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Conceptual strategies and inter-theory relations: The case of nanoscale cracks

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ABSTRACT

This paper introduces a new account of inter-theory relations in physics, which I call the conceptual strategies account. Using the example of a multiscale computer simulation model of nanoscale crack propagation in silicon, I illustrate this account and contrast it with existing reductive, emergent, and handshaking approaches. The conceptual strategies account develops the notion that relations among physical theories, and among their models, are constrained but not dictated by limitations from physics, mathematics, and computation, and that conceptual reasoning within those limits is required both to generate and to understand the relations between theories. Conceptual strategies result in a variety of types of relations between theories and models. These relations are themselves epistemic objects, like theories and models, and as such are an under-recognized part of the epistemic landscape of science.

This paper introduces a new account of inter-theory relations in physics, which I call the conceptual strategies account. This account develops the notion that relations among physical theories, and among their models, are constrained but not dictated by limitations from physics, mathematics, and computation, and that conceptual reasoning within those limits is required both to generate and to understand the relations between theories. Conceptual strategizing, by which I mean the practice of employing conceptual, computational, mathematical, or physical features of a pair of theories or models to the advantage of constructing a relation, results in a variety of types of relations between theories and models. These relations are better understood through studying the details of the conceptual strategies that generate them, than by merely labeling them either reductive or emergent. Once they are understood in this way, it becomes evident that these relations are themselves epistemic objects, like theories and models, and as such are an under-recognized part of the epistemic landscape of science.

Using the illustration of a multiscale computer simulation model of nanoscale crack propagation in silicon, I identify, by way of example, two types of conceptual strategy used to generate inter-theory relations of the sort I have in mind. I use these strategies and the contrast between them to show how other accounts of inter-theory relations have tended to obscure, rather than clarify, the epistemic landscape around inter-theory relations. Many historical accounts of inter-theory relations have focused on logical or compositional relations among two or more theories. These accounts are typically classified either as reductionist or as emergentist theories, depending on the nature of the identified relations. More recently, some philosophers of science have defended interpretations of emergent relations that do not rest solely on logical relations, such as in Batterman's (Batterman, 2001) analysis of renormalization group methods as explanatory of emergent critical phenomena, or in Mitchell's (Mitchell, 2009) account of emergence as self-organization via nonlinear dynamical feedback loops. These accounts improve on earlier attempts, and the account presented here may be seen as a continuation of the project to course-correct discussions of inter-theory relations away from the narrowly logical confines of earlier efforts.

Another view in this more recent bunch is Winsberg's (2006, 2010) example of "handshaking" relations among component models in a multiscale computer simulation model of nanoscale crack propagation. Winsberg uses this example to problematize both reductionist and emergentist analyses of the relations in the example and argues for the need for a more robust and empirically

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informed alternative, but his critique stops short of proposing an positive account. Although Winsberg aims to focus on the details of individual relations among component models in a multiscale model, his analysis does not sufficiently distinguish between the types of reasoning used to generate the algorithms that connect those component models, and so misses the central moral about inter-theory relations that can be gleaned from this example. The conceptual strategies account that I propose here centralizes these differences and their implications for understanding inter-theory relations. The result is a view in which inter-theory relations become epistemic objects subject to the same sort of philosophical and scientific analyses as theories and models themselves.

To develop this account, I proceed first in Section 1 by reviewing the details of the simulation model under consideration. With this example, I show that generating a multiscale model from a set of component models sometimes requires not just logical or empirical relations among the component models, but conceptual and mathematical strategizing, which is essential for wiring together the component models into a multiscale model. In Section 2, I critique Winberg's analysis of this simulation model and contrast his emphasis on empirical relations with my account of conceptual relations. Section 3 generalizes from this example to a broader account of inter-theory relations in physics, and Section 4 contains brief summary remarks.

1. A multiscale model of nanoscale cracks

Multiscale modeling rests on the assumption that modeling practices in science must often be able to describe the behavior of target systems across a variety of length, time, and energy scales. Multiscale descriptions of this sort are frequently, if not universally, generated by combining descriptions from component models, each describing behavior at a different characteristic scale. The component models are typically individuated by the relative scale of the dynamics they model—macroscopic, intermediate or mesoscopic, and microscopic, with additions or subtractions of additional levels as necessary. A component model of material behavior at a characteristic scale might be the macroscopic component of one multiscale model and the microscopic component of another. Importantly, the component models in a multiscale model need not and generally do not rely on the same theoretical backgrounds. So beneath the surface of multiscale models, one typically finds multiple theories contributing to the descriptions, predictions, explanations, and other inferences being generated by the multiscale model. This blooming, buzzing confusion is a ripe breeding ground for a complex of inter-theory relations. Unpacking how the component models combine in a multiscale model of a physical process can shed new light on how the theories from which the models derive are themselves related to one another.

