Institutions for Simulations: The Case of Computational Nanotechnology

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Computational nanotechnology is a simulation science; that is, a way of producing scientific knowledge dependent upon computer simulations because, for a variety of reasons, current experimental set-ups do not answer crucial questions. The resource needs of simulation science have often been obscured by two assumptions – that simulations are a 'cheap' alternative to experiment and that they are closely connected to theory – though not simply synonymous with or simple extensions of theory. This paper challenges both notions by exploring the resources - human, financial, and computational – needed to perform computational nanotechnology and by showing the close coupling between empirical data and the construction of simulations. I look specifically at three U.S. computational nanotechnology sites and projects: the NASA-Ames Research Center, the Network for Computational Nanotechnology at Purdue University, and the Chemical Industry's Roadmap for Nanostructured Materials as a protocol for nanotechnological development that specifically addresses the role of simulations.

Keywords: Nanotechnology; Computational Nanotechnology; simulations

Simulations as a Mode in the Production of Scientific Knowledge

A tremendous amount of the energy expended in the philosophy of science - the vast bulk of epistemological thought in philosophy of science - is expended on the question of what theories are; how they are, can be, or should be structured; questions about the entities that they posit; and what they do and how they do it in scientific practice. However, in the past generation or two philosophical attention to experiment has escalated and one justification for this effort is the claim that experiments constitute the bulk of scientific activity and require an epistemology of their own (Hacking, 1983; Franklin, 1989; Baird, 2004). So we have an active and sometimes conten-

tious fight about whether theory or experiment constitutes the meat of science and, perhaps more importantly, which dimension serves the other. No one claims naively that the two are not interrelated and interdependent; instead, the debate is about relative epistemological position and hierarchy. But given the actual practices of scientists and the interdependency of theory and experiment in science the debate seems territorial rather than substantive and after a generation of philosophical fights, no one seems much wiser.

This contentious, bifurcated understanding of scientific practice is also the ground into which simulation science has been planted. Consequently, what philosophical literature that even exists about simulation always seems to address the theory-experiment split (Rohrlich, 1990; Winsberg, 2003). Are simulations parts of theory-world, part of experiment-world, a third category or hybrid? The claim that simulations are theoretical stems from the view that simulations are technically-enhanced or computer-aided models (Sismondo, 1999; Dowling, 1999). According to the semantic view of theories, theories are comprised of a class of models. Therefore one could draw the inference that, a simulation, as a kind of model, is the stuff of theory. This view is buttressed by claims by simulation scientists that their work is, in fact, theory (Drexler, 1992).

Others see simulation as virtual experimentation and push simulation into the experimentation category (Humphreys, 2004). This view is particularly problematic for two reasons, one being the mathematical structure of simulations which has no parallel in experiment. Even more problematic to the view of simulation as virtual experiments are the views of experimental scientists who claim that simulations have little or nothing to do with the "real world," that is the messy, laboratory basis of experimentation, so-called "wet-work." This is often the view of practicing experimentalists and instrument designers who dismiss, with prejudice, the creation of simulations as science fiction and not science (Baird, 2005). The problem with these two views of simulations either as an extension of or a special kind of either theory or experiment leads to the third position, which is now widely accepted by science studies scholars examining simulation. This claim focuses on the position that simulations are neither an extension of theory nor of experiment and might be seen in an intermediate or hybrid position between theory and experiment. A stronger position, which claims that simulations constitute a new mode in the production of scientific knowledge with some features in common with both theory and experiment but without being reducible to either, is increasingly common (Galison, 1996; Dowling, 1999; Winsberg, 2003). If one sees simulations as a third mode of inquiry or a third dimension of scientific practice, then they need to be integrated into what Pierre Duhem calls the way "science makes itself." The aim of this paper is to look at this process by focusing on the field of computational nanotechnology and by considering the resources necessary for the creation, dissemination, integration and acceptance of simulations by computational nanotechnologists.

