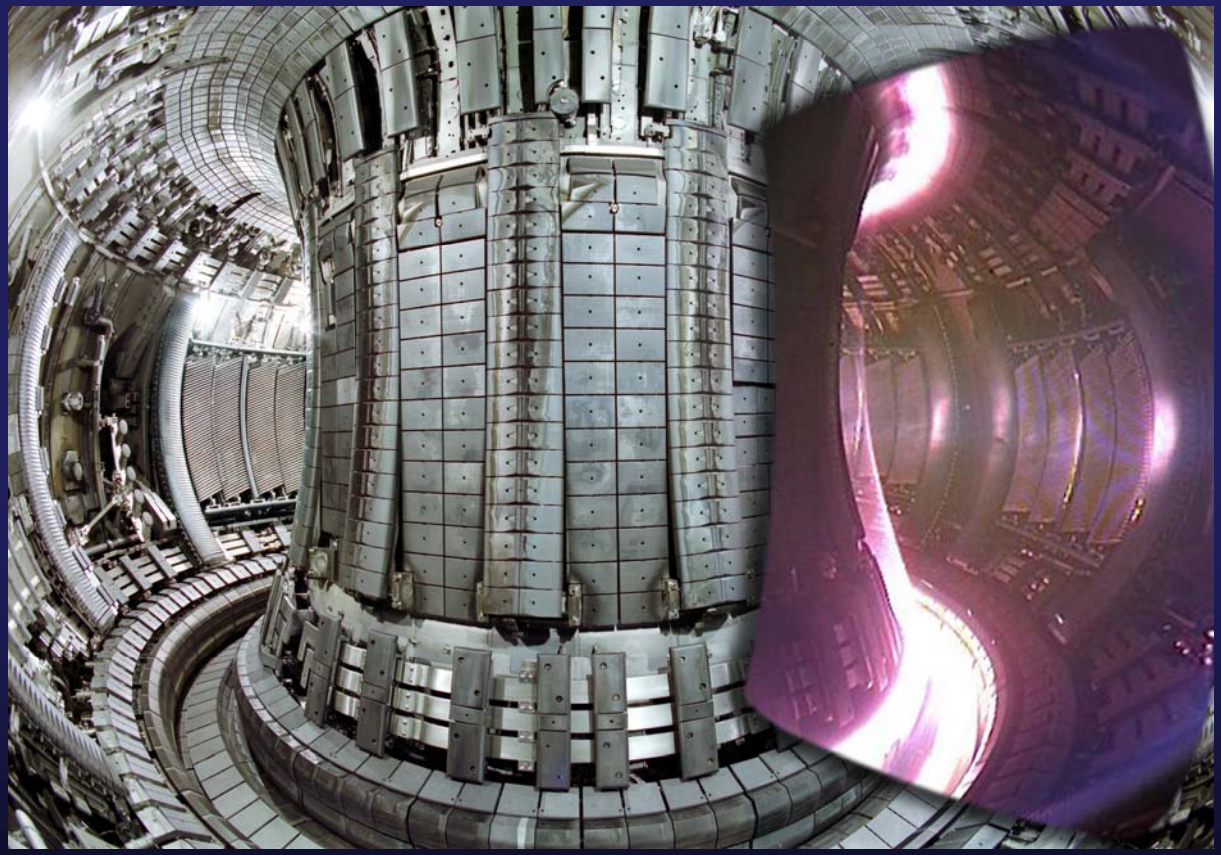


Image: EFDA-JET

Radiation Damage Cascades

- 14 MeV neutron gives high recoil energy to PKA
- Ion collisions create nanoscale region with very high temperature
- Recrystallization leaves a handful of defects
  - Vacancies coalesce into voids, dislocations entangle causing embrittlement
  - This determines mechanical properties
- Defect population affected by cooling rate
  - Heat conducted away by electrons
  - Important to understand electron-phonon coupling

