The need for an open standards, flexible and scalable multi-scale modelling capability in solid mechanics

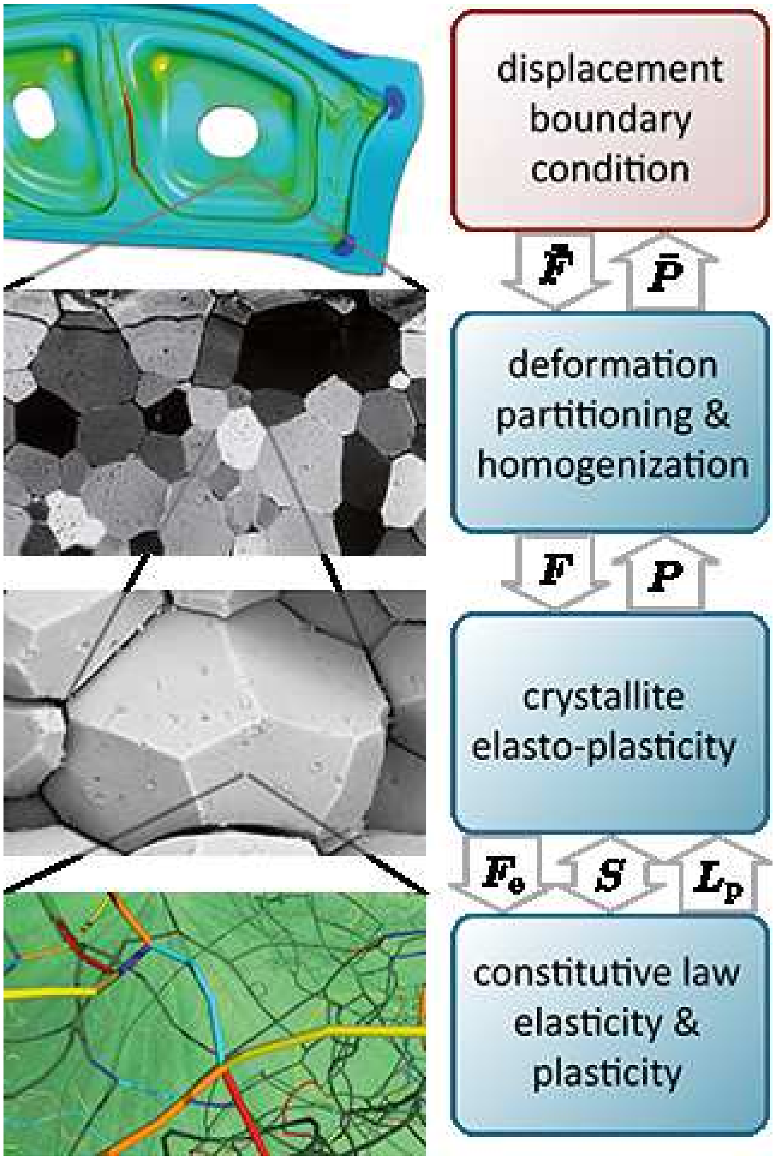
Anton Shterenlikht

Mech Eng Dept, The University of Bristol, Bristol BS8 1TR, UK
mexas@bris.ac.uk

Representative time and length scales

- Phase transformation: 10ps, 10nm.
- Dislocation nucleation and propagation: 50ps, 50nm.
- Twin formation: 1ns, 1nm.
- Interaction of dislocations: 100ns, 100nm.
- Secondary micro-crack nucleation in the process zone: 10ns, 100µm.
- Adiabatic shear: 10µs, 100µm.
- Component failure: 1s, 1m.

Linking scales: homogenisation/localisation (upscaling/down-scaling)



(From http://damask.mpie.de/)

Multi-scale solid mechanics problems:

- Armour penetration
- Explosive propagation of multiple interacting cracks in a pressure vessel
- Satellite impact
- Any large scale plastic flow

Multi-scale methods

- Coupled discrete dislocation and continuum plasticity[1]
- Voronoi polyhedra FE[2]
- X-FEM[3]
- element-free Galerkin (reproducing kernel particle)[4]
- Finite point[5]
- Free mesh[6]
- Meshless FE[7]
- Atomistic/continuum mechanics[8, 9]
- Molecular dynamics/continuum mechanics[10, 11]

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[1] M. Wallin *et al*, *J. Mech. Phys. Solids* **56**, pp. 3167-3180 (2008).

