Molecular Simulation Software

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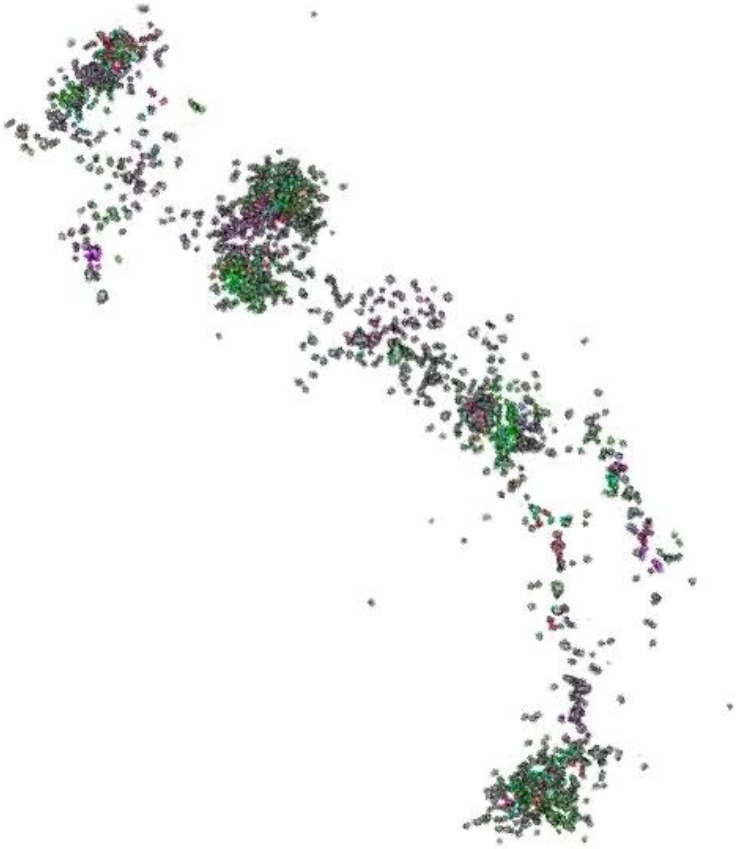
DL_POLY

Classical Molecular Dynamics Suite developed by Ilian Todorov & Bill Smith



Supported by CCP5 (EPSRC & NERC)
Cost-free to academic researchers.
Available commercially.

- Materials modelling at equilibrium
- Full-featured comprehensive force-field – SPME electostatics, instant polarisation, vdW, metals, tersoff, 3- & 4-body & bio-chemical interactions
- Particle dynamics, constraint dynamics, rigid body dynamics.

2012 statistics

- **454 citations**
- **1,650 downloads**
- **2,200 user mail-list**

K. Trachenko *et al.* - J. Phys.: Condens. Matter 25 (2013) 125402 (7pp) – 100-200 keV cascades in 100-500 million particles of Fe on 20,000-60,000 cores of Cray XE6.

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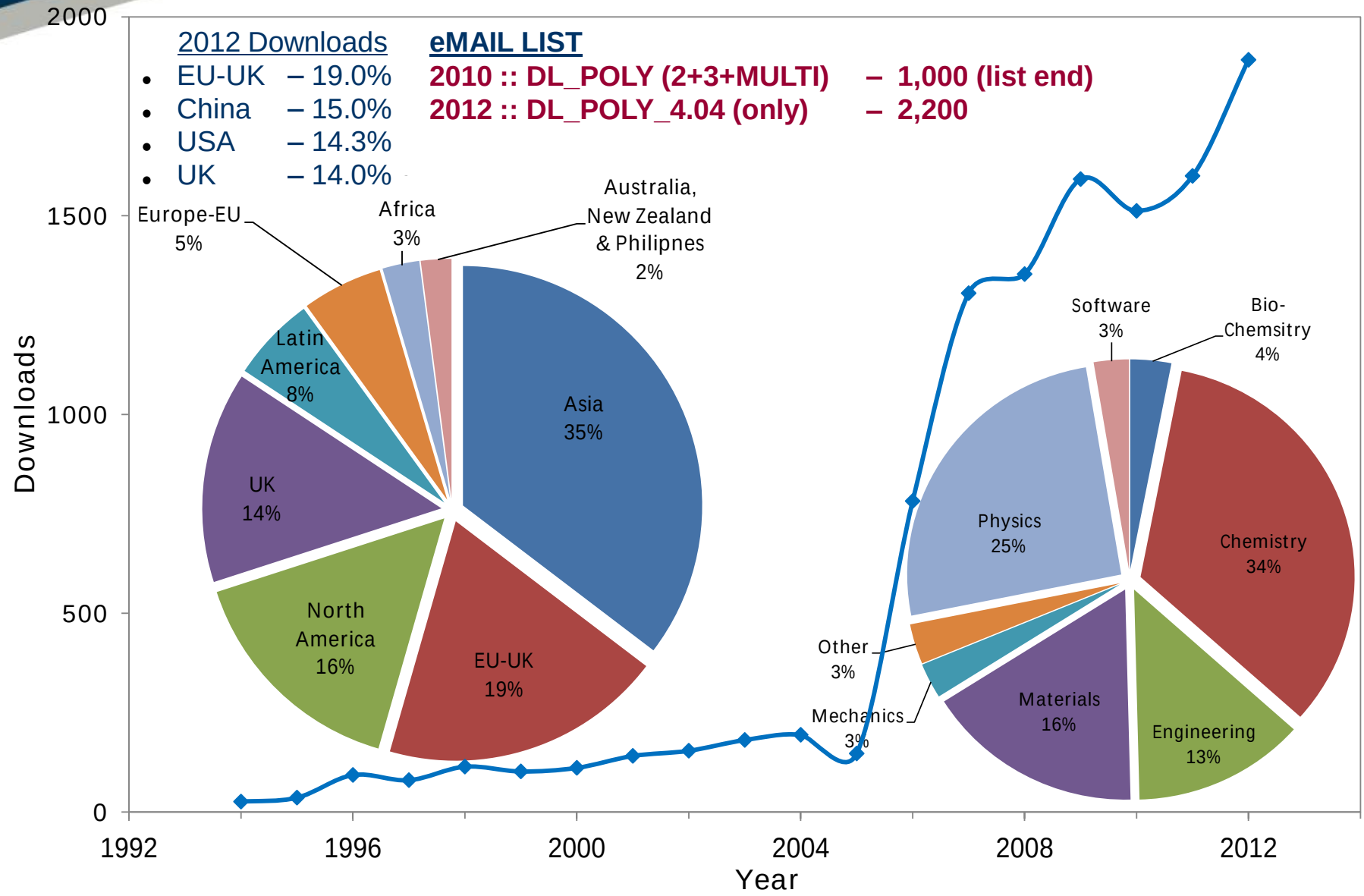
Licences



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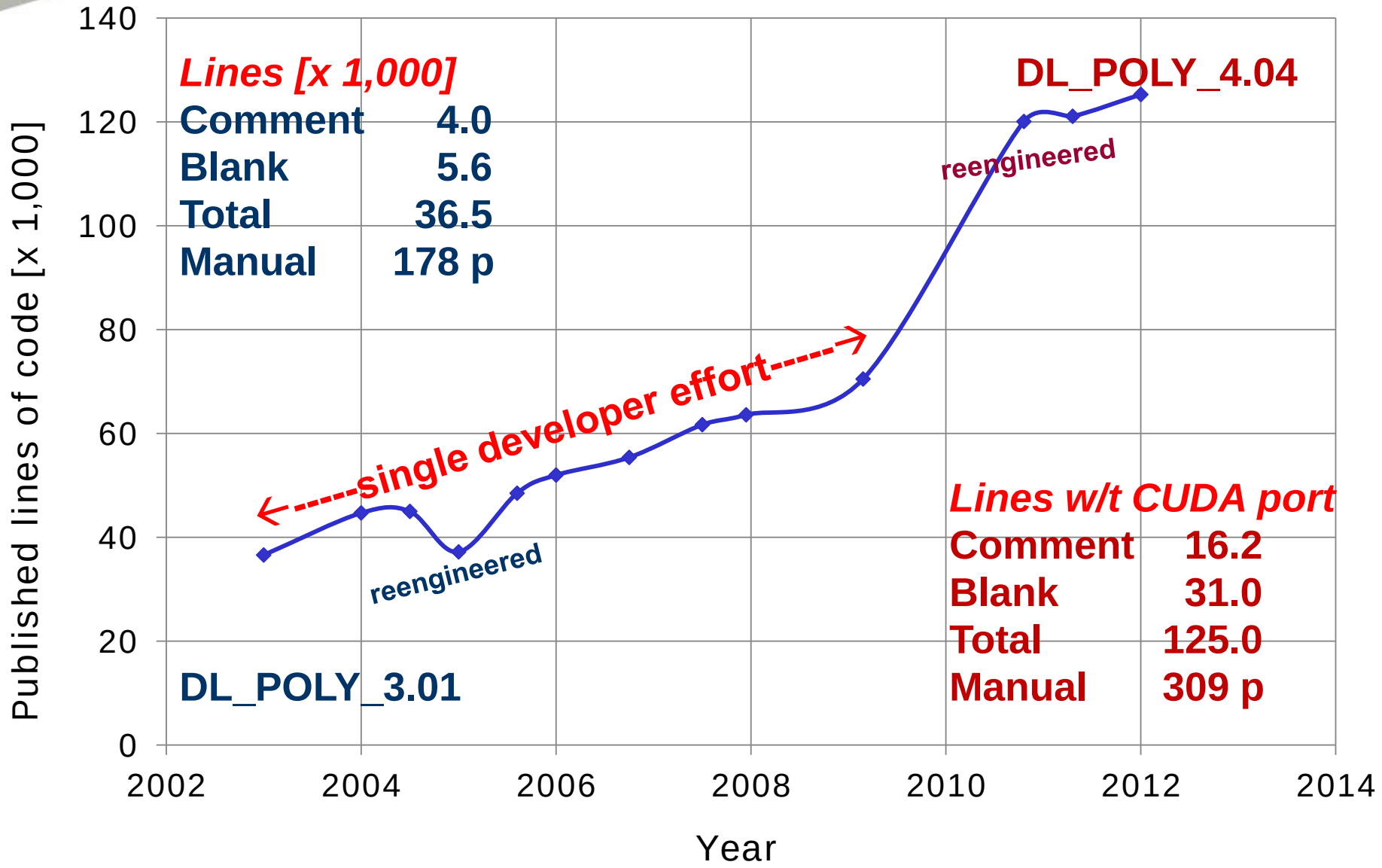
Development



