Multiscale Modeling: Beyond Non-Mereological Relations

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Abstract

Winsberg's "handshaking" account of inter-model relations is a well-known theory of multiscale modeling in physical systems. Winsberg argues that relations among the component models in a multiscale modeling system are not related mereologically, but rather by empirically determined algorithms. I argue that while the handshaking account does demonstrate the existence of non-mereological relationships among component models, Winsberg does not attend to the different ways in which handshaking algorithms are developed. By overlooking the distinct strategies employed in different handshake models, Winsberg's account fails to capture the central feature of effective multiscale modeling practices, namely, how the dominant behaviors of the modeled systems vary across the different scales, and how this variation constrains the ways modelers can combine component models. Using Winsberg's example of nanoscale crack propagation, I distinguish two modes of handshaking and show how the different modes arise from the scale-dependent physics involved in each component model.

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The basic assumption of the multiscale modeling literature is that modeling practices in science often rely on being able to describe the behavior of target systems across a variety of length, time, and energy scales. Consequently, philosophy of science should accommodate its theories of modeling, inter-theory and inter-model relations, confirmation, and explanation to multiscale modeling.

Winsberg's "handshaking" account of relations among models in certain simulation systems is a well-known theory of multiscale modeling in physical systems. The account, introduced in [Winsberg, 2006] and developed in [Winsberg, 2010], is built around a central example of multiscale computer simulation of crack propagation in nanoscale systems. From the example, Winsberg concludes that the three component models in the simulation stand in non-reductive, non-emergent relations with one another. He names this relationship the "handshake" relation, and he uses handshaking to advance a non-mereological conception of inter-model relations. Instead, he argues,

"the various scales are . . . sewn together using specially constructed algorithms to mediate between otherwise incompatible frameworks."[Winsberg, 2010, p. 73] This sewing-together occurs via the development of hybrid models.

In this paper, I argue that while the handshaking account accomplishes its non-mereological goal, Winsberg's conception of hybrid models does not supplant the mereological conception with a sufficiently robust alternative. Specifically, it does not attend to the different ways in which scales may be "sewn together." By overlooking the distinct strategies employed in different hybrid models, Winsberg's account fails to capture the central feature of effective multiscale modeling practices, namely, how the dominant behaviors of the modeled systems vary across the different scales, and how this variation constrains the ways modelers can combine component models. Using Winsberg's example of nanoscale crack propagation, I distinguish two modes of handshaking and show how the different strategies arise from the scale-dependent physics involved in each component model.

Winsberg's mature handshaking account[Winsberg, 2010, pp. 72–92] is part of his larger aim to develop an epistemology of computer simulation, and so he is interested in inter-model relations more as a means than an end. But along the way he encounters the problem of how to make sense of simulations whose component models come from a variety of theoretical backgrounds. The nanoscale simulations he discusses use three distinct computational models to describe three distinct sorts of dynamics that a nanoscale system experiences, each at characteristic length scales. *Continuum mechanics* describes large-scale behaviors of the system, *molecular dynamics* describes somewhat smaller domains that behave like classical rigid bodies, and *quantum mechanics* describes the smallest interactions among individual atoms. In the multiscale simulation Winsberg describes, the models are combined "in parallel" such that at each time-step of the simulation, each of the models contributes some mathematical quantity to the overall description of the system. The models are combined by developing computational techniques to average over boundary regions where a higher-scale model and a lower-scale model disagree on a predicted quantity. This method of combining models is the phenomenon that Winsberg, following the physicists Broughton, Abraham, Bernstein, and Kaxiras [Abraham et al., 1998, Broughton et al., 1999], calls "handshaking," and the resultant multiscale models are called "hybrids."[Winsberg, 2010, p. 74]

Winsberg argues that handshaking illustrates a non-mereological relationship between smaller-scale and larger-scale models:

> One issue that has received perennial attention from philosophers of science is 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 interlevel 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—that is, inter-theoretic relationships that flow logically from the mereological relationships between the entities posited in the two levels. But if methods that are anything like those described above become accepted as successful in nanoscale modeling, that intuition is likely to come under pressure. The reason is that parallel multiscale modeling 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 interlevel interaction—a physics that is guided but not determined by either the theories at each level or the mereology of their respective entities. Indeed, whether or not the relationships employed by Abraham and his group will turn out to be the correct ones is an empirical/physical question and not a logical/mereological one.
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> [Winsberg, 2010, p. 84–85]

Winsberg's account primarily concerns representational relationships of the sort typical to the modeling literature more than it does inter-theory relations, and so he does not prod the details of the simulation further than is needed to show that in simulations like this one, inter-level in-

teractions are empirically determined and non-mereological. This is a mistake, as it overlooks the question of *why* the simulation manages to model propagating-crack systems successfully. Part of Winsberg's epistemology-of-simulation project is to rationalize the use of simulation models to make scientific progress in just these sorts of cases, so the oversight is surprising. In the case of these crack-propagation simulations, details of the simulations—specifically, the assumptions built into the handshaking techniques—answer the related questions of (1) why these models are not mereologically combinable and (2) what licenses the non-mereological strategies that do allow them to be combined. Winsberg keys in on the first question, but does not acknowledge the second.