[2] J.-P. Mathieu *et al*, *Fatigue Fract. Engng Mat. Struct* **29**, pp. 725-737 (2006).

[3] M. Holl *et al*, *Comp. Mech* **53**, pp. 173-188 (2014).

[4] W. K. Liu, S. Li, and T. Belytschko, *Comput. Methods Appl. Mech. Eng.* **143**, pp. 113-154 (1997).

[5] E. Onate *et al*, *Int. J. Numer. Meth. Engng* **39**, pp. 3839-3866 (1996).

[6] G. Yagawa and T. Yamada, *Comput. Mech.* **18**, pp. 383-386 (1996).

[7] S. R. Idelsohn, *Int. J. Numer. Meth. Engng* **58**, pp. 893-912 (2003).

[8] J. Q. Broughton, *et al*, *Phys. Rev. B* **60**, pp. 2391-2403 (1999).

[9] W. A. Curtin and R. E. Miller, *Model. Simul. Mat. Sci. Engng* **11**, pp. R33-R68 (2003).

[10] G. J. Wagner and W. K. Liu, *J. Comput. Phys.* **190**, pp. 249-274 (2003).

[11] M. Xu and T. Belytschko, *Int. J. Numer. Meth. Engng* **76**, pp. 278-294 (2008).

Open source FE

Source: http://bnmc.caltech.edu/resources/finite_element

ADVENTURE
Aladdin
ALBERTA
CalculiX
CMISS
Code_Aster
deal.II
DOUG
DUNE
Elmer
FEA(S)T
FENICS
FELIB
FElt
FELYX
FEMLISP
FEM_Object
FEMOCTAVE
FEMSET
FFEP
freeFEM
Getfem++ HMD
Impact
IMS
kaskade
KFEM
LUGR
MiniFEM
MODFE
MODULEF
NASTRAN
NLFET
OLEFI
OOFEM
Open FEM
Open FEM (INRIA)
OpenSees
Padfem2
ParaFEM
Rheolef
SLFFEA
Sundance
TOCHNOG
VAPAS
VECFEM3
WARP3D
Z88

Common problems with open source codes

- Scaling
- Portability
- Documentation
- Flexibility
- Continuing development and future proofing
- Standard libraries
- Algorithms

Generic framework

We need:

- *Framework* for building multi-scale solid mechanics models
- *Flexible, expandable*- wide range of problems.
- *API* centred
- Opportunities for *code replacement* and *interoperability*.
- The framework must not not be linked to any particular FE code or any particular microstructure model.
- *Concurrent* simulation at all scales, with a two way information exchange.[12]
- The framework must allow for implementing *homogenisation* and *localisation* (upscaling/downscaling) algorithms, e.g. using the representative volume of material (RVE)[13] or nested homogenisation-localisation.[14]
- Multi-scale models are large. *Petascale* now and *exascale* soon.
- The aim of the framework is to allow researchers to combine their micro- or mesa-scale models with a variety of continuum mechanics FE solvers.
- *Comparison* of different multi-scale models and of different modelling results will be more rigorous and fair.

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[13] K. Pham *et al*, *J. Mech. Phys. Solids* **61**, pp. 2125-2146 (2013).

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Cellular Automata Finite Element (CAFE) simulation of transgranular cleavage in polycrystalline iron

- CAFE has been used before for solidification[15] and recrystallisation.[16]
- FE - continuum mechanics - ParaFEM[17] - stress, strain, etc.
- CA - crystal boundaries, cleavage, grain boundary fracture - CGPACK.[18, 19]
- FE → CA - stress, strain
- CA → FE - damage variable

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[15] Ch.-A. Gandin and M. Rappaz, *Acta Mat.* **42**, pp. 2233-46 (1994).

[16] C. Zheng and D. Raabe, *Acta Mat.* **61**, pp. 5504-5517 (2013).