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Features & Science

- MPI based parallelisation
- Cuda port available
- 3D FFT (DaFT) implemented within domain decomposition
- Parallel I/O (read & write)
- ASCII, netCDF (AMBER) formats
- DL_FIELD – protonated PDB to DL_POLY Force-Field format converter
- Defect detection and variable timestep
- Two-temperature thermostat
- Elastic constants and NEMD
- openMP hybridisation
- Long integers for multi-billion particle simulations
- Multiple timestepping algorithms
- Grid based Poisson solver for SPC electrostatics and advanced implicit solvent model ABNP2
- Multipolar electrostatics
- MMM@HPC – UNICORE GridBeans
- GB – shaped particle dynamics
- Biased Potential Dynamics
- Temperature Accelerated Dynamics
- Metadynamics
- Solvation Features – Spectral-Shifts

- TRAINING :2-3 W/S p.a. ~ 60 people
- MOF modes of vibration
- Gaseous permeability and retention in OF (CO_2 and N_2)
- Radiation Damage in metals & ceramics
- GABA_A receptor (ion channel) opening
- nAChR receptor dynamics (with cholesterol)
- Pressure driven reversal of halotane aggregation
- Inelastic thermal spike in Si slabs

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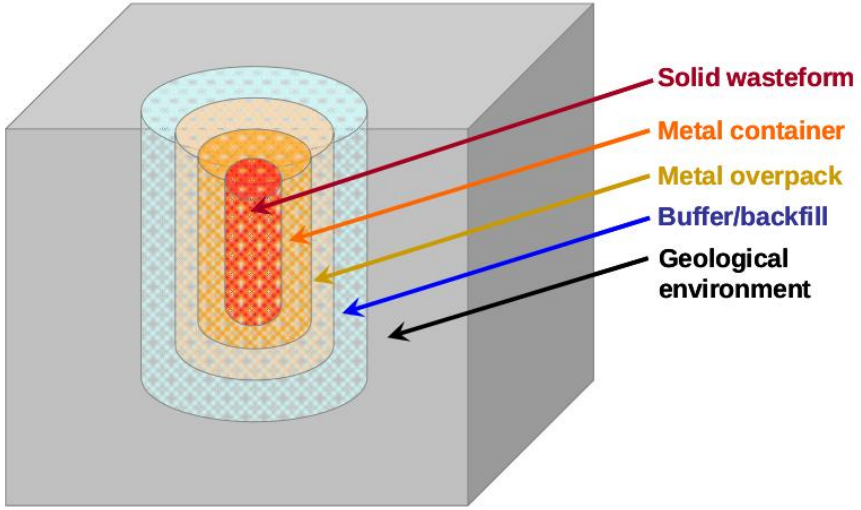
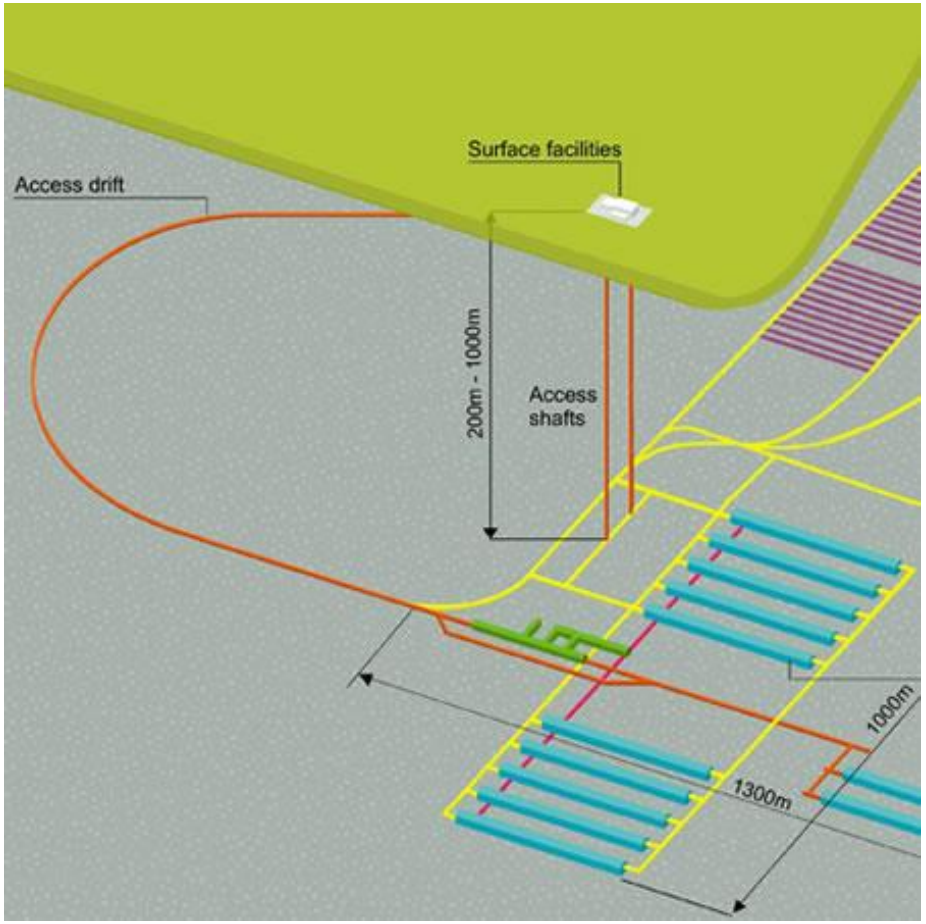
Disposal of High Level Waste





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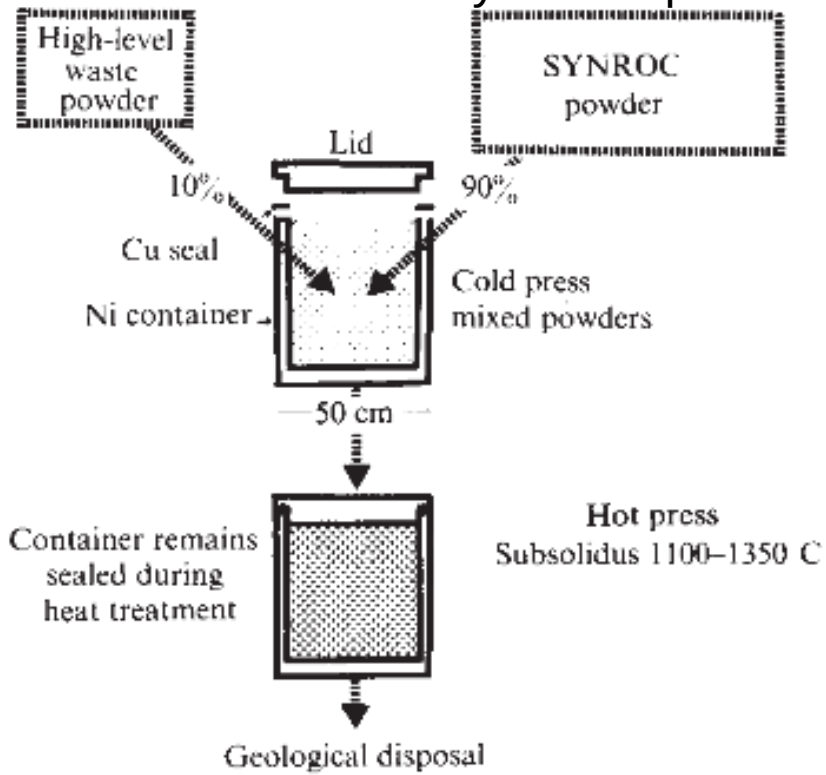
Disposal of High Level Waste

The proposed encapsulating route is through High Isostatic Pressing (HIPing). The process prevents loss of volatile fission gases as the lid seals at a lower temperature than the gases are released. Canister is then ready for disposal.



