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Abstract	The rise of computational science, which can be dated, somewhat arbitrarily, as beginning around 1945–1946, has had effects in at least three connected domains – the scientific, the philosophical, and the socio-technological context within which science is conducted.
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Abstract

This paper discusses ways in which the rise of computational science has changed the epistemology and metaphysics of science. It argues that computational science constitutes neither a Kuhnian revolution nor a `Hacking Revolution', but an emplacement revolution .

Computational Science and Its Effects

Paul Humphreys

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Introduction

The rise of computational science, which can be dated, somewhat arbitrarily, as beginning around 1945–1946,[1] has had effects in at least three connected domains – the scientific, the philosophical, and the socio-technological context within which science is conducted.[2] Some of these effects are secondary, in the sense that disciplines such as complexity theory would have remained small theoretical curiosities without access to serious computational resources. Other effects, such as the possibility of completely automated sciences, are longer term and will take decades to alter the intellectual landscape. I shall provide here some examples of fine-grained philosophical effects as well as examples of more sweeping social and intellectual consequences that will suggest both the different ways of thinking that these methods require and a hint at how far-reaching they are.

First, we need a framework. In their paper "Complex Systems, Modelling, and Simulation", Sylvain Schweber and Matthias Wächter (2000) suggested that the introduction and widespread use of computational science constitutes what they call a "Hacking Revolution" in science and that Hacking's use of "styles of reasoning", a concept which originated with the historian of science A.C. Crombie, can give us

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This is a slightly revised version of a paper that originally appeared in the *ZiF Mitteilungen*, Zentrum für interdisziplinäre Forschung, Bielefeld, 2008.

[1] I identify its origins with the use of electronic computers to perform Monte Carlo calculations at Los Alamos and John Mauchley's suggestion that ENIAC could be used for difference equation simulations, rather than for just routine arithmetical calculations. See Metropolis (1993), 127 for the second point. I do not vouch for the accuracy of Metropolis's recollections on this point although the exact historical turning point, if indeed "exact" ever makes sense in historical claims, is unimportant. For those interested in technoscience, I note that the innovation had its origins at Los Alamos and other military research institutions rather than in industrial applications.

[2] There are other domains it has affected, but I shall restrict my discussion to these three.

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it is a little remarked upon aspect of scientific realism when we access the humanly unobservable realm using instruments. Just as scientific instruments present philosophy with one form of the metaphysical problem of scientific realism and its accompanying epistemological problems, so computational science leads to philosophical problems that are both epistemological, a feature that has been emphasized by Eric Winsberg and Johannes Lenhard,[7] and metaphysical.

What Is Metaphysically Different About Computational Science

The essence of computational science is providing computationally tractable representations; objects that I have elsewhere called computational templates.[8] It is an important feature of templates that they are trans-disciplinary. The philosophical literature on scientific laws, with its emphasis on counterfactuals, nomological necessity, logical form, and so on, often does not stress the fact that the fundamental laws of a science are uniquely characteristic of that science. Although Newton's laws applied to any material object in the eighteenth century, they did not characterize biological objects qua biological objects in the way that they did characterize what it was to be a physical object. Nowadays, the Hardy-Weinberg law is a characteristic feature of population biology, and it makes no sense in chemistry or physics.[9]

I mentioned above that laws are the wrong vehicle for understanding computational science. The reason for this is connected with the fact that scientific laws are intimately tied to a particular science and its subject matter, whereas the emphasis of computational science is on trans-disciplinary representations. (There are some candidates for laws of this trans-disciplinary type in complexity theory, such as Zipf's Law, a power law that reasonably accurately describes the distribution of city sizes, network connection densities, the size of forest fires, and a number of other phenomena that are the result of scale-invariant features) Just as theory and experiment involve techniques that are to a greater or lesser extent subject matter independent, so too does computational science. This cross-disciplinary orientation has at least two consequences that are worth mentioning. First, it runs counter to the widely held view that models are local representations. It is, of course, true that many models are far less general than theories, but the existence of widely used computational templates suggests that the disunity of science thesis that often accompanies the "models are local" thesis is simply wrong about the areas of contemporary science that lend themselves to the successful use of such templates. Secondly, it runs

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[7] See e.g. Winsberg (2001, 2003) and Lenhard (2007).

[8] See Humphreys (2002, 2004/Chapter 3, 2008).

[9] To prevent misunderstanding, I note that although the term "law" is used for such things as the weak and strong laws of large numbers in probability theory, this is a courtesy use of the term "law" because these are purely mathematical results. They lack at least the nomological necessity possessed by scientific laws.

orthogonally to the traditional reductionist approach to understanding. Reduction suggests to us that we can better understand higher level systems by showing how they can be reduced to, how they can be explained in terms of, lower level systems. Computational templates suggest that we can gain understanding of systems without pursuing reduction by displaying the common structural features possessed by systems across different subject domains. In saying this, I am not claiming that these trans-disciplinary representations did not exist prior to the introduction of computational science. What the latter development did was to allow the vastly increased use of these techniques in ways that made their application feasible.