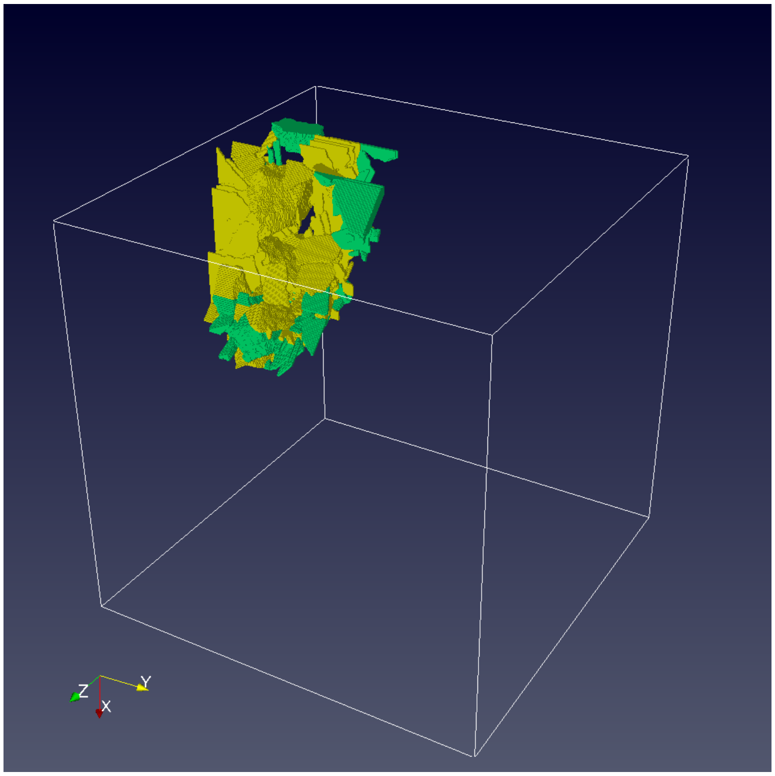
[17] Smith, Griffiths, and Margetts, *Programming the finite element method*, Wiley, 5ed (2014).

[18] A. Shterenlikht and L. Margetts, *Proc. Roy. Soc. A* (2015). in print.

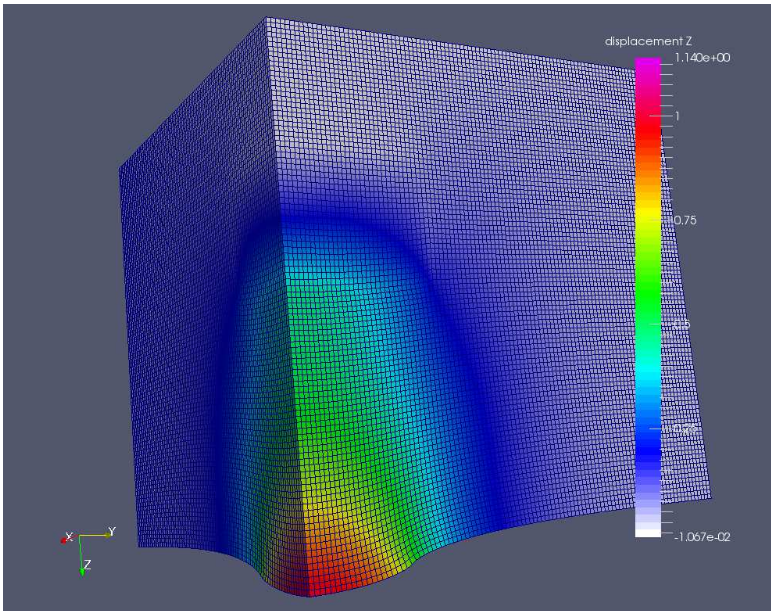
[19] A. Shterenlikht in *Proc. 7th PGAS Conf.*, The University of Edinburgh, UK (2013).

CAFE visualisation - ParaView

The macro-crack emerges as cleavage cracks in individual grains join up after crossing grain boundaries in poly-crystalline bcc iron. Green cracks - {110} planes, yellow - {100} planes.