Ringwood – Nature **278**, 1979, 219

Some ceramics are a safe and more durable alternative to glasses – $CaTiO_3$, $CaZrTi_2O_7$ (proposed, a component of most SYNROC formulations), $BaAl_2Ti_6O_{16}$ and TiO_2. Geochemically stable minerals which have immobilised uranium and thorium for billions of years. They can aslo incorporate high-level radioactive waste (Pu, Sr, Ba, Cs) as well as neutron absorbers Hf, Gd into its crystal structure.

Pyrochlore (Gd, Sm, Hf-based)-rich titanate phases for Pu encapsulation: high waste load (~50%) plus criticality control (neutron absorbants).

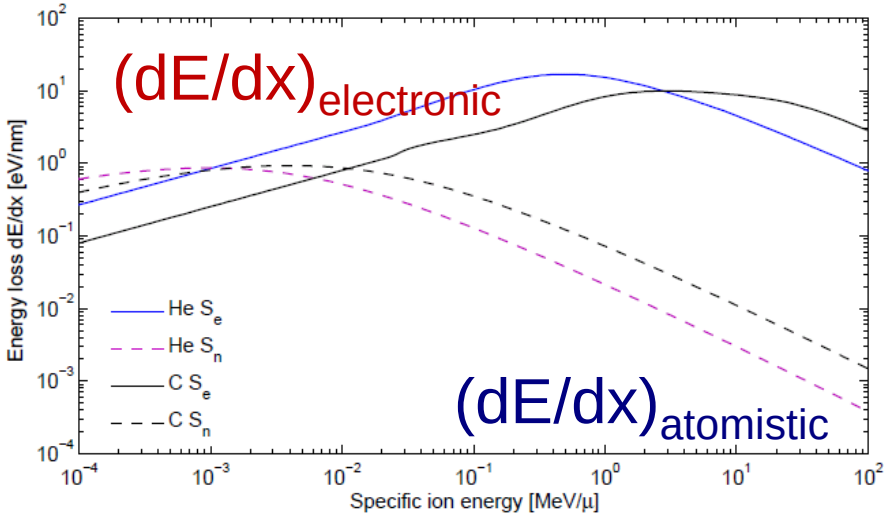
Other potential "waste forms": $ZrSiO_4$, ZrO_2, $Gd_2Zr_2O_7$, **$Gd_2Pb_2O_7$** and so on..

Swift heavy ion radiation damage

S = dE/dx (Energy/length) = $(dE/dx)_{electronic}$ + $(dE/dx)_{atomistic}$

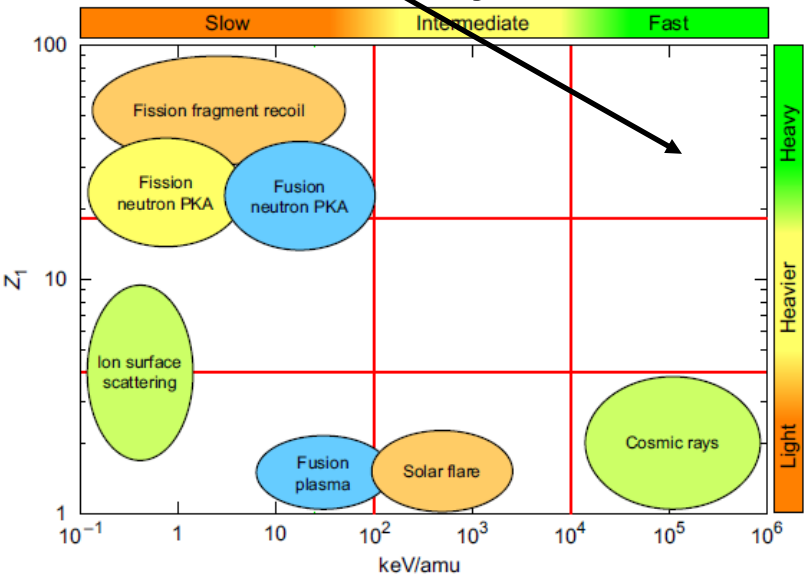
- Atomistic: elastic recoil
- Electronic: ionisation and electronic excitation

Beyond cascade simulations…



Nuclear and electronic stopping powers (solid and dashed lines, respectively) for Helium and Carbon in Silicon. Data obtained using SRIM-2008.04

Swift heavy ions



C P Race *et al* 2010 *Rep. Prog. Phys.* 73 116501

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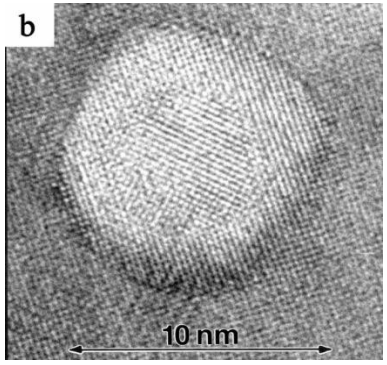
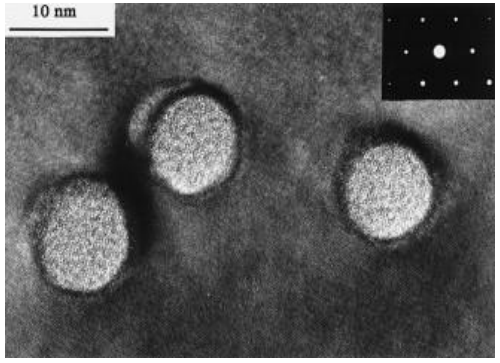
Motivation & background

Predictive radiation damage modelling for band-gap materials:

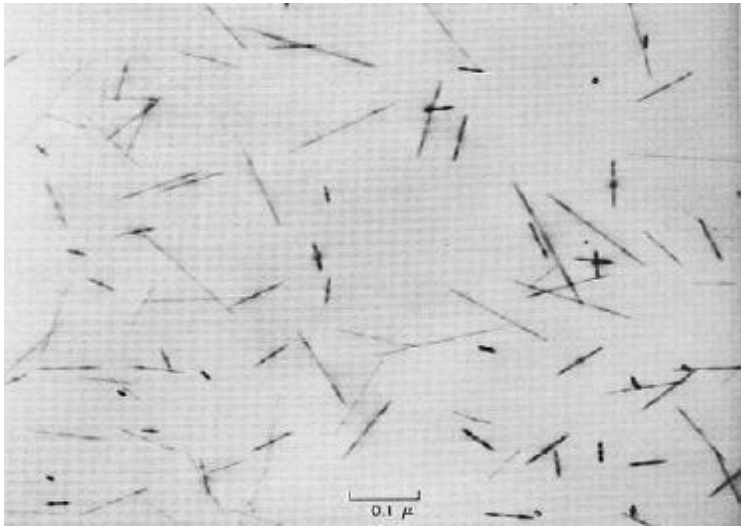
- Materials selection in nuclear industry (diagnostics)
- Nanotechnology
  - Modify nanostructures
  - Form nm-size channels
  - Change quantum wells



InSb (*E* = 1.85 MeV/amu)
G. Szenes et. al. PRB 65, 045206



Si (E = 30MeV) C_{60} cluster ions
A. Dunlop et. al. Nuclr. Instr. B 146 (1998) 302-308



Latent tracks in mica
E. Silk and R. Barnes, Acta Metallurgica 9, 558 (1961)

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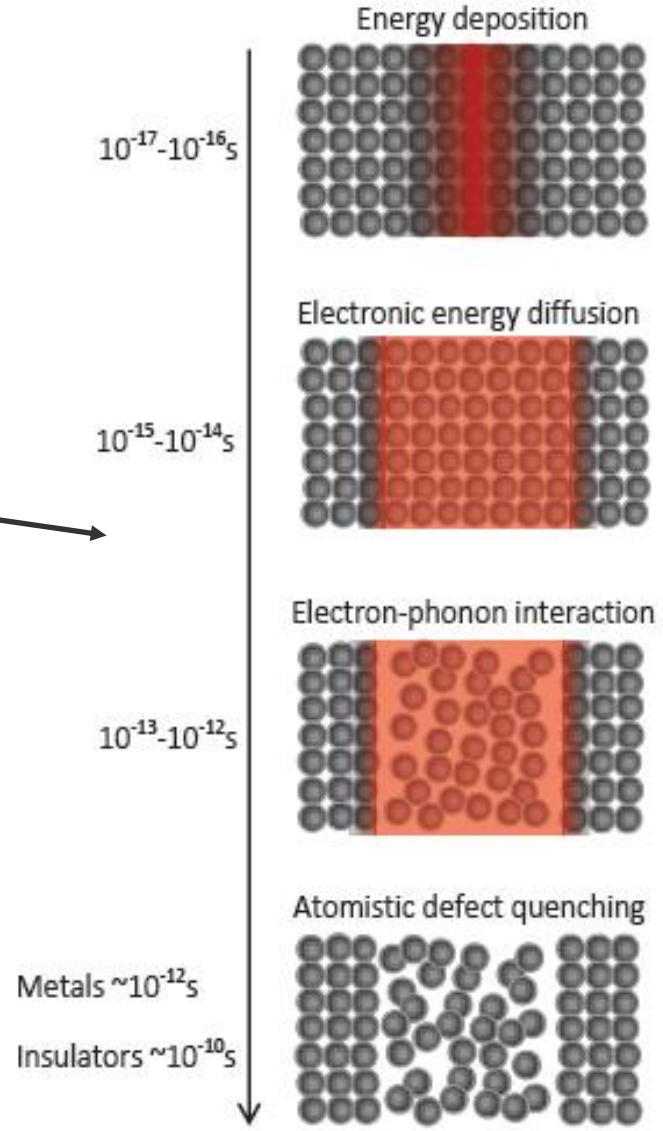
Track formation models