I can illustrate the issue involved using as an example agent based simulations. Agent based simulations are in certain ways very different from what one might call equation-based simulations. It is a common, although not universal, feature of agent based models that emergent macro-level features appear as a result of running the simulation, that these features would not appear without running the simulation, that new macro-level descriptions must be introduced to capture these features, and that the details of the process between the model and its output are inaccessible to human scientists. No traditional modeling methods address the first, second, and fourth features of these simulations . Let me elaborate a little on how the third point plays out in this context. The situation has been nicely captured by Stephen Weinberg: "After all, even if you knew everything about water molecules and you had a computer good enough to follow how every molecule in a glass of water moved in space, all you would have would be a mountain of computer tape. How in that mountain of computer tape would you ever recognize the properties that interest you about the water, properties like vorticity, turbulence, entropy, and temperature?" (Weinberg, 1987, 434). Many of the "higher level" conceptual representations needed to capture the emergence of higher level patterns do already exist in other theoretical representations; they are the starting point for what Ernest Nagel called inhomogeneous reductions (Nagel, 1974). With other agent based models the situation is different because the simulation itself will, in some cases, construct a novel macro-level feature. It is this constructivist aspect of simulations, one that runs in the opposite direction to the traditional reductionist tendency of theories, that is a characteristic feature of agent based models in particular, although it also can be a focus of equation based models. Constructivism was memorably described in Anderson (1972) and is a key element of the arguments presented in Laughlin and Pines (2000).[10] These emergent patterns in computer simulations form the basis for what Mark Bedau has characterized as "weak emergence" (Bedau, 1997) and traditional human modeling techniques will not generate them from the agent base. They can only be arrived at by simulation.

This emphasis on higher level patterns is not restricted to computational science or to emergence. It is a feature of multiply realizable systems and of physical systems in which universality is exhibited. (For a discussion of the relations between

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[10] The use of generative mechanisms as an element of constructivism is noted in Küppers and Lenhard (2006).

Here the shift is first, from the complete abstraction from practical constraints that is characteristic of much of traditional philosophy of science, and second from the kind of bounded scientific rationality that is characteristic of the work of Simon and Wimsatt (Wimsatt, 2007), within which the emphasis tends to be on accommodating the limitations of human agents. Ignoring implementation constraints can lead to inadvisable remarks. It is a philosophical fantasy to suggest, as Manfred Stöckler does that "In principle, there is nothing in a simulation that could not be worked out without computers" (2000, 368).[12]

In saying this I am not in any way suggesting that in principle results are not relevant in some areas. They clearly are; there are also other issues to which the philosophy of science needs to devote attention. One of the primary reasons for the rapid spread of simulations through the theoretically oriented sciences is that simulations allow theories and models to be applied in practice to a far greater variety of situations. Without access to simulation, applications are sometimes not possible; in other cases the theory can be applied only to a few stylized cases.

Within philosophy, there is a certain amount of resistance to including practical considerations, a resistance with which I can sympathize and I am by no means suggesting that the investigation of what can (or cannot) be done in principle is always inappropriate for the philosophy of science. One source of resistance to using in practice constraints is already present in the tension between descriptive history of science and normative philosophy of science, and in the tension between naturalistic approaches (which tend to mean different things to different people) and more traditional philosophy of science. But the appeal to in principle arguments involves a certain kind of idealization, and some idealizations are appropriate whereas others are not. A long-standing epistemological issue involves the limits of knowledge. Are there things that we cannot know, and if so, can we identify them? There surely cannot be any question that this is a genuine philosophical problem. Of course, it is not new – Kant famously gave us answers to the question. The question of what we can know, or more accurately, what we can understand, has been transformed by the rise of computational science and it is partly a question of what idealizations can legitimately be used for epistemic agents. We already have experience in what idealizations are appropriate and inappropriate for various research programmes. The move away from hyper-rational economic agents in micro-economics to less idealized agents mentioned earlier is one well-known example. For certain philosophical purposes, such as demonstrating that some kinds of knowledge are impossible even in principle, in principle arguments are fine. But just as humans cannot in principle see atoms, neither can humans in principle be given the attributes of unbounded memory and arbitrarily fast computational speed. This is the reason underlying epistemic opacity, one of the key epistemological features of the new methods.

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[12] The first versions of Thomas Schelling's agent based models of segregation, and the first versions of Conway's Game of Life were done "by hand", but almost all contemporary simulations require abilities that go ~~so~~ far beyond what is possible by the unaided human intellect.

have to be supplemented with dozens of extra terms to account for various features. They therefore employ multiple approximations and are heavily computational. So the approximations chosen in the Hartree-Fock self-consistent field approach, a standard method of calculating ground state energies in ab initio quantum chemistry, are inextricably linked with the degree to which those calculations can actually be carried out in practice. On the other side there is now a growing sense that a different problem has arisen; that new techniques need to be developed to effectively exploit the massive computational power that is now available in many areas.[14]

Conclusion

Although some scepticism has been expressed about the novelty of computer simulations and related techniques (e.g. Stöckler, 2000; Frigg and Reiss, 2008; for a response see Humphreys, 2008), there is more than enough evidence to support claims that they constitute an important addition to the techniques of science, on a par with theoretical representations and experiment. The effect of this emplacement revolution in computational methods is a rich source of philosophical problems, metaphysical, epistemological, and representational.

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