Multiscale Simulation

Modern simulation requires us to cover wide range of length and time scales. This is still a challenge in spite of ever-growing computational power. In order to understand this, let us consider an algorithm whose computational complexity grows as $O(N^2)$. This means that while the problem dimension grows twice, computational time grows four times. On the other hand, computational power grows according to the Moore's law. This means that for the algorithm above we have to wait about a 3-year when we can afford for the same time compute the problem of the doubled dimension. This means that we cannot solve a multiscale problem by merely increasing the problem dimension, that is, making modeling at the level of the lowest length and time scale.

The goal of the present paper is to demonstrate how one can treat different scales simultaneously in an intelligent way. To this end, we have selected three different approaches that will be briefly reviewed below. It should be stressed that modern research on multiscale simulation is not limited to these methods and that the choice of works to demonstrate methods is rather arbitrary.

We start with a homogenization theory when two different length scales are separated from each other. Then we consider the phase field theory that allows us to consider in the uniform way different material phases and hence the explicit treatment of the interface during grain growth becomes unnecessary. Finally, we review an approach where different modeling levels are employed simultaneously for different locations in space.

Homogenization Theory

Many materials are heterogeneous, that is, they are made form different phases. For example, a composite material (see Fig. 1) is an engineering material made from two or more constituent materials that remain separate and distinct on a macroscopic level. In a similar way one can say that a porous material (see Fig. 2 and 3) consists from a mixture of a particular material and void.

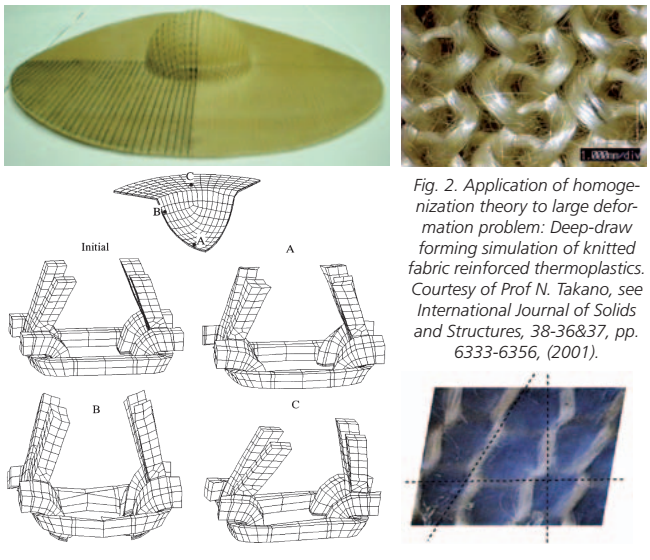

Fig. 2. Application of homogenization theory to large deformation problem: Deep-draw forming simulation of knitted fabric reinforced thermoplastics. Courtesy of Prof N. Takano, see International Journal of Solids and Structures, 38-36&37, pp. 6333-6356, (2001).

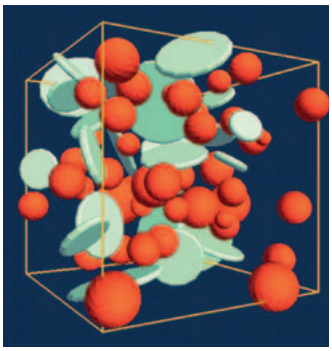

Fig. 1. A model of a composite material generated by software Palmira. Courtesy of Matsim GmbH.

This means that we have two quite different scales, first is related to the dimension of the whole object and the second is tied with the dimension of grains. As a result, the final material usually has anisotropic properties that are different from that of constituents.

If we develop a finite element model that resolves the smallest scale, we do not need make further assumptions. Yet, the dimension of the model will be very high. This is nowadays possible (see a link to micro-FE method below) but requires massive parallelism and supercomputers.

A natural idea to simulate a heterogeneous material is to average material properties. With apparent materials properties it is unnecessary to model the geometry of each particle from which the object is actually made. In this case, the dimension of the finite element model stays at feasible level but then we have a problem to extract effective constitutive equations from given information about constituent materials and their geometries.

Modern approaches based on computational homogenization define a microstructural representative volume element that is modeled in full details. Then one makes joint simulation of the whole object meshed with a coarse mesh with such a representative cell. Roughly speaking, the constitutive equations for the whole object are computed on the fly from the representative cell. Fig. 2 shows the application of the homogenization theory to a straw hat and Fig. 3 to porous ceramics after its internal structure was obtained by micro computed tomography.

Internet Links:
Homogenization theory
Homepages of Prof N. Kikuchi,
http://www-personal.engin.umich.edu/~kikuchi/

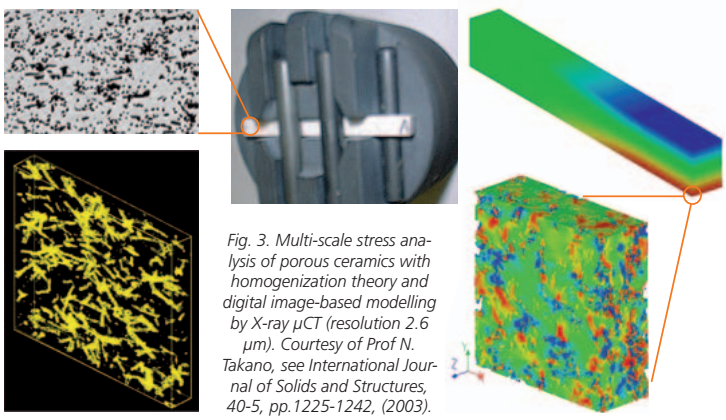

Fig. 3. Multi-scale stress analysis of porous ceramics with homogenization theory and digital image-based modelling by X-ray μCT (resolution 2.6 μm). Courtesy of Prof N. Takano, see International Journal of Solids and Structures, 40-5, pp.1225-1242, (2003).

