Towards mechanism-based simulation of impact damage using exascale computing

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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 \textsuperscript{1} coarray CA library - CGPACK, \textsuperscript{2} cgpack.sourceforge.net and coupled it with a highly scalable finite element (FE) library ParaFEM, \textsuperscript{3} parafem.org.uk

The resulting CAFE multi-scale framework\textsuperscript{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.\textsuperscript{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.\textsuperscript{7,8}

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

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).

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

References