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34. Computer Simulations and Computational Models in Science

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Computational science and computer simulations have significantly changed the face of science in recent times, even though attempts to extend our computational capacities are by no means new and computer simulations are more or less accepted across scientific fields as legitimate ways of reaching results (Sect. 34.1). Also, a great variety of computational models and computer simulations can be met across science, in terms of the types of computers, computations, computational models, or physical models involved and they can be used for various types of inquiries and in different scientific contexts (Sect. 34.2). For this reason, epistemological analyses of computer simulations are contextual for a great part. Still, computer simulations raise general questions regarding how their results are justified, how computational models are selected, which type of knowledge is thereby produced (Sect. 34.3), or how computational accounts of phenomena partly challenge traditional expectations regarding the explanation and understanding of natural systems (Sect. 34.4). Computer simulations also share various epistemological features with experiments and thought experiments; hence, the need for transversal analyses of these activities (Sect. 34.5). Finally, providing a satisfactory and fruitful definition of computer simulations turns out to be more difficult than expected, partly because this notion is at the crossroads of difficult questions like the nature of representation and computation or the success of scientific inquiries (Sect. 34.6). Overall, a pointed analysis of computer simulations in parallel requires developing insights about the evolving place of human capacities and humans within (computational) science (Sect. 34.7).

For several decades, much of science has been computational, that is, scientific activity where computers play a central and essential role. Still, computational science is larger than the set of activities resorting to computer simulations. For example, experimental science, from vast experiments in nuclear physics at the European Organization for Nuclear Research (CERN) to computational genomics, relies heavily on computers and computational models for data acquisition and their treatment, but does not seem to involve computer simulations proper. In any case, there is a great and still proliferating variety of types of computer simulations, which are used for different types of inquiries and in different types of theoretical contexts. For this reason, one should be careful when describing the philosophy of computer simulations and nonjustified generalizations should be avoided. At the same time, how much the development of computer simulations has been changing science is a legitimate question. Computer simulations raise questions about the traditional conceptualization of science in terms of experiments, theories and models, about the ways that usual scientific activities like predicting, theorizing, controlling, or explaining are carried out with the help of these new tools and, more generally, how the production of scientific knowledge by human creatures is modified by computer simulations. Importantly, while the specific philosophical analysis of computer simulations is recent (even if it was preceded by the development of the philosophical study of scientific models) and computational science is a few decades old, the development of computational tools and mathematical techniques aimed at bypassing the complexity of problems belongs to a much older tradition. This means that claims about how much computer simulations change science, and how much a closer attention to computer simulations should change our picture of scientific activity, are questions to be treated with circumspection.

34.1 Computer Simulations in Perspective

When discussing philosophical and epistemological issues related to computational models and computer simulations, different chronologies should be kept in mind. The blossoming of the philosophy of models and simulations, within the philosophy of science is something recent (Sect. 34.1.1). The development of techniques aimed at extending our inferential and computational powers corresponds to a longer trend, even if the recent invention of powerful digital machines has changed the face of computational science (Sect. 34.1.2). Finally, the acceptation of computer simulations as legitimate scientific tools across the different fields goes at various paces (Sect. 34.1.3). This means that, even if computer simulations do change the face of science, much care is needed when analyzing the aspects of science which are actually changed, and how we should modify our picture of science when we adopt a computer simulation-based perspective (Sect. 34.1.4).

34.1.1 The Recent Philosophy of Scientific Models and Computer Simulations

While the use of computer simulations in the empirical sciences, in particular physics, developed after the construction of the (ENIAC) computer during World War II [34.1], and started changing how the empirical sciences were practiced, for decades computer-related discussions among philosophers were primarily focused on the development of artificial intelligence and the analysis of human cognition. Particularly active were debates in philosophy of mind regarding the question of the *computational theory of the mind*, that is, whether the mind can be likened to a digital computer, and in particular to a classical machine employing rules and symbolic representations [34.2–6]. However, within the mainstream philosophy of science, continued interest for computational science, computational models, and digital simulations of empirical systems as such did not really start until the early 1990s, with articles by *Humphreys* [34.7, 8], *Rohrlich* [34.9] or *Hartmann* [34.10]. (Such a description of the field is necessarily unfair to earlier works about the use of computer simulations in the empirical sciences. Particular mention should be given to the works of *Bunge* [34.11] or *Simon* [34.12].) An article by *Hughes* about the investigations of the Ising model [34.13], a special issue of *Science in Context* edited by *Sismondo* [34.14] and works by *Winsberg* [34.15–17], who completed his Ph. D. in 1999 about computer simulations, also contributed to the development of this field. Finally, in 2006, the *Models and Simulations* Conference took place, which was the first of what was to become a still active conference series, which has contributed to making the issue of computational science one of the fields of philosophy of science.

Philosophical works about scientific models, a very close field, were not significantly older. The importance of the notion of set-theoretic model had been emphasized by partisans of the model-theoretic view of theories in the 1970s, but, if one puts aside works by pioneers like *Black* [34.18] or *Hesse* [34.19], this did not launch investigations about scientific models proper. Overall, the intense epistemological study of models did not start until the 1980s, with in particular a seminal article by *Redhead* about scientific models in physics [34.20]. Members of the *Stanford School* also argued against the view that science was unified and that theories played a dominant role in scientific activities such as the selection and construction of models [34.21], and conversely emphasized the autonomy of experimental and modeling practices. This context was appropriate for an independent investigation about the role of models in science, which bloomed at the end of the 1990s [34.22] and was further fed by a renewal of interest for the question of scientific representation [34.23–25]. These investigations of models paved the way for new studies focused neither on theories nor on experiments. However, while the difficulty to explore a model was already acknowledged in works by Redhead and Cartwright, interest for the actual modes of its exploration, in particular by computer simulations, was not triggered. Indeed, the focus remained on the effects of the complexity of the inquiry on scientific representations, with studies about simplifications, approximations, or idealizations (Even *Laymon*'s 1990 paper [34.26], in spite on its apparent focus on computer simulation, mainly deals with the nature of approximation and what it is to accept or believe a theory.), or how to articulate the model-theoretic view of theories and the uses of models and representations in actual scientific practices, by taking into account scientific users, qua intentional cognitive creatures [34.27, 28], and their cognitively constrained ways to handle models by means of inferences, graphs, pictures or diagrams (*Kulvicki* [34.29], *Giardino* Chap. 22, this volume; *Bechtel* Chap. 27, this volume). Overall, in spite of the close connection within scientific practice between the uses of models and their computational explorations, the issue of computational models and computer simulations was not seen clearly as a fruitful field of inquiry of its own, this trend of thought being explicitly and vividly brought to the fore in 2008 in a deliberately provocative paper by *Frigg* and *Reiss* [34.30].

