FOCUSED DISCUSSION (invited paper)
Frankenstein in Lilliput: Science at the Nanoscale

Models and Theories at the Nanoscale

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One of the most interesting things about science and engineering at the nanoscale, from the point of view of the philosophy of science, is the frequent use they make of models constructed out of theories belonging to different levels of description. We usually take it for granted that every level of description falls under the domain of its own theory. For example, we generally presume there is some fundamental level of description. And with that presumption comes the hope that we will be able to find a general theory of how things work at that level. But we also often take it for granted that at every other level of description that interests us—whether it be at the level of subatomic particles, atoms, fundamental theory molecules, fluids or mechanical solids—there will be some non-fundamental theory available to us that will be practically serviceable for explaining, predicting, and controlling the various phenomena that live at that level of description.

Nano-science challenges this assumption. And in so doing, it challenges the idea that theory is where the action is for philosophers. Much of nano-science involves the study of phenomena that exhibit themselves on a scale too large to be studied practicably using the resources of our best microscopic theories, and too small to be studied, with a reasonable degree of accuracy, using any of our standard higher-level, non-fundamental macroscopic theories. Many of the so-called "multiscale" approaches to studying phenomena at the nanoscale are predicated on a certain degree of scepticism that a coherent, unified theory of these phenomena exists to be found.

Take, for example, the field of nano-mechanics. "Nano-mechanics" is the study of solid-state materials that are too large to be manageably modelled with atomic physics, and too small to be studied using the physics of continua. Consequently, nano-sized solid-state materials are studied with hybrid models constructed out of theories from a variety of levels (Nakano et al. 2001). As such, they create models that bear interestingly novel relationships to their theoretical ancestors. So a close look at simulation methods in the nano-sciences could offer novel insights into the kinds of relationships that exist between different

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theories (at different levels of description) and between theories and their models.

If we are looking for an example of a simulation model likely to stimulate those sorts of insights, we need look no further than so called "parallel multiscale" methods of computer simulation. These methods were developed by a group of researchers interested in studying the mechanical properties (reaction to stress, strain, and temperature) of intermediate-sized solid-state materials. The particular case that I will detail below is a pioneering example of this method.[1] What makes the modelling technique "multiscale" is that it couples together the effects described by three different levels of description: quantum mechanics, molecular dynamics, and continuum mechanics.

Modellers of nanoscale solids need to use these multiscale methods—the coupling together of models built out of competing theories from different levels—because each individual theoretical framework is inadequate on its own at the scale in question. Here is why: The traditional theoretical framework for studying the mechanical behaviour of solids is the mother's milk of engineers: continuum mechanics (CM). CM provides an excellent framework for modelling macroscopic solids when they are close to equilibrium. But the theory breaks down under other conditions. CM, particularly the flavour of CM that is most computationally tractable—linear elastic theory—is no good when the dynamics of the system are too far from equilibrium. This is because linear elastic theory assumes that materials are homogeneous even at the smallest scales, when in fact we know this is far from the truth. It is an idealization; a statistical average. When modelling large samples of material, this idealization works, because the sample is large enough that one can effectively average over the heterogeneities. But as we get below the micron scale—when the bit of material we are interested in is smaller than a micron in size—the fine-grained structure begins to matter more. The "averaging" fails to be adequate. Small local variations from mean structure, such as material decohesions (actual tearings of the material) and thermal fluctuations, begin to play a significant role in the system. In sum, CM cannot be the sole theoretical foundation of "nano-mechanics"—it is inadequate for studying solids smaller than one micrometer in size (Rudd and Broughton 2000).

The ideal theoretical framework for studying the dynamics of solids far from equilibrium is classical molecular dynamics (MD). This is the level at which thermal fluctuations and material decohesions are most naturally described. But computational issues constrain MD simulations to about 10 million molecules. In linear dimensions, this corresponds to a constraint well below the micron-scale. A piece of material with linear dimension on the scale of one micron contains far too many molecules to be tractably modelled by today's computers.