The multiscale model under consideration here is a multiscale computer simulation model of a nanoscale crack propagating through a two-dimensional material. The material is a block of silicon, one of the most common materials used in the construction of microchips, diodes, solar cells, and other semiconductor technologies. If you've ever dropped a smartphone, spilled coffee on a computer, accidentally stepped on a modern holiday light, or seen hail or small animals take out rooftop solar cell panels, you have witnessed the cracking of silicon.

One of the innovations of the model, at the time of its introduction in the early 1990s, was its ability to model the propagation of nanoscale cracks at temperatures above 0° K, which paved the way for more realistic multiscale models of crack propagation in ensuing simulation models. This innovation arose from the use of both continuum and molecular component models, which allowed physicists to simulate material behavior without being forced to artificially restrict atomic motion by imposing low-temperature boundary conditions on the system. But reconciling continuum and molecular descriptions of the silicon block brought about challenges, as well, as the modelers sought to reconcile the two mutually incompatible descriptions of energy distribution in the material.

The model, developed by the physicists Jeremy Broughton, Farid Abraham, and colleagues in (Abraham, Broughton, Bernstein, & Kaxiras, 1998; Broughton, Abraham, Bernstein, and Kaxiras, 1999), was introduced to the philosophy of science literature by Winsberg in (Winsberg, 2006) and analyzed more extensively in (Winsberg, 2010). The model is built from three component models at three distinct length scales: the macro-, meso-, and micro-scale. Each component model is derived from a distinct theory of matter: the macroscale model from continuum mechanics, the mesoscale model from classical molecular dynamics, and the microscale model from quantum mechanics.

To develop the multiscale simulation model, these three component models are combined by two coupling algorithms that operate on subregions of the modeled system. These subregions are located at the interface between a region modeled by one component model and a region modeled by another component model. These coupling algorithms are called “handshakes” or “handshaking algorithms” both by Broughton et al. and by Winsberg, and I use this terminology here. In what follows, I shall be primarily concerned with the strategies employed in the development of handshaking algorithms. My aim is to show that generating these algorithms requires making choices informed by an understanding not just of logical, empirical or computational relations among the component models, but of the physical relations among the systems being modeled, as well as of the conceptual differences between representational and non-representational features of the component models. In order to examine these algorithms, some exposition on the component models is first required.

1.1. Macroscopic model: finite elements

The simulation model of the macroscopic length scale in this example concerns the regions of the silicon block that are spatially distant from the propagating crack and whose dynamics are, as a result, near equilibrium. The behavior of this region of the system is modeled by an implementation of the finite-elements (FE) method, which is derived from continuum mechanics, and specifically from the elastic theory of solids. FE is a quite widely-applicable and well-established numerical-methods approach to discretizing continuous phenomena so that they can be represented in computer models.[1] The FE method divides a continuous volume, which represents the system, into triangular cells. The cells are joined to one another at their vertices, forming a network called a mesh. The vertices are known as mesh points. Kinetic energy (displacement) and potential energy (strain) are defined at each mesh point at each timestep in the simulation. Displacement and strain throughout the system at a given timestep are represented as an integration over the mesh point network. The model postulates smooth, uniform transitions in displacement and strain values from one mesh point to its neighbors, thus preserving the treatment of the modeled space as continuous despite the discretized model.

[1] In fact, FE and other numerical methods were developed as numerical solutions to continuum problems so that analytically intractable problems in continuum mechanics could be solved numerically, which is a far greater achievement than merely offering a means of discretizing a continuous space.

The variables in the FE model—quantities associated with material behaviors such as stress and strain—represent bulk quantities. They do not apply to atoms, just as temperature and color do not. Continuum mechanics, the theoretical framework in which bulk quantities are modeled, treats the block of silicon as continuous, i.e., without atomic parts, and as uniform. In the FE simulation model, despite the discretization of the system into a network of mesh points, the assumptions of continuity and uniformity hold, and both assumptions play essential roles in developing the FE simulation of the system's behavior. These assumptions license the inferences about the smooth distribution of strain and displacement in the spaces between each mesh point, as well as the smooth evolution of system-wide strain and displacement over time. These physical quantities, strain and displacement, are the representational targets of this component model and of continuum models of cracking more generally: buildups of strain lead to new cracks, and displacement is the propagation of those cracks.

