Overview of Research Programs at the Multiscale Structural Simulations Laboratory

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Abstract:
The document provides a concise overview of activities at the multiscale structural simulations laboratory (MSSL) in the Department of Aerospace Engineering at University of Michigan. Our interests are in the areas of computational mechanics, multi-scale materials modeling and optimization with emphasis on prediction and design of properties in aerospace materials. Multi-scale models resolve interactions of material structure and mechanisms at electronic (ab-initio), atomistic (molecular dynamics), micro (mechanics of slip), meso and macro (finite element models) scales. We develop models to address key aerospace issues such as manufacturing process optimization to achieve tailored material response and prediction of material performance in moderate to extreme environments using an integrated computational materials engineering (ICME) approach.

Figure: A snapshot of research activities at MSSL lab. The particular research areas are described below:

A. Areas of research
   1. Crystal Plasticity modeling: Our group specializes in crystal plasticity modeling for modeling metallic material response at the mesoscopic scale. Most structural metallic materials are composed of aggregates of single crystals. Plastic flow in a single crystal is
anisotropic, and cannot be modeled using simple yield models. Instead, a complex material law is used, which models unit mechanisms such as slip and twin activity. Using this model, we simulate the crystallographic rotations of individual grains in a polycrystal to predict texturing, and we predict stress-strain response at the structural scale. The PRISMS DoE software center grant enabled development and distribution of an open source crystal plasticity finite element code to the broader research community. The code is publically available at https://github.com/prisms-center/plasticity

2. **Multi-scale materials design:** This project focuses on computational multi-scale design/optimization approaches for tailoring engineering properties of metallic materials. Of particular interest is the use of controlled deformation processes to tailor evolution of microstructural features such as crystallographic texture. The design problem involves prediction of process conditions (forging velocity, preform shape etc.) that lead to a desired microstructure distribution in the material. Here, micro-scale evolution is solved with crystal plasticity at the integration points of a finite element large deformation simulation. The inverse problem is by far (at least on the basis of computational complexity alone, with billion microstructural degrees of freedom) a challenging inverse problem. Highlight of our approach is a multiscale continuum sensitivity analysis scheme for rapidly computing the sensitivity of microstructural features to change in process parameters. Using this approach, we have demonstrated design of tailored 'high strength' (eg. turbine disk) or 'minimal magnetic hysteresis loss' (eg. transformer cores) structures. Our research with National Science Foundation supported theoretical and computational investigation of new thermo-mechanical processes for manufacturing low-cost polycrystalline iron-gallium alloy (Galfenol) with properties comparable to expensive single crystals. Our collaboration with UTRC is on development of the method for modeling processing of third generation aluminum lithium alloys for fan blades.

3. **Markov random fields for microstructure synthesis:** Currently available methods for microstructure synthesis such as geometry based (eg. Voronoi models), physically based (eg. Phase field models) or feature-based (eg. Simulated annealing) methods run into various difficulties when modeling complexities of microstructures such as non-equilibrium grain structures, non-convex grains, twins, second phases and cell structures that naturally arise from material processing. These features play an important role in the properties and performance of modern aerospace alloys. Further, stochasticity of microstructures lead to location-specific variability in material properties, and a single instance of a microstructure does not adequately model the property distribution in a component. In this project, we delve into a mathematical model that is expected to provide a robust alternative for microstructure synthesis: Markov random fields (MRFs). We are developing theory and software for building three dimensional (3D) microstructural maps of engineering components through Markovian inference from two dimensional (2D) measurements.

4. **Reduced order descriptors for microstructure modeling:** As a part of the 'basic research challenge'(BRC) team selected by the office of naval research, we investigated alternatives to computationally expensive crystal plasticity finite element modeling (CPFE) of polycrystalline microstructures for multiscale modeling of deformation processes. Recently, we have developed the general theory behind physics-based modeling and scale-linking of three reduced order descriptors with increasing levels of microstructural information: (i) Orientation distribution function (ODF) which contains crystallographic texture, (ii) Grain size orientation distribution function (GSODF) that contains texture as well as grain size/shape information and (iii) Conditional orientation
correlation function (COCF) and nearest neighbor orientation correlation function (NNOCF) that contains texture as well as crystal neighborhood information. The common theme in our approach is the use of Lagrangian finite element analysis to directly evolve the ‘descriptor’ (rather than the actual microstructure) during deformation. We have shown that the approach is significantly faster than CPFE and will result in orders of magnitude speed up for microstructure sensitive design of advanced titanium alloys used in aircraft and naval structures.

5. Multi-scale modeling of composites in extreme environments:
   
i. Ceramic matrix composites: We have developed a multi-scale (macro-micro) methodology to study degradation of ceramic matrix fiber reinforced composites in high temperature oxidizing environments. The method integrates multiple physics associated with microstructure degradation including thermal transport, chemical reaction kinetics, thermo-mechanical deformation, matrix damage accumulation, diffusion of oxygen/oxides and carbon fiber surface recession at the microstructural level. The macro-to-micro coupled model has the ability to quantitatively capture oxidative mass loss and mechanical behavior at high temperatures as reported in published experiments (Past support from NASA).

   ii. Energetic composites: With support from DTRA, the multiscale approach was extended to include high rate (detonation wave) physics for a HMX/polymer composite system. We include equations of state for every component, chemical reaction rates, heat generation and have developed mixture rules to model solid-gas mixing. The method has been implemented using Taylor Galerkin approach with flux limiter schemes for modeling sharp shock and detonation waves.