The Ehrenfest method

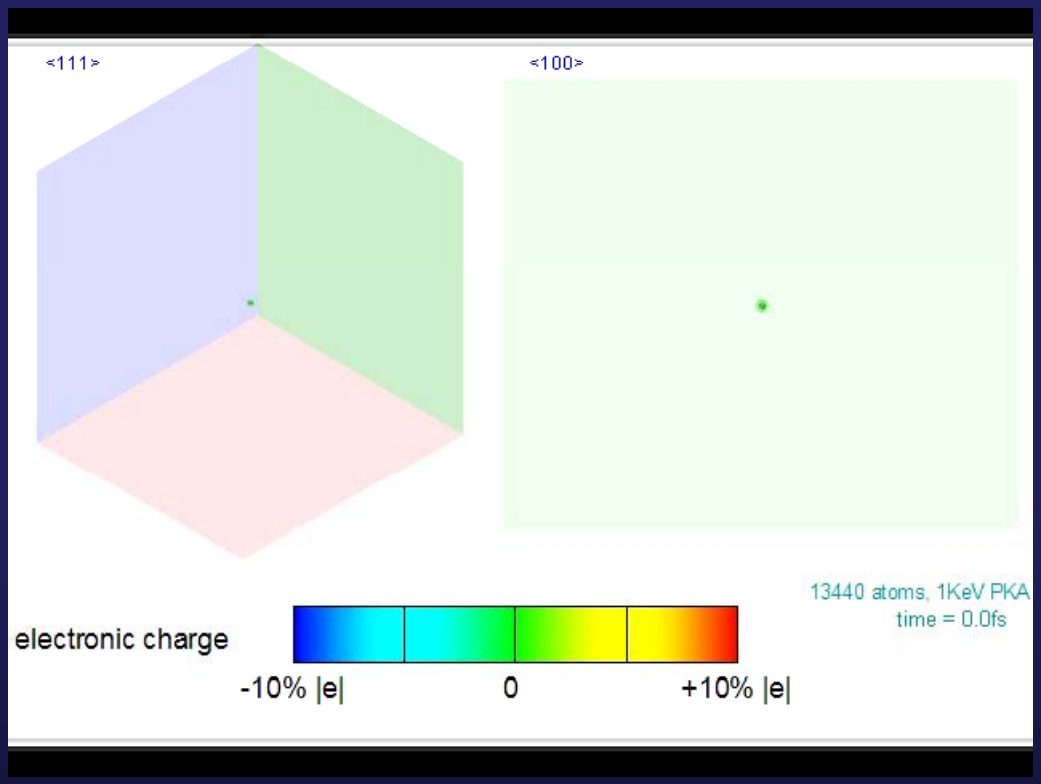
- Classical ions evolving with Newton's equations
- Quantum mechanical electrons evolving with time-dependent Schrödinger equation.
  - Quantum Liouville equation

$$i\hbar\frac{d\rho}{dt} = [H, \rho]$$

  - Electrons not kept in ground state.
- Electronic excitation measured by comparison to ground state.

• J. le Page, D.R. Mason and W.M.C. Foulkes 2008, *J. Phys.: Cond. Matt.* 20, 125212
• D.R. Mason *et al.* 2007, *J. Phys.: Cond. Matt.* 19, 436209

1keV cascade



13440 atoms, 64 processors, 72h

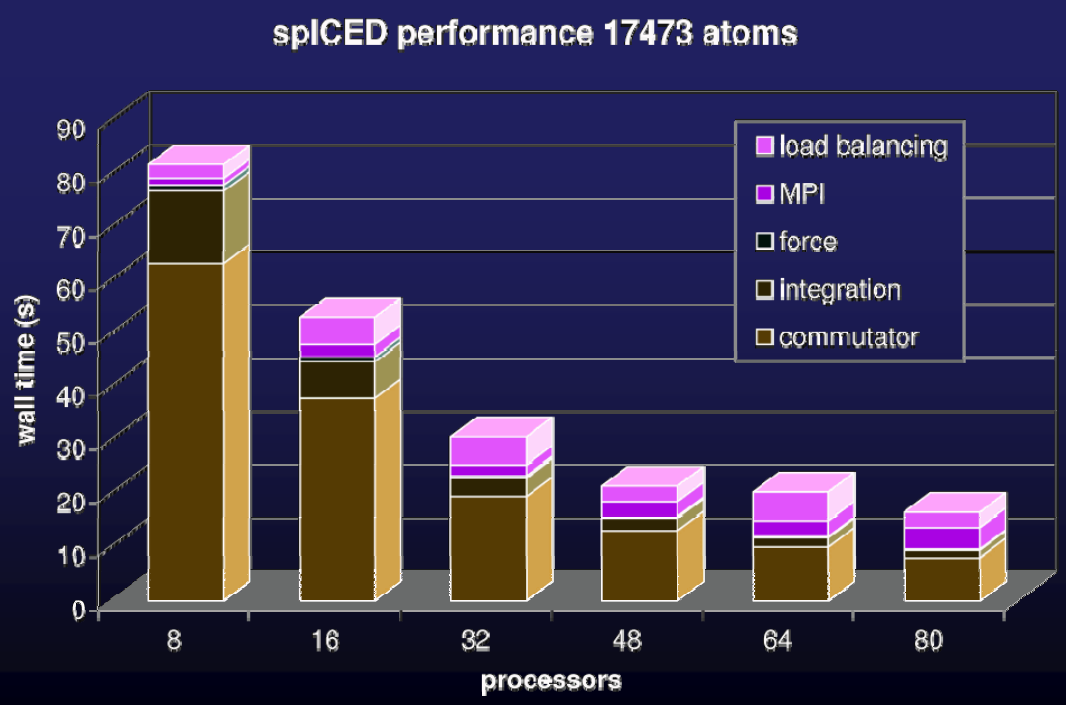
Simulation challenges

- Thousands of atoms to contain even a low energy cascade.
- ps of simulated time for cascade evolution
- Delocalised electrons in a metal: $\hat{\rho}$ is dense
- Atoms move around
- Memory M^2N^2. Floating ops zM^3N^2.
  - M: orbitals per atom, N: atoms, z: coordination.