Dispelling some Myths about Simulation Science

A science studies literature about simulations is just beginning to develop. As a matter of course, in this paper when I refer to science studies, I do so in a broadly inclusive way that includes the history and philosophy of science, as well as social science-based STS. The philosophical and epistemological literature of simulations is probably the best developed, owing largely to the important foundational work of Winsberg (1999; 2003), coupled with longer term attention to the production of scientific models from Cartwright (1983), Hacking (1983), Morgan and Morrison (1999). Consequently, to date, there has been only minimal examination of the social, institutional and financial resources needed to make simulations. However, addressing this practical dimension of simulation science does require the dismissal of at least one myth about simulations. It is not uncommon to find a claim that one of the chief values of simulations in present-day science is that they constitute a cheaper alternative to expensive and labour-intensive laboratory work (Humphreys, 2004). This claim is widely made by simulation scientists themselves (Merkle, 1991; King, 2000). Yet it is problematic for two different reasons, both of which need examination before any substantially new examination of the resources necessary for simulations can begin. The most important is the question of whether simulations are or can ever be epistemologically equivalent to experiments; that is, do simulations effectively replace laboratory experiments? As discussed above, the notion that they do is widely challenged in the nascent science studies literature of simulations (see particularly Winsberg, 2003), and articles on the epistemology of simulation are much more likely to describe simulations as a new mode of scientific production, rather than as a modification or extension of either theory or experiment. In short, the assumption that simulations replace laboratory work implies that simulations produce the same kinds of data as laboratory work, an implication that again fails to cohere with any examination of simulation as a scientific activity. Simulations are themselves based on laboratory data and only in the process of verification do simulations duplicate laboratory data.

In fact, no models or simulations are truly *ab initio* – that is, relying entirely on calculations from first principles (Scerri, 2004). Simulations are nearly always semi-empirical to a greater or lesser extent, even when not noted as such.[1] Simulations are normally used to calculate values not easily retrievable from purely theoretical models. If theories produced desired quantitative outputs, then simulations would scarcely be necessary. But simulations are often used as models to extend theoretical models to accommodate new empirical findings and to extend empirical data into new regions where empirical data do not exist for a variety of reasons that will be discussed later. Hence, nearly all simulations are, in fact, semi-empirical – more theoretically informed than completely empirical curve-fitting exercises, but not simply calculations from first principles. Furthermore, semi-empirical models and simulations ought not to be seen as epistemologically inferior to *ab initio* models, since this dimension of

being partially derived from theoretical principles and partly derived from empirical data is what makes these models both useful and valid. Claiming *ab initio* simulations to be better models makes sense only in a particular mode of the philosophy of science, wherein scientific knowledge or even science itself is defined as theory, full-stop.[2] From the more recent perspective of the epistemology of simulations, semi-empirical simulations are ideal, extending both experimental AND theoretical knowledge. Furthermore, being semi-empirical is what allows simulations to stand in for laboratory work when that work is not feasible; simulations are bound up with the "real" world to varying extents. The most common use of simulations and their chief value is that they can be done where laboratory work is limited. Laboratory work can be limited for all sorts of reasons. In the case of computational nanotechnology, instruments do not (perhaps, yet) exist that will allow nanotechnologists to either measure or manipulate all the nanoscale elements they would like. Simulations can be built from what is known from experiment and can extend those results into the dimensions which are instrumentally intractable. Other simulations are used to produce data which stands in for fully empirical data when experimentation will never be possible, as in the cases of meteorology, economics or evolutionary theory. Yet, despite the closer relationship, the dependence even, of simulation and experiment, I do not advocate the position that they replace experiment. Simulations simply do not do the same work as experiments. They do, however, rely on experimental knowledge for their creation. Nor do simulation scientists aspire for their work to replace experiment. Mathematical chemist Bruce King makes this clear in his argument that present day chemistry is comprised of a trichotomy of activities – experimental, theoretical and computational (King, 2000). Computational chemistry is not reducible to chemical theory, nor is it a weak stand-in for experiment.

Even having dismissed the claim that simulations are an unproblematic alternative to experiment, there is another questionable dimension to the assertion that simulations are a cheaper alternative to experiment. Are they, in fact, cheaper? This might seem a straightforward enough question about the cost of running a simulation facility versus the cost of running a laboratory, but in fact, there are a variety of resources that simulation production depends upon. Calculating the costs of all of these resources amounts to something quite a bit trickier than simply adding the cost of servers, software, programmers and information technology technicians and post-docs and comparing them to scientific instruments, laboratory technicians and post-docs. The main problem with a calculation, is the interdependence of simulations and laboratory science; fully accounting for the "cost" of simulations would require counting the cost of the laboratory work needed to construct the semi-empirical simulations. Similarly, doing a full accounting of the cost of laboratory work would include the salaries and equipment of the simulation scientists that are a part of nearly every nanotechnology laboratory - even those focused primarily on the development of instrumentation, such as Stanford's Center for Probing the

Nanoscale. If simulation and experimentation really are two integrally related activities, then separating and comparing their costs, is in actuality a rather dubious project. Accounting for the cost of simulating in such a simplistic way is actually based on a fictional understanding of the relation of simulation to scientific knowledge. Simulations are simply not a stand alone mode of producing scientific knowledge, but then again neither is theory or experiment. Examining the actual practices of simulation may very well lead to the conclusion that they are not a cost-effective alternative to experiment, but this also coheres with the epistemological claims that they do not simply replace experiment. Questions about the resources necessary for simulation science must spring from a fuller understanding of the place of simulation in the production of scientific and technological knowledge.

