Multiscale phenomena and techniques

Offered by:	Departments W, TN and W&I
Language:	English
Aimed at:	W, TN, Stand W&I (primarily) and BMT, Bk, EE (secondarily)
Prior knowledge:	Calculus + additional requirements per course (see below)
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Contents

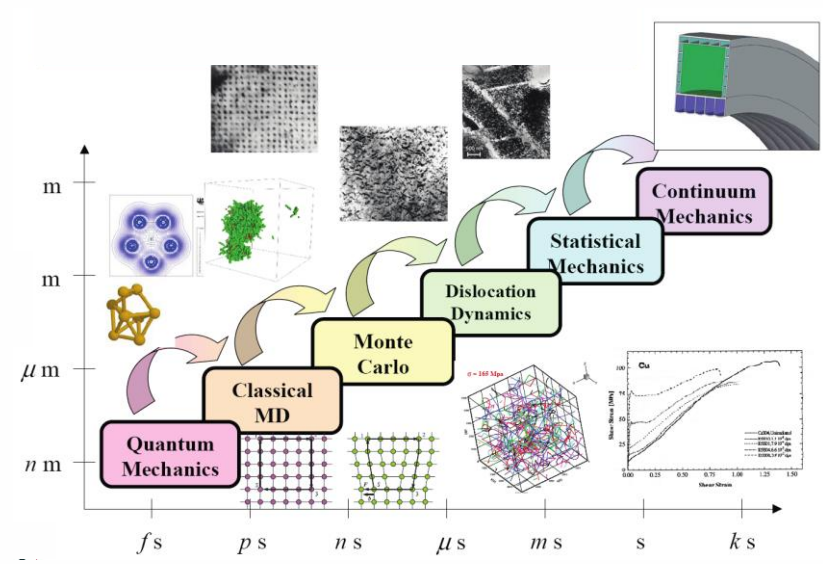
Reductionism is one of the basic principles of exact sciences: to understand complex systems (materials, processes, etc.), a system is subdivided in smaller parts that can be considered separately . The power of reductionism is its recursive character: if the parts in turn are too complex, they can subdivided once more. This process can be continued until one's left with only simple components. Four examples of reduction of a complex system are:

1. material - crystal - molecule - atom
2. organism - organ - tissue - cell - molecule
3. crowd - individual
4. country - city - urban area - building

tissue crowd urban area

The applicability of the reductionistic approach reduces as the number of components increases. A typical property of many systems however is that they show emergent behavior, i.e. to describe the behavior of the complete system it is not necessary to know the exact behavior of the underlying parts. This is concisely summarized by the quote of Nobel Prize winner P.W. Anderson: "More is different".

Emergent behavior appears because parts of a complex system show a typical behavior on time and length scales much smaller than those of the original system; see figure below. Because of this so called multiscale behavior only the "average" of the lower scale parts is of importance.



The coherent package *Multiscale Phenomena and Techniques* is an inter-faculty package, aimed at students from Mechanical Engineering, Technical Physics, Chemical Engineering and Mathematics (primarily) and students from Building physics, Electrical Engineering and Bio-Medical Engineering (secondarily). The goal of this package is to introduce students to the fundamental "multiscale" concept, with associated phenomena in different applications and with special modelling and computational techniques for problems with a multiscale character.

The package offers a selection of 4 courses, of which students choose 3 in consultation with the coordinator, depending on prior knowledge and further course planning.

The first course, *Introduction asymptotic techniques*, lays the mathematical foundation to understand, model and analyze multiscale problems.

The other courses focus on multiscale phenomena and techniques in particular applications:

- *Chemically reacting flows*: interplay between flow and fast chemical reaction
- *Statistical Mechanics and Molecular Simulation*: molecular models and continuum models to computationally describe molecular processes
- *Strength and Structure*: multiscale phenomena in solid materials.