34.1.2 Numerical Methods and Computational Science: An Old Tradition

The second relevant chronology is that of the advancement in attempts to solve complex mathematical problems by developing computing machines and mathematical methods. Importantly, while the development of digital computers in the mid-twentieth century changed the face of scientific computation, humans did not wait for this decisive breakthrough to extend their mathematical and computational powers. Further, as *Mahoney* wrote it, "the computer is not one thing, but many different things, and the same holds true of computing" [34.31], and it is only in the twentieth century that different historical strands related to logic, mathematics, or technologies came together. On the one hand, early mathematical procedures, like Newton's method to find the roots of real-valued functions, or Euler's method to solve ordinary differential equations, were developed to provide numerical approximations for problems in numerical analysis. This field was already important to investigate physical systems but, with the advent of digital computers, it became a crucial part of (computational) science. On the other hand, mechanical calculating tools, such as abacuses or slide rules, were used from the Antiquity through the centuries. The invention by Pascal of a device (the *Pascaline*) to perform additions and subtractions, and the conceptualization by Babbage of mechanical computing systems fed by punched cards, were important additional steps. *Human computers* were also used. For example, in 1758, Clairaut predicted the return of Halley's comet, by dividing the computational work with other colleagues [34.32]. Gaspard de Prony produced the logarithm and trigonometric tables in the early nineteenth century by dividing the computational tasks into elementary operations, which were carried out by unemployed hairdressers with little education. Human computers were used during World

War I to compute artillery tables and World War II to help with the Manhattan project [34.33, 34]. Finally, mechanical analog computers were developed for scientific purposes by engineers and scientists like Thomson or Kelvin, in the late nineteenth century, Vannevar Bush, between the two World Wars, or Enrico Fermi, in 1947, and such computers were used till the 1960s. Finally, even in the digital era, new technological change can have a large impact. For decades, access to computational resources was difficult and only possible in the framework of big projects. Typically, *Schelling*'s first simulations of residential segregation [34.35] were hand made. An important recent step has been the development of personal computers, which has brought more flexibility and may have triggered the development of new modeling practices [34.36].

34.1.3 A More or Less Recent Adoption Across Scientific Fields

The development of computational science and the use of computational models and simulation methods vary from one field to another. Since the 1940s onward, computer simulations have been used in physics, and computers were also used in artificial intelligence as early as the late 1950s. However, some fields have resisted such methods, and still do, as far as commonly accepted mainstream methods are concerned. Typically, the development of computational models and computer simulations in the human and social sciences, with the possibility of analyzing diachronic interactions between agents (versus static models describing equilibria) is much more recent. As emphasized earlier, Schelling's initial dynamic model of segregation was first run manually in 1969. Attempts to use computational science to predict social and economic behavior were globally met with suspicion in the 1960s and 1970s, all the more since these studies were often carried out by scholars who did not belong to well-entrenched traditions in these fields (such as scientists studying complexity, including human behavior, in institutions like the Santa Fe Institute). Overall, in economics, computer simulations are still not accepted [34.37]. Similarly, the development of a specific (and still somewhat distinct) subfield using computational methods to analyze social phenomena is recent, with the edition by *Hegselmann* et al. of the volume *Modelling and Simulation in the Social Sciences from the Philosophy of Science Point of View* [34.38], the need felt to create, in 1998, the *Journal of Artificial Societies and Social Simulation* and the publication in 2005 of the handbook *Simulation for the Social Scientist* by *Gilbert* and *Troitzsch* [34.39].

34.1.4 Methodological Caveat

These different chronological perspectives call for the following comments.

First, philosophers should be careful when developing an epistemology of computational models and computer simulations. Modeling and simulating practices have been developed in various epistemic contexts in scientific fields in which well-entrenched theories are more or less present and which have different methodological and scientific norms. Thus, the role of computer simulations and their epistemological assessment can significantly differ from one case to another, and bold generalizations should be carefully justified or avoided. As just mentioned, the use of computer simulations is central and accepted in fields like climate science (even if it raises important problems) but is still regarded with great suspicion in fields like economics [34.37, 40].

Second, how much computational models and computer simulations correspond to epistemologically different practices, which should be described in terms of some *computational turn*, cannot be assumed, but should be investigated on a case-by-case basis regarding all potentially relevant aspects. This can be illustrated with the question of the tractability of scientific models. *Humphreys*, in his 2004 book *Extending Ourselves*, proposes the following two principles to analyze science: "It is the invention and deployment of tractable mathematics that drives much progress in the physical sciences"; and its converse version: "most scientific models are specifically tailored to fit, and hence are constrained by, the available mathematics" [34.41, pp. 55–56]. These two principles suggest both a continuist and discontinuist reading of the development of science. First, students of science need to assess which precise aspects of scientific practices have been changed by the development of computers and whether these changes should be seen as a scientific revolution, or simply as an extension of existing modes of reasoning [34.42]. In this perspective, questions about the tractability and complexity of models can no longer be ignored, and may be crucial to an understanding of how new branches of modeling and computational practices can develop and of how the dynamics of science can be qualitatively different [34.43]. At the same time, scientific practices were also constrained by the available mathematics before the advent of computers, and new findings in mathematics already paved the way for the development of new scientific practices. For example, *Lakatos* emphasizes that [34.44, p. 137]

> "the greatness of the Newtonian programme comes partly from the development – by Newtonians of

classical infinitesimal analysis which was a crucial precondition for its success."