Onto a New, Institutional Understanding of Simulation Practices

If simulations are to be seen as a new mode of producing scientific knowledge, then substantive questions should be asked on how knowledge is produced in this mode. While philosophers like Winsberg have begun work on the epistemology of simulations and ethnographers like Dowling (1999) and Merz (1999) have begun studies of simulation scientists and their work, this paper focuses on an intermediate level of examination between epistemology and ethnography. I will examine simulations less abstractly and universally than philosophy usually does, but not as closely as a participant-observer would in an ethnographic project. Here I am looking more specifically at environments where simulations are situated and produced, and the resources which sustain these environments. Over the past decade, a complex of institutional arrangements has been created to facilitate and support the production of simulation science, particularly in nanotechnology. Rather than a run-down of the funding sources, amounts, and the machines and programs which characterize the field of computational nanotechnology - which would tell us very little about the socio-epistemological structures underlying the production of simulations, I will focus on different kinds of institutions. The three in particular I will examine are an NSF center, a government lab and an industry cooperative: the Network for Computational Nanotechnology, a multi-university NSF network (hereafter, NCN); the NASA-Ames Computational Nanotechnology group, a government laboratory; and the Chemical Industry Vision2020 Technology Partnership, an industry partnership. While all of these organizations are unique, they are also all representative of the kinds of institutions that back the development of simulations of the nanoscale.

The reason for examining the resources behind computational nanotechnology stems from a belief, well developed in science studies, as well as among academics in other disciplines, that resources shape and constrain the development of knowledge. By "resources," I do not mean to restrict my gaze to purely financial matters; rather, I include intellectual and human resources, as well as, the obviously impor-

tant class of technological resources. Resources directed to particular problems raise the status of those problems, increasing their attractiveness to graduate students and young scholars who are in the process of building their careers. At the same time, focusing resources on a particular, new set of problems usually implies that those resources were diverted away from other problems, making work in those areas less attractive and with scarcer rewards. Yet this ebb and flow is on-going and reversals occur. Furthermore, by attracting certain scientists and engineers at certain times to work on particular problems resource allocation shapes the multi-disciplinarity of the field (among other dimensions), which, in turn, shapes the work being done and the solutions presented. The result is that resources push and pull communities, privileging certain kinds of work at the expense of others. Social and epistemological factors are intertwined and both are dependent on resource allocation.

A Brief History of Computational Nanotechnology

There are at least two stories to tell about the origins of nanotechnology. While both reach back to Richard Feynman's 1959 speech "There's Plenty of Room at the Bottom" as a founding myth, the two stories diverge in the 1980s. The more common origination story follows the development of scientific instruments like the scanning tunnelling microscope as a way of instrumentally accessing the nanoscale world (Baird and Shew, 2004). The other, less common story details the development of computational methods for modelling the nanoscale (Bueno, 2004). There are multiple complicated reasons for the preference of the instrumental story over the computational, some of which are actually instructive for the study of simulations. Simplistically, the instrumental story is a success story, culminating in the 1986 Nobel Prize in physics for the inventors of the scanning tunneling machine, Gerd Binnig and Heinrich Rohrer. It also appeals to the science studies community, because of its instrumental basis; that is, it is a useful case study in the conceptual power of instruments (Baird and Shew, 2004). The computational story on the other hand remains a yet-to-be-realized dream - and experimental practitioners in nanoscale science often dismiss computation as somehow less "real" than instrumental manipulation at the nanoscale, which incidentally itself remains incapable of achieving the vision Feynman put forth in "Plenty of Room" (Baird, 2005). In addition, the actor at the center of the computational story is K. Eric Drexler, a figure who remains an outspoken proponent of a version of molecular manufacturing that is commonly ridiculed by chemists and instrumentalists (Smalley, 2003). At the core of this argument, whether the more legitimate origins of nanotechnology are instrumental or computational, is an argument about the relation of experiment to simulation as competing techniques for scientific development. Experimentalists deny the importance of computation because it isn't "real" (Baird, 2005). Computational nanotechnologists want credit for leading the science, for shaping the experimental pursuit of nanoscale manipulation (Drexler, 2003). Neither side is incorrect in their interpretation; both reflect the ethos and the stakes of their communities. The competition

for the ownership of nano is an instructive one for showing the ways that experiment and simulation are intertwined.

