1
Introduction

1.1 Examples of multiscale problems

Whether we explicitly recognize it or not, multiscale phenomena are part of our daily lives. We organize our time in days, months and years, as a result of the multiscale dynamics of the solar system. Our society is organized in a hierarchical structure, from towns to states, countries and continents. Such a structure has its historical and political origins but it is also a reflection of the multiscale geographical structure of the earth. Moving into the realm of modeling, an important method for studying functions, signals or geometrical shapes is to decompose them according to their components at different scales, as in Fourier or wavelet expansion. From the viewpoint of physics all materials at the microscale are made up of nuclei and electrons, whose structure and dynamics are responsible for the macroscale behavior of the material, such as its transport and wave propagation properties and its deformation and failure.

In fact, it is not an easy task to think of a situation that does not involve multiscale characteristics. Therefore, broadly speaking, it is not incorrect to say that multiscale modeling encompasses almost every aspect of modeling [29]. However, adopting such a position would make it impossible to carry out serious discussion in any kind of depth. Therefore we will take a narrower view and focus on a number of issues for which the multiscale character is the dominating issue and is exploited in the modeling process. This includes analytical and numerical techniques that exploit the disparity of scales, as well as multi-physics problems. Here the term "multi-physics problems" is perhaps a misnomer; what we have in mind are problems that involve physical laws at different levels of detail,

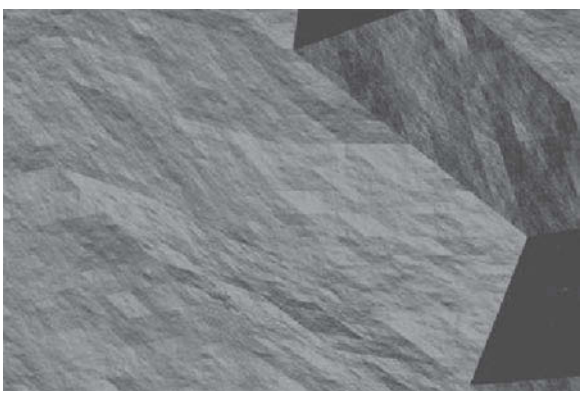

Figure 1.1. An image with large-scale edges and small-scale textures (from 3D Nature's Visual Nature Studio, used with permission).

such as quantum mechanics and continuum models. We will start with some simple examples.

1.1.1 Multiscale data and their representation

A basic multiscale phenomenon is that signals (functions, curves, images) often contain components at disparate scales. One such example is shown in Figure 1.1, which displays an image that contains large-scale edges as well as textures with small scale features. Such an observation motivates the decomposition of signals into different components according to their scales. Classical examples of this include Fourier and wavelet decomposition [21].

1.1.2 Differential equations with multiscale data

Propagation of wave packets Consider the wave equation

$$\partial_t^2 u = \Delta u. \tag{1.1.1}$$

This is a rather innocent-looking differential equation that describes wave propagation. Consider now the propagation of a wave packet that is a solution of (1.1.1) with initial condition

$$u(\mathbf{x}, 0) = A(\mathbf{x}) e^{iS(\mathbf{x})/\varepsilon} \tag{1.1.2}$$

where A, S are smooth functions (see Figure 1.2). As always, we will assume that the scale parameter $\varepsilon \ll 1$. There are clearly two scales in this