- Coulomb explosion
  - Narrow positively charged core
  - Few results: mainly surface effects
- Inelastic thermal spike
  - Energy deposition on electronic subsystem; e-p coupling; local melting and quenching
  - Quantitative results: metals
- Structure relaxation methods
  - Modified (Te dependent) interatomic potentials



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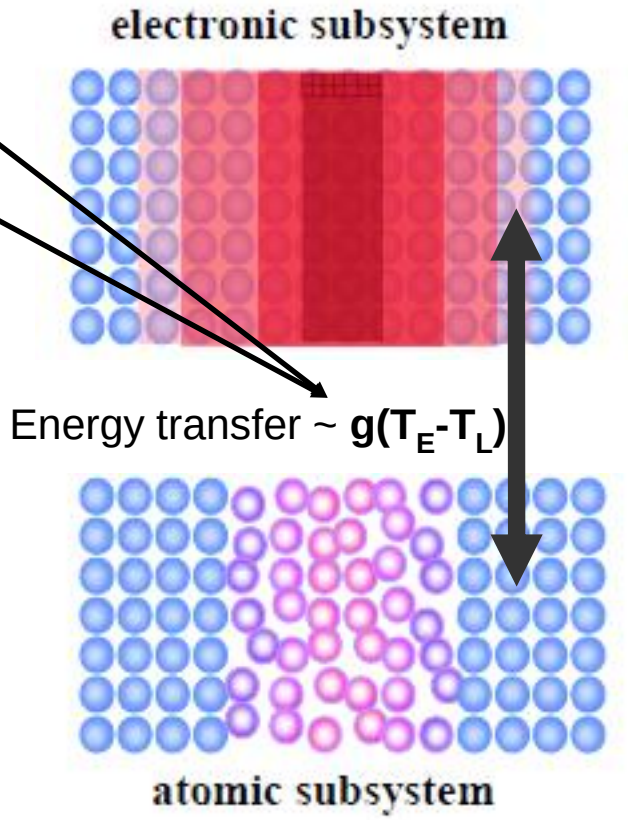
The inelastic thermal spike model (i-TS)

$$C_E(T_E)\frac{\partial T_E}{\partial t} = \nabla K_E \nabla T_E - g(T_E - T_L) + A(r[\alpha_R], t)$$

$$C_L(T_L)\frac{\partial T_L}{\partial t} = \nabla K_L \nabla T_L + g(T_E - T_L)$$

- Based on TTM approach
- Applied to: metals, insulators*[1], semiconductors*[2]
- Amorphised region predictions
- Coupled to MD (for metals)[3]



1. A.Meftah et al. Nucl. Instr. Meth. Phys. Res. B 237 (2005) 563
2. A. Chettah et al. Nucl. Instr. Meth. Phys. Res. B, 267 (2009) 2719
3. D. M. Duffy and A. M. Rutherford, J. Phys: Conden. Matt. 19 (2007) 016207

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Band-gap materials model extension

Must include a conservation equation for e-h carriers

Based on approach used in laser-ablation studies

NEW Carrier number conservation

$$\frac{\partial N}{\partial t} + \nabla \cdot J = G_e - R_e$$

Carrier energy conservation

$$\frac{\partial U}{\partial t} + \nabla W = A(r[\alpha_R], t) - U_L$$

Lattice heat

$$\frac{\partial T_L}{\partial t} - \left(\frac{\kappa_L}{c_L \rho_L}\right) \nabla^2 T_L = \frac{U_L}{c_L \rho_L}$$

Carrier energy flux density

$$W = (E_g + 2k_B T_E) J - (\kappa_e + \kappa_h) \nabla T_E$$

Carrier current

$$J = D(T_L) \left(\nabla N + \frac{2N}{k_B T_L} \nabla E_g + \frac{N}{2T_E} \nabla T_E \right)$$

Carrier total energy

$$U = N E_g + 3 N k_B T_E$$

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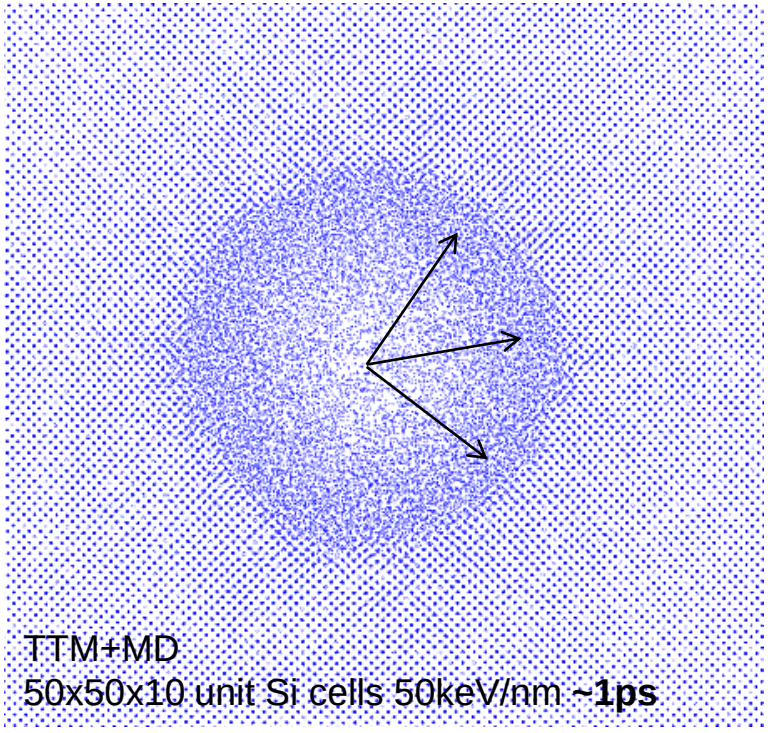
Towards MD

Superheating? Lattice temperature above the melting temperature with no track formation[1]. Continuum models cannot give accurate track radii; require MD-coupling!

- Continuum neglects lattice straining and emission of shock waves (carry away some energy). C_L in continuum is neither identical with C_v or C_p.
- Volume change by a phase transition is not included, i.e. Silicon shrinks upon melting



1. D.M. Duffy, N. Itoh, A.M. Rutherford and A.M. Stoneham, *J. Phys: Condens. Matt.* **20** (2008), p. 082201

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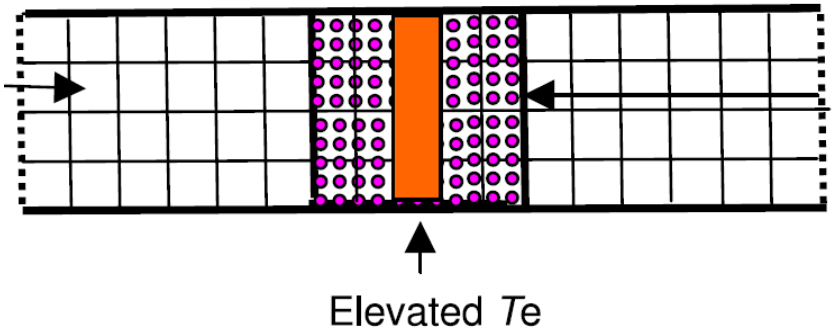
Towards MD

MD additions:

- Coarse-grained T-cells
- Choice of boundary conditions…
  - Periodic for the atomistic lattice
  - Electronic system: z-dir von-Neumann, xy-dir infinite sink



Inhomogeneous Langevin thermostat

- Mechanism for electronic energy transfer to the lattice
- Depends on the local electronic temperature

Continuum

$$C_e \frac{\partial T_e}{\partial t} = \nabla \cdot (\kappa \nabla T_e) - g_p(T_e - T_l)$$

or $$\frac{\partial U}{\partial t} + \nabla \cdot W = A(r[v_{ion}], t) - g(T_e - T_l)$$

Molecular dynamics

$$m \frac{\partial \boldsymbol{v}_i}{\partial t} = \boldsymbol{F}_i(t) - \gamma_i \boldsymbol{v}_i + \tilde{\boldsymbol{F}}_i(t)$$

$$\tilde{\boldsymbol{F}}_i(t) = \sqrt{\Gamma}\, \tilde{\boldsymbol{A}}_i(t) \quad \Gamma = 2\gamma_p m_i k_B T_e$$