• D. Dundas, E.J. McEniry, D.R. Mason and L. Stella 2007, *Capability Computing* 10 ,12-14

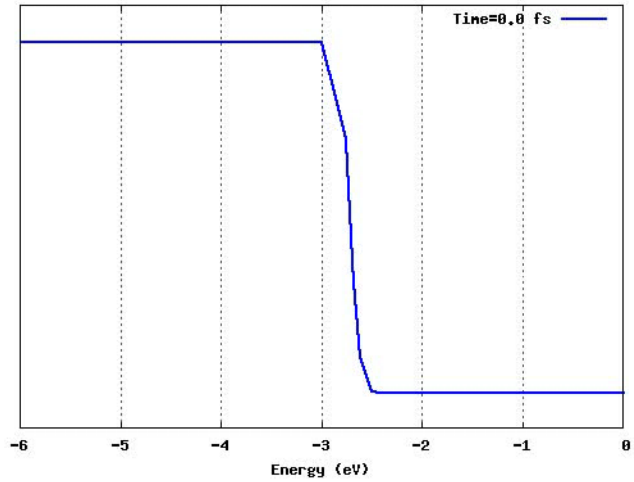
Computational strategy

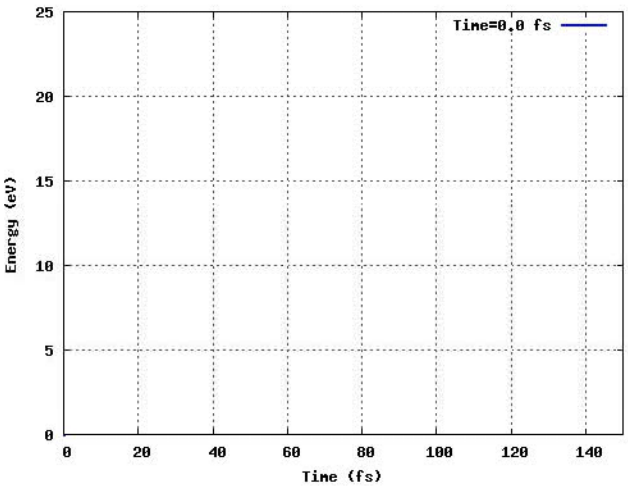
- $\hat{H}$ sparse, $\hat{\rho}$ dense. Both Hermitian
- 1d spatial decomposition
  - Processor computes a slice of $\hat{H}$, f
  - Upper triangle of $\hat{\rho}$ stored as blocks

