Computational Models

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A different way of thinking about how the sciences are organized is suggested by the use of cross-disciplinary computational methods as the organizing unit of science, here called computational templates. The structure of computational models is articulated using the concepts of construction assumptions and correction sets. The existence of these features indicates that certain conventionalist views are incorrect, in particular it suggests that computational models come with an interpretation that cannot be removed as well as a prior justification. A form of selective realism is described which denies that one can simply read the ontological commitments from the theory itself.

1. Introduction. What are the correct units of analysis to use when we are thinking about how scientific knowledge is applied to the world? Historically, the most popular choice has been theories, variously reconstructed, with larger units such as research programs and paradigms also being important candidates. Those with finer-grained interests and tastes have chosen sentences, laws, terms, or concepts as the items of investigation. Recently, models have grown in popularity. Which unit of analysis we choose influences how we see the organization of science. Theories tend to be subject-specific objects and this subject-specificity tends to mirror the familiar ontological hierarchy of the sciences based on the mereological inclusion of the subjects of one theory within the subjects of another. Elementary particle physics underpins nuclear physics, which in turn

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forms the basis for atomic physics. Thence to simple molecules, macromolecules, biochemistry, and on up to at least population biology.

In contrast, certain broadly conceived theories can have applications across subject matters, as we have when quantum mechanics is used in elementary particle physics, physical chemistry, and astrophysics. The usual explanation for this versatility is that in the background lies the familiar kind of ontological hierarchy I have just mentioned. Without this background picture, the same theory will not usually occur in, say, both physics and biology. A successful theory of the electro-weak interaction is just that; it will not also be a theory, successful or otherwise, of organism/parasite interactions or of anything else in the biological realm. Although they are broader units, the same point holds of research programs and paradigms, unless they are so general, as in corpuscularianism, that they become methodological directives and, if not reductionist, at least unifying.

In contrast, even though much of the literature on modelling has quite correctly tended to emphasize the particularity of models, one of the characteristic features of mathematical models is that the same model, in a sense to be explained, can occur in, and be successfully employed in, fields with quite different subject matters. This feature has significant consequences for the organization of science and suggests a re-organization that is not simply hypothetical but is now occurring in some of the more intensively computational areas of modelling.

In this paper I shall try to capture a broad and increasingly important type of applied unit—the *computational model.* Although these have been around at least since the work of Hipparchus of Nicaea, their peculiar advantages can be seen most clearly in the explosively growing enterprise of contemporary computational science.

At the heart of a computational model lies its *computational template.*[1] Familiar examples of such templates are differential equation types, such as Laplace's equation and the Lotka-Volterra equations; statistical models such as the Poisson process and its various extensions; and specifically computational models such as cellular automata and spin-glass models. Such computational templates are common in mathematically formulated sciences, although they frequently occur at a quite abstract level and require the specification of free parameters before they can be applied. Some examples are Schrödinger's Equation, $\mathbf{H}\,\Psi = \mathrm{E}\,\Psi$, which requires a specification of both the Hamiltonian $\mathbf{H}$ and the state function Ψ in order to be used and Maxwell's equations: $\nabla\cdot\mathbf{D} = 4\pi\rho$ (Coulomb's Law), $\nabla \times \mathbf{H} = (4\pi/c)\mathbf{J} + (1/c)\partial\mathbf{D}/\partial t$ (Ampere's Law), $\nabla \times \mathbf{E} + (1/c)\partial\mathbf{B}/\partial t = 0$ (Far-

1. The need for computational templates was explored in Humphreys 1991, although the term itself is not used in that paper.

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aday's Law), $\nabla \cdot \mathbf{B} = 0$ (Absence of free magnetic poles), where **D** is the displacement, **B** is the magnetic induction, **H** is the magnetic field, **E** is the electric field, and **J** is the current density—each requiring a specification of component physical quantities before it can be brought to bear on a given problem, despite the fact that three of the examples I have just cited are often given the honorific status of representing a law of nature. In much the same way, probability 'theory' is a computational template for which a specific measure or distribution function must be provided before the template can be used.