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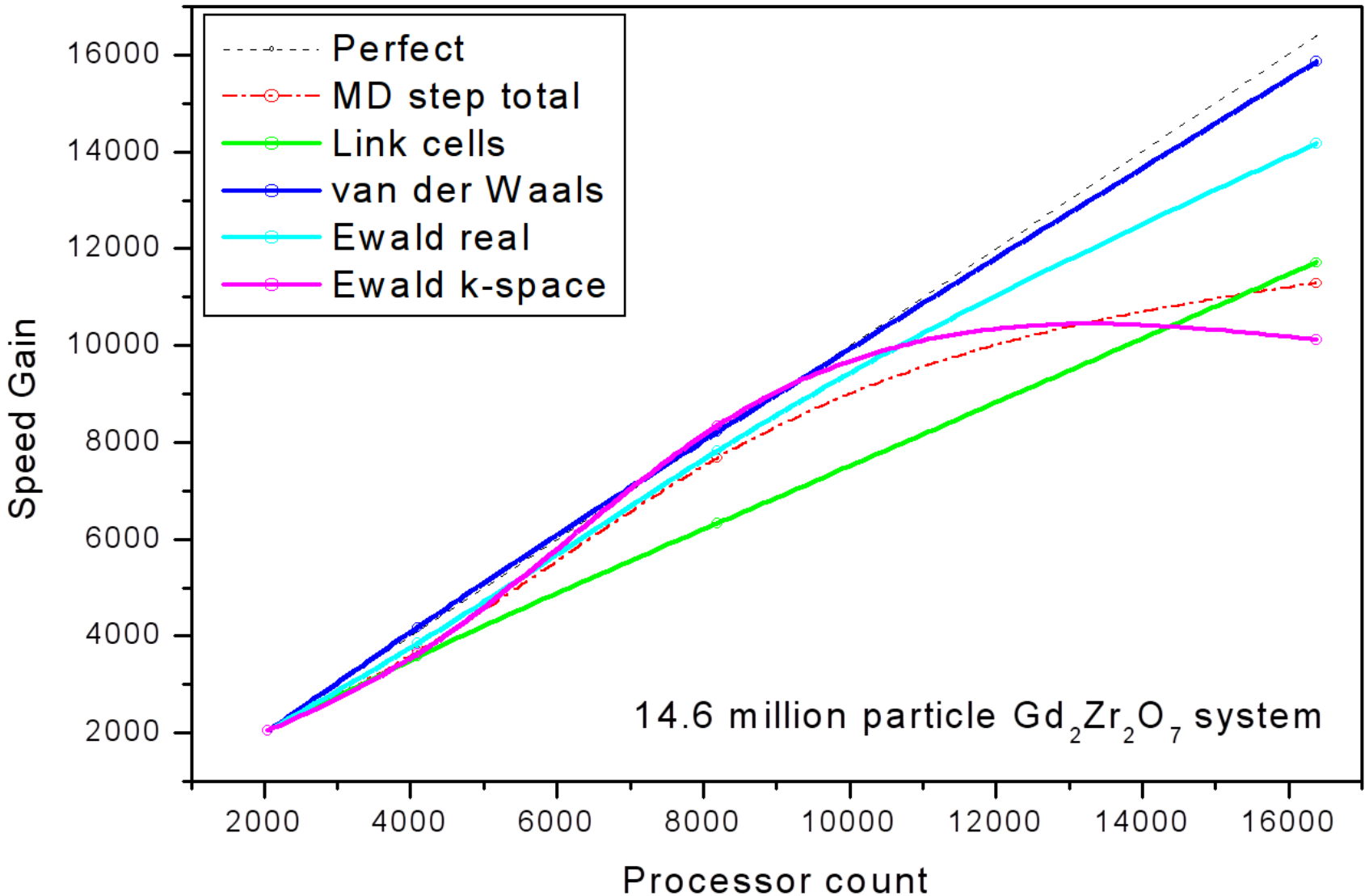
HPC Parallel Scaling

STRONG



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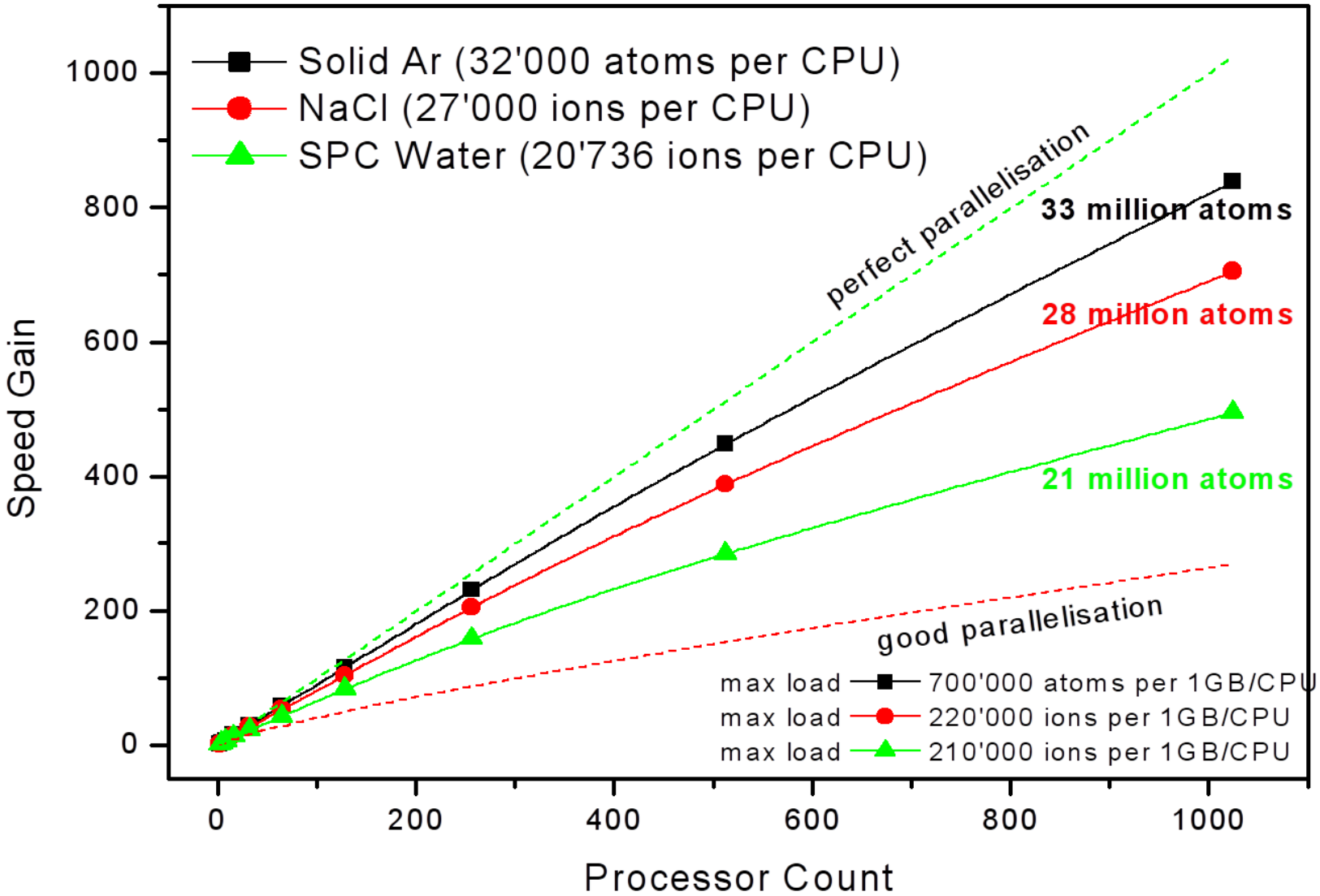
HPC Parallel Scaling