To put the point another way, if one attempted to model the same system using classical atomistic methods, the model would represent the motion of atoms in space over time. Strain would be recast as a set of changes in the inter-atom distance between two or more atoms in a subregion of the modeled system. Consequently, where an individual atom was placed in the system would matter to the overall distribution of inter-atom spacings. This is exactly the constraint that mesh points avoid: because of the continuum-derived assumptions of uniformity and continuity, where a particular mesh point is placed in a subregion of the modeled system can change without changing the distribution of strain. Changing the distribution of mesh points is like changing the units on the coordinate system in a Cartesian graph: while both actions can generate increased or decreased precision and reveal new and useful information, neither will interrupt the function or the properties being modeled. Conversely, changing the distribution of atoms in an atomistic model is like changing the exponent on a function's dependent variable: even the smallest disturbance results in a different function. Call this ability of mesh points to be redistributed without impacting the physical properties of the modeled system a non-representational feature of the FE model. More pointedly (pardon the pun), the mesh points do not represent atomic centers or any other physically discrete feature of a physical system, such as a grain boundary or crystal lattice spacing. The mesh points are solely figments of the need for discretized representations of a continuous space in the computer simulation; conceptually, the domain modeled by the FE component model is still continuous.

The non-representational character of the mesh points issues from the continuum and uniformity assumptions, and as I shall discuss shortly, that non-representational character is precisely the conceptual particularity of the FE model that licenses the handshake between the FE model and the adjoining mesoscale model. Keep in mind that mesh points may be placed arbitrarily throughout the spatial region described by the FE model, although distributing the mesh points more narrowly will generate a finer-grained description of the energy distribution of the system. To generate the FE dynamical simulation, one calculates differences between the values at each vertex and its nearest neighbors, and then advances the simulation forward one time-step to view changes over time in the overall displacement and strain of the system.

1.2. Mesoscopic model (molecular dynamics) and first handshake

The simulation model of the mesoscopic length scale in this example concerns the regions of the silicon block that are nearby, but not at the leading tip of, the propagating crack. In other words, the mesoscale model 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 most 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 a classical (semi-Newtonian) model of the movement of individual atoms or molecules. Since the model is of a solid, it is populated as a lattice of atoms whose movement—the vibration and rotation of bonds—is described by interatomic electronic potentials. Think of a network of balls connected by springs. In the MD model, unlike in the FE model, spatial features of the points on which the calculations are performed are representational. The points themselves stand for rigid-body models of atoms, which interact elastically and whose inter-point distances are derived empirically from the known inter-atomic spacing of atoms of silicon in a block.

To develop a handshaking algorithm for these two models, and to reconcile the apparently incompatible descriptions of the nature of the modeled material, Broughton et al. begin by partitioning off a region described by the FE model from the one described by the MD model. They draw a plane boundary between the last set of FE mesh points and the first layer of the MD lattice points. Next, they run the simulation on both sets of points first as if they were FE mesh points, and then as if they were MD lattice points. Finally, they average the resulting values, and the averaged values are recorded as the energy of the system across the plane boundary. This is the action of the handshaking algorithm.

From a conceptual standpoint, the action of this algorithm is mundane, though, as shall be discussed later, non-reductive. However, it is not the action—that is, the averaging computation—but the conceptual steps taken during the set-up of the algorithm that gets the algorithm off the ground. Since the FE mesh describes continuously distributed matter, the mesh points can be lined up anywhere along the plane boundary—including at a spacing that matches the inter-atomic spacing in the lattice of MD interatomic potentials. As Broughton puts it, what the algorithm needs in order for the handshake to work is a “one-to-one mapping of a mesh point to an atom site.” [Broughton, Abraham, Bernstein, and Kaxiras, 1999, p. 2396] Farther away from the handshake interface, the mesh can be spaced out for computational efficiency, allowing individual cells to cover larger spatial regions. It is the exploitation of the fact that mesh point spacing is non-representational that licenses the handshake between the continuum and molecular descriptions of the system. In other words, it is a particularity of the way the continuum region was discretized that explains *how* the two models, and the theories they encode, are able to shake hands. Selecting and exploiting this feature of the continuum model as the one that will carry information over into the molecular model justifies the development of the FE/MD handshaking algorithm.

Averaging the energy from the FE and MD component models to obtain the handshake 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 subregion interface. That alignment is possible in the first place because the FE mesh describes a region of the system where continuum mechanics is the appropriate description of physical behavior. The macroscopic scale, and associated near-equilibrium, of the FE-modeled region of the system is what licenses the use of continuum methods to describe it. The continuous deformability of the mesh, a property derived from continuum mechanics, is what allows modelers to line mesh points up with the MD lattice, because it ensures that the mesh points are non-representational.

Manipulating this non-representational feature of the FE model is the sort of epistemic activity I characterize as a conceptual strategy. Deforming the FE mesh to align with the MD lattice is what makes possible the handshake at the interface between the component models. Deforming the FE mesh is not a merely computational activity, nor a merely logical one. Recognizing that it will not change what the model means to deform the FE mesh, and that by deforming it one can then hook it onto the MD framework, requires sensitivity to and understanding of both the component models and the physics that they represent. Further, it is possible to get the deformation wrong, at an empirical or a computational level, and it is possible to characterize and compare the kinds of conceptual strategies used to connect models across distinct theoretical frameworks. The strategy described here, which I will rather cumbersomely dub "manipulating non-representational features of a model," or MNRF, is distinct from the strategy used to connect the MD model to its other neighbor in this multiscale model, as I shall discuss below.