6. Atomistic modeling of epoxy resins and nanocomposites: We specialize in molecular dynamics simulations of polymer nanocomposites. These simulations are used to computationally determine the thermomechanical properties of cured thermoset or thermoplastic resins reinforced with pristine or covalently functionalized nanostructures. The thermoset structure building is performed using the ‘dendrimer’ growth approach that leads to equilibrated atomistic structures with properties that closely reproduce measurable engineering properties such as stiffness, thermal expansion and conductivity. By adding nanostructures with different chemical functionalizations, these techniques allow design of polymers even before they are synthesized. Micromechanical theories are used to obtain the properties of larger-scale isotropic system of oriented nanotubes in epoxy. Theoretical models show substantial improvements of functionalized nanocomposites over plain epoxy in terms of higher stiffness (200% increase) and lower thermal expansion (32% reduction).

7. Uncertainty quantification for materials science: Although there has been extensive work on multiscale modeling of materials, an understanding of the effect of intrinsic microstructure uncertainties on macro-scale engineering properties is still lacking. In this work, we aim to bridge this gap by developing stochastic analysis tools (specifically, markov random field approach for microstructure probability estimation and analytical methods for uncertainty propagation). We are also working on an efficient multi-scale stochastic sensitivity analysis technique in the context of managing uncertainties in materials-by-design approaches. We have developed uncertainty quantification and design techniques to optimize these reduced order descriptors to obtain microstructures with desired property distributions.
8. **Metallic Fracture and Fatigue**: Multi-scale analysis is used for computation of failure of metals under static/cyclic loads and external environment. Computational themes include crystal plasticity, dislocation dynamics, molecular dynamics and density functional theory. In an ONR program, we developed models for environmentally assisted failure based on cohesive energies computed from DFT calculations. We have used molecular dynamics to compute failure along grain boundaries and its effect of intergranular decohesion and failure. We couple crystal plasticity finite element method with variational multiscale method for modeling arbitrary crack paths (both transgranular and intergranular). In the DoE software center, we employ dislocation dynamics simulations to inform cyclic crystal plasticity models for simulation of low cycle fatigue failure.

9. **Nonlocal theories and peridynamics**: Unlike local theories, non-local elasticity theories take into account the multi-atom interactions that determine stress state at the nano-scale. Non-local theories may overcome several issues associated with local models, for example, local elasticity predicts infinite stresses at a crack tip and does not predict size effect in elastic properties at the nanoscale. In collaboration with Dr. Anthony M. Waas, we worked on methods to directly build accurate non-local models of Carbon nanotubes from dispersion curves obtained from molecular simulations. A collaborative paper was published discussing the physical properties of the non-local kernel. The project was supported by Boeing Company.

   i. Recent work has continued development of non-local models based on the peridynamic formulation. Peridynamics is a non-local formulation of continuum mechanics that is promising for modeling fracture and gradient effects. We developed the first implementation of crystal plasticity within state-based peridynamics theory and have developed new algorithms based on both explicit and implicit methods for integration of peridynamic equations of motion.

10. **Materials informatics**: Data-mining techniques are eminently suitable for materials design since optimal microstructures can be selected based on available information from a large database relating processes, properties, and microstructures. A hierarchical X-means classifier and support vector machines algorithm have been developed to enable automated identification of such relationships by mining over a database of microstructural signatures. These methods were employed for multiscale design of Galfronol and Titanium alloys in an AFOSR funded MURI in collaboration with Northwestern University.

B. **Software dissemination**: As part of a broad software dissemination effort, we have gradually transitioned our computational work to a fully open-source parallel C++ format based on open MPI and the PETSc platform.

List of other computational packages developed by our group are listed here:

- **PRISMS Plasticity**: An open source Crystal plasticity finite element code based on Dealii library. [https://github.com/prisms-center/plasticity](https://github.com/prisms-center/plasticity)
- **MicroFract**: An image based code for microstructural fracture, open source code at [http://umich.edu/~veeras/projects/MicroFract.html](http://umich.edu/~veeras/projects/MicroFract.html)
- **Polycrystal plasticity using probabilistic descriptors**: A material point simulator for polycrystal plasticity in Rodrigues space for FCC, BCC and HCP metals, extension to modeling GSODFs and COCFs for planar crystals.
Multiscale Deformation Process Modeling: A Petsc based library for multi-scale modeling of deformation processes using polycrystal plasticity within a Rodrigues representation as well as using discrete aggregates. It includes texture and grain size effects as well as tools for meshing of realistic 3D polycrystals.

Design of Deformation Processes: A Petsc based code for the design of multi-stage deformation processes (forging, extrusion, etc.) including texture evolution via the ODF formulation for controlling location-specific microstructure-sensitive properties.

Level Set Modeling of oxidative degradation of composites: A Petsc based level set computation of carbon fiber oxidation in an porous matrix at high temperatures.

Reactive hydrodynamics model of energetic composites: A Petsc based finite element library for computation of detonation and shock waves in energetic composites.

Data driven models of microstructures: A stand alone C++ package for unsupervised clustering of microstructural features using X-means algorithm for identification of feature-property relationships, a Markov random field approach for 3D microstructure reconstruction.

Fracture/Fatigue modeling: A variational multiscale cohesive zone method for modeling fracture at microstructural scale, extension of the approach for fatigue modeling, a new peristatics approach for modeling shear bands in polycrystals.

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