From this point of view, a continuist reading is also required.

Third, the computational perspective may require partly revising the philosophical treatment of questions about science, and scientific representation in particular. Computer simulations are *actual* activities of investigation of scientific models, and, for this reason, the tractability and computational constraints that they face can hardly be ignored when analyzing them. They force us to adopt an in practice perspective, where what matters is not the logical content of representations (that is, the information which agents can access in principle, with unlimited resources), but the results and conclusions which agents can in practice reach with the inferential resources they have [34.41, §5.5]. By contrasts, traditional analyses of scientific models adopt an in-principle stance: the question of their exploration and of the tractability of the methods used to explore them is one question among others, and is implicitly idealized away when discussing other issues. This implies surreptitiously smuggling in the unjustified claim that the distinction between what is possible in principle and what is possible in practice can be ignored for the investigation of these other issues, which may sometimes be controversial.

At the same time, philosophers of science draw their examples from the scientific literature, which, by definition, presents successful investigations of models which must have been found to be, one way or another, tractable enough regarding the inquiries pursued. In brief, discussions about the scientific models which are found in scientific practices are ipso facto concerning computationally tractable models, or models having computationally tractable versions.

How much these remarks imply that existing analyses about scientific models have been discretely skewed, or on the contrary that the constraints of tractability have already been taken into account, needs to be ascertained, and the answer may be different depending on the question investigated. For example, for decades the question of the relations between fields has mainly been treated in terms of relations between theories. While this perspective is in part legitimate, recent investigations suggest that tractable models may also be a relevant unit to analyze scientific theoretical, methodological or practical transfers between fields [34.41, §3.3], [34.45, 46]. In any case, when discussing questions related to scientific representation, explanation, or confirmation, philosophers of science must watch out that answers may sometimes differ for the models that scientists work with daily (and which more and more require computers to be investigated), and for simple analytically solvable models, which philosophers more naturally focus upon, and which may have a specific scientific status regarding the construction of knowledge and the development of families of models in each field.

34.2 The Variety of Computer Simulations and Computational Models

Computer simulations involve the use of computers to represent and investigate the behavior of physical systems (Sect. 34.2.1). Beyond this simple characterization, various types of computer simulations can be met in science, each with its specificities, and, it is important to distinguish them to avoid undue extrapolations. Differences can be met at various levels of description. Computing machines can be digital or analog (Sect. 34.2.2). Digital computers are usually used to carry out numerical computations (Sect. 34.2.3), even if all computer simulations do not involve operations on numbers (Sect. 34.2.4). In both cases, computations may be deterministic or nondeterministic (Sect. 34.2.5). Finally, various types of mathematical and physical computational models can be met across science, such as equation-based models, agent-based models, coupled models or multiscale models, but, not all important computational methods or mathematical frameworks are used to carry out computer simulations (Sect. 34.2.6).

My purpose in this section is to present and characterize different important types of simulations, which are used in scientific practice and will regularly be referred to in the following sections, and to highlight some specific epistemological questions related to them.

34.2.1 Working Characterization

In science, computer simulations are based on the use of computers. A computer is a physical apparatus which can reliably be used to carry out logical and mathematical operations. A computer simulation corresponds to the actual use of a computer to investigate a physical system S, by computationally generating the description of some of the states of one of the potential trajectories of S in the state space of a computational model of S (*working characterization*).

This characterization is not meant as a full-blown definition (Sect. 34.6) but as a synthetic presentation of important features of computer simulations.

First, it emphasizes that the development of computers is a central step in the recent evolution of science, which was made possible by steady conceptual and technical progresses in the twentieth century. It can therefore be expected that computational aspects are often, though not necessarily always, central for the epistemological analysis of computational science and computer simulations (Sect. 34.3). Second, the working definition is meant to emphasize that all uses of computers in science cannot be seen as computer simulations. Typically, the use of computers to analyze big data is not considered as a computer simulation since the dynamics of the target system is not represented. Third, the characterization remains neutral regarding the question of whether in science there are simulations that are not based on the use of computers (whatever these could be). It is not incompatible with the claim that computer simulations are some sort of experimental activity, even if people willing to endorse such claims need to explain and justify in which sense the corresponding uses of computers can be considered as *experimental* (Sect. 34.5). Finally, since different types of computers exist, computer simulations may correspond to various types of objects. The working definition emphasizes that, in order to analyze actual science, the emphasis should be primarily on models of computations that can have an *actual* physical realization, and on physical systems that can be *used in practice* for scientific purposes – even if investigations about potential machines, and how some physical systems could instantiate them, may be relevant for foundational issues.

I now turn to the description of important types of computer simulations that have been, or still are, used in science and that figure in epistemological discussions about computer simulations.

34.2.2 Analog Simulations and Their Specificities

Analog computers were important tools for scientific computing till the late 1960s, during which with handbooks of analog computation were still being written [34.47, 48], and attempts were made in the early 1970s to link analog and digital computers. Analog simulations and physical analog systems are still occasionally used to investigate physical systems.