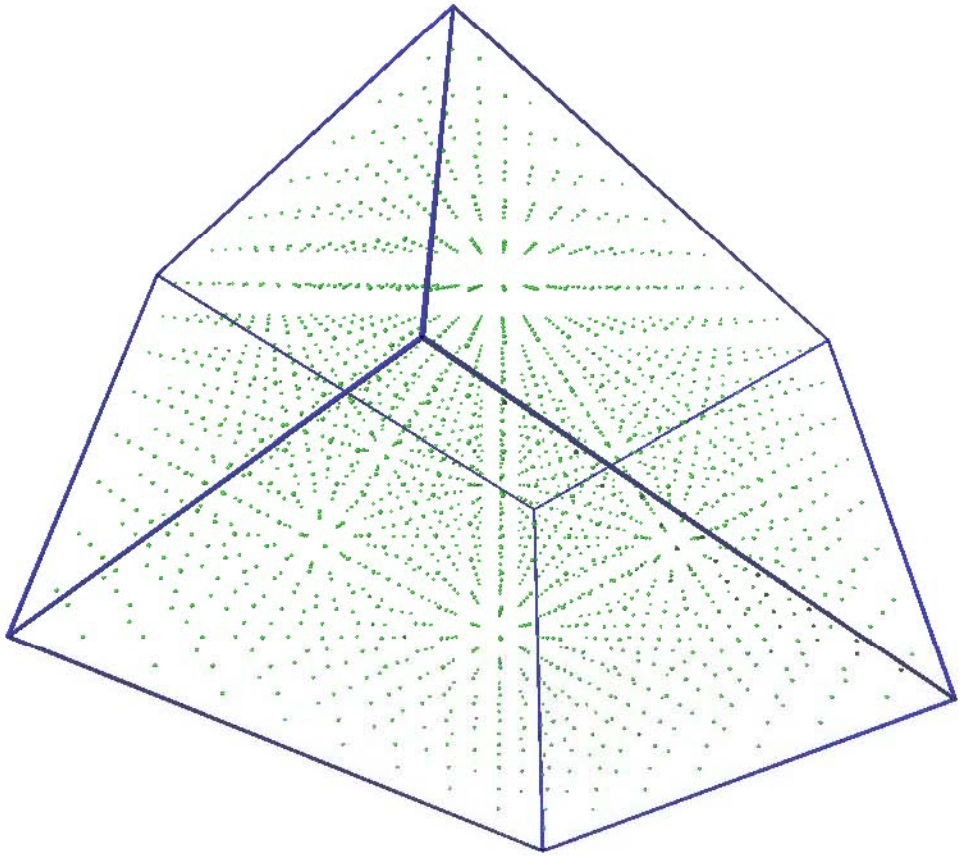


Excitation as temperature rise

Electronic occupations





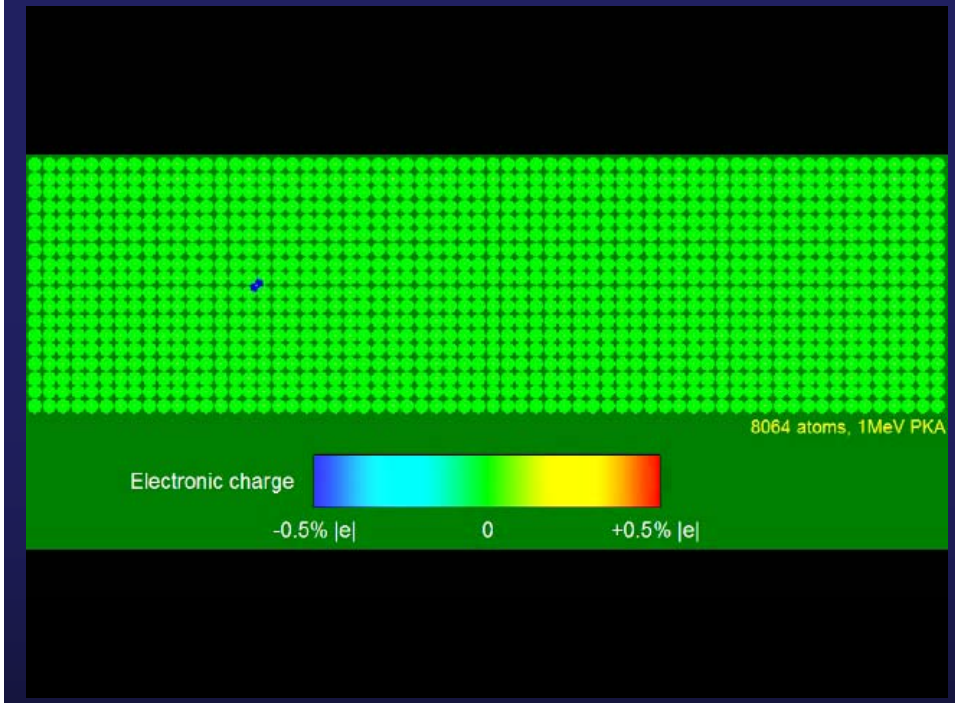


Energy transfer

Atoms displaced > 0.1A

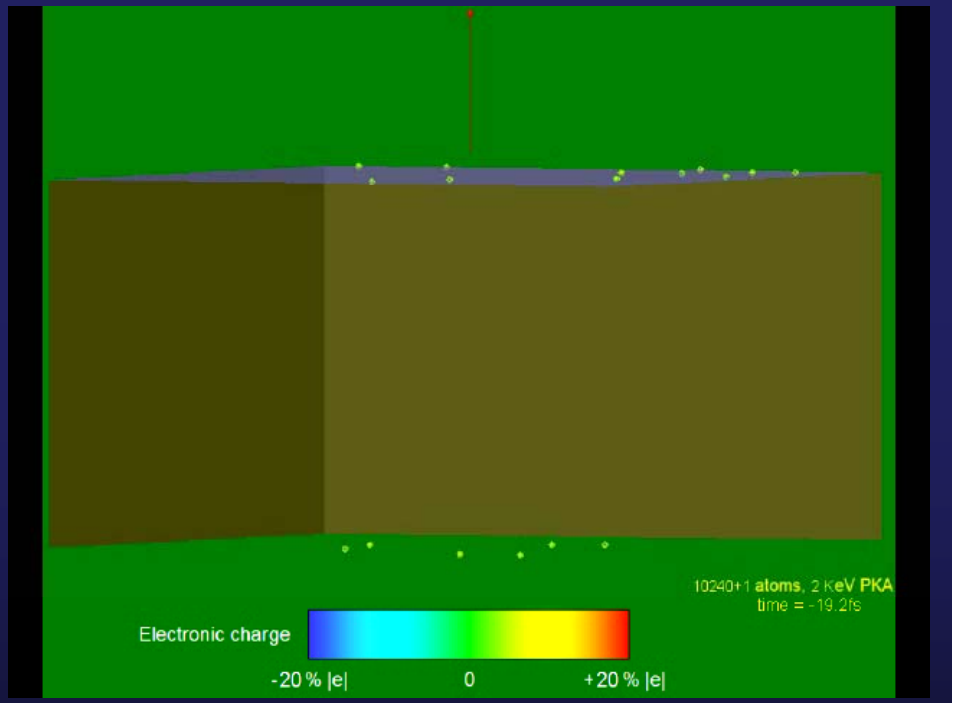
Ongoing work

- Channelling



  - 1MeV ion loses energy by Coulomb interaction

- Sputtering



  - Impact on surface causes ejection of ions

Thanks to…

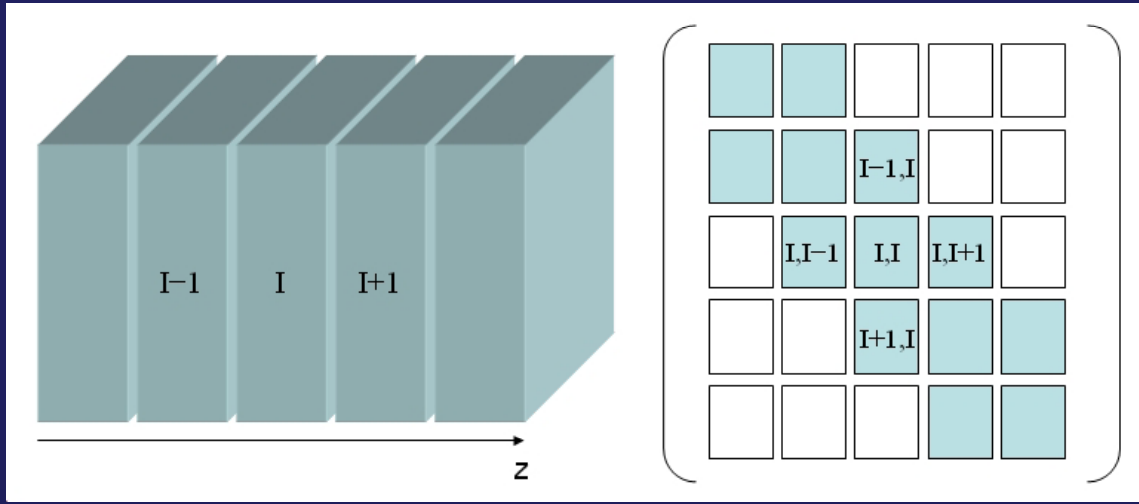