So MD methods are too computationally expensive, and CM methods are insufficiently accurate, for studying solids that are on the order of one micron in

[1] Good review literature on parallel multiscale simulation methods for nanomechanics can be found in (Abraham, et. al, 1998), (Broughton et. al., 1999), and (Rudd and Broughton, 2000).

diameter. On the other hand, parts of the solid in which the far-from-equilibrium dynamics take place are usually confined to regions small enough to be manageably modelled by MD methods. So the idea behind multiscale methods is that a division of labour might be possible—use MD to model the regions where the non-equilibrium action is, and use CM for the surrounding regions, where things remain close enough to equilibrium for CM to be effective.

There is a further complication. When cracks propagate through a solid, the splitting at the tip of the crack involves the breaking of chemical bonds. But the breaking of bonds involves the fundamental electronic structure of atomic interaction. So methods from MD, (which use a classical model of the energetic interaction between atoms), are unreliable right near the tip of a propagating crack. Building a good model of bond breaking in crack propagation requires a quantum mechanical (QM) approach. Of course, QM modelling methods, which were designed by chemists for studying individual molecules, are orders of magnitude more computationally expensive than MD. Not even the far-from-equilibrium sub-region of the solid can be modelled, in its entirety, using a QM model.

The upshot is that it takes three separate theoretical frameworks to model the mechanics of crack propagation in solid structures on the order of one micron in size. Multiscale models couple together the three theories by dividing the material to be simulated into three roughly concentric spatial regions. At the centre is a very small region of atoms surrounding a crack tip, modelled by the methods of computational QM. In this region, bonds are broken and distorted as the crack tip propagates through the solid. Surrounding this small region is a larger region of atoms modelled by classical MD. In that region, material dislocations evolve and move, and thermal fluctuations play an important role in the dynamics. The far-from-equilibrium dynamics of the MD region is driven by the energetics of the breaking bonds in the inner region. In the outer region, elastic energy in dissipated smoothly and close to equilibrium, on length scales that are well-modelled by the linear-elastic, continuum dynamical domain. In turn, it is the stresses and strains applied on the longest scales that drive the propagation of the cracks on the shortest scales.

It is the interactions between the effects on these different scales that lead students of these phenomena to describe them as "*inherently* multiscale" (Broughton et. al. 1999, 2391). What they mean by this is that there is significant feedback between the three regions. All of these effects, each one of which is best understood at its own unique scale of description, are strongly coupled together. Since all of these effects interact simultaneously, it means that all three of the different modelling regions have to be coupled together and modelled simultaneously. The fact that three different theories at three different levels of description need to be employed makes the models "multiscale". The

fact that these different regions interact simultaneously, that they are strongly coupled together, means that the models have to be "parallel multiscale."

An instructive way to think about the meaning of the phrase "parallel multiscale" is to compare two different ways of going about integrating different scales of description into one simulation. The first more traditional method is what is sometimes, in contrast, called "serial multiscale". The idea of serial multiscale is to choose a region, simulate it at the lower level of description, summarize the results into a set of parameters digestible by the higher-level description, and then pass those results up to a simulation of the higher level.

But serial multiscale methods will not be effective when the different scales are strongly coupled together:

> There is a large class of problems for which the physics is inherently multiscale; that is the different scales interact strongly to produce the observed behavior. It is necessary to know what is happening simultaneously in each region since one is strongly coupled to another. (Broughton et. al. 1999, 2391)

What seems to be required for simulating an inherently multiscale problem is an approach that simulates each region simultaneously, at its appropriate level of description, and then allows each modelling domain to continuously pass relevant information back and forth between regions—in effect, a model that seamlessly combines all three theoretical approaches. Sticking to language borrowed from computer science, Abraham's group refers to this method as "parallel multiscale" modelling. They also refer to it as "concurrent coupling of length scales." A parallel multiscale model is one that builds a single Hamiltonian for the entire system, but where the Hamiltonian is motivated by theories at more than one scale.

One issue that has received perennial attention from philosophers of science has been that of the relationship between different levels of description. Traditionally, the focus of this inquiry has been debate about whether or not, and to what extent or in what respect, laws or theories at higher levels of description are reducible to those at a lower level.