To shift the focus here to the computational story, it is necessary to remember that nanotechnology has always been closely associated with computational methods, in part because of its recent development. Even its instrumental developments rely on the development of computers for control systems and for the graphical output of the microscopes, which themselves generate algorithmic images "drawn" by computers. Nanotechnology is a field of inquiry which has developed more recently than the personal computer - since the mid-1980s. There was no nanotechnology before digital computers; one need not be concerned with how nanotechnology became computerised, in contrast to the application of the computer in, say, physics where one can see the way computers change what is calculable in physics, by examining a series of episodes in physics where the computer facilitates the production of new knowledge, for example, the development of Monte Carlo simulations or Ising models. As a result, nano is a particularly good case study for ways science and engineering develop completely within the realm of relatively inexpensive digital computers. Despite referring to his work as "theoretical applied science," Drexler is obviously a simulation scientist. In Drexler's vision of nanotechnology, "design calculations and computational experiments enable the theoretical study of these devices, independent of the technologies needed to implement them" (Drexler, 1992). This is a vision which privileges simulation over experimentation. Ralph Merkle, an early adherent of Drexler's vision and a computational scientist at Xerox PARC in the 1980s, shared Drexler's vision. Both Merkle's and Drexler's simulations and their hopes for simulations focused on bringing together the computational tools of chemistry and mechanical engineering. Thus the roots of computational nanotechnology are found in two predecessor simulation-based sciences: computational chemistry and computer-aided engineering.

It was Ralph Merkle who coined the term "computational nanotechnology" in a 1991 article in the journal, *Nanotechnology.* Merkle drew both the term and its methods from computational chemistry. From the beginning, computational nanotechnology has depended on three different levels of computer-aided modelling tools from computational chemistry. At the largest scale, classical molecular dynamics show the relationships of molecules using classical calculations without any consideration of quantum mechanics. Classical molecular dynamics models can be quite large – modelling the collective behaviour of hundreds of thousands of atoms – without becoming computationally intractable. However, they are not useful for modelling detailed changes in chemical bonds, and therefore are limited in their description of chemical behaviour. Moving to a smaller scale of investigation, semi-empirical methods include tight-binding molecular dynamics models, which begin to consider density functional theory and quantum effects, but draw these effects from empirical data rather than first principles' calculations. At the finest-grained level of examination, *ab initio* models are built up from

first principles to a much greater extent, keeping in mind Scerri's (2004) well-stated skepticism about the feasibility and legitimacy of complete dependence on first principles' calculations. *Ab initio* simulations usually account for full quantum behaviour, but end up being computationally intractable for anything other than very small molecular systems – systems involving so few molecules as to be uninteresting to many nanotechnologists. Obviously, bridging between scales was and is a central concern in nanoscale simulation, and scale bridging depends on making these models computationally coherent and tractable, despite the fact that they are obviously theoretically incommensurate as they move between classical and quantum worlds. Merkle's interest in computational models of molecular systems came from nanotechnologists' inability to build any of the molecules he wanted to design in 1991. The computer screen acted as the only experimental space that would allow Merkle to design molecular machines. Merkle believed it was simply a matter of developing more computing power before large scale *ab initio* calculations would be able to model the nanoscale accurately. Merkle argued that this time of great computing power would come, the result of a few more generations of Moore's Law increasing computational capacity. The job of the computational scientist was to be ready for this eventuality rather than sitting and waiting for it happen.

Being prepared for advances in information technology entailed modelling systems which were computationally tractable, even if that meant the level of detail was less than ideal. Merkle justified the use of computer-aided molecular design in a very specific way. He argued from his experience in computer science that computer-generated models in a number of fields had proven to be reliable indicators of the feasibility of various mechanical configurations. According to Merkle, knowing that a system will be feasible even though the technology to actually construct it does not yet exist, will accelerate the process of developing the technology to build molecular machines. Computer simulations allow the development of assembler technology to be carried out in a parallel, modular process, instead of a linear, serial one. In this way computer simulations promise to accelerate the development of actual assembler technology, by pinpointing the best routes to development. Merkle writes:

> Doing things in the simple and most obvious way often takes a lot longer than is needed. If we were to approach the design and construction of an assembler using the simple serial method, it would take a great deal longer than if we systematically attacked and simultaneously solved the problems that arise at all levels of the design at once and the same time. That is, by using methods similar to those used to design a modern computer, including intensive computational modelling of individual components and sub-systems, we can greatly shorten the time required to design and build complex molecular machines (Merkle, 1991).