An analog computer is a physical machine which is able to carry out algebraic and integrodifferential operations upon continuous physical signals. Thus, operations that would be difficult to program on a digital computer are immediately possible on an analog machine. The specificity of analog machines is that they contain physical elements whose dynamics decisively contribute to the dynamic instantiation of these mathematical operations. For a machine to be used as an analog computer, its physical dynamics must be explicitly known and completely under control so that there is no uncertainty about the operations which are carried out. While systems like wind tunnels cannot be made to compute several different dynamics, mechanical analog computers like the differential analyzer and electrical analog computers can be used as general-purpose computational tools.

Even if analog computers and analog simulations are seldom used nowadays, understanding them is epistemologically important. For instance, while quantum computation is an extension of classical digital computation, quantum analog computing, which involves no binary encoding, may prove useful for the purpose of the quantum simulation of physical systems [34.49]. Analog computers are considered to be potentially more powerful than digital machines *and* to be actually instantiated by physical systems, even if we are unable to use them to the full extent of their capacities because of analog noise or the impossibility of precisely extracting the information they process. The analysis of analog computability is also important for foundational studies aimed at determining which types of actual computers devices could be used for the purposes of computer simulations, how much resources we may need to simulate physical systems or what natural systems can compute [34.50–52]. For example, the General Purpose Analog Computer was introduced by Shannon as a model of the differential analyzer, which was used from the 1930s to 1960s.

Finally, understanding how analog computers work is important to understand analog simulations and how they differ from digital simulations. As is pitifully emphasized by *Arnold* [34.53, p. 52], the failure to distinguish properly between digital computer simulations and analog simulations can be (and has recently been) a major source of error in the philosophical discussions of computer simulations. Analog computers physically instantiate the mathematical dynamics which they are used to investigate. Therefore, the analog computational model that is analyzed is instantiated both by the physical computer and by the target system that is being simulated. Thus, the simulating and simulated processes share a common structure and are isomorphic [34.54], which need not be the case for digital simulations (Sect. 34.5.3). Importantly, this common structure is purely mathematical, and involves dimensionless quantities [34.55, Chap. 8]. While the need to describe systems in terms of dimensionless quantities is a general one in the empirical sciences [34.56–58], and is also crucial for digital simulations, here it is specifically important to understand the type of reasoning involved in analog simulations. Indeed, the physical description of the simulating and simulated systems matter only in so far as one needs to justify that they instantiate a common dimensionless dynamical structure. In brief, such analogical reasoning does not involve any direct comparison between the physical material properties of the simulating and simulated systems: the mathematical structure mediates the comparison. In other words, even with analog simulations, an analysis of the similarities of the two systems is irrelevant once one knows which analog computation is being carried out by both systems.

34.2.3 Digital Machines, Numerical Physics, and Types of Equivalence

In digital machines, information is processed discretely, coded in binary digits (1 or 0), and stored in transistors. Computations involve the transition between computational states. These transitions are described in terms of logical rules between the states. If these rules can be described in a general form, they may be described in terms of equations involving variables. Digital computers can have various types of architecture with different computational performances. Traditionally, software was written for sequential computation, in which one instruction is executed at a time. In contrast, modern supercomputers are designed to solve tasks in parallel, and parallelism can be supported at different levels of architecture, which often implies the need to adapt algorithms, if not models, to parallel computation [34.59].

Digital machines can be used to develop different types of computer simulations. Much computational science is numerical: binary sequences code for numbers and computers carry out numerical operations on these numbers by processing the binary strings. Since computers can only devote limited memory to represent numbers (e.g., with floating-point representation), numerical science usually involves numerical approximations. In other words, computer simulations do not provide exact solutions to equations – even if the notion of an exact solution is not as straightforward as philosophers usually take it to be [34.60].

Different types of equivalence between computations, and, by extension, computer simulations, should be distinguished beyond equivalence at the bit level [34.61]. Logical and mathematical expressions and algorithms can be mathematically equivalent when they refer to, or compute, the same mathematical object or some of its properties. Because of floating-point representation, round-off errors cannot be avoided in simulations. When algorithms result in small cumulative errors, they are stable and two such stable algorithms may be considered as numerically equivalent – although they need not be computationally equivalent in terms of their computational efficiency. Finally, based on the type of inquiry pursued, wider notions of representational equivalence can be defined at the computational model or computer simulation level. Typically, two computations yielding the same average quantity, or describing the same topology of a trajectory, may be considered as equivalent. Overall, this shows that analyses of the failures and predictive or explanatory successes of computer simulations must often be rooted in the technical details of computational practices [34.62]. From this point of view, an important part of computational science can be seen as the continuation of the numerical analysis tradition presented in Sect. 34.1.2.

34.2.4 Non-Numerical Digital Models

A large part of science gives a central role to scientific theories couched in terms of differential equations relating continuous functions with their derivatives. For this reason, much of computational science is based on finite-difference equations aimed at finding approximate numerical solutions to differential equations. However this theory- and equation-oriented picture does not exhaust actual practices in computational science. First, computer simulations can be carried out in the absence of theories – which turns out to be a problem when it comes to the explanatory value of computer simulations (Sect. 34.4). Second, even when equation-based theories exist, computational models are not necessarily completely determined by these theories and by mathematical results describing how to discretize equations appropriately (Sect. 34.3.2). Finally, even when well entrenched, equation-based, theories exist, digital, but non-numerical, computer simulations can be developed. This perspective was advocated in the 1980s by computer scientists like Fredkin, Toffoli, or Margolus. Building on the idea previously expressed by *Feynman*, that maybe "nature, at some extremely microscopic scale, operates exactly like discrete computer logic" [34.63], they wanted to develop "a less roundabout way to make nature model itself" [34.64, p. 121] than the use of computers to obtain approximate numerical solutions of equations. The idea was to represent more directly physical processes by means of *physically minded* models, with interactions on a spatial lattice providing an emulation "of the spatial locality of physical law" [34.65] and to use exact models obeying discrete symbolic dynamics to dispense with numerical approximations. In practice, this resulted in the renewed development of cellular automata (hereafter CA) studies and their use for empirical investigations. A CA involves cells in a specific geometry; each cell can be in one of a finite set of states, and evolves following a synchronous local update rule based on the states of the neighboring cells. The field of CA was pioneered in the 1940s by Ulam's works on lattice networks and von Neumann's works on self-replicating automata. It was shown over the decades that such models, though apparently over-simplistic, can not only be successfully used in fields as different as the social sciences [34.66] and artificial life [34.67], but also physics, in which they were shown in the late 1970s and 1980s to be mesoscopic alternate to Navier–Stokes macroscopic equations [34.68].