- Funding: EPSRC EP/C524403
  States of Guernsey
- Computer time: HPCx
  IC-HPC

Equations of motion

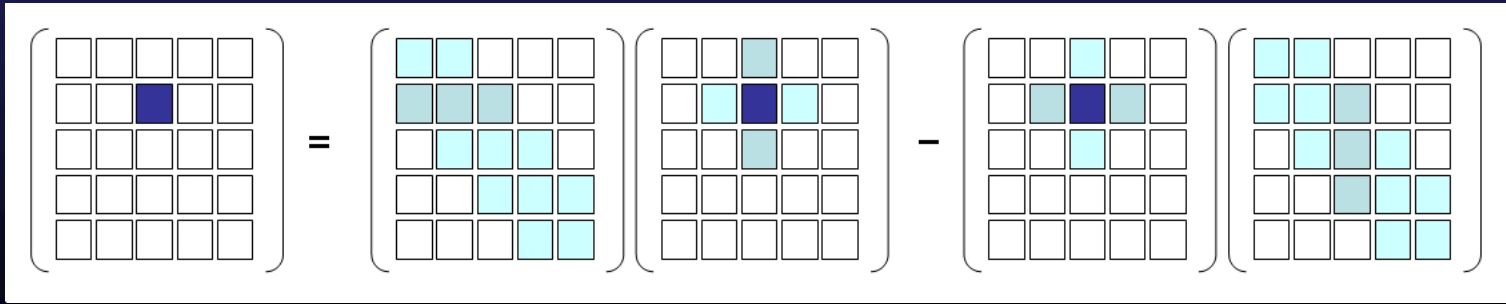
- Electronic energy $$E = \langle \Psi(t) | \hat{H} | \Psi(t) \rangle$$
- Electronic Force $$F = \langle \Psi(t) | \hat{F} | \Psi(t) \rangle$$
- Quantum Liouville equation $$i\hbar \frac{d\hat{\rho}}{dt} = \left[\hat{H} + \frac{\delta \varepsilon}{\delta \hat{\rho}^{*}}, \hat{\rho} \right]$$