Institutions for Computational Nanotechnology: NASA-Ames

In the early 1990s Merkle generated interest for computational nanotechnology in Silicon Valley, and his work, at least in part, led to the creation

of a computational nanotechnology research group in the Numerical Aerodynamic Simulation Systems Division (NAS) at NASA's Ames Laboratory at Moffett Field in Silicon Valley. At Ames NASA has developed techniques for modelling nanosystems, particularly novel nanomaterials and nanomachines that have not only extended computational chemistry techniques, but also transformed these tools by adding other simulation methods from other disciplines. While Merkle claimed that the existing commercial computational chemistry software packages in 1991 were sufficient to design and test a number of critical components for the construction of molecular machines (on the computer, that is), the subsequent development of new techniques has made that claim look increasingly naive (Musgrave *et al.*, 1991). Over the decade of the 1990s, computational nanotechnology research evolved its own computer-aided methods that were more than simply borrowed techniques from chemistry, bringing in ideas, theories, and software largely from engineering and computer science.

In 1998, Merkle co-authored a paper on "NASA applications of molecular nanotechnology" in the *Journal of the British Interplanetary Society* (Globus *et al.*, 1998). His six co-authors all worked at the NASA Ames Research Laboratory. The paper laid out a number of products and materials which NASA researchers were working on, all of which promised great importance in space research and travel. Most of the developments named in the article were to take advantage of significantly improved strength-to-weight ratios of nano-manufactured, diamond-like carbon materials. While the 1998 article was not exclusively devoted to computational methods, the importance of computer models was reinforced in the article's conclusion:

> ...it is clear that computation will play a major role regardless of which approach... is ultimately successful. Computation has already played a major role in many advances in chemistry, SPM manipulation, and biochemistry. As we design and fabricate more complex atomically precise structures, modeling and computer-aided design will inevitably play a critical role. Not only is computation critical to all paths to nanotechnology, but for the most part the same or similar computational chemistry software and expertise supports all roads to molecular nanotechnology. Thus, even if NASA's computational molecular nanotechnology efforts should pursue an unproductive path, the expertise and capabilities can be quickly refocused on more promising avenues as they become apparent (Globus *et al.*, 1998).

In 1997, the year before the appearance of this article, a research team for computational nanotechnology had been created at Ames. Locating the team at Ames was an important step, since Ames is NASA's high speed computing research facility. The Ames location facilitated cross fertilization between nanotechnology and developments in computer science and programming. In addition, computational nanotechnologists would be able to access easily and freely the high-end supercomputing and parallel computing facilities at NASA.

Yet, these visions of the capacity of computational models remain unrealized in 2006. Nearly a decade after Merkle's 1998 statements about the feasibility of computational chemistry tools, the systems he was most inter-

ested in modelling have not been made tractable by developments in memory and parallel computing to be able to include full quantum effects. Other techniques, from engineering, have been blended with computational chemistry in order to simplify molecular machines and make their properties manageable. The last thing Merkle or NASA advocated was waiting for developments in computing technology to catch up with the kinds of problems they were interested in solving. Problems needed instead to be re-parsed in ways that would make them tractable. They found many resources for this process in the fact that mechanical engineers had been doing this kind of simplification for decades.

From the perspective of resources for simulation, there are several important dimensions to the research enterprise at NASA-Ames. First is its location. Scientists and engineers at Ames have excellent access to state of the art supercomputers and massively parallel computer clusters. This diverts speculation of what would be possible given access to better computing and focuses their research efforts on the greatest existing capacity for computation. The Silicon Valley location also matters for the ease of bringing in new programming tools from the private sector, as well as other computing institutions in the area, from Xerox PARC to Stanford. Since programmers are easily "jobbed-in" to work on specific projects, new ideas about programming flow in and out of NASA-Ames in a way that is predicated on its location in the heart of computing research. NASA's space orientation also matters as a resource for the development of computational nanotechnology at Ames. The kinds of projects NASA works on often have to do with nanostructured materials, particularly smart materials, wherein electronic and chemical capabilities are included in structural materials. The potential weight savings of such materials with a variety of capacities is very attractive to NASA. This privileges certain kinds of research while disadvantaging others. As a result, some of the most significant work at Ames focuses on the interdependent chemical, electrical and mechanical properties of the carbon nanotube. While computational nanotechnologists work on simulating nanotube behaviour under a variety of different kinds of stresses, others, mostly chemists, work on laboratory and manufacturing techniques to produce these nanotubes in bulk. Neither the computational nor the laboratory work stands alone – each side gains from NASA's success in the other venue. NASA's laboratory was one of the first government laboratory programs in computational nano, and has become a model for other government labs that combine experimental and computational research programs, such as the theory group at Argonne's National Laboratory's Center for Nanoscale Materials, a Department of Energy centre that brings together nanostructured materials research with a historic focus on high-end computing.