34.2.5 Nondeterministic Simulations

Another important distinction is between deterministic and nondeterministic algorithms. From the onset, computers were used to execute nondeterministic algorithms, which may behave differently for different runs.

Nondeterministic simulations involve using random number generators, which can be based on random signals produced by random physical processes, or on algorithms producing pseudorandom numbers with good randomness properties. Overall, the treatment of randomness in computer simulations is a tricky issue since generating truly random signals, with no spurious regularities which may spoil the results by introducing unwanted patterns, turns out to be difficult.

Monte Carlo methods, also called Monte Carlo experiments, are a widely used type of nondeterministic simulations. They were central to the Manhattan project, which led to the production of the first nuclear bombs and contributed heavily to the development of computer simulations. They can be used for various purposes such as the calculation of mathematical quantities like Pi or the assessment of average quantities in statistical physics by appropriately sampling some interval or region of a state space. These practices are hard to classify and, depending on the case, seem to correspond to computational methods, experiments, or full-blown computer simulations. *Metropolis* and *Ulam* [34.69] is a seminal work, *Galison* [34.70, 71] correspond to historical studies, and *Humphreys* [34.8], *Beisbart* and *Norton* [34.72]) to epistemological analyses.

34.2.6 Other Types of Computer Simulations

It is difficult to do justice to all the kinds of simulations that are seen in scientific practice. New computational methods are regularly invented, and these often challenge previous attempts to provide rational typologies. Further, the features presented in the previous sections are often mixed in complex ways. For example, CA-based methods in fluid dynamics, which were not originally supposed to involve numbers or offer exact computations, were finally turned into lattice Boltzmann methods, which involve making local averages [34.73]. Here, I shall merely present types of computer simulations that are widely discussed in the philosophical literature.

Agent-Based Methods

Agent-based methods involve the microlevel description of agents and their local interactions (in contrast to global descriptions like balance or equilibrium equations), and provide tools to analyze the microscopic generation of phenomena. They are often opposed to equation-based approaches, but the distinction is not completely sharp, since equations do not need to describe global behaviors and, when discretized, often yield local update rules. Agent-based models and simulations are used across fields to analyze artificial, social, biological, etc., agents. CA models like the Schelling model of segregation can be seen as agent-based models even though most such agent-based also involve numbers in the descriptions of local interactions. Because they rely on microscopic descriptions, agent-based simulations are often at the core of debates about issues such as emergence [34.74], explanation [34.75], or methodological individualism in science [34.76].

Coupled and Multiscale Models

Extremely elaborate computational models, developed and studied by large numbers of scientists, are increasingly used to investigate complex systems such as Earth's atmosphere, be it for the purpose of precise predictions and weather forecasting or for the analysis of larger less precise trends of climate studies. While in fluid dynamics, it is sometimes possible to carry out *direct simulations*, where the whole range of spatial and temporal scales from the dissipation to the integral scale are represented [34.77, Chap. 9], such methods are too costly for atmosphere simulations, in which subgrid models of turbulence or cloud formation need to be included (see *Edwards* [34.78] and *Heymann* [34.79] for accessible and clear introductions). Also, different models sometimes need to be coupled like in the case of global coupled ocean-atmosphere general circulation models.

These complex computer simulations raise a number of epistemological issues. First, in the case of multiscale or coupled models, the physical and computational compatibility of the different models can be a tricky issue, and one must be careful that it does not create spurious behavior in the computer simulation (see *Winsberg* [34.16, 80], *Humphreys* [34.41, 81] for more analyses about such models). Second, since there are various ways of taking into account subgrid phenomena, pluralism in the modeling approaches cannot be avoided [34.82]. Importantly, the existence of different incompatible models need not be seen as a problem, and scientists can try to learn by comparing their results or elaborate ensemble methods to try to deal with uncertainties [34.83]. The development of investigations of such large-scale phenomena requires collective work, both within and between research teams. Typically, not only the interpretation of the models, their justification, the numerical codes [34.84], but also the standard of results [34.78, 85] must be shared by members of the corresponding communities. An important but still unexplored question is how much the collective dimension of these activities influences epistemologically how they are carried out. From this point of view, the epistemology and philosophy of computational models and computer simulations can be seen as another chapter of the analysis of the collective dimension of science.

Computational Methods versus Computer Simulations

Not all major families of mathematical and computational methods are used to produce computational models or computer simulations of empirical systems. Evolutionary algorithms are used for the investigation of artificial worlds, or of foundational issues about evolution, and they have important applications in the field of optimization methods. Artificial neural networks are used in the field of machine learning and data learning and to predict the behavior of physical systems out of large databases. Bayesian networks are helpful to model knowledge, develop reasoning methods, or to treat data. Overall, all these computational methods have clear practical applications. They can be used for scientific tasks, sometimes concurrently with computer simulations in the case of predictive tasks. However, no genuine representations of physical systems and their dynamics seem to be attached to their use – even if, as the development of CA-based simulations has shown, novel formal settings may eventually have unexpected applications for modeling purposes in the empirical sciences.

