Connecting mesoscale structure to macroscopic material performance

Opportunity

Evolving mesoscale features in materials connect directly to material performance and are in turn driven by loading conditions dictated by material performance.

Developments in Multiple Process/Multiple Data (MPMD) parallel computing provides a framework for describing complex multi-scale modeling frameworks.

Exascale computing infrastructure (ExMatEx) provides an opportunity for running MPMD programs at previously inaccessible length and time scales.

A renewed focus on employing predictive simulations for accelerating property-driven materials design as laid out in the Materials Genome Initiative.

Meso Challenge

These structures generally require non-spatial statistical descriptions, as well as reduced dimensional bases for implementation in multi-scale modeling frameworks.

Self-consistent sampling, projection, and evolution of these distributions in the context of multi-scale/multi-physics materials models is non-trivial, and is often the "weak link" in current efforts.

Outliers and nucleation driven events are often linked to feature networks – with interactions – at the mesoscale (*e.g.* voids, grain boundaries, etc…).

Approach

Explore bases for upscale/downscale projection of statistical distributions describing structural heterogeneity (*e.g.* lattice orientations, morphology, boundary networks, damage, etc…) and develop methods for evolving distributions characterizing the mesoscale.

Implement mesoscale homogenization in existing multiscale modeling frameworks, using high fidelity characterization experiments for validation and verification.

Integrate with commensurate development of statistical and topological frameworks for extracting "material DNA."

Impact

Greatly advancing the predictive ability for assessing the suitability of different materials systems to complex performance needs, including the effects of evolving mesoscale state during the material's life cycle.

Gaining the ability to capture performance limiting "rare events" arising from the evolution of mesoscale feature networks.

Advancing the goal of critical property optimization and manufacturing feedback for accelerated materials design under the paradigm of Integrated Computational Materials Engineering.

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LLNL-PRES-557153

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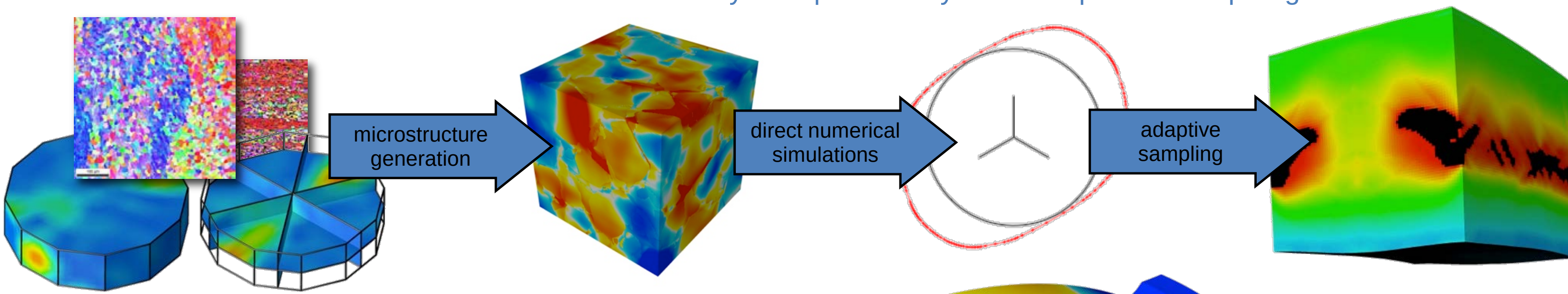
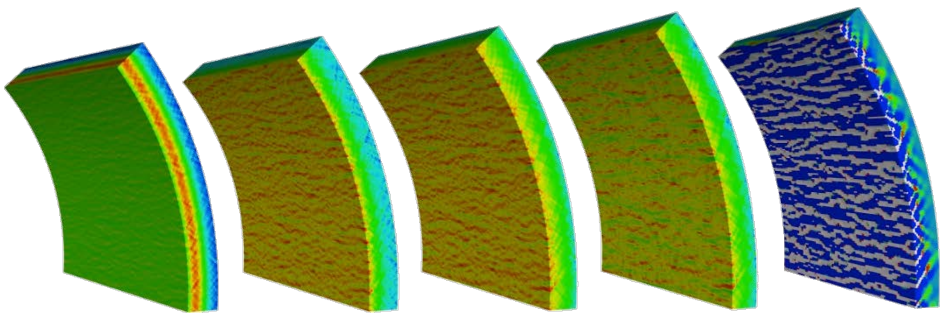
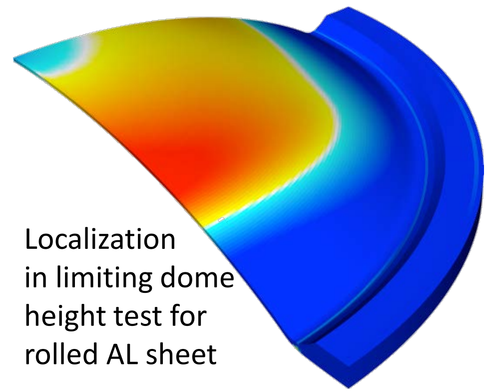
Crystal plasticity via embedded adaptive sampling has been successful in a variety of applications

Framework for embedded crystal plasticity via adaptive sampling



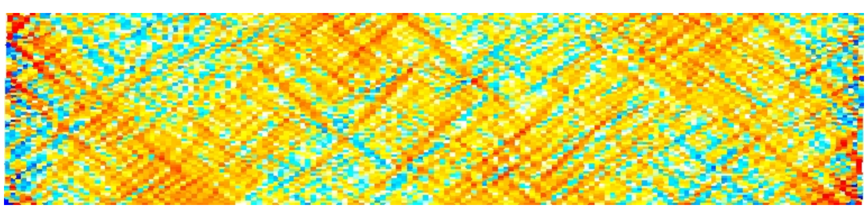


Fragmentation of rapidly expanding cylinder

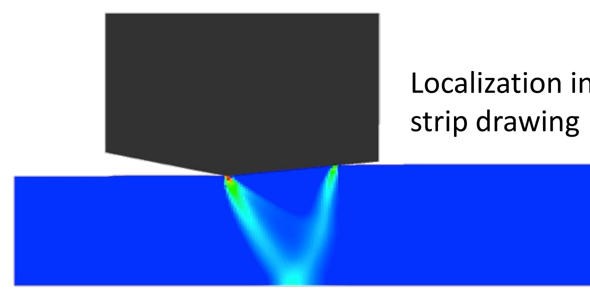


Localization in limiting dome height test for rolled AL sheet

Earing in cup forming



Localization of deformation under plane-strain compression



Localization in dynamic strip drawing

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For some of the foregoing: Arsenlis *et al.*, *CMAME*, 2006; Barton *et al.*, *IJP*, 2008; Knap *et al.*, *IJNME*, 2008; Bernier *et al.*, *JEMT*, 2008; Barton *et al.*, *IJNME*, 2011

LLNL-PRES-557153