Studies in History and Philosophy of Modern Physics xxx (2017) 1–8

Contents lists available at ScienceDirect

Studies in History and Philosophy of Modern Physics

journal homepage: www.elsevier.com/locate/shpsb

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

Julia R. Bursten

Department of Philosophy, University of Kentucky, 1415 Patterson Office Tower, Lexington, KY 40506, USA

ARTICLE INFO

Article history:
Received 24 February 2017
Received in revised form
24 July 2017
Accepted 5 September 2017
Available online xxx

Keywords:
Reductionism
Emergence
Inter-theory relations
Models in physics
Nanoscience
Quantum physics
Classical physics
Conceptual strategies

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

E-mail address: jrbursten@uky.edu.

http://dx.doi.org/10.1016/j.shpsb.2017.09.001
1355-2198/

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.

Please cite this article in press as: Bursten, J. R., Conceptual strategies and inter-theory relations: The case of nanoscale cracks, Studies in History and Philosophy of Modern Physics (2017), http://dx.doi.org/10.1016/j.shpsb.2017.09.001