Bachelor/Semester/Master's thesis topics

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Atomistic modeling of materials

This project involves the computational simulation of materials at the level of atoms/molecules. Molecular dynamics simulations afford a tremendous level of resolution of various mechanical/physical/chemical processes and enable the derivation of the macroscopic behavior from first principles. Molecular dynamics are simple in concept: one considers a large number of particles and exploits Newton's equation of motion that links acceleration to interatomic forces. Students will get familiar with modeling and computational issues, will employ existing software (e.g. LAMMPS, GROMACS) and will ultimately be able to predict material properties (e.g. elastic modulus) at the atomistic level.

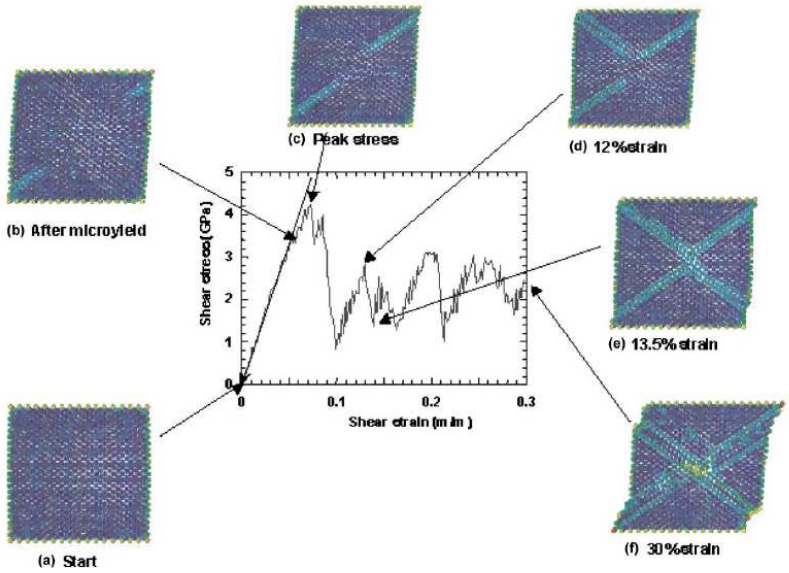


Figure 1: from *Computational nanoscale plasticity simulations using embedded atom potentials* by M.F. Horstemeyer et al. 2001

Model-based damage detection of dynamical systems

This project aims at investigating data-driven, model-based, damage identification techniques for mechanical systems. It combines computational models for the time evolution of systems with state estimation techniques. It will attempt to answer the following questions:

- how can we combine models with data?
- how much information do measurements contain about the state of our system?
- can we use incomplete measurements to infer the complete state of our system?
- can we use noisy measurements to infer accurately the state of our system?
- how certain can we be in our predictions?

Students will get familiar with modeling and computational issues and will write or use existing software in test problems.

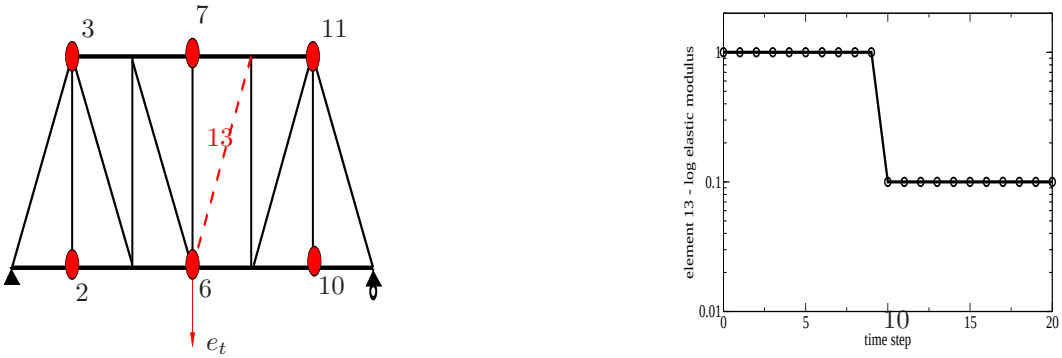
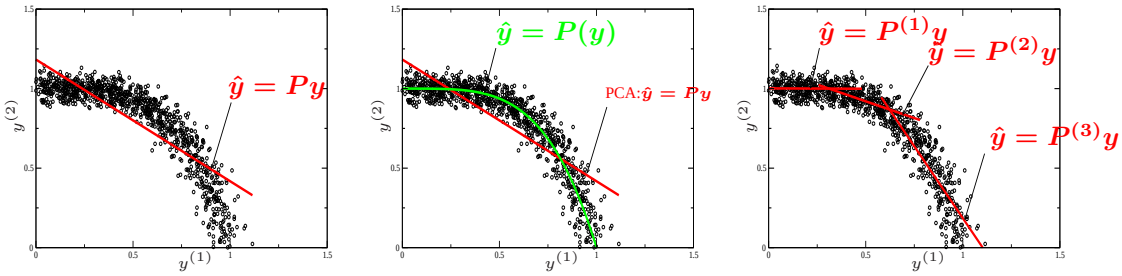