Underlying all of this debate, I believe, has been a common intuition: The basis for understanding inter-level interaction—to the extent that it is possible—is just applied mereology. In other words, to the extent that the literature in philosophy of science about levels of description has focused on whether and how one level is reducible to another, it has implicitly assumed that the only interesting possible relationships are logical ones—i.e. inter-theoretic relationships that flow logically from the mereological relationships between the entities posited in the two levels.[2]

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[2] An important exception is the recent work of Robert Batterman (2002).

But if methods that are anything like those described above become accepted as successful in nanoscale modelling, that intuition is likely to come under pressure. The reason is that so called "parallel" multiscale modelling methods are forced to develop relationships between the different levels that are perhaps suggested, but certainly not logically determined, by their mereology. Rather, developing the appropriate relationships, in Abraham's words, "requires physical insight".

What this suggests is that there can be a substantial physics of inter-level interaction; a physics which is guided, but not by no means determined by either the theories at each level or the mereology of their respective entities. Indeed, whether or not the relationships employed by this group will turn out to be the correct ones is an empirical/physical question, and not a logical/mereological one.

But this also means the models that are built in science and engineering at the nanoscale are, and are likely to continue to be, built out inconsistent sets of laws. This is an issue that has begun to receive attention only recently, particularly in the work of Mathias Frisch (2004). Using classical electrodynamics (CED) as an example, Frisch has challenged a common philosophical intuition about scientific theories: that the internal consistency of its laws is a necessary condition that all successful theories have to satisfy. I want to make a similar point here. In this case, the example of multiscale modelling seems to put pressure on a closely related, if somewhat weaker, intuition: that an inconsistent set of laws can have no models.

In a formal setting, this claim is obviously true; indeed it is true by definition. But rarely in scientific practice do we actually deal with models that have a clear formal relationship to the laws that inspire them. Most likely, the intuition that inconsistent laws cannot produce a coherent model in everyday scientific practice rests as much on pragmatic considerations as it does on the analogy to formal systems: how, in practice, could mutually conflicting sets of laws guide the construction of a coherent and successful model?

If Frisch is right, than CED would be a great place to look, and CED has a longer and more distinguished history than multiscale models in nano-science. In most models of CED, each respective model draws from only one of the two mutually inconsistent laws of the theory (Maxwell's laws on the one hand, and Lorentz' force law on the other). This technique works for most applications, but there are exceptions where the method fails. Models of synchrotron radiation, for example, necessarily involve both mutually inconsistent parts of the theory.

There are problems, in other words, that require us to calculate the field from the charges, as well as to calculate the motion of the charges from the fields. But the solution method, even in the synchrotron case as Frisch describes it, is still a form of segregation. The segregation is temporal. You break the

problem up into time steps: in one time step the Lorentz equation are used, in the next, the Maxwell equations, and so on.

A form of segregation is employed in multiscale modelling as well, but it is forced to break down at the boundaries. Each of the three theoretical approaches is confined to its own spatial region of the system. But the fact that there are significant simultaneous and back-and-forth interactions between the physics in each of these regions means that the strategy of segregation cannot be entirely effective. *Parallel* multiscale methods require the modeller to apply, in the handshaking region, two different sets of laws. The laws in Abrahams model, moreover, are each pair-wise inconsistent. They offer conflicting descriptions of matter, and conflicting accounts of the energetic interactions between the constituents of that matter. But the construction of the model in the handshaking regions is guided by both members of the pair. When you include the handshaking regions, parallel multiscale models are—all at once—*models of an inconsistent set of laws*.

The methods developed by these researches for overcoming these inconsistencies (what they call the "handshaking algorithms") may or may not turn out to be too crude to provide a reliable modelling approach. But by paying close attention to developments in the field of nanoscale modelling, a field in which the models are almost certainly going to be required to involve hybrids of classical, quantum and continuum mechanics, philosophers are likely to learn a great deal about how inconsistencies are managed. In the process, we will be forced to develop richer accounts of the relationships between theories and their models—richer accounts, in any case, than the one suggested by the analogy to formal systems.

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