Homepages of Prof N. Takano,
http://www.ritsumei.ac.jp/~takano/index-e.html

Micro finite element method

Homepage of Prof B. van Rietbergen,
http://www.mate.tue.nl/mate/showemp.php/75

Related Software

Palmira, http://www.matsim.ch/
Voxelcon, http://www.quint.co.jp/eng/index.html

Phase Field Theory

It happens that modeling single-phase metal/alloy is also complicated. Although formally speaking in this case material is homogenous, it is actually made of small and randomly oriented grains, that is, it has still some microstructure. The size of grains depends on the solidification conditions and at the same time the mechanical and electrical properties of a metal ingot strongly depends on the microstructure formation.

Engineers have great experience and intuition to predict microstructures based on previous experimental results. Yet, there is growing tendency to switch to a physically based microstructure modeling and to reduce the dependence on intuition.

An interesting phenomenon during solidification is dendrite formation (see Fig. 4). A dendrite has a multi-branching tree-like form and let us imagine what happens if we need during simulation to follow its form explicitly. This again will lead to a very high dimensional problem.

Phase field theory allows us to consider melt and crystal as a single computational object by means of new variable, phase field. It changes from 0 to 1, for example 0 for solid and 1 for melt and describes a diffuse interface between melt a solid (intermediate values of the variable). As a result, it is unnecessary explicitly to follow the interface and this greatly simplifies simulation. Two examples of phase field simulation made with software MICRESS® are shown in Fig. 4 and 5.

Internet Links:

Dendrites in Wikipedia

http://en.wikipedia.org/wiki/Dendrite_%28metal%29
http://en.wikipedia.org/wiki/Dendrite_%28crystal%29

Dendritic solidification by H. K. D. H. Bhadeshia

http://www.msm.cam.ac.uk/phase-trans/dendrites.html

Phase field theory

H. K. D. H. Bhadeshia,
http://www.msm.cam.ac.uk/phase-trans/mphil/MP6-15.pdf

Related Software

MICRESS®, http://www.micress.de/

Coupling of Different Length Scales

There are applications when objects with different scales are separated spatially. For example, a modern microresonator is made just from 1 million atoms and assumptions of continuum mechanics are no longer applicable to describe its movements. This number of atoms can be modeled by molecular mechanics with the use of empirical potentials to describe atom interactions. However, simulation must include mircroresonator supports that are much bigger than the microresonator. Simulation of both the microresonator and support at atomistic level is no longer feasible. What is possible is to couple two simulations together: molecular dynamics for the microresonator and finite elements for the support. This way we preserve the right level of modeling for the microresonator and computational feasibility for the whole simulation.

Crack propagation is another example. During crack propagation there is breaking of chemical bonds and in principle the right level of modeling is quantum mechanics. However, at this level one can afford to consider just a few thousands atom. As a result, the computational domain can be split to three different parts: the very beginning of the crack treated by quantum mechanics, some intermediate region around treated by molecular dynamics and the rest treated by finite elements. Again, we preserve the right modeling level thought computational domain and at the same time make simulation possible.

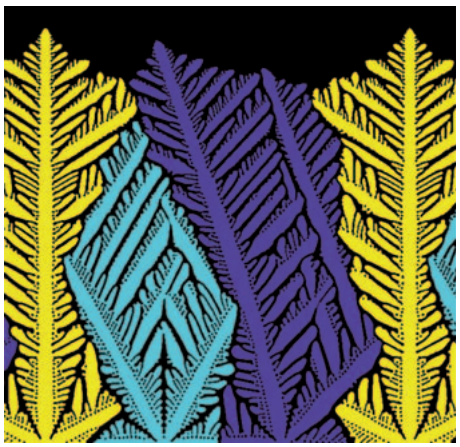

*Fig. 4. Directional growth of a ternary Mg-alloy (Al-Zn-Mg). Simulation made with MICRESS®. Note the hexagonal symmetry of the dendrites. Picture size corresponds to an area of approximately 1*1 mm².*

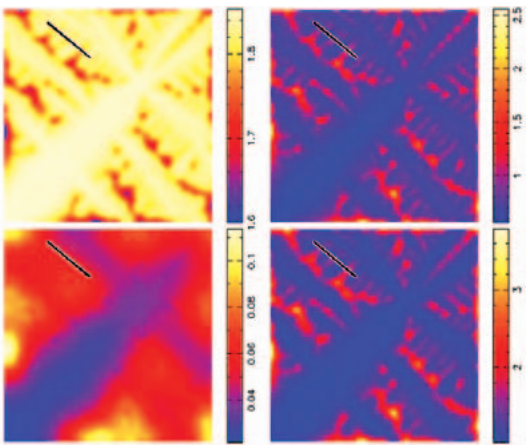

*Fig. 5. Distributions of chemical elements (C upper left, Mn upper right, P lower left and Si lower right) in a simulated cross-section of a quinternary steel Fe-C-Mn-Si-P. Simulation made with MICRESS®. Area of the sections shown is approximately 1*1 mm².*

Internet Links:

Home pages of Dr R. E. Rudd

http://www-phys.llnl.gov/Research/Metals_Alloys/People/Rudd/

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