Sparse-dense commutator

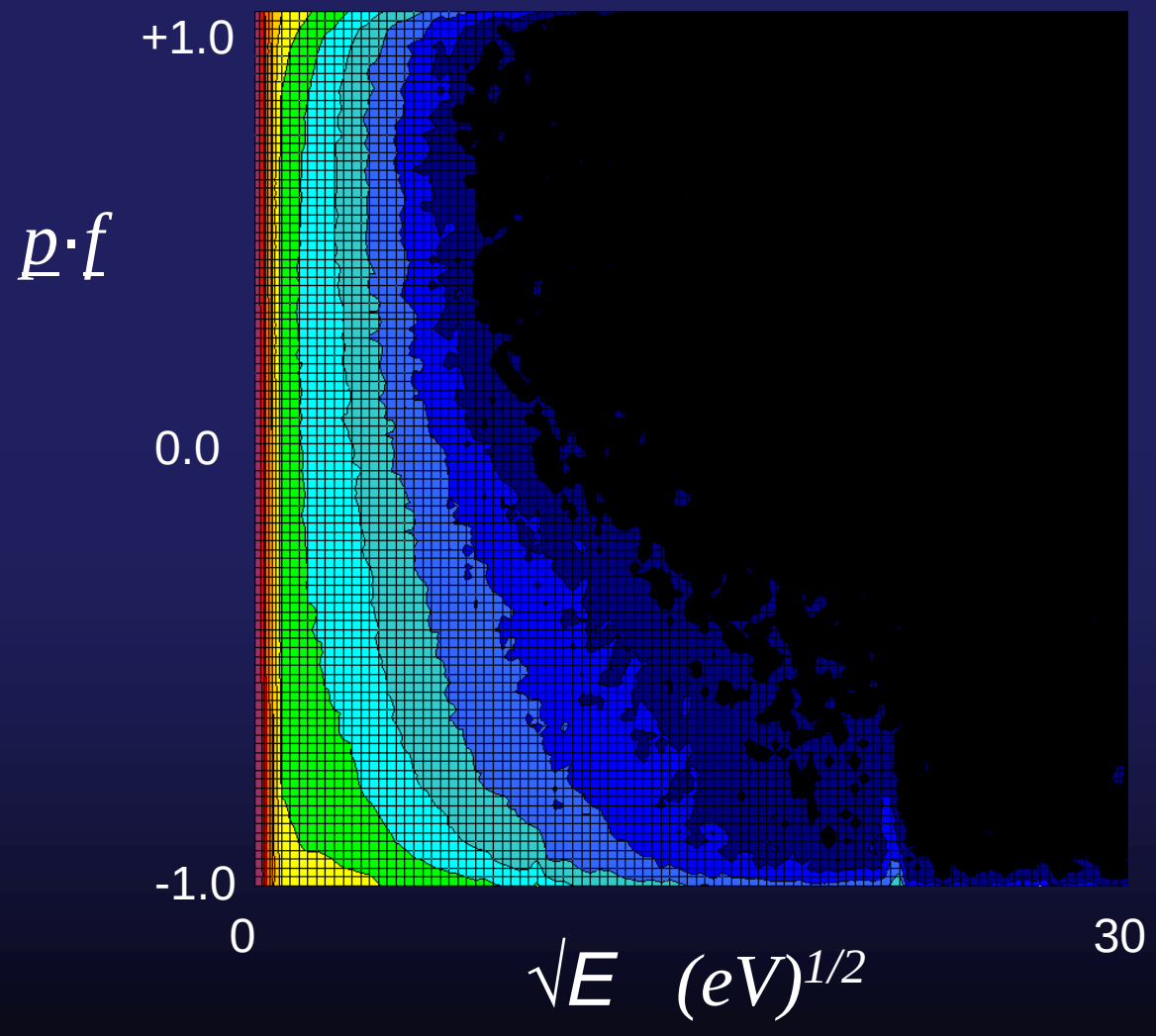
- A 1-d domain decomposition…



… means only local message passing



Direction of non-adiabatic force



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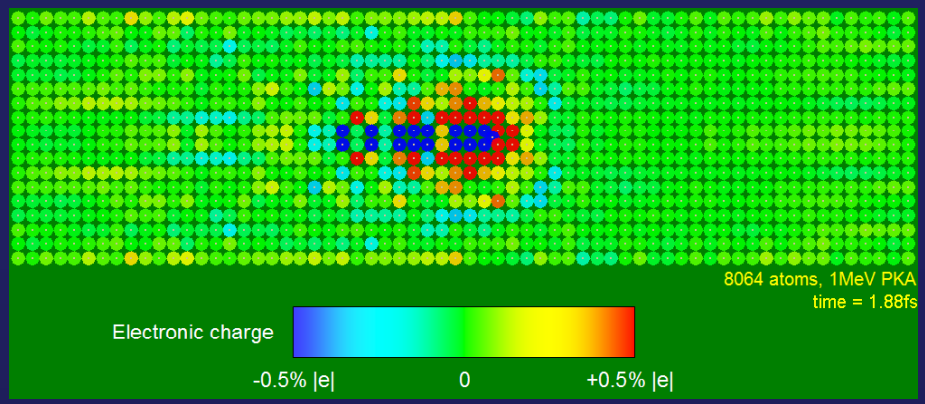