WEAK



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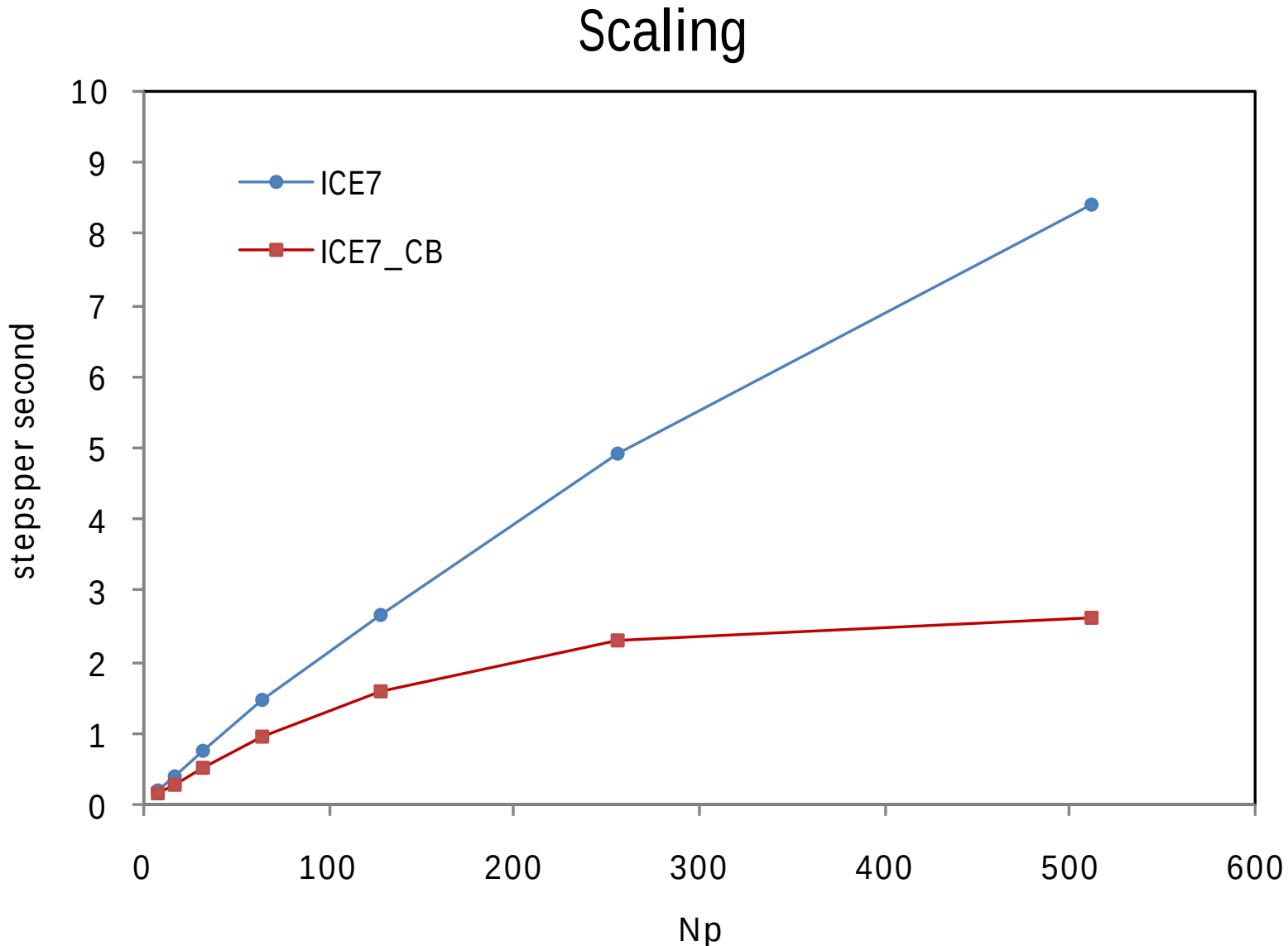
RB v/s CB 450,000 particles



I/O Solutions

1. **Serial read and write (sorted/unsorted)** – where only a single MPI task, the master, handles it all and all the rest communicate in turn to or get broadcasted to while the master completes writing a configuration of the time evolution.

2. **Parallel write via direct access or MPI-I/O (sorted/unsorted)** – where **ALL / SOME** MPI tasks print in the same file in some orderly manner so (no overlapping occurs using Fortran direct access printing. However, it should be noted that the behaviour of this method is not defined by the Fortran standard, and in particular we have experienced problems when disk cache is not coherent with the memory).

3. **Parallel read via MPI-I/O or Fortran**

4. **Serial NetCDF read and write** using NetCDF libraries for machine-independent data formats of array-based, scientific data (widely used by various scientific communities).

MPI-I/O Write Performance for 216,000 Ions of NaCl on XT5

		3.09	3.10	3.09	3.10
Cores	I/O Procs	Time/s	Time/s	Mbyte/s	Mbyte/s
32	32	143.30	1.27	0.44	49.78
64	64	48.99	0.49	1.29	128.46
128	128	39.59	0.53	1.59	118.11
256	128	68.08	0.43	0.93	147.71
512	256	113.97	1.33	0.55	47.60
1024	256	112.79	1.20	0.56	52.47
2048	512	135.97	0.95	0.46	66.39

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MPI-I/O Read Performance for 216,000 Ions of NaCl on XT5

		3.10	New	3.10	New
Cores	I/O Procs	Time/s	Time/s	Mbyte/s	Mbyte/s
32	16	3.71	0.29	17.01	219.76
64	16	3.65	0.30	17.28	211.65
128	32	3.56	0.22	17.74	290.65
256	32	3.71	0.30	16.98	213.08
512	64	3.60	0.48	17.53	130.31
1024	64	3.64	0.71	17.32	88.96
2048	128	3.75	1.28	16.84	49.31

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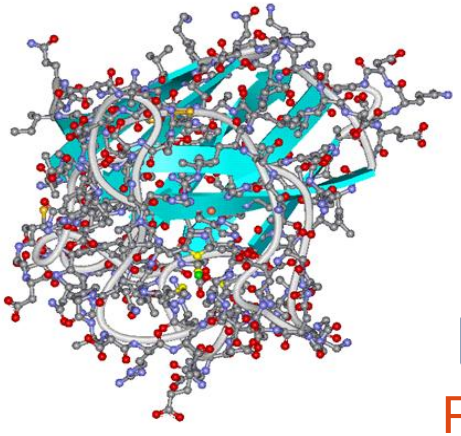
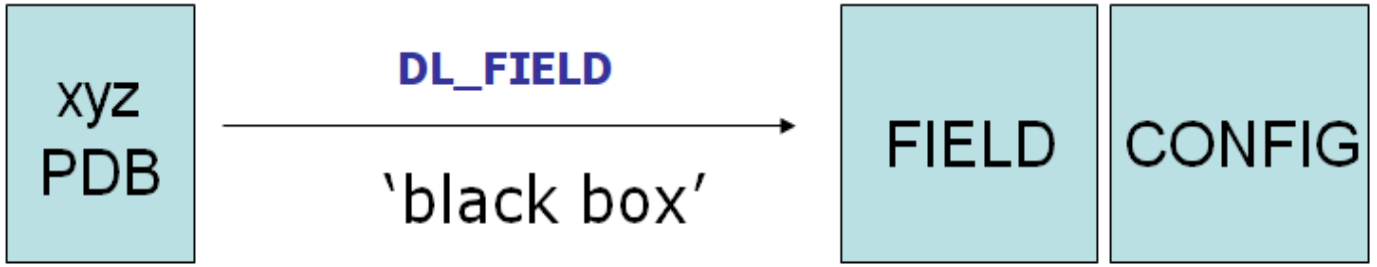
DL_FIELD

Force field generator
developed by Chin Yong





Protonated

Force field schemes

(1) CHARMM – protein, saccharides, some lipids, organic molecules
(2) AMBER – proteins, Glycam – sugars, glycans.
(3) OPLSAA – proteins
(4) PCFF – small organic molecules, organic polymers.
(5) DREIDNG – general force fields for organic and other covalent molecules.
(united atom, CHARMM19)

4,382	atoms
19,400	two-body
7,993	three-body
13,000	four body
730	vdw

2012 statistics

- **350 downloads**
- **400 user mail-list**

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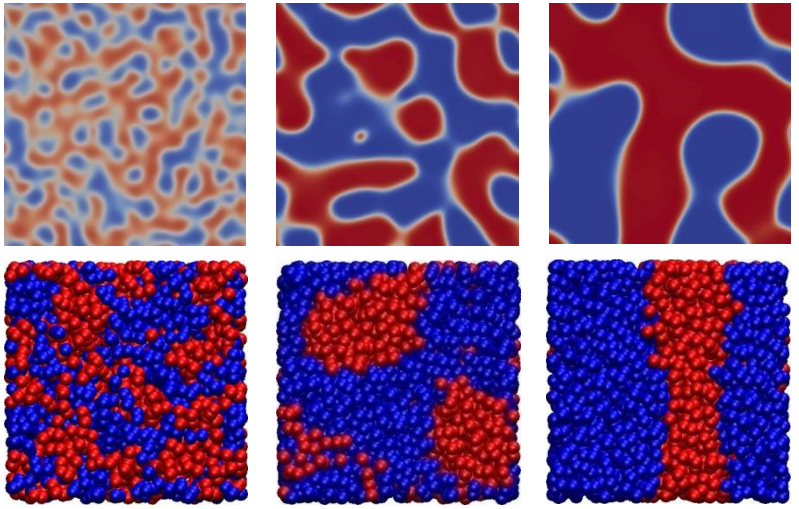
DL_MESO

Mesoscale Modelling Suite
developed by Michael Seaton & Bill Smith

Supported by CCP5 (EPSRC)
Cost-free to academic researchers.
Available commercially.