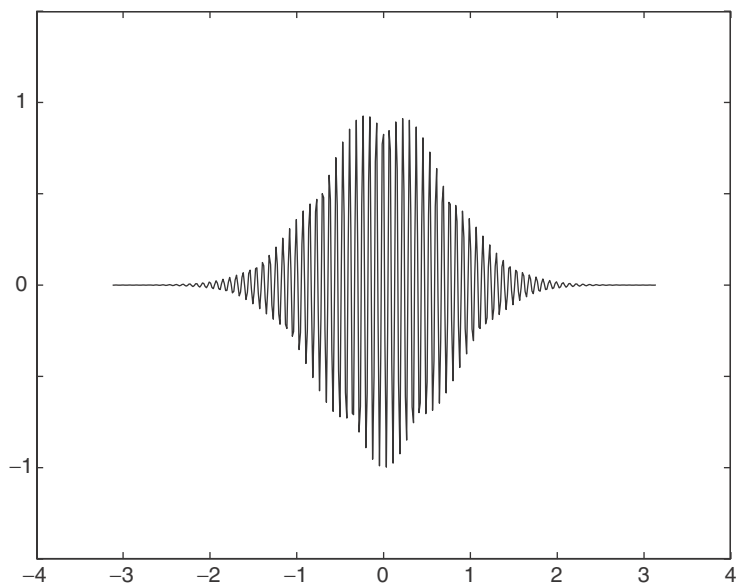

Figure 1.2. An example of a wave packet.

problem: the short wavelength ε and the scale of the envelope $A(\mathbf{x})$ of the wave packet, which is $\mathcal{O}(1)$. One can exploit this disparity between the two scales to find a simplified treatment of the problem, as is done in geometric optics. For a review of the different numerical algorithms for treating this kind of problem, we refer to [40].

Mechanics of composite materials The mechanical deformation of a material is described by the equations of elasticity theory:

$$\begin{aligned} \nabla \cdot \boldsymbol{\tau} &= 0, \\ \boldsymbol{\tau} &= \lambda(\nabla \cdot \mathbf{u})\mathbf{I} + \mu\big(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}}\big), \end{aligned}$$

where $\mathbf{u}$ is the displacement field and $\boldsymbol{\tau}$ is the stress tensor. The first equation describes the force balance. The second equation is the constitutive relation, in which λ and μ are the Lamé constants that characterize the material.

To model composite materials we may simply take

$$\lambda(\mathbf{x}) = \lambda^{\varepsilon}(\mathbf{x}), \quad \mu(\mathbf{x}) = \mu^{\varepsilon}(\mathbf{x}),$$

where ε is again a small parameter that measures the scale of the heterogeneity of the material. For example, for a two-phase composite

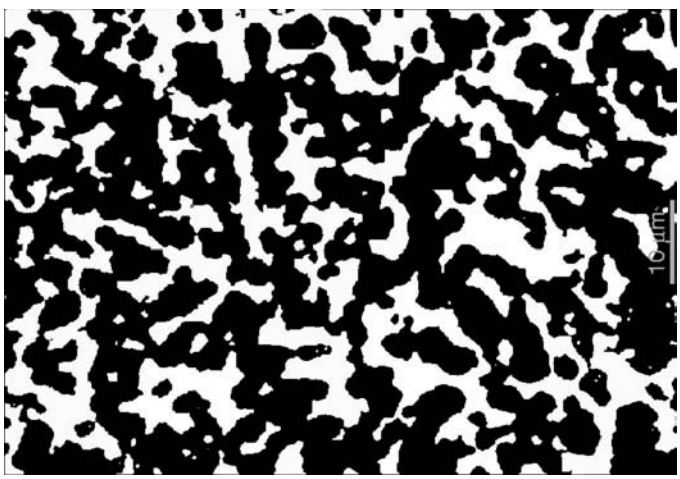

Figure 1.3. An example of a two-phase composite material (courtesy of Sal Torquato).

(see Figure 1.3), λ and μ take one set of values in one phase and another set of values in the other phase. If the microstructure happens to be periodic, then we have

$$\lambda^\varepsilon(\mathbf{x}) = A\left(\frac{\mathbf{x}}{\varepsilon}\right), \quad \mu^\varepsilon(\mathbf{x}) = B\left(\frac{\mathbf{x}}{\varepsilon}\right),$$

where A and B are periodic functions. However, in most cases in practice, the microstructure tends to be random rather than periodic. A detailed account of such issues can be found in [45].