Institutions for Nanotechnology: Network for Computational Nanotechnology

While computational nanotechnology research was well underway in the twilight of the twentieth century, nanotechnology exploded onto the political agenda with the creation in 2000 of the National Nanotechnology Initiative

(hereafter, NNI) in the U.S.. Europe and Japan had both simultaneous initiatives and nearly immediate responses to the NNI; other nanotechnology participants in Asia – primarily India, China, and South Korea – also followed suit. Computational work has hardly been ignored in these new funding and policy regimes. In 2001 the National Science Foundation, acting under the aegis of the National Nanotechnology Initiative, put out a call for proposals for a centre for computational nanotechnology. Mihail Roco is quoted describing the vision for the centre in the following way:

> We envision a national center of excellence where academic and industry nanotechnologists will share the most advanced simulation tools for understanding and designing novel materials, catalysts, electronics, pharmaceuticals, molecular manufacturing technologies, energy conversion devices and many other things that would not have been possible otherwise. (Lundstrom, 2002)

The centre was awarded to a network of universities including Northwestern, Morgan State University, the University of Illinois at Urbana-Champaign, the University of Florida, the University of Texas at El Paso, Stanford, and based at Purdue University in Indiana. While this network is the only one in the U.S. National Nanotechnology Initiative focusing explicitly on simulations, it is clear from the NCN's self-descriptions that it does not focus solely on simulations or see simulation as a stand-alone producer of new scientific knowledge. For example, in the award abstract, the NSF established the NCN "with a three-fold mission:

> 1. to catalyze the formation of theorists, computational scientists, and experimentalists in research that addresses key challenges in realizing novel nanosystems;
>
> 2. to support the research and the broader National Nanotechnology Initiative with an infrastructure that provide ready access to high-performance computing and visualization, facilities coordination, delivers simulation services, and enables solutions to large multiscale problems by assembling standard open-sources components that are available to the entire community; and
>
> 3. to develop educational packages that can be incorporated into the curricula to train students, scientists, and engineers." (NSF, 2004)

While visions offered in abstracts can have multiple motives, once the grant is secured the institution develops a track record to which the actual commitments of the institution can be compared. This rhetoric of multiple modes of knowledge production continues in NCN's descriptions since the award has been made and is reflected in the publications which credit the NCN for support. Mark Lundstrom, Principle Investigator and Director of the NCN, has emphasized his interest in extending nanoscale simulation research in many directions, crossing disciplines and length scales. However, this extension is always done in ways that "tightly couples computational experts and experimentalists" (Lundstrom, 2002). The vision of the NCN is not one that sends simulations way out in the "wild blue yonder" of science fiction, while the experimentalists stay tied securely to reality. Instead the vision of the NCN is to advance simulation and extend what can be feasibly produced and

scaled up in a lockstep manner. As a result, network members provide not only simulation scientists and facilities, but also the concurrent commitment to bridging between experiment and simulation, with the hope that keeping the two activities closely coupled would shorten the development times on a wide variety of nanoscale research projects. Merkle's vision of computational models shortening laboratory development time is also repeated by the leaders of the NCN. In order to have the best chance of showing results, the main resources of the NCN have been focused in three general areas of simulation: nanoelectronics, including both carbon nanotubes and molecular devices; nano-electro-mechanical systems (NEMS); and Nano-bio transport modelling. Each of these areas has a multidisciplinary team of researchers from NCN host institutions. On all four teams at least 25% of the personnel (on average, 2 out of 8) are experimentalists whose work will closely lead, follow or cohere to trajectory of developments in simulations.