- Lattice Boltzmann Equation (LBE) & Dissipative Particle Dynamics (DPD) methods
- Serial and highly parallelized (domain decomposed) codes in Fortran90 and C++
- Bridges gap between atomistic (e.g. classical MD) and continuum methods



Statistics and information

- 128 downloads in 2012 (28% EU-UK, 20% China, 15% USA, 11% UK)
- Currently 475 users on mailing list

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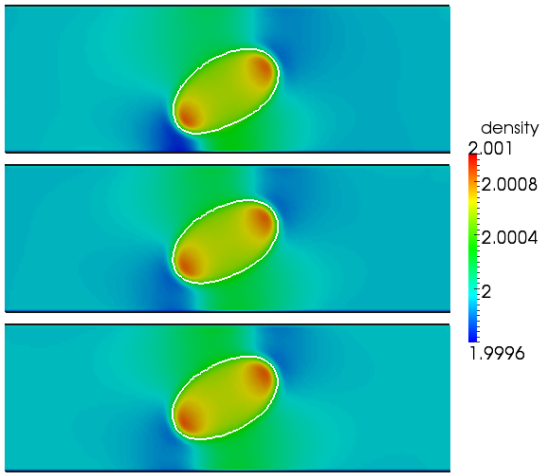
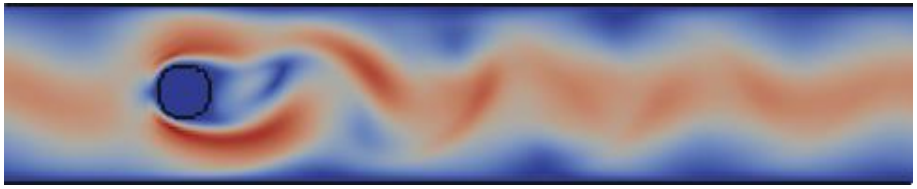
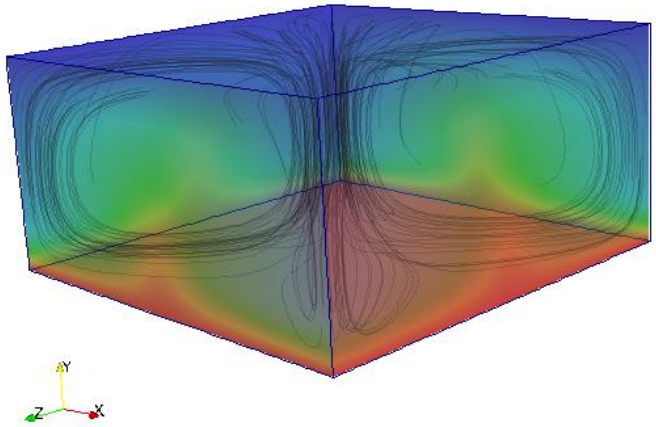
Features & Science

Lattice Boltzmann Equation

- Grid-based solution of Boltzmann equation: emergent Navier-Stokes behaviour
- Collision schemes for application of fluid viscosity: range from simplicity to greater numerical stability
- Complex boundary conditions possible using simple procedures
- Plug-and-play nature of additional physics:
  - Multiple phase/fluid algorithms based on applying interfacial tensions or equations of state
  - Mass/heat transfers – can be applied with reaction kinetics
- Future features: immersed boundary method, CUDA port







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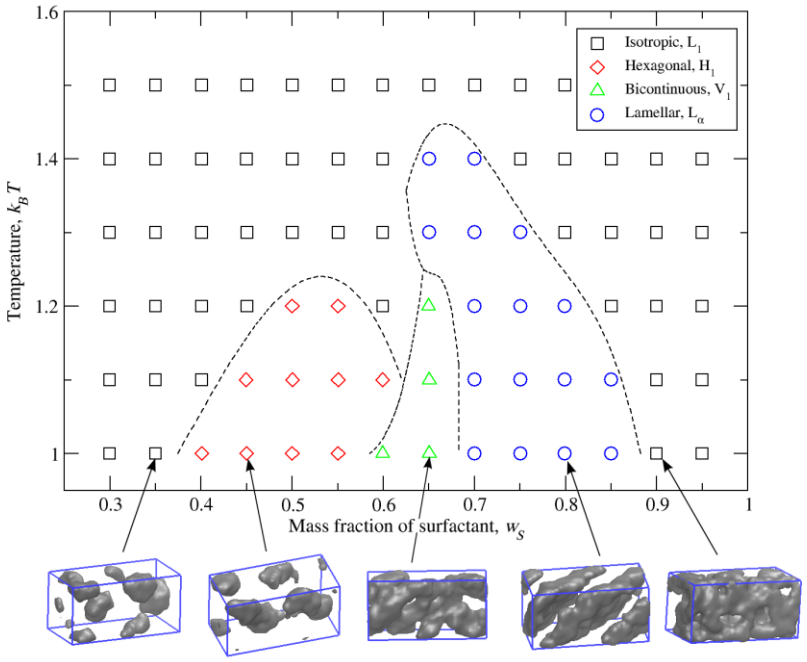
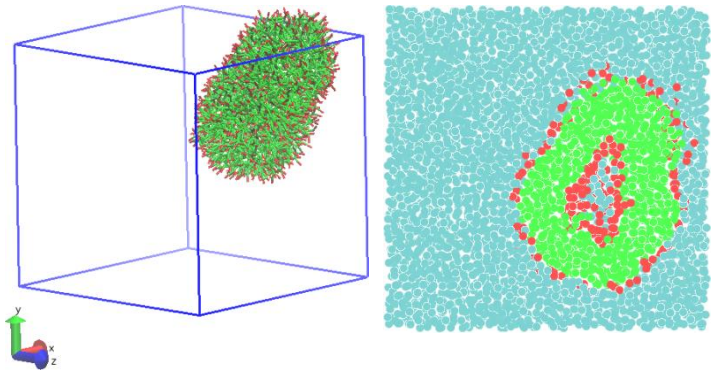
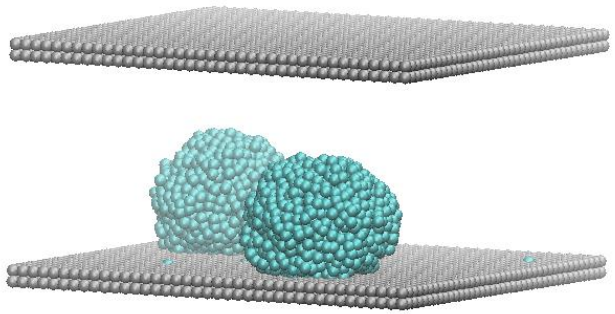
Features & Science

Dissipative Particle Dynamics

- Soft potentials for fast equilibration, including many-body DPD (gives vapour/liquid systems)
- Bond interactions and Ewald electrostatics with smeared charges
- Pairwise thermostats (DPD and alternatives): give correct hydrodynamic behaviour
- Barostats for NPT ensembles
- Boundary conditions: periodic, Lees-Edwards shear, adsorbing hard walls, frozen bead walls
- Future plans: improved scalability for thermostats and electrostatics







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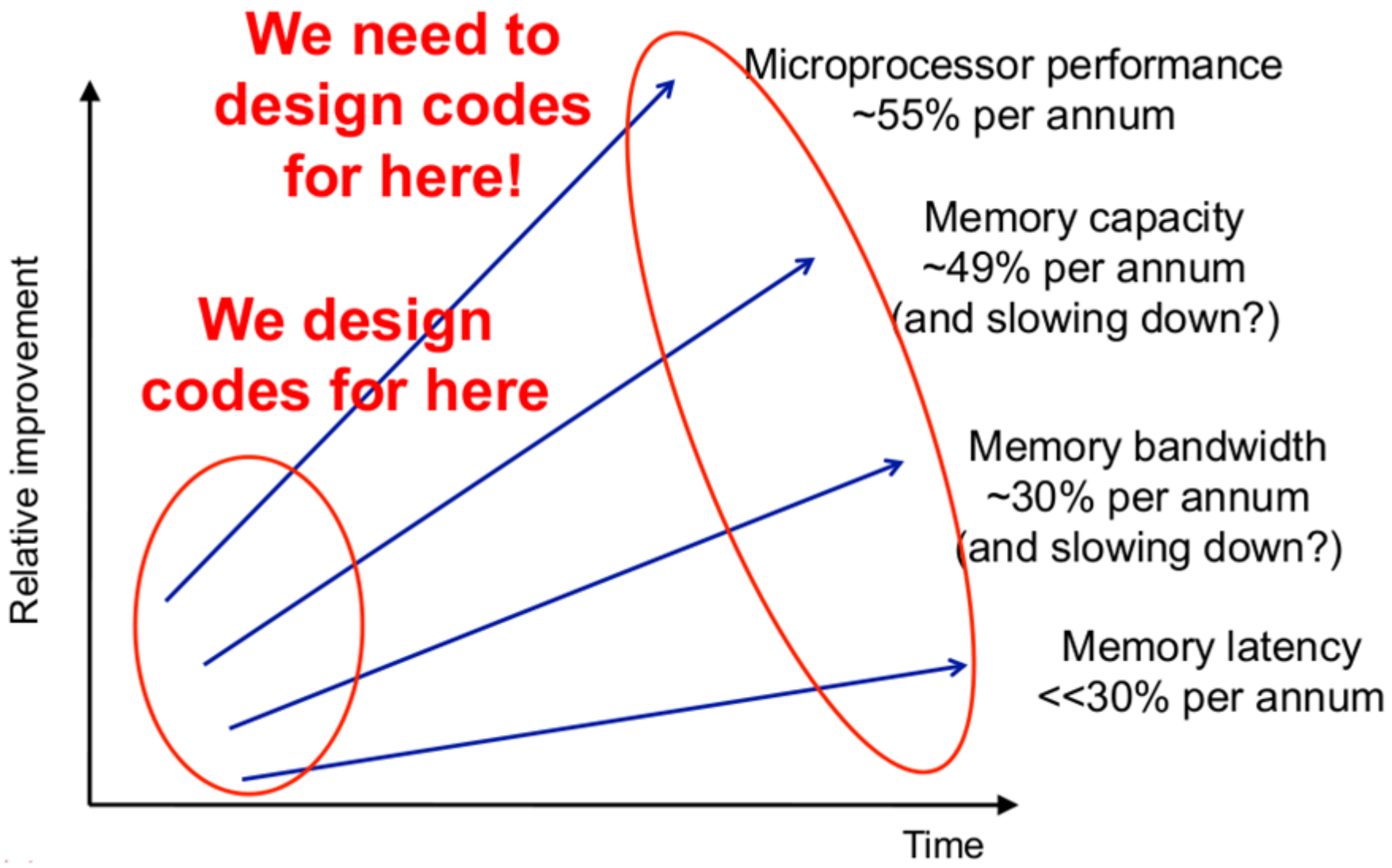
?!? FUTURE ?!?