1.1.3 Differential equations with small parameters

Consider the Navier–Stokes equation for incompressible flows at large Reynolds numbers:

$$\rho_0(\partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u}) + \nabla p = \frac{1}{\mathrm{Re}}\Delta\mathbf{u},$$
$$\nabla\cdot\mathbf{u} = 0.$$

Here $\mathbf{u}$ is the velocity field, p is the pressure field, ρ_0 is the (constant) density of the fluid and $\mathrm{Re} \gg 1$ is the Reynolds number. In this example the highest-order derivative in the differential equation has a small coefficient. This has some rather important consequences. These include:

(1) the occurrence of boundary layers;
(2) the occurrence of turbulent flows with vortices over a large range of scales.

Partial differential equations of this type, in which the highest-order derivatives have small coefficients, are examples of singular perturbation problems. In most cases the solutions to such problems contain features at disparate scales.

1.2 Multi-physics problems

1.2.1 Examples of scale-dependent phenomena

We will now discuss some well-known examples in which the system response exhibits a transition as a function of the scales involved.

Black-body radiation Our first example is black-body radiation. Let $e_T(\lambda)$ be the energy density of the radiation of a black body at temperature T and wavelength λ. Classical statistical mechanics considerations lead to Rayleigh's formula

$$e_T(\lambda) = \frac{8\pi}{\lambda^4} k_{\mathrm{B}} T,$$

where k_{B} is the Boltzmann constant. This result fits very well with experimental results for long wavelengths but fails drastically at short wavelengths. The reason, as was discovered by Planck, is that at short wavelengths quantum effects become important. Planck postulated that the energy of a photon has to be an integer multiple of $h\nu$, where h is now known as the Planck constant and ν is the frequency of the photon. If quantum effects are taken into consideration, one arrives at Planck's formula

$$e_T(\lambda) = \frac{8\pi hc}{\lambda^5} \frac{1}{e^{hc/(k_{\mathrm{B}} T\lambda)} - 1},$$

where c is the speed of light. This result agrees very well with experimental results at all wavelengths [35]. Note that Planck's formula reduces to Rayleigh's formula at long wavelengths.

Knudsen-number dependence of the heat flux in channel flows Consider a gas flowing between two parallel plates, one of which is stationary and the other moving with a constant speed. The two plates are held

at uniform temperatures T_0 and T_1 respectively. We are interested in the heat flux across the channel as a function of the Knudsen number, which is the ratio between the mean free path of the gas particles (the average distance that a gas particle travels before colliding with another gas particle) and the channel width. What is interesting is that the dependence of the heat flux as a function of the Knudsen number is non-monotonic: it is an increasing function for small values of the Knudsen number but a decreasing function at large values [43]. This phenomenon can be understood as follows. When the Knudsen number is very small, there is little heat conduction since in this case the gas is very close to local equilibrium. In this regime the dynamics of the gas is very well described by Euler's equations of gas dynamics; heat conduction is a higher-order effect (see Section 4.3). If the Knudsen number is very large then effectively the gas particles undergo free streaming. There is little momentum exchange between the particles since collisions are rare. Hence there is not much heat flux either. In this case the dynamics of the gas can be found by solving Boltzmann's equation with the collision term neglected (see Section 4.3). We see that the origins of the reduced heat conduction in the two regimes are very different.

The reverse Hall–Petch effect In the early 1950s, Hall and Petch independently found that, as the size of the grains that make up a material decreases, the yield strength of the material increases according to the equation

$$\sigma = \sigma_0 + \frac{k}{\sqrt{d}},$$

where k is a strengthening coefficient characteristic of the material and d is the characteristic grain size [31]. Roughly speaking, this is due to the fact that grain boundaries impede dislocation motion.

Recent experiments on many nanocrystalline materials demonstrate that if the grains reach a critical size, which is typically less than 100 nm, the yield stress either remains constant or decreases with decreasing grain size (see Figure 1.4) [20, 42]. This is called the *reverse Hall–Petch effect*. The exact mechanism may depend on the specific material. For example, in copper it is thought that the mechanical response changes from dislocation-mediated plasticity to grain boundary sliding as the grain size is decreased to about 10 to 15 nanometers [42].