In the example from Broughton et al [Broughton et al., 1999] that Winsberg considers, there are three length scales of interest and, therefore, two handshaking algorithms. The macroscopic length scale describes regions of a solid-state system whose dynamics are close to equilibrium, and it is modeled by finite-element (FE) methods, which are derived from the elastic theory of solids. The model divides a continuous volume of the system into cells and describes the kinetic energy (displacement) and potential energy (strain) on individual cells (hence, finite elements). These cells are joined together into a mesh, and cell borders are called mesh points. One of the authors' innovations is their particular method for determining overall displacement and strain as a function of values of those quantities at the mesh points. So their model discretizes the continuum description.

The mesoscopic length scale describes regions of the system that are slightly perturbed from equilibrium but which are nonetheless not dynamically central to the simulation—these are not the areas where bonds are breaking and forming, but instead the trailing wake of dynamical disturbance left by a propagating crack. These regions are modeled by molecular dynamics (MD). Molecular dynamics is what it sounds like, that is, a model of the movement of individual atoms or molecules. It is a classical (non-quantum) model. Since the model is of a solid, it is populated as a lattice of atoms whose movement (vibration, rotation, and the breaking and forming of bonds) is described by interatomic electronic potentials. Think of a network of balls connected by springs.

To develop a handshaking algorithm for these two models, Broughton[1] begins by drawing an

[1]For narrative ease, I refer to the first author of [Broughton et al., 1999] in this explication.

imaginary surface between a region described by the FE model and one described by the MD model. The interatomic potentials governing the movement of atoms in the MD model range across that surface into the region described by the FE model. Since the FE mesh describes continuously distributed matter, the mesh points can be lined up anywhere along the surface—including right along the lattice of MD interatomic potentials. As Broughton puts it, what the algorithm needs is a "one-to-one mapping of a mesh point to an atom site." [Broughton et al., 1999, p. 2396] Farther away from the handshake interface, the mesh can be spaced out for computational efficiency, allowing individual cells to cover greater spatial regions. The energy at a point in the interfacial (handshake) region is calculated by taking the arithmetic mean of predictions from each model.

The effectiveness of the energy-averaging strategy the physicists end up with is contingent both on features about the world and on features about the computational models. Averaging the energy is effective exactly because the MD lattice has been lined up with the FE mesh at the contact region; otherwise there would not be commensurable values along the imaginary surface at the interface. That alignment is possible because the FE mesh describes a region of the system where continuum mechanics is the appropriate description of physical behavior. The continuous deformability of the mesh is what allows modelers to line mesh points up with the MD lattice. In other words, the macroscopic scale, and associated near-equilibrium, of the FE-modeled region of the system, is what licenses the use of continuum (FE) methods to describe it.

The physics of the system constrains the application of different models to different portions of the system. The physical and computational details of the models in turn constrain the handshaking strategies available; if the FE mesh were not continuously deformable, Broughton would have had to devise an alternative sort of algorithm to average the energy in the interfacial region, and the resulting handshaking strategy would differ both computationally and in the representational relationships between the component models and their target physical behaviors. In fact, this is exactly what happens in this example's other handshake region.

One of the distinctions with which Broughton begins the discussion of the MD/TB handshake algorithm is that the MD and TB models both proceed under assumptions of atomicity, whereas in the FE/MD region the FE model's mesh points are not meant to represent spatial points—indeed

just the opposite, mesh points are meant as abstractions away from spatial details of material behavior. Without continuous deformability in one model, the problem of connecting the spatial regions of the system that are being represented by the different models cannot be solved as it was in the MD/FE case.

Both MD and TB can model atoms in a lattice and their electronic interactions. This is the area of representational overlap between the models on which Broughton bases the MD/TB handshake. The MD/TB handshake is constructed from the electronic interactions of a carefully-defined set of fictional "atoms." The material modeled in this example is made of silicon, and the fictional "atoms," called "silogens," are assigned some silicon-like properties and some hydrogen-like properties. The latter properties are introduced for the sake of localizing electronic behavior so it can be modeled by MD, and they are properties that silicon atoms could not have—hence, the silogens' status as fictional entities. The handshake is effective because of how the modelers assign properties to the silogens. Some properties, such as the spacing in a crystal lattice, are defined by the the MD model. Other properties, such as reduced electronic symmetries, come from TB. The result is a messy, chimeric dynamical entity in the interfacial region, but it is one that both MD and TB can analyze, and thus it is one from which a picture of the energetic behavior at the interface can be developed.