The computational template has certain characteristic features. Its computational features are usually essentially dependent upon a particular syntactic formulation. Thus, the Heisenberg, Schrödinger, and Dirac representations of classical quantum mechanics all have distinct templates even though there are transformations that will take each into the others. Similarly, representations of classical mechanical systems in polar co-ordinates often give different templates than do representations in rectilinear co-ordinates. The reason for this is simple. Computational tractability is the primary reason for adopting a particular computational model and it is the computational template that initially provides this. For certain purposes the Dirac representation is computationally superior, whereas for others the Schrödinger representation is better.

The importance of syntax to applications, and especially to computational tractability, is something that the semantic account of theories, for all its virtues, is essentially incapable of capturing. This is because one of the main points of the semantic view is to abstract from the particular syntactic representation and to identify the theory with an underlying abstract structure.[2] Important as the semantic approach is for baring the underlying abstract structure of a theory, it moves us in exactly the opposite direction from where we should be when we apply computational models. Syntax matters.

A key feature of computational templates is their ability to be applied across a number of different scientific disciplines. Variations of the basic Lotka-Volterra equations can be used to represent the growth and decline of predator-prey populations in biology and botany and to represent arms races (the Richardson model) and, perhaps, to represent the outbreak of political revolutions.[3] Variations of the Poisson process template have been used to represent carcinogenesis, the flow of calls at a telephone exchange, radioactive decay, and many other phenomena.[4] Laplace's

2. See e.g. Suppes 1970; van Fraassen 1972.

3. For the arms race models, see Epstein 1997, chap. 3 and for the models of revolution, see Epstein 1997, chap. 4.

4. See e.g. Feller 1968.

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equation in two dimensions represents the flow of viscous fluid between parallel sheets as well as the flow of electricity in a plane.

The drive for computational tractability also explains the enormous importance of a relatively small number of computational templates in the quantitatively oriented sciences. In physics, there is the mathematically convenient fact that three fundamental kinds of partial differential equations—elliptic (e.g. Laplace's equation), parabolic (e.g. the diffusion equation), and hyperbolic (e.g. the wave equation)—are used to model an enormous variety of physical phenomena.[5] This emphasis on a few central templates is not restricted to physics. William Feller, the statistician, makes a similar point about statistical models:

> We have here [for the Poisson distribution] a special case of the remarkable fact that there exist a few distributions of great universality which occur in a surprisingly great variety of problems. The three principal distributions, with ramifications throughout probability theory, are the binomial distribution, the normal distribution . . . and the Poisson distribution. . . . (Feller 1968, 156)

So, too, in engineering:

> It develops that the equations for most field problems of interest to engineers take no more than five or six characteristic forms. It therefore appears logical to classify engineering field problems according to the form of the characteristic equations and to discuss the method of solution of each category as a whole. (Karplus 1959, 11)[6]

Some phenomena that are covered by the same template have something in common. For example, the Rayleigh-Taylor instability is found in astrophysics, magnetohydrodynamics, boiling, and detonation. But some do not—there are phenomena described by the same template that seem to have nothing in common 'physically.' The motion of a flexible string embedded in a thin sheet of rubber is described by the Klein-Gordon equation

$$1/c^2\ \partial^2\Psi/\partial t^2 = \partial^2\Psi/\partial x^2 + \mu^2\ \Psi$$

but so too is the wave equation for a relativistic spinless particle in a null electromagnetic field. For another example of subject divergence, this time drawn from Monte Carlo theory, suppose we have a problem in electromagnetic theory that requires an exact solution to Laplace's equation, subject to certain boundary conditions that make it not amenable to an-

5. See e.g. Morse and Feshbach 1953.

6. I have deliberately chosen older, classic, texts to illustrate the point that this is not at all a new phenomenon.

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alytic techniques. Since Laplace's equation can also be used to model particles that diffuse randomly in a region with absorbing boundaries, by representing the behavior of particles by random numbers it is possible to solve the special case of Laplace's equation for these boundary conditions.[7] And of course this multiple applicability of formal descriptions formed the basis of analog computers that modelled mechanical systems with electronic systems, both systems being covered by the same computational template. Let the analog computer solve one and you automatically have a solution to the other.