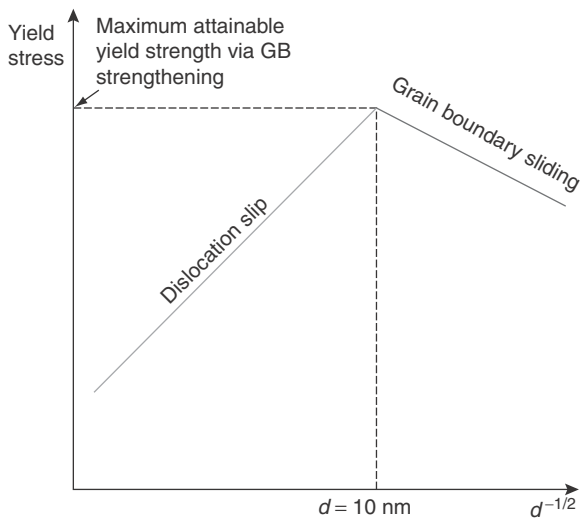

Figure 1.4. Yield stress vs. $d^{-1/2}$, where d is the grain size, illustrating the Hall–Petch and reverse Hall–Petch effects (adapted from Wikipedia).

All three examples discussed above exhibit a change in behavior as the scales involved change. The change in behavior is the result of the change in the dominating physical effects in the system.

1.2.2 Deficiencies of the traditional approaches to modeling

Central to any kind of coarse-grained model is a constitutive relation, which represents the effect of the microscopic processes at the macroscopic level. In engineering applications the constitutive relations are often empirically based on very simple considerations such as:

(1) the second law of thermodynamics;
(2) symmetry and invariance properties;
(3) linearization or Taylor expansion.

Such empirical models have been very successful in applications. However, in many cases they are inadequate, either because of the complexity of the system or because they lack crucial information about how the microstructure influences the macroscale behavior of the system.

Take incompressible fluid flow as an example. Conservation of mass and momentum gives

$$\rho_0(\partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u}) = \nabla\cdot\boldsymbol{\tau}, \tag{1.2.1}$$

$$\nabla\cdot\mathbf{u} = 0, \tag{1.2.2}$$

where $\mathbf{u}$ is the velocity field. Here, in order to write down the momentum conservation equation we have introduced $\boldsymbol{\tau}$, the stress tensor. This is an object introduced at the continuum level to represent the short-range interactions between the molecules. Imagine a small piece of surface inside the continuous medium: the stress $\boldsymbol{\tau}$ represents the force due to the interaction between the molecules on each side of the surface. Ideally the value of $\boldsymbol{\tau}$ should be obtained from information about the dynamics of the molecules that make up the fluid. This would be a rather difficult task. Therefore in practice $\boldsymbol{\tau}$ is often modeled empirically, through intelligent guesses and calibration with experimental data. For a simple isotropic fluid, say one made up of spherical particles, isotropy and Galilean invariance implies that τ should not depend on $\mathbf{u}$. Hence a simple guess is that $\boldsymbol{\tau}$ is a function of $\nabla\mathbf{u}$. In the absence of further information about the behavior of the system, it is natural to start with the very simplest choice, namely that $\boldsymbol{\tau}$ is a linear function of $\nabla\mathbf{u}$. In any case, every function is approximately linear in appropriate regimes. Using isotropy, we arrive at the *constitutive relation* for *Newtonian fluids*:

$$\boldsymbol{\tau} = -p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}) \tag{1.2.3}$$

where p is the pressure. Substituting this constitutive relation into the conservation laws leads to the well-known *Navier–Stokes equation*.

It is remarkable that such simple-minded considerations yield a model, namely the Navier–Stokes equation, which has proven to be very accurate in describing the dynamics of simple fluids under a very wide range of conditions. Partly for this reason, considerable effort has gone into extending such an approach to the modeling of complex fluids such as polymeric fluids. However, the results there are rather mixed [12]. The accuracy of the constitutive laws is often questionable; in many cases, they become quite complicated since many parameters need to be fitted and their physical meaning becomes obscure. Consequently the original appeal of their simplicity and universality is lost. In addition, there is no systematic way of developing such empirical constitutive relations. So a constitutive relation obtained by calibrating against one set of experimental data may not

be useful in a different experimental setting. More importantly, such an approach does not contain any explicit information about the interaction between fluid flow and the conformation of the molecules, which might be exactly the kind of information in which we are most interested.