34.3 Epistemology of Computational Models and Computer Simulations

Epistemologists analyze whether and how much knowledge claims are justified. In this case, it requires analyzing the specific roles played by computer simulations in the production and generation of items of knowledge (Sect. 34.3.1). Different levels of description and analysis can be relevant when investigating the epistemology of computer simulations, in addition to that of the computational model and how it is theoretically or experimentally justified (Sect. 34.3.2). Importantly, how computer simulations are justified, and why specific computational models are used by scientists, are overlapping (though not identical) questions. For example, field- or inquiry-specific explanations of the use of computer simulations fail to account for cross-disciplinary recurrences in the use of computational models, which may have more general mathematical or computational explanations (Sect. 34.3.3). Overall, computer simulations are one of the main sources of knowledge and data in contemporary science, even if the sense in which they produce new data and knowledge is often misunderstood (Sect. 34.3.4).

34.3.1 Computer Simulations and Their Scientific Roles

Science, as an institution, aims to reach epistemic goals of various sorts, both propositional (like reaching some epistemic states, typically justified true beliefs) and practical (like being able to reliably manipulate some physical systems). Epistemologically analyzing science requires the study of the reliability and efficiency of scientific procedures to reach these goals. Accordingly, to develop the epistemology of computer simulations, one first needs to single out their different scientific goals.

Even if they also serve pedagogical or expository purposes, most computer simulations can be described as activities aimed to develop knowledge. There exist various types of scientific knowledge (see *Humphreys* [34.81] for an overview), which raise specific problems, and, conversely, various types of knowledge can be produced by computer simulations.

Typically, items of knowledge may differ in how they are justified (theoretically, experimentally, inductively, etc.), and whether they were reached by a priori or a posteriori investigations. They may also differ regarding the activities needed to produce them and the type of information that they provide. For example, predictive or explanatory knowledge, or knowledge about how systems behave and can be controlled are of different types. Some scientific roles can be general (*predicting*) and others are very specific. For example, computer simulations are used to develop evidential standards in physics by simulating detection procedures and identifying patterns of data (*signatures*) [34.86]. Overall, developing a coherent and fine-grained epistemology of computer simulations would require drawing a map of their various roles to see how much their epistemological features are general or contextual and role specific.

Let us now be more specific. In the twentieth century, the role of experiments, as sources of empirical evidence about nature and guides in the selection of theories, was repeatedly, if not exclusively, emphasized by empiricist philosophers of science. Conversely, activities which did not provide such evidence were mainly seen as serving theoretical purposes. Typically, models were first seen as being primarily of a theoretical nature [34.20, §5]. In this perspective, *Models as Mediators*, in 1999, represented a significant advance. Morgan and Morrison, by presenting a more precise "account of what [models] do" in science [34.20, p. 18], offered a more nuanced epistemological picture, where models were shown to have functions as diverse as investigating theories and the world, intervening, helping for measurement purposes, etc. Since an important role of computer simulations is to demonstrate the content of models [34.13] or unfold well-defined scenarios [34.87], computer simulations can be expected to have, or contribute to, similar roles to those described by Morgan and Morrison and to potentially share these roles with other demonstrative activities like argumentation or mental simulations.

Importantly, such a description of science, where items or activities as diverse as theories, models, computer simulations, thought experiments, or experiments may serve partly overlapping purposes, remains compatible with empiricism provided that experiments are seen as, in the architecture of knowledge, the only ultimate source of primary evidence about the nature of physical systems. It is also compatible with the claim that secondary, derived sources of knowledge, like theories, models, or simulations, can sometimes be more reliable than experiments to provide information about how systems behave, in particular in cases in which experimental evidence is hard to come by (Sect. 34.5.4).

Overall, it is unlikely that there is such a thing as *the* epistemology of computational models and simulations. If the various roles of computer simulations are specific cases of general functions, like demonstrating or unfolding, there may be such a thing as a general, but incomplete, epistemology of computer simulations, corresponding to the general epistemological problems raised by such general functions. In any case, to complete the picture, one needs to go deeper into the analysis of the roles that computer simulations serve within scientific practices and how they fulfill these roles in various types of contexts. This program is not incompatible with the philosophical perspectives of some of the advocates of the so-called *practice turn* in science [34.88], and in particular of authors who put contextually described scientific activities at the core of their description of science [34.89, 90].

34.3.2 Aspects of the Epistemological Analysis of Computer Simulations

A Multilayered Epistemology

Epistemology analyzes the types of justifications that we have for entertaining knowledge claims, and investigates how and why we epistemically fail or succeed. In the case of computer simulations, failure may take place at various levels, from the material implementation of the computation to the physical model that is at the core of the inquiry, and at all the intermediate semantic levels of interpretation that are needed to use computers for the investigation of models (see *Barberousse* et al. [34.91] for a general description and *Grim* et al. [34.92] for a discussion of some specific failures found in computer simulations). Overall, the epistemology of computer simulations involves discussing the reasons that we have for claiming:

1. The computers that we use work correctly.
2. The programs or algorithms do what we want them to do.
3. The computer simulations, *qua physical representations*, correctly depict what we want them to represent.

Steps 1 and 2 correspond to questions related to engineering and computer science. I shall not discuss these at length but will simply illustrate them to show how serious they are in this context. For example, at the architectural level, parallel computing requires coordination the different cores of computers so that all potential write-conflicts in the memory are solved. At the program level, when trying to solve a problem P with an unknown solution S, scientists need to prove the correctness of the algorithms they use and to verify that the programs written do indeed execute these algorithms. Many such verification problems are undecidable, which means that no general versatile procedure can be found to make this verification for all cases. However, this does not imply that proofs of the correctness of the algorithm cannot sometimes be provided for specific problems. Overall, scientists in this field still actively investigate and debate how much algorithms can be verified (see *Fetzer* [34.93], *Asperti* et al. [34.94] and *Oberkampf* and *Roy* [34.95] for discussions). At a higher mathematical level, as we saw earlier, many computational methods provide numerical methods for approximately solving problems, and the stability of algorithms can be a source of concern, which means that analyzing computational errors is part of the epistemology of simulations [34.62].