1.3. Microscopic model (tight binding) and second handshake

The simulation model of the microscopic length scale in this multiscale model concerns the region of the silicon block at the propagating tip of the crack, a region around 5 Å in diameter. This model employs quantum mechanics in order to account for changes in the distribution of energy throughout the modeled region of the system as bonds break and form. Broughton et al. explain the need for this component model aptly: "Since it is a region where bonds are breaking it requires a quantum-mechanical description; empirical interatomic potentials are prone to be untrustworthy in such cases" [Broughton et al., 1999, p. 2392] The implementation of quantum mechanics used in the simulation is called tight binding (TB). Like the MD model, the TB model is atomic, but unlike the MD model, calculations are performed not on classical nearest-neighbor interactions but instead on a parameterization of the total energy of the modeled region of the system. The parameterization separates component electron–electron repulsive interactions and combines them using a linear combination of basis functions, similar to the linear combination of atomic orbitals method for computing electron distribution in molecules via combination of electron distribution of the molecule's component atoms. The pairwise interactions, rather than single-electron states, make up the elements of the matrix that forms the mathematical model.

While the computations in the MD and TB component models both concern the distribution of energy around atomic centers, MD is an essentially classical, force-driven model while TB treats the distribution of energy as a product of the distribution of electronic orbitals. Despite this conceptual difference, both MD and TB are models that are essentially about, or representing, atoms in a lattice and their electronic interactions. This is the area of representational overlap between the models on which Broughton et al. base the MD/TB handshake. The MD/TB handshake is constructed from the electronic interactions of a carefully-defined set of fictional "atoms." The fictional "atoms," called "silogens," are assigned some silicon-like properties and some hydrogen-like properties. Specifically, silogens are entities with the inter-atomic spacing of silicon and the electronic symmetry of hydrogen. The hydrogen-like electronic symmetry is introduced for the sake of localizing electronic behavior so it can be modeled by MD. This is a symmetry that silicon atoms could not have—hence, the silogens' status as necessarily fictional entities.[2]

As in the FE/MD handshake, the action of the MD/TB algorithm is, again, to compute a simple average. However, instead of drawing a plane boundary between mesh points and lattice points, as in the FE/MD handshake, the MD/TB handshake performs calculations on a plane boundary consisting of points. These points are occupied by the silogens, and the handshake is achieved by computing the energy at each silogen first in MD and then in TB, and then averaging the values. Also like the FE/MD handshake, the MD/TB handshake is effective because of the ways in which the modelers assign properties to the silogens. 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. By reducing electronic symmetries while maintaining the inter-atomic spacing of silicon—a physically, though contingently, impossible conjunction of properties—the component models can produce 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. The MD/TB handshake generates the silogen, a contrived, un-physical fiction, in order to describe the local energetic behavior of the interfacial region. Generating this fiction is a rather different sort of conceptual strategy than the MNRF approach described in the previous subsection, and that difference will be a focal point of the present discussion.

2. Conceptual strategies, or, how theories shake hands

When the handshakes and component models in this simulation model are put together, each time-step of the simulation is a snapshot of the distribution of energy in the system at a moment. The snapshot is built of five components: the FE model, the FE/MD handshake, the MD model, the MD/TB handshake, and the TB model. It so happens that this snapshot reveals quite a lot about how the component models, and the theories from which they derive, are related. However, viewing the snapshot in the right light requires some development. In this section, I discuss three possible ways of developing the snapshot—a hypothetical reductionist analysis, a hypothetical emergentist analysis, and Winsberg's analysis—and present objections to all three. As a more promising alternative, I present my conceptual-strategies analysis of the picture.

First, consider a rather crude but instructive caricature of the reductionist analysis of this simulation. Such an analysis would favor the TB model's description of the system as the one that best describes the "real" physics of the situation; the other four component models may be considered merely computational conveniences, or approximations that are good enough for the present but from which one should withhold ascriptions of truth. Tight binding, and moreover the quantum mechanics that it encodes, is the genuine theory of matter from which users should derive their understanding of material behavior, and the other components serve to support and ease the burden of the quantum-mechanical computations. What is happening at the quantum level is what is "really" happening, so the snapshot of relations among the components is developed from a quantum theory of material behavior. The snapshot reveals that the four component models besides the TB model fade into the background, and that what the model is representing, what it is about, is a set of relations among quantum-mechanical phenomena.

[2] It is worth noting that the way in which silogens are fictional is different from the way in which the classical silicon atoms in the MD model are fictional. Silogens cannot, in principle, be de-idealized into a more realistic entity and retain their status as silogens, since their properties are drawn from distinct kinds of materials. By analogy, a dog that is purple is a fiction, but a somewhat different sort of fiction than a dog that is a bird. Silogens are like dogs that are birds.

