Multiscale Modeling and Emergence

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ABSTRACTS

Surface Tensions: Scale-Dependence in Nanoscience and Philosophy of Science

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A traditional view of the structure of scientific theories, on which philosophers of science have based their accounts of explanation, modeling, and inter-theory relations, holds that scientific theories are composed of universal natural laws coupled with initial and boundary conditions. In this picture, universal laws play the most significant role in scientific reasoning. Initial and boundary conditions are rarely differentiated and their role in reasoning is largely overlooked. In this talk, I use the problem of modeling surfaces in nanoscience to show why this dismissal is deeply problematic both for philosophers of science and for scientists themselves.

In macroscopic-scale modeling, surfaces are treated as boundaries in the mathematical sense-that is, as infinitesimally thin borders of a system that confine its interior. As such, surface structure and behavior is usually modeled in an idealized manner that ignores most of the physics and chemistry occurring there. At the nanoscale, however, the structure and behavior of these surfaces significantly constrains the structure and behavior of the interior in more complex ways. Three important conclusions emerge:

1. The very concept surface changes as a function of scale, and other central concepts in nanoscience also behave in this scale-dependent manner.
2. The traditional view of theory described above does not adequately capture the nature of nanomaterials modeling, which requires attention to multiple models constructed at different characteristic scales. These component models do not comport well with a single set of universal laws, as the standard view suggests. Instead, boundary behaviors become crucial and models are designed to capture these behaviors.
3. The projects of nanomaterials modeling and synthesis dictate that divisions between boundaries and interiors must be continually adjusted. Overlooking this problem has led to failures of experimental design and interpretation of data.

An Introduction to Homogenization

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Homogenization theory aims at providing a macroscopic description of materials that are microscopically heterogeneous. Roughly speaking, the heterogeneous material is replaced by an ``ad-hoc" homogeneous one, identified mathematically, and whose properties are a good approximation on those of the original material. In this talk I will present a brief introduction to the mathematical theory of homogenization, as well as to the main techniques.

An introduction to Gamma convergence

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In this talk we introduce the notion of Gamma convergence and present some of its applications.

Colloidal Nanoparticle Alloys

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From bronze to steel, alloyed materials have defined the technological capabilities of their times. Like their monometallic counterparts, alloys can experience dramatic changes in physical and chemical properties at the nanoscale. Multimetallic nanoparticles promise to provide improved catalysts for efficient use of fossil fuel resources, as well as serving in a variety of biomedical functions from diagnostics to treatment of disease. One of the central challenges of research into alloyed nanomaterials is to devise effective methods for synthesizing materials with tunable properties, such as photoluminescence. Current preparation methods afford scientists limited ability to tune materials to exhibit desired properties. Our group investigates the roles of surface chemistry and composition in tuning the photoluminescence of nanoscale alloys, and we have produced some of the first observations of nanoscale alloy luminescence in the near-infrared, which is a particularly useful energy range for medical use, as it is transparent to human skin. One outcome of this research is new insight into dramatic differences between the ways metals mix at macroscopic scales and the ways they mix at the nanoscale, and further differences even within in the nanometer length scale itself, where metals may combine differently when the material has dimensions between 2-5 nm and 5-100 nm. This research points toward a critical challenge in nanomaterial structure-function design and study where models for atom and bulk matter behavior must be bridged or redeveloped as a function of the material size.

Turbulent Flows, Universality and Emergence

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Turbulent flows are paradigm cases of complex systems where multi-scale modelling is required. The fundamental problems in the field are strong fluctuations and couplings – problems that are also present in condensed matter physics (CMP) and field theory. Like the latter two areas of physics, renormalization group methods have been used to treat some of the theoretical difficulties with turbulent flows. However, unlike CMP where universality is reasonably clearly understood, it is less than straightforward in cases of turbulence. I examine some of these issues in an attempt to clarify how we might understand emergence in the context of turbulent flows.

The Greediness of Scales

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The methodological problem to be discussed is an old one that has influenced metaphysical thinking in the past considerably (especially Leibniz). In modern form, it runs like this. Scientists know a lot about the internal structures of complex materials upon different length scales and have framed very effective models of the key behaviors witnessed. But these treatments all employ differential equations, which inherently operate upon an infinitesimal size scale, despite the fact that their targeted behaviors only emerge upon much longer characteristic lengths. Such modeling policies engender descriptive inconsistencies between the different treatments that prevent them from working together in a mutually beneficial way (upon a computer, say). Unfortunately, these clashes can't be easily rectified without spoiling the utility of the models altogether. Recent advances in multi-scalar methods have uncovered policies that evade these syntactic inconsistencies by persuading the different models to "talk to one another' in strikingly novel ways. These innovations raise important philosophical questions about "truth value" in physical theory and how directly such accounts relate to the world they describe. As such, philosophy of science is returned to the basic concerns that Leibniz weighed in his writings on "the labyrinth of the continuum." In consequence, modern metaphysicians should recognize that "determining the ontology of a theory" may not follow the simple contours suggested by Quine in "On What There Is" and may require a deeper engagement with the actual details of effective applied mathematics.