Finally, one needs to assess whether the approximations in the solution, as well as the representational inadequacies of the model, are acceptable regarding the physical inquiry pursued. At this interpretational level, because of the variety of theoretical contexts in which computer simulations are carried out, there is no single and general way in which the reliability of the results they provide can be analyzed. The credentials of computer simulations will be different depending on whether a sound theory is being used, how much uncertainty there is about the initial conditions, how complex the target system is, whether drastic simplification assumptions have been made etc. Also, depending on what the simulation is used for, and what type of knowledge it is meant to provide, the justificatory requirements will be more or less stringent. It takes different arguments to justify that based on a simulation one knows how to represent, control, predict, explain, or understand the behavior of the system (see Sect. 34.4 for a discussion of the last two cases, and [34.96] for similar analyses). Similarly, precise quantitative spatial-temporal predictions are in need of much pointed justifications than computer simulations aimed at studying average quantities or qualitative behaviors of systems. Importantly, this discussion of the reliability of computer simulations overlaps significantly with that of the epistemology of physical models, and with how the results issued from approximate, idealized, coarse grained, or simply partly false models can still be scientifically valuable (see *Portides* Chap. 2, this volume; *Frigg* and *Nguyen* Chap. 3, this volume). However, in the present context, it is important to emphasize that, even if the content of models obviously constrains the reliability of the information that can be extracted from them, models do not by themselves produce results – only procedures which investigate them do. In this perspective, the epistemology of computer simulations is a reminder that reliability primarily characterizes practices or activities that produce knowledge and that models, taken alone, are not such practices. In other words, epistemological discussions about the reliability of models as knowledge providers make sense only by explicitly reintroducing such practices or when it can be assumed that reliably extracting all their content is possible, an assumption that, in the framework of computational science, is often not plausible.

From Theoretical to Empirical Justifications

Computer simulations have often been viewed as ways of exploring theories by hypothetico-deductive methods. This characterization captures a part of the truth, since existing theories are often a starting point for the construction of computer simulations. In simple cases, computer simulations can mainly be determined by theories, like in the case of *direct simulations* [34.77] in fluid dynamics, which derive from Navier–Stokes equations, and in which all relevant scales are simulated and no turbulence model is involved.

However, taken as a general description, this view misrepresents how computer simulations are often produced and their validity justified. As emphasized by *Lenhard* [34.97], even when theoretical equations are in the background, computer simulations often result from some cooperation between theory and experiments. For example, in 1955 when Norman Phillips managed to reproduce atmospheric wind and pressure relations with a six-equation model, which arrangement of equations could lead to an adequate model of the global atmosphere was uncertain and the need for experimental validation was primordial to confirm his speculative modeling assumptions. Overall, the role of empirical inputs in simulation studies is usually crucial to develop phenomenological modules of models, parameterize simulations, or investigate their reliability based on their empirical successes [34.15, 17].

At the same time, since computer simulations are used precisely in cases where empirical data are absent, sparse, or unreliable [34.16], sufficient data to build up and empirically validate a computational model may be missing. In brief, in some cases, computer simulations can be sufficiently constrained neither by theories nor by data and are somewhat autonomous. From an epistemological point of view, this potential situation of theoretical and experimental under-determination is not something to be hailed, since it undermines the scientific value of their results (see also Sect. 34.4.2).

The Epistemology of Complex Systems

Because computer simulations are generally used to analyze complex systems, their epistemology partly overlaps that of complex systems and their modeling. It involves the analysis of simplification procedures at the representational or demonstration levels and of how various theoretical or experimental justifications are often used concomitantly. Overall, when it comes to investigating complex systems, obtaining reliable knowledge is difficult. Thus, any trick or procedure that works is welcome and the result is often what Winsberg has labeled a *motley* epistemology [34.16].

At the same time, sweeping generalizations should be avoided. Philosophers studying computer simulations have too often cashed in their epistemology in terms of that of the most complex cases, such as computer simulations in climate science, which are characterized by extreme uncertainties and the complexity of their dynamics. But computer simulations are used to investigate systems that have various types and degrees of complexity, and whose investigation meets different sorts of difficulties. It is completely legitimate, and politically important, that philosophers epistemologically analyze computational models and computer simulations in climate science (see, e.g., [34.98] for an early influential article). However, to obtain a finer grained and more disentangled picture of the epistemology of computer simulations, and not to put everything in the same boat, a more analytic methodology should be applied. More specifically, one should first analyze how the results are justified in more simple cases of computer simulations where specific scientific difficulties are met independently. In a second step, it can be analyzed how adding up scientific difficulties changes justificatory strategies and when exactly more holistic epistemological analyses are appropriate [34.99]. In this perspective, much remains to be done.

Epistemic Opacity

Epistemic opacity is present in computer simulations to various degrees and has various origins.

Models are often said to be white, gray, or black boxes depending on how they represent their target system. White-box models describe the fundamental laws or causal mechanisms of systems whereas black-box models simply correctly connect different aspects of their behavior. This distinction partly overlaps with that of theoretical and phenomenological models (see *Barberousse* and *Imbert* [34.100, §3.2] for sharper distinctions about these last notions). Computer simulations can be based on all types of such models, which may affect the understanding that they yield [34.101] (see also Sect. 34.4).