The situation described above is to some extent generic. Indeed, empirical modeling by constitutive relations is a very popular tool and is used in many areas, including:

(1) elasticity and plasticity in the theory of solids;
(2) empirical potentials in molecular dynamics;
(3) empirical models of reaction kinetics;
(4) hopping rates in kinetic Monte Carlo models;
(5) collision cross sections in the kinetic theory of gases.

These constitutive relations are typically quite adequate for simple systems, such as small deformations of solids, but fail for complex systems. When empirical models become inadequate, we have to replace them by more accurate models that rely more on a detailed description of the microscopic processes.

The other extreme is *quantum many-body theory*, which could be said to be the true first principle. Assume that our system of interest has M nuclei and N electrons. At the level of quantum mechanics, this system (neglecting spin) is described by a wavefunction of the form

$$\Psi = \Psi(\mathbf{R}_1, \ldots, \mathbf{R}_M, \mathbf{r}_1, \ldots, \mathbf{r}_N)$$

The Hamiltonian for this system is given by

$$\begin{aligned}\mathcal{H} = &-\sum_{J=1}^{M} \frac{\hbar^2}{2M_J}\nabla^2_{\mathbf{R}_J} - \sum_{k=1}^{N} \frac{\hbar^2}{2m_e}\nabla^2_{\mathbf{r}_k} \\ &+ \sum_{J<K} \frac{Z_J Z_K}{|\mathbf{R}_J - \mathbf{R}_K|} - \sum_{J,k} \frac{Z_J}{|\mathbf{R}_J - \mathbf{r}_k|} + \sum_{i<j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \end{aligned} \tag{1.2.4}$$

where Z_J is the nuclear charge of the Jth nucleus. Here all we need in order to analyze a given system is to input the atomic numbers Z_J for the atoms in the system and then solve the Schrödinger equation. There are no empirical parameters to fit! The difficulty, however, lies in the complexity of its mathematics. This situation is very well summarized by the following remark of Paul Dirac, made shortly after the discovery of quantum mechanics [22]:

The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.

The mathematical complexity noted by Dirac is indeed quite daunting: wave functions have as many (or, rather, three times as many) independent variables as the number of electrons and nuclei in the system. If the system has 10^{30} electrons, then the wave function has 3×10^{30} independent variables. Obtaining accurate information for such a function is a quite impossible task. In addition, such a description often gives far too much information, most of which is not really of any interest. Getting the relevant information from this vast amount of data would also be quite a challenge.

This dichotomy is the kind of situation that we encounter for many problems. On the one hand, empirically obtained macroscale models are very efficient but are often not accurate enough or lack crucial microstructural information in which we are interested. Microscopic models, on the other hand, may offer better accuracy but they are often too expensive to be used to model systems of real interest. It would be nice to have a strategy that combines the efficiency of macroscale models and the accuracy of microscale models. This is a tall order but is precisely the motivation for multiscale modeling.

1.2.3 The multi-physics modeling hierarchy

Between macroscale models and the quantum many-body problem lie a hierarchy of other models, which are better suited at the appropriate scales. This is illustrated in Figure 1.5. A more detailed description of this modeling hierarchy is shown in Table 1.1.

In traditional approaches to modeling we tend to focus on one particular scale: the effects of smaller scales are modeled through the constitutive relation; the effects of larger scales are neglected by assuming that the system is homogeneous at these scales. The philosophy of multiscale, multi-physics modeling is the opposite. It is based on two ideas.

(1) Any system of interest can always be described by a *hierarchy of models of different complexity*. This allows us to think about more detailed models when a coarse-grained model is no longer adequate. It also gives us a basis for understanding coarse-grained