Center for Multiscale Modeling for Engineering Materials
CM^2EM

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ICES President's Advisory Board

Vision

- Quantitative understanding of materials from the smallest to the largest relevant scales, with special emphasis on *emergent* behavior in complex materials systems to enable better design of applications with existing engineering materials and to engineer new materials with targeted functionality

Multiscale Modeling for Engineering Materials

- Use mathematical and computer modeling to understand deformation, flow, and fracture of solids under complex loading conditions
  - Mechanical response is different, but related, depending upon scale (spatial and temporal) of observation

- *Goal*
  - *Deduce physically-sound descriptions at individual scales by understanding the interaction between response at smaller and larger scales*
    - *Physics at smallest scale may be well-known; but by itself, it is of little practical value for physics at larger scales*

- One of the most important intellectual challenges of modern-day science, with direct link to technology
  - Fatigue in jet engine/electronic storage components
  - Design and reliability of (N)MEMS devices
  - High rate deformation in armor/weapons
  - Forming of high strength-high ductility metallic glasses & alloys
  - Response of soils and rocks;
  - High-frequency response in earthquake rupture dynamics;
  - Granular flow in fluidized beds and material handling applications,
  - Ball milling……

Center Goals

- Prediction of properties and performance of existing engineering materials systems under varied operational conditions
- Engineer new materials for targeted functionality
- Serve as a primary hub for materials *modeling* activity at CMU providing
  - a point of common reference
  - greater visibility
  - support to other Centers involved primarily with materials development and characterization

Motivation

- Set up a mechanism for coordinated
  - research and
  - educational

  activities in Multiscale Materials Modeling across CMU colleges of Engineering and Science

- Idea has significant support among
  - CIT and MCS faculty
  - CIT Dean, Dept. Heads (CEE, MSE, ME), and Center Directors (ICES, MRSEC, CNXT)

Participants (31)

CEE

Acharya
Bielak
Dayal
Maloney
Soibelman

ECE

Fedder
Li
Pileggi
Towe (MSE)

Math

Ta'asan
Tartar
Walkington

Physics

Sekerka
Suter
Swendsen
Widom

ChemE

Islam (MSE)
Kitchin
Ydstie

MSE

Barmak
DeGraef
Rohrer
Rollett
Seetharaman

MechE

Aubry
De Boer
Higgs
LeDuc
McGaughey
Ozdoganlar

PSC

Wang

Mission

- Develop new theory and simulation tools for engineering and scientific applications that often require multiscale physics e.g.,
  - Stress management in metallic and semiconductor heterostructures
  - Earthquake rupture dynamics
  - Influence of atomic scale grain boundary structures in the macroscopic response of polycrystalline materials
  - Mechanical behavior of granular materials from the solid to the liquid regimes
  - Nucleation and kinetics of phase boundary motion and their effect on macroscopic response (e.g. reliability of ferroelectrics; TRIP, AHSS steels)
  - Phase field modeling of free boundary problems
  - Colloidal systems
  - Rheology of soft/polymeric materials (e.g. paints and plastic composites)
  - Macroscopic response of metallic glasses
  - Dynamics of specified observables of a system for real-time control

- Emphasis: not only physics but engineering
    - e.g., Effects of finite geometries, boundary conditions, loadings and bifurcations due to such parameters

Mission

- Educate next generation of students in engineering, that will be well-versed in
  - Nonlinear continuum mechanics
  - Relevant aspects of Physics
    - Equilibrium and non-equilibrium statistical mechanics
    - Quantum mechanics – electronic density functional theory
  - Mathematics
    - Homogenization – weak convergence methods,….
    - Dynamical systems - averaging, invariant manifold theory, nonlinear dynamics of time series…..
    - Stochastic Analysis
  - Each of the above topics can be subject of life-time study, but we believe working knowledge required for appreciating core-issues of multiscale physics and computation can be distilled into 1 or 2 courses.
  - Scientific and engineering computing
- This educational approach would provide an important niche, as this viewpoint is not part of present training, even though it is essential for dealing with the challenges facing modern engineering

Activities

- Strong seminar series
  - Internal
  - External
- Target research funding opportunities in focused groups
  - DOE, DARPA, DOD, NASA, NSF, …..
- Seek industrial collaboration to strengthen funding opportunities, provide outlets for research results and test beds for algorithms and methods
- Phase in a curriculum in *M²EM*
  - Existing courses in Colleges of Science & Eng.

