A High-Performance Crystal Plasticity Solver for CPU-GPU Architectures

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ABSTRACT

We present a crystal plasticity (CP) solver that scales efficiently on heterogeneous computing clusters composed of CPUs and graphics processing units (GPUs). The approach makes use of a database containing a spectral decomposition of CP simulations performed using a conventional iterative solver over a parameter space of crystal orientations and applied velocity gradients. Only the largest components in the decomposition are used in the subsequent simulations, with sufficiently many chosen to satisfy a prescribed error tolerance.

The solver begins by dividing the macroscopic domain amongst computational nodes using standard techniques from distributed memory finite element (FE) schemes. On a given node, the crystal grains corresponding to those macroscopic points are then divided evenly amongst the cores of all the GPUs on the node. At each timestep, the GPUs use the spectral database to perform the grain-level calculations, which are then homogenized to produce the macroscopic responses. These responses are then used in the FE simulation, carried out by the CPU cores on each node.

We find that this approach exhibits excellent parallel scaling on problems in the hundreds of millions of crystal grains, on computational configurations achieving over 100 teraflops.

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