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DL_MONTE

DL_MONTE is FORTRAN 95 Monte Carlo simulation package developed by John Purton (john.purton@stfc.ac.uk). It uses DL_POLY style input and output and is able to use DL_POLY's java based Graphical User Interface (GUI). At present DL_MONTE is capable of Metropolis sampling only!

Force fields available are:

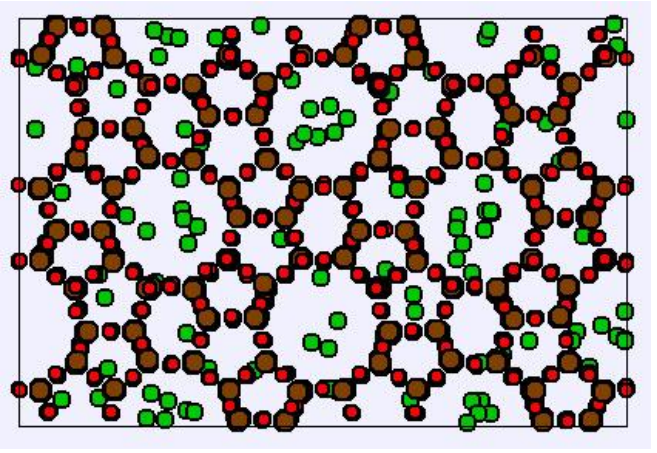
- Ewald sum, Two-body (vdw and bonded), Three-body (bonded and non-bonded), Tersoff, Metals (Sutton/Chen, EAM and Gupta)

The available ensembles are:

- NVT, NPT
- Gibbs Ensemble, Grand Canonical and Semi Grand Canonical
- Transmutation
- Parallel Replica exchange on multiple cores

Plans

- Additional potentials from DL_POLY_4
- A routine for external potentials.
- Inclusion of configurational bias (with Dmytro Antypov at Liverpool).
- Development of distributed data parallelisation.



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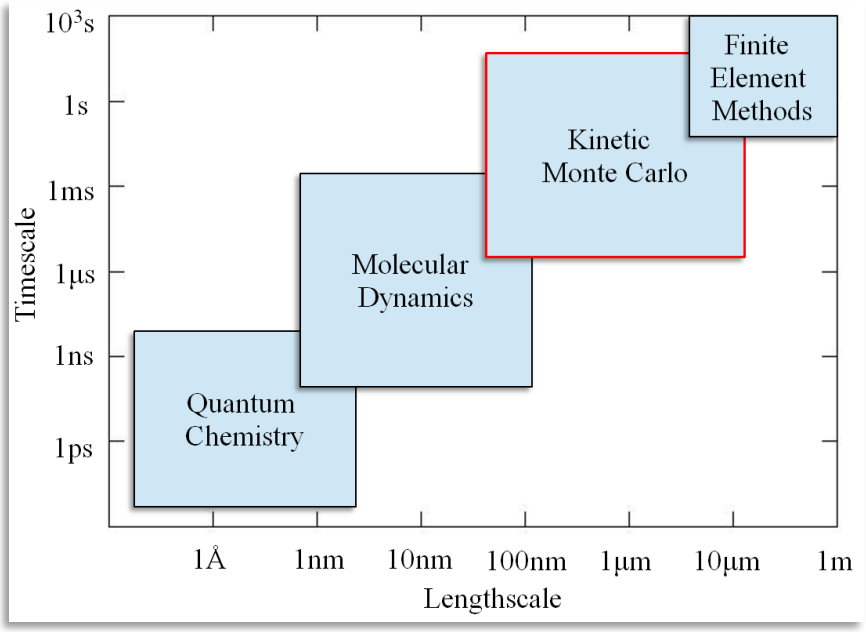
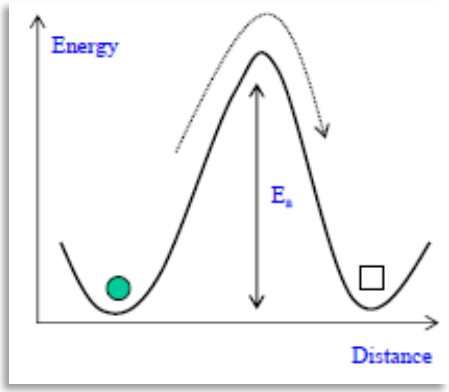
Kinetic Monte Carlo

- Kinetic Monte Carlo (KMC) is a method for simulating the state-to-state dynamics of a rare event system.
- Rare events correspond to the thermal activation of atoms from one energy basin to another on the potential energy surface.
- If the rates of these transitions are known, KMC can be used to simulate dynamics over long time scales.





$$k_{TST} = n_p \nu \exp\left(-\frac{E_a}{kT}\right)$$

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Adaptive Kinetic Monte Carlo

Adaptive Kinetic Monte Carlo (aKMC) is a method for determining all of the transitions from each state on the fly, eliminating the need to use a pre-defined rate-list.

DL_AKMC:

- Uses MD-type potentials (e.g. Buckingham, Tersoff, EAM etc.)
- Dimer method for finding transition states, from DL_FIND
- DL_POLY-type input files
- Simulation times reaching the level of seconds
- First release due 30th September 2013
- Runs on small workstations and large HPCs

Uses:

- Diffusion across/to surfaces and bulk
- Surface growth
- Defect mobility and clustering
- Simulation of infrequent event kinetics

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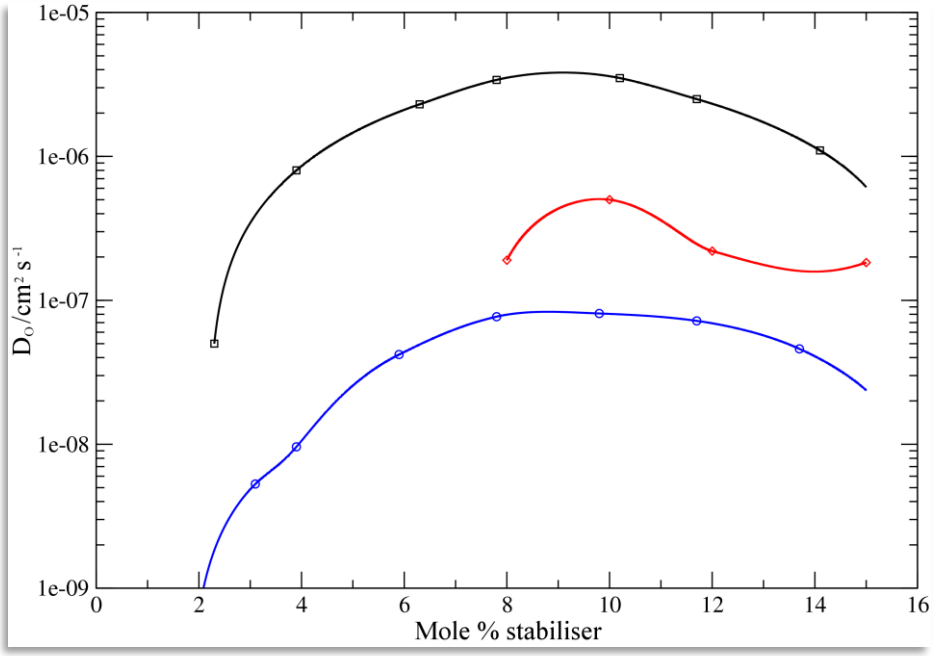
DL_AKMC examples

Oxygen self diffusion in fuel cell electrolytes:

- YSZ is used as an electrolyte in solid oxide fuel cells
- One of the requirements for such materials is to have a high ionic conductivity, and the level of doping affects this.
- DL_AKMC simulation of diffusion of oxygen in YSZ (black line) over several milliseconds matches well with experiment (red line) and finds the same optimum doping level found in experiment (just under 10 %)

Peak doping level of YSZ using DL_AKMC (black line) matches experiment (red line).
DL_AKMC of CSZ (blue line) has a diffusivity roughly two orders of magnitude lower than YSZ, but similar doping profile.



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