The problem with this analysis is that, beyond the computational limits associated with the TB model, and beyond the fact that the TB model is itself a simplification of quantum mechanics developed to be more computationally tractable than a full quantum theory, the TB model does not have the conceptual resources to account for many of the features of interest of the simulated system. There are phenomena captured in the snapshot that quantum mechanics cannot resolve with its lens. Pressure waves, elastic strain, and thermal fluctuations in a solid are macroscopic, or occasionally mesoscopic, phenomena. Thermal fluctuations in particular simply cannot be tracked by quantum-mechanical descriptions of a system, and to deny their genuine reality, as this reductionist lens would, is to willfully ignore how materials really behave—and to lose the ability to model the nanoscale cracking behavior of silicon, which was, after all, the point of the exercise.

Next, an emergentist analysis of this simulation would generate a somewhat more vivid snapshot of the relations between component models. Where the reductionist caricature emphasized the role of the TB model in representing the "real" physics the model aims to represent, an emergentist alternative would bring the MD and FE models into focus alongside the TB model. For this analysis, I want to consider a classical emergentist snapshot. Here I have in mind an account such as the one sketched in Fodor's seminal "Special Sciences" paper series, in which multiple lower-level realizers of the same higher-level phenomenon are, in at least some cases, related to each other solely through their membership in the same class, namely as instantiators of the higher-level phenomenon. Fodor's classic case (Fodor, 1974) is of the physical realizers of a simple economic transaction, such as the transfer of a dollar from me to you. This could occur via one paper bill, four quarters, a paper check, a PayPal or Venmo transaction, etc. The only thing these different physical transactions have in common is that they each result in you possessing, in some fashion, a dollar that used to belong to me. There are no interesting physical generalizations to make about these transactions; there are, however, interesting economic generalizations to make. In a similar vein, a classical emergentist view of the simulation model would recognize, e.g., that different configurations of atoms in the MD model may generate the same overall quantity of elastic strain, which would be apparent in the FE model. It would not, however (assuming elastic strain were considered an emergent property) seek generalizations about or commonalities among those different MD configurations as a means of gaining insight into the FE phenomenon.

This snapshot of relations among component models emphasizes the autonomy and independence of different levels of physical behavior, producing a picture with all three component models as subjects. Importantly, though, the handshake algorithms still have not come into focus. Each of the three component models stands on its own as a partial representation, or as a representation only of the level it describes. This emergentist snapshot is able to track higher-level phenomena, such as pressure waves and elastic strain, on their own terms. On this account, at least, it fares better than the reductionist picture. Further, each component model is governed by a distinct theoretical framework—the TB model describes quantum behavior of electrons, the MD model describes classical elastic atomic interactions, and the FE model describes stress and strain on a material continuum—and each of these frameworks genuinely contributes to the physics in the simulation. Different phenomena in the modeled system may only be apparent in one of the component models' representations, and a phenomenon does not have to appear in the TB model to be counted as real.

Acknowledging the mechanics of each model as genuine and autonomous is an improvement, but it is merely the beginning of a discussion of how this multiscale model operates. Importantly, it says nothing about two epistemic projects that are central to the success of the simulation model: first, the project of rationalizing or warranting the handshaking algorithms, which will in turn provide warrant for the full multiscale model, and second, the project of justifying the model as a representation of its target, real-world system.[3] Some picture of the relations among the component models is needed to get either project, but especially the first one, off the ground, and neither the emergentist nor the reductionist account will suffice. Winsberg recognizes these shortcomings, and his handshaking analysis does bring the relations between the component models back into the picture, but it does not go on to provide a portrait of the epistemic role these connective algorithms play.

Winsberg addresses this simulation model most extensively in a chapter of his (Winsberg, 2010) called, "When Theories Shake Hands." In that chapter, he likewise points out the failures of both reductive and emergent analyses of this model, arguing that a clear view of the contributions of each component model, plus the contributions of the handshaking algorithms, at each time-step, problematize both the view of the higher-level models as in-principle reducible to the TB model, and the view of each component model as autonomous from its counterparts. The preceding discussions of the classical reductionist and emergentist snapshots have rehearsed these points.

In Winsberg's analysis, the problem can be ascribed to the idea that both the reductive and emergent accounts rely on so-called logical or mereological relations between levels of description, and that the relationships among the component models in this example are empirical, not merely logical nor reducible to mereology. He writes,

> 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.

[3] I thank Johannes Lenhard for bringing the distinction between these two epistemic projects to my attention.

[Winsberg, 2010, p. 84–85].

