The atomic hypothesis, which has its origins in the observations of the ancient Greek philosopher Demokritos, is the basis of our modern understanding of the material world. No scientist would doubt that all phenomena we observe in our everyday lives are ultimately related to how atoms move and interact at the nanometer scale. However, establishing the link between the atomic scale and the scale of our daily experiences—which, by our sensory abilities, is confined to the macroscopic (a fraction of a millimeter and higher) regime—is a nontrivial task.

It is literally impossible (and will probably remain so for the foreseeable future) to describe the behavior of macroscopic objects, such as solids, in terms of the motion of all atoms involved. In fact, we wouldn’t even want to do so, because most atoms in a typical solid undergo boring motion, consisting of tiny excursions from their equilibrium positions. What really matters for macroscopic behavior is either the uniform collective response of atoms—as in a solid’s elastic deformation, where the details of the atomic motion are not important—or the dramatic changes in the state of a small fraction of the atoms—as in brittle fracture or plastic deformation. The description of phenomena related to uniform collective behavior of all the atoms in a solid is handled by approaches that view macroscopic objects as single entities, making no reference to the un-
nderlying atomic degrees of freedom. A case in point is continuum elasticity theory for modeling elastic deformation of solids.

Such approaches have let us make spectacular advances in the last century: witness the marvel of engineering that modern jet aircraft represent, carrying hundreds of passengers and tons of cargo at a good fraction of the speed of sound. However, phenomena that are due to dramatic changes in the state of relatively few atoms, yet are manifested at the macroscopic scale, are still the subject of intense scientific inquiry. In fact, some of these phenomena, such as corrosion and fatigue, put severe limitations on the lifespan of airplanes and might even cause the occasional catastrophic failure. The satisfactory description and prediction of such phenomena remains an open issue.

Connecting the atomic and the macroscopic

The question becomes how to identify this small fraction of atoms whose state is significantly affected, how to properly model their behavior at the nanometer scale, and how to connect this behavior to the solid’s macroscopic response. Of those three aspects, the connection between the atomic and macroscopic scales, both in time and in space, is particularly bothersome. Not only do these scales differ by many orders of magnitude, but they also involve disparate methodologies. In most situations, the description at the atomic scale must rely on quantum mechanics, the only successful theory for handling the interactions between the atomic cores and the electrons responsible for cohesion in molecules and solids.

Yet, at the macroscopic scale it is desirable to have a classical description, which we can ultimately comprehend through our everyday experience.

This issue

These challenges become more pronounced in the context of problems posed by modern technology, where control of nanoscale behavior becomes crucial in achieving our technological goals. In this special issue of CiSE, three articles address these challenges in different but not unrelated fields.

The first article, by Peter Kratzer and Matthias Scheffler, addresses the question of controlling crystal growth in semiconductors. These systems are obviously of crucial importance in electronic device applications. Controlling their growth at the atomic level is a prerequisite for manufacturing devices with desirable features and characteristics, as current and future technological needs demand. The objective of the methodology Kratzer and Scheffler outline is to replace the trial-and-error approach to growth by intelligent design of the growth conditions. This is achieved by combining kinetic Monte Carlo techniques with ab initio dynamics of the atoms, which bridges the relevant time and length scales in the context of growth mechanisms.

The second article, by Sauro Succi, Olga Filippova, Greg Smith, and me, concerns a different physical system in which similar issues of activity at the atomic scale are crucial and need to be coupled to the macroscopic scale. The physical system here has to do with reactant flow carried by an inert fluid around a substrate’s macroscopic features. The methodology adopted is the Lattice Boltzmann equation, a computational tool capable of handling large-scale fluid dynamics while receiving input from a finer scale. Its capabilities are first demonstrated in a classic example of flow around an airfoil and then tested in the context of reactive flow in a channel with micron-sized obstacles. These case studies illustrate what the method can achieve in terms of integrating various length scales in reactive flow.

The last article, by Steven Johnson, Attila Mekis, Shanhui Fan, and John Joannopoulos, considers yet another physical system with some of the same themes as the previous article. In this case, the authors consider the flow of light in a medium whose dielectric properties change on an “atomic” scale. The “atoms” here are not the Periodic Table’s familiar elements but larger units that can be arranged in crystalline structures. The relevant equations are neither the Navier-Stokes equations of macroscopic fluid flow nor the Schrödinger equation of electron waves in solids but Maxwell’s equations for the electromagnetic field. Nevertheless, computational techniques are again indispensable in determining the dynamics of the physically interesting quantity (light) in a complex environment that involves novel three-dimensional crystals and their defects.

In a real sense, the computational approaches described in the three featured articles are the modern incarnation of what Feynman called “a little imagination and thinking,” necessary to reconcile our macroscopic observations of everyday phenomena with the atomic hypothesis.

Efthimios Kaxiras’ bio appears on p.45