    + new to provide the unique necessary background

        - (e.g. will try out a new CEE seminar course)
  - Consider a formally recognized specialization attached to conventional individual Dept. degree

Administration

- Center within ICES
  - Director – Amit Acharya (CEE)
  - Associate Director – Michael Widom (Physics)
  - Utilize ICES support infrastructure and enthusiasm!

Recent Activities

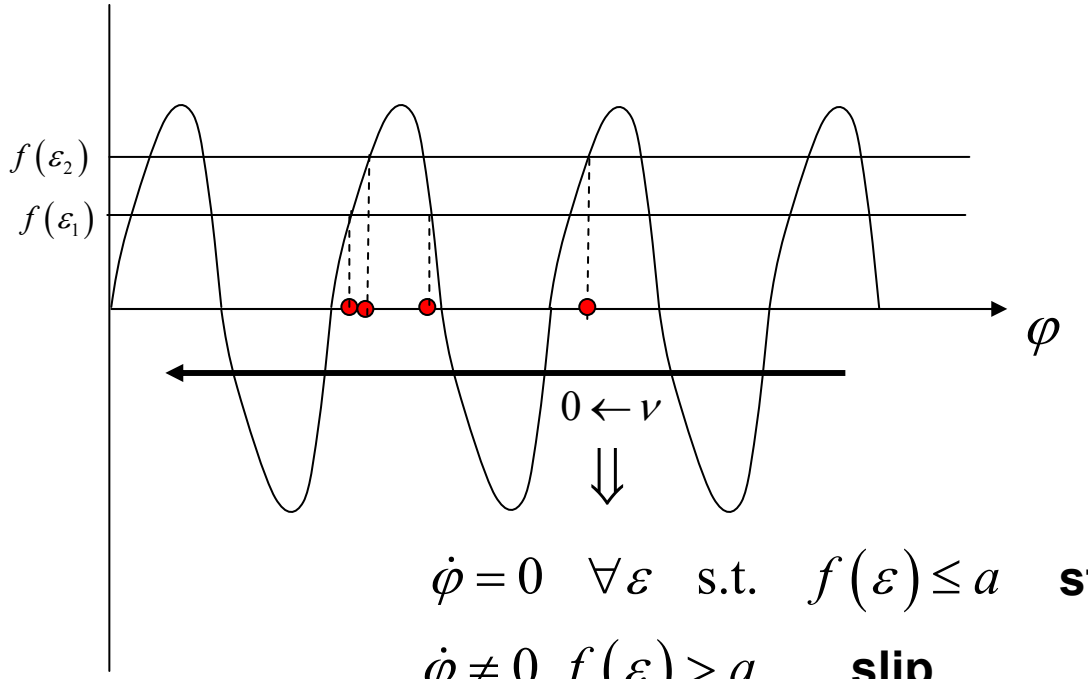
- Seminar series
  - February 28 **Amit Acharya**, CEE - Center Introduction & A simple example of sequential scale transition in dynamics
  - March 13 **Maarten DeBoer**, ME - Adhesion and Friction Experiments in Microscale Systems
  - March 27 **Bob Swendsen**, Physics - Optimized Monte Carlo simulations
  - April 10 **Luc Tartar**, Mathematics - What is "the general theory of homogenization"?
  - April 17 **Greg Rohrer**, MSE - The onset of three dimensional microstructural observations: analysis and simulation challenges (NOTE: off the bi-weekly schedule)
  - May 8 **Mike Widom**, Physics - Thermodynamics from First Principles
  - May 19 Retreat

- First proposal submitted

  - NSF CDI full proposal competition – “Slow response of fast dynamics” $2.7mil/4yrs
    - CM^2EM participants - Acharya, Dayal, Maloney, Soibelman, Tartar, Ydstie
    - Nystrom PSC; Gorban UK; Radulescu Fr.

M²EM is Computational Materials, but more!

Emergent behavior



$$\dot{\varphi} = 0 \quad \forall \varepsilon \quad \text{s.t.} \quad f(\varepsilon) \le a \qquad \textbf{stick}$$

$$\dot{\varphi} \neq 0 \quad f(\varepsilon) > a \qquad \textbf{slip}$$

$$\dot{\varphi} = f(\varepsilon) - a \sin\left(\frac{\varphi}{\nu}\right)$$

Microscopic motion

e.g. Abeyaratne, Chu, James 1996, Phil. Mag.

Macroscopic stick-slip

Questions?

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