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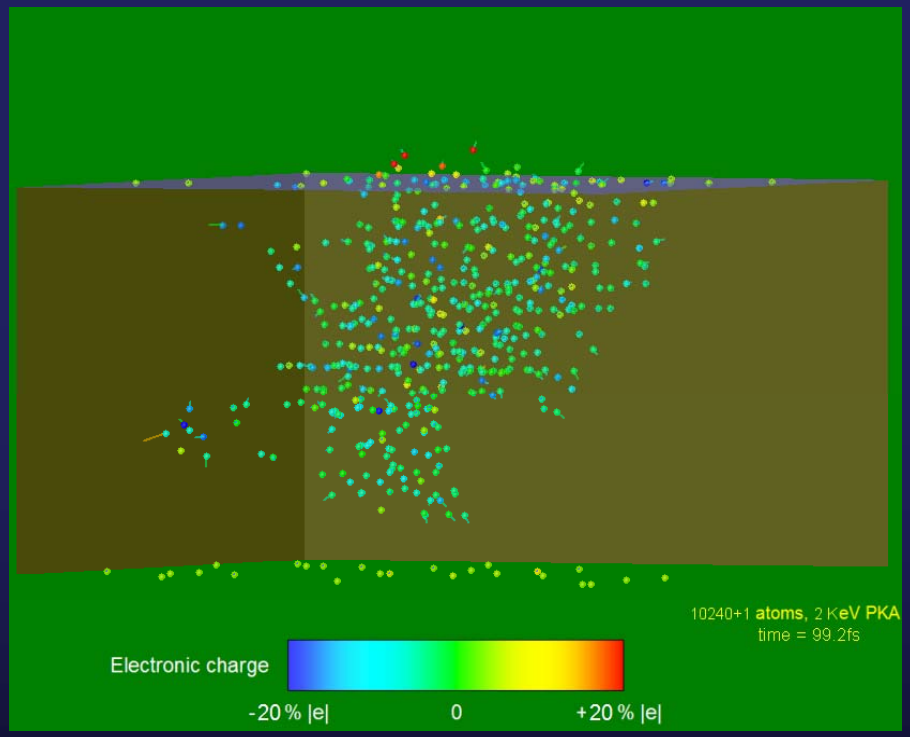

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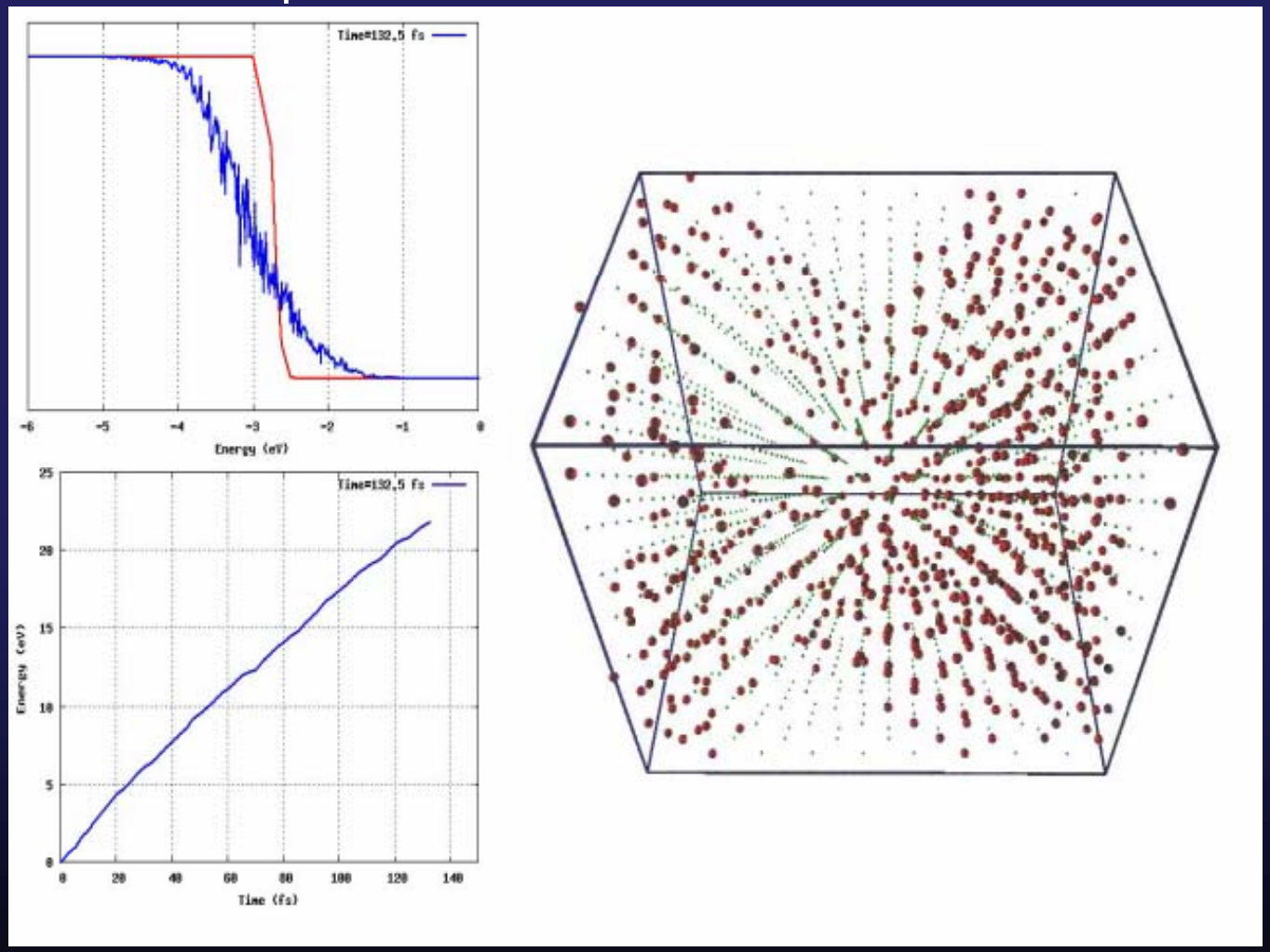

