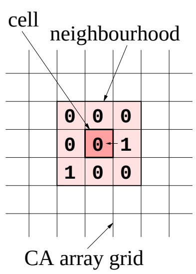
Towards mechanism-based simulation of impact damage using exascale computing

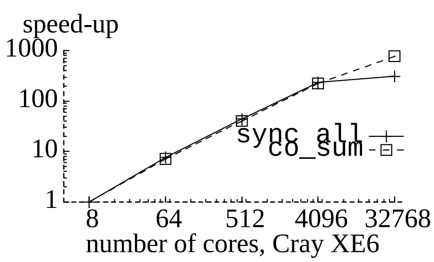
Anton Shterenlikht[1], *Lee Margetts*[2], *Samuel McDonald*[2], *Neil Bourne*[2]

[1]The University of Bristol, UK
[2]The University of Manchester, UK

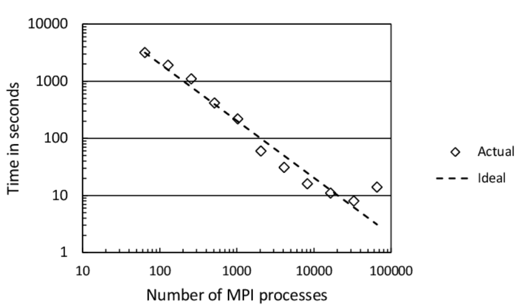
We have designed a framework for building multi-scale deformation and fracture models for supercomputers. Material microstructure evolution is implemented via cellular automata (CA).



We have developed a scalable Fortran 2008 [1] coarray CA library - CGPACK,[2]
`cgpack.sourceforge.net`



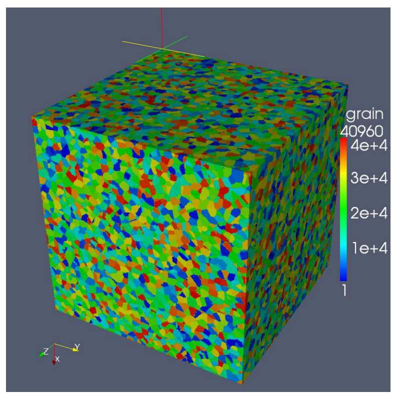
and coupled it with a highly scalable finite element (FE) library ParaFEM,[3]
`parafem.org.uk`



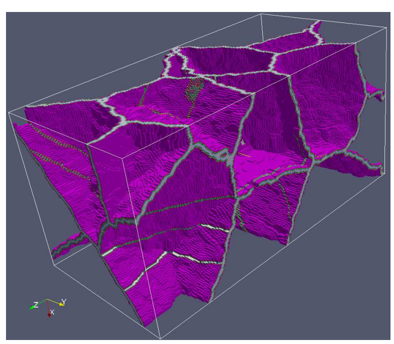
The resulting CAFE multi-scale framework[4, 5] is suitable for modelling microstructure/structure interaction problems, such as dynamic fracture.

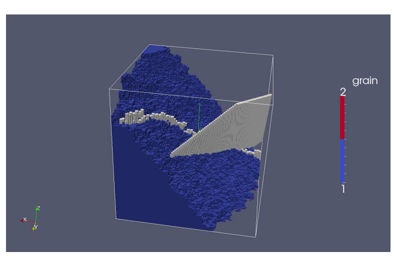
The framework implements simulation at all scales concurrently with a two way information exchange.[6] It is flexible, expandable and can be adapted to other problems. The framework is similar to the idea of a representative volume of material (RVE). It can accommodate different homogenisation and localisation (upscaling/downscaling) algorithms.[7, 8]

Large volumes of microstructure can be analysed. Image below shows a model with over 4×10^5 bcc grains, at a resolution of 10^5 CA cells per grain, i.e. over 4×10^9 cells in total.

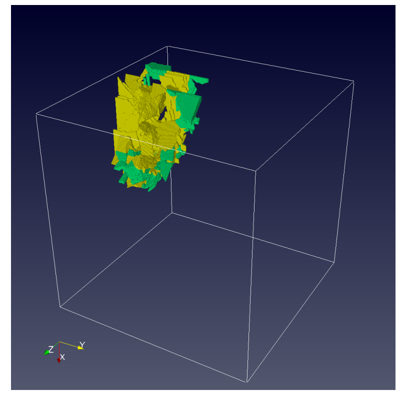


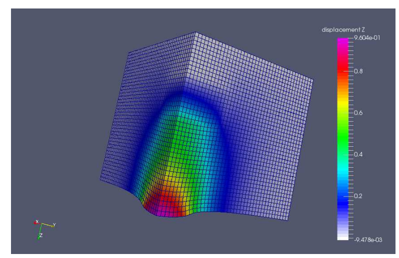
Grain boundaries (GB), crack propagation across GB and GB accommodation fracture can be studied.





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 CA. The process is driven by the FE stress fields on the macro-scale (bottom image).





References

1. A. Shterenlikht, L. Margetts, L. Cebamanos, and D. Henty, *ACM SIGPLAN Fortran Forum* **34**, pp. 10-30 (2015).
2. A. Shterenlikht in *Proc. 7th PGAS Conf.*, The University of Edinburgh, UK (2013).
3. I. M. Smith, D. V. Griffiths, and L. Margetts, *Programming the finite element method*, Wiley, 5ed (2014).
4. A. Shterenlikht and L. Margetts, *Proc. Roy. Soc. A* **471**, p. 20150039 (2015).
5. A. Shterenlikht and I. C. Howard, *Fatigue Fract. Eng. Mat. and Struct.* **29**, pp. 770-787 (2006).
6. V. Kouznetsova *et al*, *Comp. Mech.* **27**, pp. 37-48 (2001).
7. K. Pham *et al*, *J. Mech. Phys. Solids* **61**, pp. 2125-2146 (2013).
8. E. W. C. Coenen *et al*, *Int. J. Fract.* **178**, pp. 157-178 (2012).