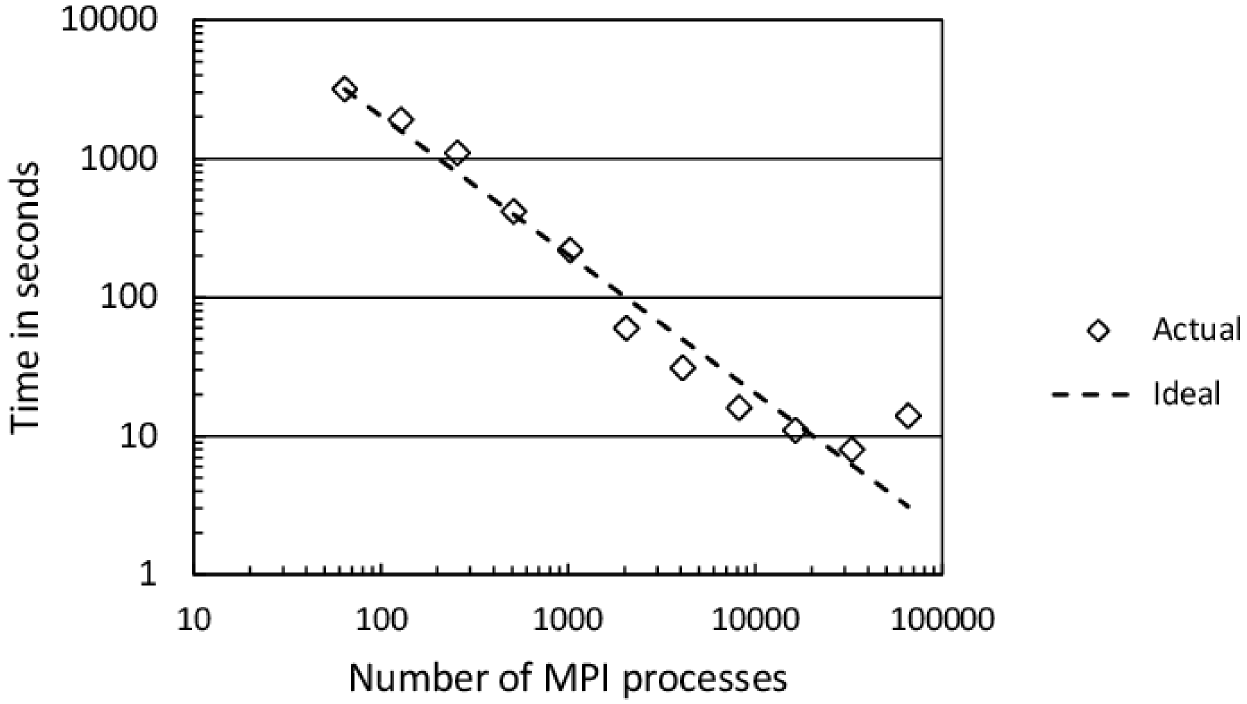


The process is driven by the FE stress fields on the macro-scale.