The cost of supporting both simulations and experiment is reflected in the budget of the NCN, which is $2,848,333 in 2005 (NSF, 2005). The average annual budget for the 14 NSF nanotechnology centres (not including figures from the first year of operation) is $2,370,865 (NSF, 2005). While it is obviously meaningless to derive any scale of importance based on single year budgets, it is important that the NCN is comparable to virtually every other NSF centre for nanotechnology with the one exception of the obviously larger National Nanotechnology Infrastructure Network ($7 million in 2005). As is true in much research and development, the primary cost of a centre for nanotechnology of any kind, simulation-oriented or not, is personnel. However, at the NCN the research mission is coupled to an equally important effort in making the tools developed at NCN and other centres available to the computational nanotechnology community. At the NCN this is done through the Nanohub, a website which facilitates remote access of simulation tools. In addition to serving remote users, Nanohub also makes available open source codes for incorporation into new simulation tools being developed by users of the Nanohub both within and outside of the NCN. In September 2005, the site received over a half-million hits. The programs run analyses on computer clusters located at Purdue. The primary cluster is a 200 CPU parallel Linux cluster called Superman, which was purchased using two US Department of Defence grants (Purdue Computational Electronics, 2005). Jobs on the Nanohub are managed by a portal called PUNCH which allocates computing resources and "allows the transparent use of workstations, supercomputers and linux clusters" (Goasguen, 2003). The targeted users of Nanohub are not the scientists and engineers involved in the research mission of the NCN; rather, 80% of Nanohub users are undergraduates (Goasguen, 2003). This reflects the educational goal of the NCN. The explicitly educational goals of the NCN are indicative of growing demand for the scientists and engineers who will create the next generation of simulations and will be able to bring together the interdisciplinary resources along with an understanding of the needs to maintain the relationship

between simulation and experiment.

In examining the organizational structure of the NCN, as is common in many centres for nanotechnology, one notices quickly that organizational lines are not drawn between disciplines, but are, instead, problem-oriented as in the research teams detailed above. In the case of the NCN the construction of both the research areas and the organization of Nanohub are multidisciplinary and oriented toward particular problems which have not been solved within existing socio-institutional arrangements, such as academic departments or disciplinary centres. For example, in the nano-bio research field, the main project is to use simulations for carrier transport in semiconductors as models for simulations of transport in ion channel bio transport systems (NCN, 2005). This field is so clearly multidisciplinary that an institution like the NCN is uniquely able to bring together simulation resources – particularly human resources – to bridge science and engineering; "wet" chemistry and electrical engineering; molecular biology and algorithm design; simulation predictions to laboratory achievement. Thus, the lessons drawn from NCN again points to the difficulty of separating simulation from experiment, undermining claims of simulation as science fiction or of an independent third mode of scientific knowledge production.

Institutions for Nanotechnology: The Chemical Industry Roadmap

On December 12, 2003 a U.S.-based chemical industry consortium named The Chemical Industry Vision2020 Technology Partnership released a report titled "R&D Roadmap for Nanomaterials by Design" (Chemical Industry, 2003). As a third kind of institutional resource, this roadmap shapes and constrains the kinds of simulations created for nanotechnology. The purpose of the roadmap is to coordinate research in nanostructured materials so that development will be more rational, direct, and faster. This is also the goal or purpose of the NCN and of NASA-Ames, though not so explicitly and without the profit motivations of the chemical industry so clearly in view. But the roadmap is also a resource in that it aims to organize effort and labour and more importantly sets benchmarks for developments in different modes of scientific knowledge production. Organized into four concurrent research areas: fundamental knowledge, tools, modelling, and manufacturing capability, the Roadmap claims to be an attempt to move problem solving to an application-driven basis, instead of a discovery-based activity.

However, this contrast only works if a naive, Vannevar Bush version of "pure science" is used as a foil. Clearly the move to "application-based problem solving" happened centuries ago in the engineering profession and at least a century ago in the chemical industry itself in the origins of the industrial research laboratory. What is more novel about the Roadmap is its vision of the interconnectedness and interdependence of the four modes of knowledge production it breaks science into. In distinction to claims about theory versus experiment versus simulation, the Roadmap's version is much more organic claiming,

> "The nature of working at the nanoscale dictates the need to simultane-

> ously integrate R&D in fundamentals and synthesis, manufacturing, tools and modelling. Breakthroughs in each area will provide capabilities to enable progress in other areas, ultimately leading to cost-effective manufacturing and integration into applications (i.e., fundamentals to function). An exceptionally high degree of interdependent, multidisciplinary R&D performed by diverse stakeholders is required, amounting to a cultural change in the way science and technology are pursued" (Chemical Industry, 2003).

For a document produced by industry and aiming at manufacturing this rhetoric of cultural change in science is, to say the least, unexpected. At the same time, the language and the vision are clearly borrowed from the U.S. National Nanotechnology Initiative, which ultimately justified an annual nanotechnology budget by the US federal government of more than one billion dollars.

