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Multiscale CAFE for Fracture in Heterogeneous Materials under Dynamic Loading Conditions

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The motivation of the authors is to develop a general purpose open source framework capable of multi-physics and multi-scale modelling on high performance computing systems. This paper describes one of the latest components developed in this framework, achieved through the integration of the cellular automata library CGPACK, modelling fracture at the grain scale to the finite element library ParaFEM, simulating engineering structures the continuum scale. The specific program is a mini-app[1], based on previous work by Shterenlikht and Margetts[2], adapted to model fracture in a three dimensional structure under dynamic loading conditions.

Simulations of this nature can involve both a large number of finite elements and cellular automata, so scalability is essential. ParaFEM and CGPACK use the Message Passing Interface and Fortran coarrays respectively for parallel communication, with both packages having been shown to scale to large core counts[3, 4]. The numerical results and parallel performance of the new application has been evaluated using a simple test problem on a Cray XC30 machine. Results highlight the fracture at the meso-scale and time-displacement plots, show the evolution of the localised fracture, which leads to macroscopic cracks and ultimately a non-linear response to dynamic loading.

This mini-app is part of a growing tool kit being developed by the authors. This application provides capabilities to capture both the meso-scale and macro-scale mechanics in deforming structures, subject to dynamic loading and in future work, this will be used in fluid-structure interaction problems[5].

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