Multiscale Modeling

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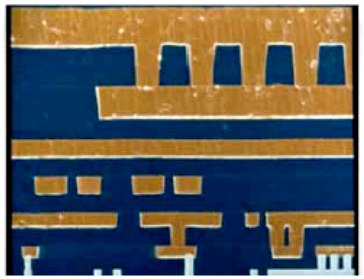
- **Integrated computational approach for predictive modeling of complex systems behavior**
  - **Disparate length and time scales**
  - **Heterogeneous and diverse phenomena**
- **Theoretical Goal: Establish rigorous links between different theoretical formalisms representing widely disparate length scales, time scales, and nonlinear phenomena**
- **Computational Goal: Develop computational enabling technologies, software tools, and supporting infrastructure for efficient implementation of multiscale models**
- **Applications Goal: Derive process-structure-function-system response relationships to enable optimal engineering strategies**

Example: Chemical/Materials Processing & Function. Core Capabilities

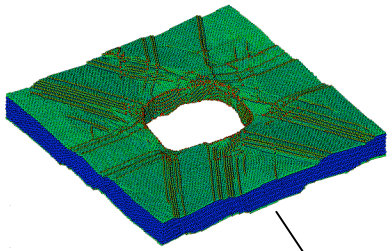


Supply Chain Modeling:
- Planning & Scheduling
- Mixed Integer Linear Programming

→ **Global logistics**

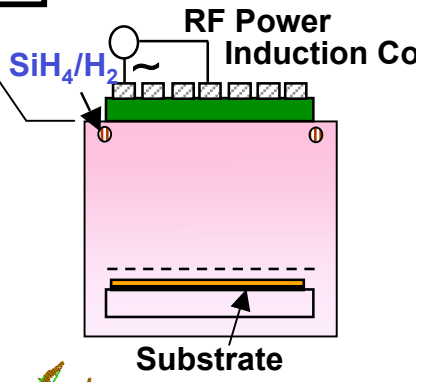
Process Simulation:
- Equation-Based Models
- Control and Optimization

→ **Processing units/facilities**



Continuum Mechanics:
- Finite-Element & -Difference Methods
- Boundary-Integral Methods

→ **Macroscopic modeling**

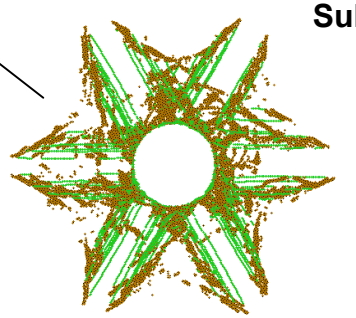


Mesoscopic Scale:
- Coarse-grained Quantum and Statistical Mechanics
- Quasi-Continuum Methods

→ **Mesoscale modeling**

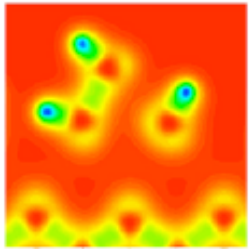
Statistical Mechanics:
- Semi-empirical Hamiltonians
- Molecular Statics, Lattice Dynamics, Molecular Dynamics, Monte Carlo

→ **Modeling for mechanistic understanding**



Quantum Mechanics:
- *Ab initio,* electronic structure
- Density Functional Theory,
- First-principles Molecular Dynamics

→ **Accurate calculations of materials properties**



Length

Time

Today's Talks

Equation-Free Modeling for Complex Systems
Yannis G. Kevrekidis, Professor, Department of Chemical Engineering, Program in Applied & Computational Mathematics, and Department of Mathematics, Princeton University

Modeling Complex Materials: Do We Need All of the Atoms?
Rob Phillips, Professor of Mechanical Engineering and Applied Physics, Division of Engineering & Applied Science, California Institute of Technology

Balancing Scales in the Use of Biological Models
Adam P. Arkin, Assistant Investigator, Howard Hughes Medical Institute; Assistant Professor, Department of Bioengineering, U. C. Berkeley; Faculty Scientist, Physical Biosciences, E. O. Lawrence Berkeley National Laboratory

Small-Scale Processes and Large-Scale Simulations of the Climate System
Bjorn Stevens, Associate Professor, Department of Atmospheric and Oceanic Sciences, University of California - Los Angeles