So, out with the reductionist's bridge principles and the emergentist's disjunctively related multiple realizers alike. Importantly, Winsberg goes on to argue that the handshaking strategies discussed above do not rely solely on logical relations between the models or the theories from which they are derived, and he is absolutely correct on this point. Winsberg interprets the action of the handshaking algorithms as physical, rather than logical, particularly by describing the algorithms as expressions that "define the energetic interactions between, for example, the matter in the continuum mechanical region with the matter in the molecular dynamical region," [Winsberg, 2010, p. 80] and the resulting dynamics as containing "significant simultaneous and back-and-forth interactions between the physics in each of [the spatial] regions [modeled by each component model]." [Winsberg, 2010, p.86].

For Winsberg, and the physicists who developed the model, there is physics in the handshakes. I agree. However, I think there is more, as well. Abraham's and Winsberg's notion of "physical insight," if understood as strictly physical—as opposed to as a part of the concepts and models used to represent the physics—is too narrow. There is certainly significant back-and-forth between the models, but it is not a straightforward exchange of energy or other strictly empirical determinables; it is an exchange of ideas constrained and moderated by the computational, mathematical, and yes, also, physical limits of the component models' frameworks. This exchange certainly requires more than mere logic, or mereology. But it also requires more than just an understanding of the physics, since mesh points and silogens are not physical objects. Developing these handshaking algorithms requires conceptual insight, beyond the brute physics, in order to notice and take advantage of the continuous deformability of the finite-element mesh, or the fact that the molecular dynamics model can arbitrarily reduce the symmetries on atoms at the edge of its lattice.

In the FE/MD handshake, the non-representationality of the FE mesh points permits modelers to permute the locations of these points such that they line up with the—representational—interatomic spacing of the MD model. This strategy takes advantage of a very different set of features of each component model than the MD/TB handshake, which relies on the construction of a fictional entity, the silogen, upon which both MD and TB calculations be performed. Broadly, these two strategies may be thought of respectively as relying on manipulating non-representational features of the model and on constructing fictions. Both strategies are widespread in the development and use of multiscale models of materials, and each has been characterized in some detail in contemporary philosophical literature on scientific explanation. Winsberg, for instance, conducts an extensive and informative investigation of fictions through a study on the silogen in this example.

Notice, though, how constructing a fiction differs from the strategy employed by the FE/MD handshake, the MNRF strategy. In the MNRF handshake, no additional computational objects are introduced into the model at the site of the handshake. There is, consequently, no need to probe new computational objects for representationality, nor ask whether de-idealizing them would generate a better, worse, or different model. It's not even clear how such questions could be posed of a piece of the mathematical background conditions of a computer model. One could, though, test the placement of mesh points at slightly different spacings to see if resolution of the simulation improves, if the macro- or mesoscale dynamics are affected, or if other differences appear in the model's physics. In the MNRF handshake, one component model remains essentially unchanged at the handshake site while the other is manipulated. In the silogen handshake, the dynamics of both component models remain fixed, while the object being run through the dynamics changes.

More differences appear for epistemic investigation, as well. In the silogen handshake, there is not a fundamental conceptual incompatibility between the models that needs to be overcome; both component models are models about atoms, although they disagree on the representation of electronic structure. Tools to address that disagreement are widely available and deeply entrenched in modern quantum chemistry, where one might turn if one wanted to refine this handshake. In the MNRF handshake, on the other hand, topology might provide a better reference point for further study.

Winsberg groups the upshot of these handshaking algorithms together, epistemically, as the collective means by which the model threads the needle between reduction and emergence. This snapshot allows the handshakes to come into focus, and to bridge the distances between the component models left in the emergentist picture. But the resolution is still too coarse, and it does not allow the handshakes to be distinguished from one another. Further, Winsberg takes as the moral of his analysis that the model is built of internally inconsistent parts, an insight that has implications for the nature of consistency in physical laws and which motivates the very useful discussion of fictions he gives next. While this moral is not wrong, it seems to miss the point for the discussion of inter-theory relations: if there weren't inconsistencies between the laws of the different theories in the first place, the physicists would not need multiple component models to generate the multiscale simulation model.

What Winsberg takes as a conclusion should have been a premise, and when understood as such, it is a restatement of a central challenge for inter-theory relations in physics, namely how to reconcile apparently competing accounts of material behavior, when each account is successful at modeling behavior at its native, characteristic length scale. By study of the conceptual strategies involved in the generation of the two algorithms, the contours of the handshakes can be differentiated, and they can be individually and jointly understood and analyzed. Winsberg's own account of fictions, as well as other recent accounts such as Bokulich's explanatory-fictions account (Bokulich, 2012), can be used to probe the silogen and answer questions about whether and how this definitively un-physical fiction, which is a Frankenstein's monster built of genuinely physical parts, is in any sense real, or explanatory, or confirmable, or exportable to other modeling contexts. But answering these questions about silogens will not immediately produce answers to parallel questions about the MNRF strategy, in no small part because there are no parallel objects about which to ask those questions in the mesh-point setting. Viewing the multiscale model through the lens of conceptual strategies reveals the difference between the MNRF strategy of moving around the mesh points and the fictions-based strategy of constructing the silogen. This new portrait offers, in return, a more robust view of the multiscale model, not as merely full of fictions, but—to don a new metaphor—as sewn together with threads as conceptually complex as the fabrics of the component models, threads that can themselves be held up to the light for philosophical inspection.