The MD/TB handshake assigns contrived, un-physical electronic behaviors to silogens, and to their near neighbors, in order to generate predictions about the local energetic behavior of the interfacial region. By reducing electronic symmetries, the models allow a localized description of the energetic behavior of the handshake region, whereas in the non-handshake region of the quantum-mechanical TB model, energetic interactions are delocalized.

Both this handshake and the FE/MD one are certainly examples of non-mereological relationships among the component models. In both the models are constrained by the physics: here, the genuinely quantum behavior of the TB region cannot be classically predicted. And in both, some features of the interface are manipulated to form the handshake. However, the ways in which the two handshakes are constructed differ in what sort of feature of the models is selected as the object of manipulation. In the FE/MD case, the FE mesh is deformed to line up with the MD lattice: this

is a mere computational device, and it doesn't introduce any explicitly unphysical assumptions. In the MD/TB handshake, however, an unphysical entity (the silogen) is introduced to both models, and computations are performed as usual on the unusual entity.

Broughton puts the point thus:

> In contradistinction to the FE/MD handshake algorithm, where a plane between rows of atoms was defined, the MD/TB handshaking takes place conceptually across a plane consisting of atoms. This different approach is necessitated because it is difficult to apportion (localize) energy in a computationally efficient way to specific bonds in an electronic structure calculation. The total energy is a property of the entire system. Attempts to define a 50/50 Hamiltonian, such as was used for the FE/MD interface, run into issues ...
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> [Broughton et al., 1999, p. 2398]

The basic idea is this: one can treat computations of the modeled system's energy as *conceptually* the same between the MD and FE regions, although the *entities* that produce changes in that energy differ. However, the conceptions of energy required to make sense of the MD and TB models are really quite different from one another, but the *entities* are, while not identical, both discretized and inter-relatable. So to combine the MD and TB models, different strategies are needed than those used to combine FE and TB—and those strategies require different conceptual resources.

As Winsberg pointed out, in neither of the handshakes is one model conceived of as containing "truer," "more correct," or "better" physics. There is something non-mereological going on here. What Winsberg did not point out is that in both handshakes, each component model is conceptually and computationally compromised in a systematic and physically-constrained way in order to combine the models. The handshakes are similar in that physical details of the modeled behaviors at each characteristic length scale in the system constrain the ways in which interfacial algorithms can be developed. But the conceptual underpinnings of the handshakes differ greatly from case to case.

Winsberg is right to identify that the relationships between these three component models

are better understood as multiscale, rather than reductive or emergent. There is no fundamental model that either represents most accurately or explains most lucidly the behavior of the target simulated system. However, by lumping the relations between Broughton's models into one category of theoretical activity, Winsberg overlooks the intricate system of physical, computational, and pragmatic constraints upon the individual handshake algorithms. By attending to precisely these differences, one can glean that the handshakes contain different strategies for combining models across scales. These strategies in turn generate different representational content, as well as different ways of rationalizing both the permissibility and effectiveness of modeling the crack propagation behavior in this multiscale model. The present example has produced two sorts of handshaking strategies; further analysis of additional examples will surely produce others.

The reason there exist different handshaking strategies is that physical systems are scale-dependent, that is, the dominant behaviors—and therefore the dominant theoretical and modeling infrastructure—of physical systems is indexed to the characteristic length, time, and energy scales of the system. Multiscale modeling itself is an outgrowth of the multiscale nature of the physical world. This point has been made before (e.g. in [Batterman, 2012, Wilson, 2012], and Morrison [Morrison, 2015] has lately shown that in addition to multiscale behavior, systems must demonstrate *scale separation* in order to get multiscale modeling strategies such as Broughton's off the ground.

One final point worth noting is that in developing both the FE/MD and the MD/TB algorithms, Broughton needed to attend to the boundary-region behavior of the component models. Indeed, these boundary regions are, more or less by definition, where the handshakes occurred. The challenge of developing a multiscale model lay in accounting for the behavior at the boundary between regions of the system modeled by a higher-scale model and regions modeled by a lower-scale model. In this way, Winsberg's 'lumpy' handshaking account did pick out a useful feature of multiscale models: while there are many differences in the specific physical, computational, and pragmatic constraints associated with combining models across scales, these constraints all inter-mingle in an attempt to solve the same sort of problem, namely how to account for behavior in the boundary regions of modeled systems.

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