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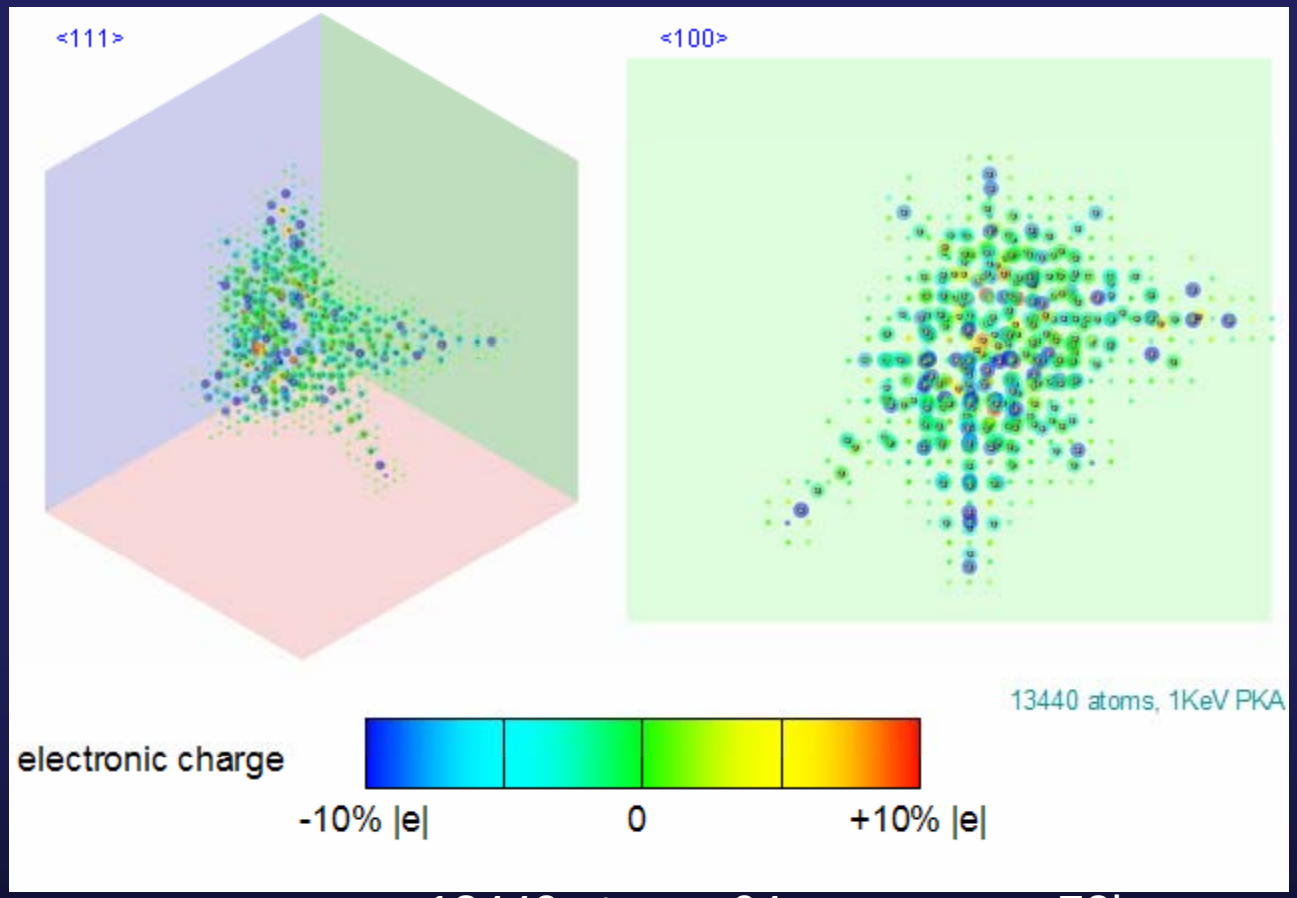

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