Rather than emphasizing, as Winsberg's analysis did, the essentially negative similarities between the strategies—both are non-reductive, non-logical or non-merelogical—the analysis I present here offers a positive view of the differences between these strategies, which paves the way for an account of what these non-logical inter-level relations in fact are. They are conceptual strategies, tools of modeling and theorizing that can be studied individually and in groups, and interrogated by the usual philosophical means applied to theories and models. Those methods of investigation can be used to establish a range of relations two (or more)

models or theories may have to one another, and characterizing that variety will provide a more productive framework for understanding inter-theory relations than reductionist or emergentist approaches, and will fill the negative space left by Winsberg's handshaking account. Grouping the handshaking algorithms together obscured precisely the conceptual differences between the two strategies, generated by the constraints imposed from the physics, the mathematics, and the computation, which rationalized the particular strategies employed in each handshake. It is not when, but how, theories shake hands that matters.

3. From multiscale models to inter-theory relations

So far, this discussion has centered around multiscale simulation models. I have shown that the two strategies I am calling manipulating non-representational features, or MNRF, and generating fictions, each underlie one of the two handshaking algorithms in the Broughton et al. model of nanoscale crack propagation. Further, these strategies are two among a handful of conceptual and inferential tools employed in the project of developing the physical insight necessary to bridge scales in modeling situations similar to the one at hand; others include abstraction and idealization. Many of these conceptual strategies are already commonly discussed in the modeling literature (e.g. in (Batterman and Batterman, 2012; Bokulich, 2012; Cartwright, 1983; Morrison, 2015), but they are not widely recognized as the means by which component models are connected into a multiscale model, description, or explanation of a system.

This has been a discussion of models up to this point, and largely of very particular implementations of models in a computer-simulation environment. Questions of reduction, emergence, and their limits, however, are more often asked of inter-theory relations than of relations among models or their implementations. So, to make a broader point about the nature of relations among theories, it is necessary to investigate how the conceptual strategies I have identified in this example relied not only on the implementation of the component models in the particular computer simulation, but on the theories from which those models are derived.

Consider first the MNRF strategy from the FE/MD handshake. The problem that this handshake faced was that there was a fundamental conceptual mismatch between the FE and MD component models, namely that one was about continuously distributed matter and the other was about a discrete set of atoms in a lattice. The solution to this problem, the MNRF strategy, was to use this mismatch to the model's advantage, by moving around the mesh points in the FE model so that they aligned with the lattice spacing of the MD model. This strategy would not get off the ground if the FE model were not a model of continuous matter, because it is the uniformity and continuity assumptions that make the spacing of the mesh points non-representational in the first place. If the FE model had been derived from atomic theory, as the MD model is, then the spacing of the mesh points would have inherited different constraints from that theory. Assumptions from continuum mechanics about how materials behave are what license the use of the MNRF strategy in this handshake.

Next, consider the silogen strategy from the MD/TB handshake. Here the problem was to reconcile two different accounts of the nature of electronic interactions. However, in this handshake, there is a shared conception of matter as composed of atoms and their electronic interactions, which each component model inherits from its respective theory; both classical molecular theory and quantum theory are about the electronic behavior of atoms. This shared conception suggests the construction of an object, composed of atoms and electrons, that both models can manipulate. The silogen is a physical fiction, rather than a mathematical or computational one. Some of its features are derived from the classical theory that supports the MD model, such as the spacing of silogens in an array, which it gets from classical data for silicon. Other features are derived directly from the TB model and other quantum models like it, such as the use of hydrogen-like electronic symmetry, which is implied by the fact that only hydrogen-like symmetries are separable (and therefore able to be linked to separable atoms in an MD model) in TB-type models. In this case, then, assumptions both from the TB model itself and from both the quantum and classical theories of matter license the construction of the silogen in this handshake.

In both cases, the handshakes are thoughtfully constructed from constraints, imposed in part although not *in toto* by physical theories, on how two models can be related. As Winsberg argued and as I've elaborated, these relations are not merely logical. But neither are they merely physical, as Winberg's interpretation seems to suggest. They are conceptual: they are born from reasoning within a set of mathematical, computational, and physical constraints, derived from theories and their models. This is not to say that those constraints dictate the construction of the handshakes; rather, the practice that I've called conceptual strategizing is required to navigate the channels carved out by these constraints. The resulting relations, constructed via conceptual strategizing, are themselves epistemic objects: silogens and conveniently-spaced mesh points are things that can succeed or fail in a model, and about which questions of representation, confirmation, and reference may be asked. They are not merely semantic principles aiming to bridge the logical gap between theories; they are themselves a robust part of the conceptual structure of science.