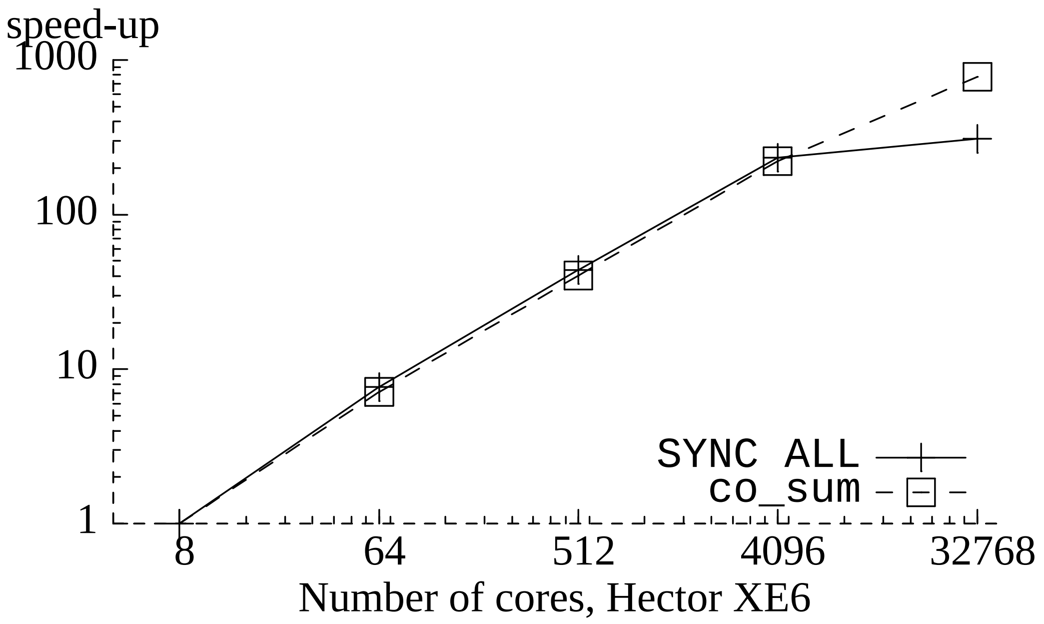


ParaFEM and CGPACK scaling on HECToR

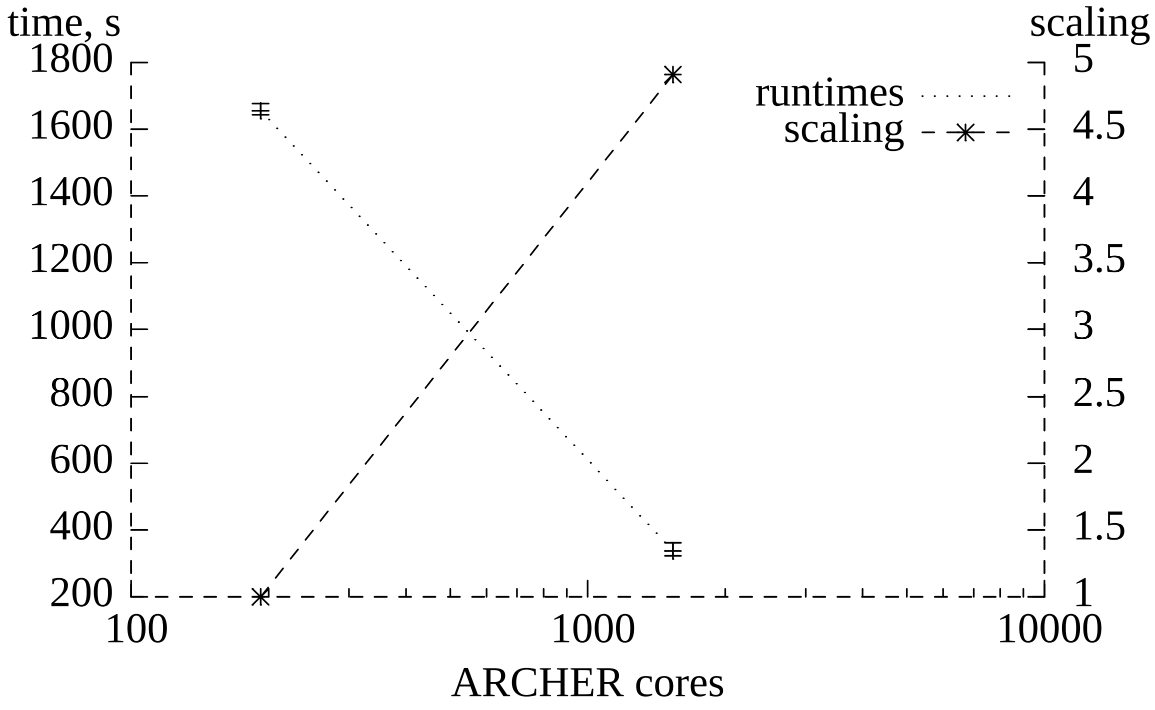
ParaFEM scaling for a 3D implicit transient heat conduction analysis in time with 125 million equations.



CGPACK scaling for a 3D solidification problem with 1 billion cells.



ParaFEM/CGPACK CAFE Scaling on ARCHER



- Good scaling: 192 → 1536 cores => scaled 5 times. Parallel efficiency of > 60%.
- ParaFEM - MPI
- CA - CGPACK - Fortran 2008 coarrays
- Hybrid MPI/coarray - novel, risky
- Cray only, poor portability
- Poor documentation
- API just emerging
- But ... 2 libraries - very flexible and expandable