In the section on modelling and simulation, the need to maintain ties between simulations and the laboratory is just as explicit as it is in the NCN. After giving a list of fifteen different disciplines necessary to produce the simulations of 2020, the report claims,

> "A new modeling paradigm is needed to combine lessons learned from experiments across the field of nanotechnology. It will be used to extrapolate properties (such as electronic, chemical, structural, toxicological, and environmental) from known conditions and apply them to novel cases. These models will be able to help design experiments, increase the efficiency of research, recognize and assess emergent properties, accurately predict performance, reduce the required number of design iterations and experiments, and reduce the number of tools for design" (Chemical Industry, 2003)

Given the nearly half-century long history of producing simulations, much of which is characterized by the kind of give and take implied by the chemical industry, calling this interaction a new paradigm seems, at best, a stretch. Yet the existence of the roadmap, which is modelled conceptually if not formally on the Sematech roadmap, that is the semiconductor industry's consortium, is an indication that something is new about the role of the interactions of theory, experiment and simulation. The Roadmap is a corporate attempt to rationalise the production of science by making the process linear which in practice is often characterized by apparently endless feedback loops between what simulations predict and experimental refutations and confirmations.

The Roadmap also sets three priority areas in modelling and simulation: developing better predictive models with a 20-year timeframe; developing new methods and approaches to bridge length scales and tie existing models together over the next 20 years; and improving the research infrastructure to support simulation, particularly through an educated workforce, over the next decade. Yet the importance of experiment and theory to simulation is not a one-way street. In the section on Characterization Tools, several simulation and information technology desiderata are presented showing that experimentalists are explicitly looking to simulation for improvements (as is also the case with the incorporation of simulation science at the instrument-oriented Stanford University Center for the Probing the Nanoscale).

Even though the explicit organization of the Chemical Industry's roadmap

separates theory, experiment and simulation, upon closer inspection it too generates resources to bring simulation and experiment, in particular, together. It is also geared toward using simulation as a catalyst for experiment and manufacturing, repeating the explicit hopes of Merkle and Drexler and the mission and vision of the NCN. Yet the chemical industry, both as a commercial enterprise and as a roadmap constitutes a different kind of institutional resource from the previous two, since it is laying out a coordinated timeline of activities rather than a funding scheme. Yet, the timeline and the coordination is, in some senses, indicative of the new three-headed hydra of scientific knowledge production, and the chemical industry seems to have rightly identified the problem as one of coordination rather than simple funding.

Conclusion

Nearly a century ago, in *The Aim and Structure of Scientific Theory*, physicist and philosopher Pierre Duhem (1954) saw the iterative relationship between theory and experiment as the dynamic through which science makes itself. Yet, these iterations were also hierarchical in Duhem's thinking - theory was the outcome; experiment simply an instrument to produce theory. In this paper I have asked how nanotechnology simulations (and the institutions necessary to support them) in the United States affect the dynamics through which science makes itself. In one sense, we clearly add a dimension and therefore a layer of complexity. Science makes itself through the interactions of theory, instruments, simulations, and manufacturing, at least according to the Chemical Industry's Nanomaterial Roadmap. This is not a strictly epistemological question, but rather one which requires attention to institutions, infrastructure, and the social construction of scientific knowledge. But the change represented by simulations in science is more than one of a more complex dynamic with more dimensions. In fact, Duhem's notion of science no longer fits. Science making itself in the age of nanotechnology has to do with making products (in a general sense here, molecules are the products). Producing those products looks a lot more like engineering, which has since the 1950s proceeded through a complex interaction of theory (or what Walter Vincenti more accurately refers to as "theoretical tools"), mathematical models which can be computer-aided - therefore simulations - and the material world. Science studies scholars from John Ziman to Helga Nowotny have examined what they see as newly commercialized modes of scientific production, but Duhem's problem remains. How does science make itself? The rub is that we need to be clear about what that science is. In the case of nanotechnology that science involves a significant design quotient, which is not unique to nanotechnology but which further complicates the disciplines and institutions nanotechnology must straddle, in that it sits between science and engineering, and this gap clearly requires institutional scaffolding to span.

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Notes

1 It is also important to note that scientists, particularly chemists, use the term "semi-empirical" themselves, and they do not necessarily use it with the epistemological specificity of philosophers of science.

2 Fortunately, this mode is becoming rarer and rarer as philosophers of science respond to the practice turn in science studies.

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