Building conceptual strategies, such as the manipulating the non-representational features of a model or constructing a fiction with unphysical combinations of physical properties, looks a lot more like theory construction than the derivation of a proof. It is part of the epistemic structure of science, and one that has been overlooked so far in discussions of inter-theory relations. One can perform all of the usual tasks of epistemology on the algorithms that tie theories and their models together: constructing models to describe the handshakes; testing their predictive accuracy; generating explanations of phenomena on the basis of them; and so forth. So, I contend that understanding inter-theory relations as built from techniques of this sort provides a richer and more useful alternative to reductive bridge laws or emergentist accounts of genuinely novel dynamics acting at each new scale. This alternative provides a more robust understanding of how different theories in physics are, in fact, related, and opens up new avenues for both scientific and philosophical investigation into the means and methods of those relations.

4. Conclusions

It is not merely logical relations that undergird inter-theory relations in physics. It is both possible and, for the purposes of multi-scale modeling, necessary, to develop accounts of how different theories at different scales can be constructively combined to model material behavior. The conceptual-strategies account of inter-theory relations that I have presented here is offered as an alternative both to standard views of inter-theory relations—which fail to offer a satisfactory account of the conceptual transition, in a given explanation, prediction, or simulation, from one theory to another—and to Winsberg's handshaking account of physical relations between component models in a multiscale model.

I have argued that relations between theories in physics, such as between continuum and molecular classical mechanics, and between classical and quantum mechanics, rely on conceptual

strategizing, a practice of reasoning within computational, mathematical, and physical constraints, which is exemplified by techniques such as the MNRF and silogen strategies used in this paper's central example of a nanoscale crack propagating through a block of silicon. These techniques, called handshaking algorithms, are instances of a few common conceptual strategies; other conceptual strategies include idealization and abstraction, among others. In philosophy of science, these strategies have been discussed primarily in the context of the epistemology of models, and one aim of this essay has been to show that these strategies are relevant to a wider variety of debates and contexts. By modeling (if you will) an account of inter-theory relations after successful strategies for constructing multiscale models, I have uncovered a more robust picture of how theories can collaborate to generation predictions and explanations in physics.

The example used throughout this essay to motivate this account has been a multiscale computer simulation of a nanoscale crack propagating through a block of silicon. This example is particularly salient because of its use of two distinct strategies for connecting theories across widely differing length scales. The first strategy, used to connect the models of the mesoscopic and microscopic length scales of the system, was to construct a fictional entity on which calculations from both contributing models could be performed, and the results averaged. This entity, the silogen, is neither an idealization of any realistic atom, nor is it a straightforward abstraction. As a piece of epistemic equipment, it is more closely akin to the construction of an explicitly un-physical fiction, such as the classical trajectories ascribed to electrons in quantum dots discussed by Bokulich (Bokulich, 2008; Bokulich, 2012).

The second strategy, used to connect the macroscopic and mesoscopic length scales of the system, was to manipulate a non-representational mathematical feature of the macroscopic model, namely the distribution in space of the mesh points used to discretize the continuum model of the system, in order to license the algorithm that was used to bridge the models of the macroscopic and mesoscopic scales. I have suggested that this strategy, which I called MNRF, is a more general one that may be found in many instances of modeling across length, time, and energy scales in physics, and likely in other sciences as well. In the modeling of critical phenomena via the renormalization group, for instance, Kadanoff's block-spin parameterization manipulates features of the model—the blocks—that are not meant to be representational of any physical phenomenon or behavior; it is another instance of the MNRF strategy. This conceptual strategy is distinct from abstraction, idealization, and constructing a fiction, which are nonetheless additional means of connecting theories across scales.

More broadly, my aim has been to show that conceptual strategies such as these are sometimes necessary to bridge scales, and that when they are used in this context they should be studied in the same ways that they are studied in more general modeling contexts; fictions, for instance, do not stop being fictions when they are called upon to ground an inter-theory relation, and what we know of fictions can help us to understand their uses as inter-theory relations. Importantly, this panoply of strategies is not reducible to the articulation of logical relations. These strategies are the tools used to justify inferences, predictions, and explanations that require contributions from across multiple scales or theoretical frameworks. Consequently, these strategies are an essential epistemic feature of inter-theory relations, and they have, with a few exceptions, been largely overlooked as a means of unpacking relationships among theories in physics and beyond. By correcting course and re-examining inter-theory relations in the richer context of conceptual strategizing across scales, I have laid the groundwork for a more robust and realistic account of how scientific theories work—and how they work together—in physics and beyond.[4]

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