This flexibility suggests that we look at scientific organization rather differently. Instead of the ontological hierarchy based on mereology that gives us the usual ordering of the natural sciences from physics through chemistry and biology we can see a reshaping of the scientific enterprise that takes place when activities are grouped according to the computational templates that they use. While there has long been a certain amount of borrowing of techniques across fields—mostly from physics into sociology, neuroscience, and economics; from statistics into physics; from biology into economics and anthropology—this regrouping is being accelerated by the increasing availability of computer-assisted solutions to computational templates. This is because many familiar templates are solvable only in very specific situations, where clean initial and boundary conditions hold that are found only in certain sorts of physical and astrophysical systems. The enormously increased flexibility introduced by computationally based methods makes a relaxation of these traditional constraints feasible with a consequently broadened set of applications.

For all these reasons, it is worth taking seriously the idea that computational templates can serve as a basic organizational unit of scientific research.

2. Construction Assumptions and Correction Sets. Computational templates can be taken as black box units, 'off-the-shelf' tools to be used as is deemed appropriate. This sort of use is common, but methodologically, the more important use of the templates comes when their construction is taken into account. Aside from a few cases, all computational templates are constructed, even though at the textbook level, or when an application has become routine, this construction may be concealed. I shall not go into the details of the construction process here, but simply note that it will ordinarily involve both mathematical and substantive approximations, idealizations, constraints (which include initial and boundary conditions as well as laws), and abstractions with the primary goal being computational tractability of the template.[8] Just as chemical processes that

7. This example is drawn from Hammersley and Handscomb 1964, 4.

8. For details, see Humphreys 1995.

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can be reproduced in the laboratory but not scaled up to industrial production are theoretically but not practically interesting, so intractable templates are of little interest to computational science. I shall call the assumptions used in the template construction the *Construction Assumptions* and represent them by the quadruple <Idealizations, Abstractions, Constraints, Approximations>.

The second main component of a computational model, which is also often formulated during the construction process but is not used at that point, is its *Correction Set.* Unlike the computational template, where solvability is primary, approach to the truth is the aim of the correction set. The components of this set will vary depending upon the construction that was used for the computational template, but the most important are:

(1) Relaxation of idealizations (e.g. moving from considering the Sun as a perfect sphere to considering it as an oblate spheroid).
(2) Relaxation of abstractions (e.g. adding previously omitted variables to the template, such as introducing a treatment of friction into a template that initially represented motion over a frictionless surface; increasing the number of individuals in an ecological simulation).
(3) Relaxation of constraints (e.g. moving from a conductor within which heat is conserved to one that has heat flowing across its boundary).
(4) Refinement of approximations (e.g. reducing the grid size in finite difference approximations to continuous models).

The construction process, including the construction assumptions, together with the correction set lead to three distinctive features of computational modelling. These are:

A) The construction process provides a prior justification for the model even before it is tested against data. Rather than the model being merely hypothetical, there are ordinarily reasons, albeit reasons modulated by the correction set, for adopting the various assumptions that go into the construction of the model. The justification can come from a variety of sources: a medium may be known to be discrete on the basis of independent investigations, linear friction terms for laminar fluid flow may be an empirically determined generalization, lattice spacings may be experimentally measured.

