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

Many solid mechanics problems must take material microstructure into account. Examples are armour penetration or explosive propagation of multiple interacting cracks in a pressure vessel. Inevitably multi-scale approach is needed. The representative time and length scales are: 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).

Popular multi-scale methods include coupled discrete dislocation and continuum plasticity,[1] Voronoi polyhedra FE,[2] X-FEM,[3] element-free Galerkin (reproducing kernel particle),[4] etc.

Many multi-scale codes are seemingly abandoned as soon as the results have been achieved and the articles published. Often the code sole purpose was to solve a particular single scientific task. As a result, multi-scale codes are often badly written, with poor portability, performance, flexibility, documentation and continuity. There's little opportunity for others to use these codes.

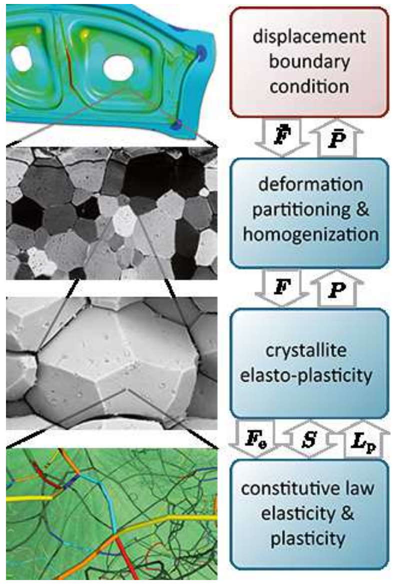
What is needed now is a generic *framework* for building multi-scale solid mechanics models.

[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).



Source: http://damask.mpie.de/

The framework must be *flexible* and *expandable* to be useful for a wide range of problems. It must be centred around clearly defined and documented *API*, so that each part of the framework can be replaced by another implementation, as long as the interfaces are matching. The framework must not not be linked to any particular FE code or any particular microstructure model. 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. This opens opportunities for code replacement and interoperability.

The framework must allow for *concurrent* simulation at all scales, with a two way information exchange.[5]

The framework must allow for implementing *homogenisation* and *localisation* (upscaling/downscaling) algorithms, e.g. using the representative volume of material (RVE)[6] or nested homogenisation-localisation.[7]

Such framework will make comparison of different multi-scale models and of different modelling results more rigorous and fair. This will produce a step change to the current state of the art, where developments are often so disparate that comparison is not possible.

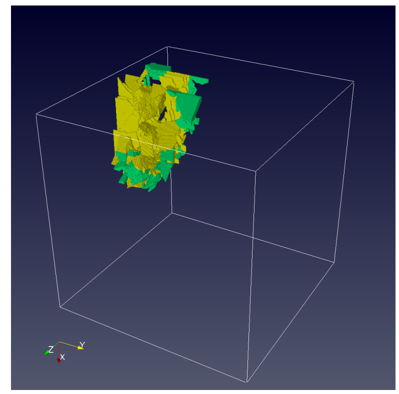
[5] V. Kouznetsova *et al*, *Comp. Mech.* **27**, pp. 37-48 (2001).

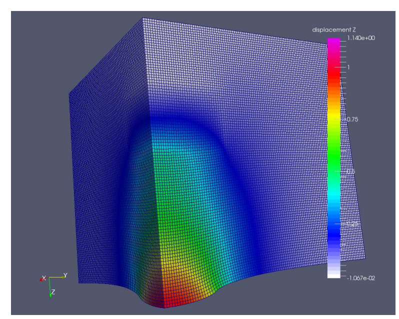
[6] K. Pham *et al*, *J. Mech. Phys. Solids* **61**, pp. 2125-2146 (2013).

[7] E. W. C. Coenen *et al*, *Int. J. Fract.* **178**, pp. 157-178 (2012).

Multi-scale models are large. The framework must be aimed at *petascale* (current) and *exascale* (future) systems.

Below is a simulation of a cleavage crack propagation in poly-crystalline bcc iron (top image). The macro-crack emerges as cleavage cracks in individual grains join up after crossing grain boundaries. Green cracks are on {110} planes, yellow are on {100} planes. Cleavage modelling is done on meso-scale with cellular automata (CA). The process is driven by the FE stress fields on the macro-scale (bottom image). These results were achieved with the ParaFEM[8] FE and the CGPACK[9, 10] CA libraries.





Similar CAFE multi-scale models have been used for solidification[11] and recrystallisation.[12]

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

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

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

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

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