Figure 2: Damage detection in truss under dynamic excitation e_t

Reduced-order modeling in computational simulations

Over the past few decades all sciences have seen an explosion of the use of computer simulations to the point where computational methods stand alongside theoretical and experimental methods. The use of large scale computational models involving millions or billions of degrees of freedom provides unprecedented level of resolution to a wide range of physical processes and into the behavior of a variety of engineering systems.

On many occasions these models must be solved several times under different conditions or for different values of model parameters as is the case in design/optimization. This results in long and impractical computational times. To enable such tasks, one must find reduced descriptions, involving much fewer unknowns, that nevertheless preserve the accuracy of the full-scale model. Students will get familiar with modeling and computational issues, methods for dimensionality and model-order reduction and will write or use existing software in test problems.



(a) PCA (b) Nonlinear PCA (c) Mixture PCA

Figure 3: Various linear and non-linear dimensionality reduction techniques. Illustration in two dimensions

Uncertainty quantification in computational modeling

Mathematical modeling of physical systems has by-and-large focused on deterministic formulations which omit or misrepresent the role of uncertainties, and as a result limit their predictive ability. In mechanical engineering in particular the role of uncertainties is quite pronounced, as they encompass material properties (i.e. stochastic spatio/temporal variations of constitutive parameters), loading (i.e. mechanical excitations), as well as manufacturing imperfections. Traditionally, their effect has been buried within ad hoc safety factors. This project aims at developing rigorous formulations that account for various sources of uncertainty, quantifying their effect on the system's response and assessing the system's reliability.

Students will get familiar with probabilistic modeling and associated computational techniques and investigate the role of uncertainties in the analysis and design/optimization of engineering systems.

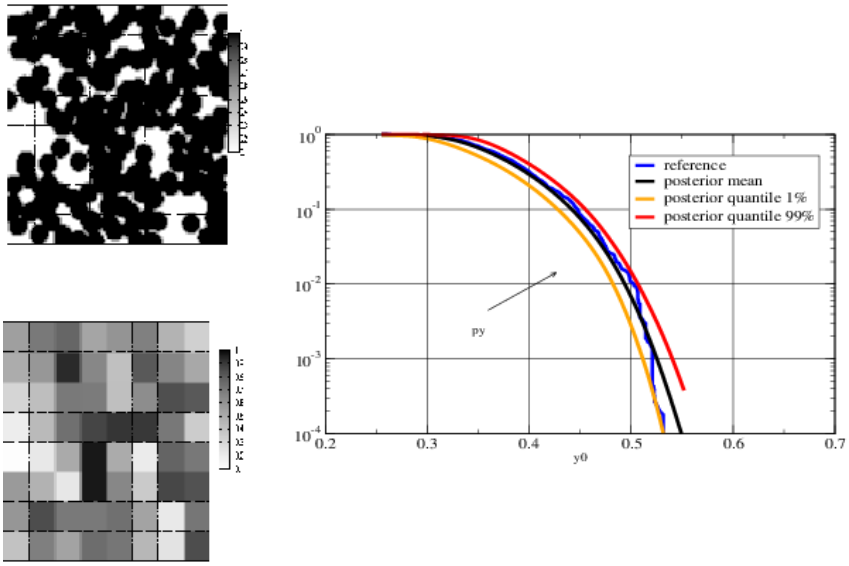


Figure 4: from *Accurate uncertainty quantification using inaccurate models* by P.S. Koutsourelakis 2009