B) The model comes with an interpretation. This interpretation cannot be stripped off and the bare formalism re-interpreted because it is the original interpretation that underpins the justification just mentioned. Because the same computational template can be used to model more than one system type, and those system types can be radically different in subject matter, of course there are re-interpretations of the formalism. But

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few of those re-interpretations will legitimate the use of the template for the specific system to which it is being applied. Moreover, other, syntactically isomorphic, templates with different interpretations are not reinterpretations of the same model, but are different computational models entirely. For example, as I mentioned, the Klein-Gordon equation can be applied both to the motions of a flexible string embedded in a thin sheet of rubber and to the motions of a relativistic spinless particle in a null electromagnetic field. But the assumptions of continuity that are required for the first application are simply inapplicable to the second application.

A few more words are needed about this issue. Although one can view the computational templates consisting of a string of formal syntax together with a separate interpretation, this is a misrepresentation of the construction process. The computational language is interpreted at the outset and any abstraction process that leads to a purely syntactic computational template occurs at an intermediate point in the construction. The substantive simplifying assumptions come first, then their formal mathematical analogues.

C) The construction process and the correction set usually mandate a selective realism viz-a-viz components of the syntactic template. Rather than reading off the realist commitments from the syntax, or being committed to every putatively referring term of a well-confirmed template denoting an element of reality, what realist commitments there are will be made by the user of the template, usually on the basis of which construction is used. The user often knows in advance which parts of his model are fictional and which parts are intended to be taken realistically.

To emphasize the importance of solvability within these computational models is not to adopt instrumentalism. Overall, such models are almost always false because of the presence of the correction set. But by asserting their falsity, we have already rejected an instrumentalist interpretation. Moreover, parts of the model often are true and some of the terms do refer. This is why one needs to be a selective realist.

3. Selective Realism. Realism is often taken to concern theories viewed in abstraction from our attitude toward them; in particular about whether those theories are true or false, or whether certain terms of well-confirmed theories refer to real entities. But realism is ordinarily an attitude taken by a user toward parts of a theory and neither the theories nor their constituent terms intrinsically display their realist commitments. Quine's famous theory of ontological commitment is often taken to be a clear statement of such a theory-oriented position. "To be is to be the value of a variable" is the slogan; a more refined statement is "In general, entities of a given sort are assumed by a theory if and only if some of them must be counted among the values of the variables in order that the statements

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affirmed in the theory be true" (Quine 1961, 103). Yet even this doctrine does not commit us to having our theories dictate our ontology to us. For Quine goes on to say "One way in which a man may fail to share the ontological commitments of his discourse is, obviously, by taking an attitude of frivolity. The parent who tells the Cinderella story is no more committed to admitting a fairy godmother and a pumpkin coach into his own ontology than to admitting the story as true. Another and more serious case in which a man frees himself from ontological commitments of his discourse is this: he shows how some particular use which he makes of quantification, involving a prima facie commitment to certain objects, can be expanded into an idiom innocent of such commitments" (1961, 103). This is an admirably wholesome concession to our freedom of association: it is we who choose our ontological friends, not our theories or models.

Our initial realist commitments will be amended as the correction set is brought into play or a more refined construction process is used, as will the interpretation. For example, taking Ohm's Law as a primitive relation between voltage, resistance, and current, no commitment to the underlying nature of current need be made. But when Ohm's Law is derived from a set of assumptions about current density, then a conception of current as atomistic units of charge is made possible, although certainly not mandatory. When using finite difference approximations to continuous processes in numerical simulations, there is an explicit commitment to the falsity of the discrete model. A position of ontological non-commitment is always possible, but positive commitments must be specific, not general. Perhaps most importantly, one can view some parts of the computational template as simply fictional and other parts as having genuine realistic content. Such considerations break the connection between a well-confirmed model and its truth. Many of the finite difference models just mentioned are very well confirmed by data, but no user construes that to require commitment to the truth of the model, *simpliciter*. The grid size of a numerical simulation is frequently determined by constraints such as processor speed and memory capacity, not by our commitment to the truth of a rather crude finite approximation.

A second conclusion to be drawn is that because the idealizations and approximations used enter directly into the construction of the equation, no "ceteris paribus" conditions are required for the statement of the law, because the restrictions on the use of the law have already been explicitly incorporated into the justificatory conditions for the equation.