Course code	Course name
2WAK0	Introduction asymptotic techniques
4BC00	Chemically reacting flows
3FOX0	Modeling and simulation at the (bio)molecular scale
4LB00	Strength and structure

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Description courses

Introduction to Asymptotic Techniques (2WAK0)

Required prior knowledge: calculus, differential equations, some basics of physics

A model (in the natural sciences) is the mathematical materialization of the way we see (for a given problem) reality. A model consists of a description of minimal elements and their relations. A good model contains only the relevant, and as little as possible the unnecessary and complicating, components. Modelling is a process where we start with a crude, intuitive model, which is then refined by making a distinction between what is important and what is unimportant. We do this by recognizing (in one sense or another) what is "small" and what is "large". Not sufficient but necessary is that we scale in our model all the quantities on some inherent length, time, etc. units. (This is a form of non-dimensionalization.) The resulting dimensionless parameters tell us something about the important and unimportant effects.
Sometimes in a problem there are several scales, which are still all important. For example: the microscopic scale of molecular exchange of energy and the macroscopic scale on which this appears to us as heat and mass diffusion; the thin boundary layer of a viscous flow where the viscous forces take effect, and the main flow; the slowly varying atmosphere and the fast fluctuating refracting light wave. We can make a model that describes one scale and include the other scale as a modelling assumption. In a "multiscale" approach we consider both scales and their coupling.
Essential for the course is therefore understanding of scales and the effect of large and small parameters. The calculus with large or small parameters is called asymptotics, or asymptotic analysis. Modelling with small or large parameters is called perturbation methods.

Chemically reacting flows (4BC00)

Recommended prior knowledge: thermodynamics, heat and flow

Chemically reacting flows play an important role in energy systems such as engines, gas turbines and boilers. The fundamental physical and chemical processes and the models that describe them, are introduced and subsequently used to analyse energy and combustion systems. This knowledge and these skills are essential for the design of systems that convert future sustainable fuels into energy in a clean and efficient way.
After successfully completing this course, the student is aware of the role of chemically reacting flows in energy systems. He/she understands the most important fundamental chemical and physical processes and can describe them with mathematical models. The student can use these models for the analysis of simple chemical reactors and premixed and non-premixed flame structures. The student can analyse and design combustion systems with the aid of numerical tools.

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Modeling and Simulation at the (Bio)molecular scale (3FOX0)
Required prior knowledge: calculus

Monte Carlo Sampling and Molecular Dynamics are the two most important simulation approaches for the microscopic description of phase behavior and dynamics of (bio)physical systems. As such, they are key tools for understanding e.g. mechanical properties of DNA molecules, effects of osmotic pressure, and depletion interactions in biological systems. In this course, we first introduce statistical mechanics, providing the mathematical foundation for these simulation methods. In the second part of the course the student will apply these simulation methods to study particle-based models for biophysical phenomena.
Topics:

- Background of Monte Carlo simulations: Getting statistical information out of ensemble averages, Metropolis algorithm.
- Practical: Setting up and executing a Monte Carlo simulation of a biopolymer using Mathematica.
- Background of Molecular Dynamics: Verlet-algorithm, calculating of forces, thermostats.
- Practical: Executing an MD simulation of a membrane using LAMMPS.

Strength and Structure (4LB00)
Required prior knowledge: solid mechanics

During the design of a product, it is crucial to know where, when and how a material fails. You can think of applications in automotive (energy absorption in crash), energy (failure behavior of wind turbine blades, batteries) or microsystems (flexible electronics) or biomedical (prostheses, in-body devices) or safety (laminated and / or bulletproof glass) but also lifetime predictions of load and load-bearing structures.

To that end, in order to quantitatively describe failure behavior, we make use of computer simulations. This course mainly focuses on the two most relevant aspects. First you learn how plastic deformation is implemented in 3D macroscopic (continuum) material models (in essence a continuation of what you have learned, in 1D, during the course Solid Mechanics). The second aspect concerns the multi-scale modeling of materials, aiming at the coupling of macroscopic behavior to processes that occur in the microstructure. You will realize that understanding and quantifying these underlying processes explains where, when and how a material, on the macroscopic level, plastically fails.