A third point, one that is characteristic of the trial and error methods often involved in solution procedures, is that a clear and transparent understanding of the deductive relations between fundamental theory and specific application is not necessary in order for a good fit to ultimately be achieved between theory and data. To put it in a characteristically

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philosophical way, there has been a long tradition in epistemology that every step in a derivation from fundamental principles should be individually open to inspection to ensure correctness. What is characteristic of many solution methods is that such transparency is not available and that the virtues of a model, such as stability under perturbations of boundary conditions, scale invariance, and conformity to analytic solutions where available can be achieved by trial and error procedures treating the connections between the computational model and its solutions as an opaque process that has to be run on a real machine for the solution to emerge.[9] There is nothing illegitimate about this opaqueness of the solution process as long as the motivation for the construction process seen above is well founded. For example, one may have excellent reasons for holding that a particular parametric family of models is applicable to the case at hand, yet have only empirical methods available for deciding which parametric values are the right ones. In fact, the justification of scientific models on theoretical grounds rarely legitimates anything more than such a parametric family, and the adjustments in the fine structure by empirical data are simply an enhancement of the empirical input traditionally used to pin down the models more precisely.

Of course a hypothetico-deductivist can reinterpret what I have said in more traditional ways: that model building is just a deductive process from very basic principles and that the equations we take as the starting point are themselves amenable to a deductive construction. This is certainly true, but to leave it at this would be to miss the point. Conventionalists frequently, perhaps universally, write as if incorrect predictions leave everything, logically, open to revision, with only pragmatic considerations motivating the decision. This is, for most situations, a serious underdescription of the situation. Model builders usually have a quite refined sense of which of the components that go into a model are well-justified and which are not. They often have, in advance of testing, a clear idea of which parts of the construction will be the first to be revised when the model fails to give accurate predictions. This is the essence of the correction set. We selectively target parts of the construction process for revision and this is done on the basis of subject-specific knowledge. Because a particular construction process will be chosen on the basis of the underlying ontology of the system, for exactly the same equation the revisions will take a different form when the template is based on different construction processes.

4. Computational Models. The final component of a computational model is the Output Representation. This will sometimes consist of familiar prop-

9. For an example of this, see Humphreys 1994.

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ositional forms, but other kinds of representations such as data arrays and especially visualizations are common and often preferable.

The sextuple <Computational Template, Construction Assumptions, Correction Set, Interpretation, Initial Justification, Output Representation> constitutes a *computational model,* which can be an autonomous object of study. As the template remains constant and the other components vary, we can recover some of the more traditional, subject-specific organizational structure of the sciences that is lost with the versatility of the computational template. Yet with these models, the knowledge is contained in the entire sextuple—it is not contained simply within an axiomatically formulated theory.

One of the central questions with representations is the degree to which their use is subject-matter specific. Probably few people have seriously believed that there was a fully subject-independent method for applying science to the world, even though some more formally inclined philosophers of science write that way. The more interesting issue is: at what points in the process of the construction and evaluation of computational models does subject-specific knowledge enter? Here I preserve the distinction between a template that may not be subject dependent (in the sense that it applies across a variety of subject matters) and the knowledge that is needed to apply that template to a given subject matter, which is. Are there any subject-matter unspecific applications of models? Not if the model is to be applied for predictive purposes. For induction itself is subject matter specific. You need to have concrete information about the constancy of the generating conditions for the data in order to effectively use inductive reasoning and that constancy or otherwise requires knowledge of the subject matter. The correction set is also always subject-dependent and so, despite its flexibility, is the template itself. This is in part because of the inseparability of the template and its interpretation, in part because of the connection between the construction of the template and the correction set. Which substantive idealizations and approximations are justifiable is always a subject-dependent issue—this is in part why scientists are willing to justify, on substantive grounds, the use of approximations that are formally unjustifiable.

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