Opacity can also be present at the computational model or computational process level. *Global epistemic opacity* may arise from the complexity of the computation when it is not possible for an agent to inspect and verify all steps of the process [34.41, §3.7], [34.102]. It is in part contingent since it is rooted in our limitations as epistemic creatures, but it may be in part intrinsic in the sense that the complexity of the computation may be irreducible (see Sect. 34.4.3). Importantly, it is compatible with *local epistemic transparency*, when *any* step of the process can be inspected by a human mind – which may prove useful in cases in which problems can be located by testing parts of the process and applying a dichotomy procedure. Local transparency requires that all details of the physical models and computational algorithms used be transparent, which may be more or less the case. Usually, computer simulations make heavy use of mathematical resource libraries such as code lines, routines, functions, algorithms, etc. In applied science, more or less opaque computational software can be proposed to simulate various types of systems, for example, in computational fluid dynamics [34.91, p. 567]. This raises epistemological problems since black-box software is built on physical models with limited domains of physical validity, and results will usually be returned even when users unknowingly apply such software outside these domains of validity.

Another form of epistemic opacity for individual scientists arises from the fact that investigating natural systems by computer simulations may require different types of experts, both from the empirical and mathematical sciences. As a result, no single scientist has a thorough understanding of all the details of the computational model and computational dynamics. Such type of opacity is not specific to computer simulations, since it is a consequence of the epistemic dependence between scientists within collaborations [34.103].

34.3.3 Selecting Computational Models and Practices

How do individual scientists decide to pursue specific theories, and, in particular, what types of sociological, psychological, or epistemic factors play a role in such processes? Conversely, do selected theories share specific features or properties? Mutatis mutandis, similar questions can be asked about other elements of science, such as research programs, experiments, models, practices, and, in the present case, computational models and computer simulations. Philosophers have mainly analyzed these questions by focusing on the explicit scientific justifications of individual practices, and the content of the representations involved. As we shall see, this is only a part of the story.

Explanation of Uses versus Justification of Uses

A helpful distinction is that between the explanation (and context) of use of a practice and its scientific justification within a scientific inquiry aimed at reaching specific purposes. To use words close to *Reichenbach*'s [34.104, pp. 36–37], while the latter deals with the objective relation that scientists consciously try to establish between these given <activities> (simulations, experiments, etc.,) and the conclusions that are obtained from them, other aspects of material, computational, cognitive, or social natures, potentially unknown to the scientific agents involved in the inquiry, may play a role to explain that these activities were actually carried out. For example, in the case of the Millennium Run (a costly simulation in astrophysics), the results were made publicly accessible. Scientists who were not involved in the process leading to the decision to carry out this simulation could try to make the best of it since it was already there and milk it as much as possible for different purposes. Or, some scientists may decide to study biological entities like proteins or membranes by means of Monte Carlo simulations, because members of their teams happen to be familiar with these tools. However, once they have decided to do so, they must still justify how their computer simulations support their conclusions.

In the perspective of explaining actual scientific uses, one also needs to distinguish between explanations aimed to account for specific uses (e.g., *Why was the millennium simulation carried out in 2005 by the Virgo consortium?*) and those aimed to explain more general patterns, corresponding to the use of practices of a given type, within or across several fields of science (e.g., *Why are Monte Carlo simulations regularly used in this area of physics?*, *Why are they used regularly in science?*). Importantly, since different instantiations of a pattern may have different explanations, the aggregated frequency of a scientific practice, like that of the use of the Ising model across science, may be the combined effect of general transversal factors and of inquiry- or field-specific features [34.105].

Field-Specific versus Cross-Disciplinary Explanations

A tempting move has often been to answer that scientific choices are primarily, if not completely, theory driven – and are therefore field specific. After all, theories guide scientists in their predictive and explanatory activities by fueling the content of their representations of natural systems. However, a reason to look for additional elements of explanations is that the spectrum of actual modeling and computational practices is smaller than our scientific knowledge and goals would allow [34.21, 41, 106]. For example, why do the harmonic oscillator, the Ising model, the Lotka–Volterra model, Monte Carlo simulations, etc., play such prominent roles throughout science?

As highlighted by *Barberousse* and *Imbert* [34.105], a variety of significantly different explanations of the greater or lesser use of models of a given type, and of scientific practices, can be found, beyond the straightforward suggestion that there are regularities in nature, which are mirrored by modeling and computational practices.

Local Factors

The explanation may be rooted in the specificities of modeling and computational activities. In particular, if explaining is better achieved by limiting the number of (types) of (computational) models [34.21, pp. 144–5], or explanatory argument patterns [34.107], it is no surprise that often the same computational models and practices are met. Also, scientists may feel the need to avoid dispersion of their efforts in cases when research programs need to be pursued for a long time before good results can be reached and it is more profitable to exploit a local mine than to go digging somewhere else [34.106, Chaps. 4 and 5], [34.21, pp. 143–4]. More generally, the recurrence of computational practices may be viewed as another example of the benefits of adopting scientific standards [34.108]. One may also, in the Kuhnian tradition, put the emphasis on the education of scientists, who are taught to see new problems through the lens of specific problems or exemplars [34.106, p. 189], and emphasize that this education has a massive influence on the lineages of models or practices which are later developed. This story can have a more or less contingentist version, depending on why the original models or practices at the lineage seeds are adopted in the first place, and why these uses are perpetuated and scientists do not emancipate from them after schooling.

Theories may also play an indirect role in the selection of computational models. For example, models naturally couched in the standard formalism of a theory may be easier to use, even if the same physics can also be put to work by using other models. *Barberousse* and *Imbert* [34.100] analyze the case of lattice methods for fluid simulations in depth, which, though significantly different from approaches based on Navier–Stokes differential equations, can be used for the same purposes, even if this requires spending time learning and harnessing new methods and formalisms, which physicists may be reluctant to do.

Computational and Mathematical Explanations

As seen in Sect. 34.1.4, *Humphreys* [34.41, 81], suggests that most scientific models are tailored to fit the available mathematics, hence the importance in scientific practice of tractable models (see *Humphreys*'s notion of computational template [34.41, §3.4], and further analyses in [34.45]). Even if one grants the potential importance of such mathematical and computational factors, cashing out in detail the corresponding explanation is not straightforward. *Barberousse* and

Imbert [34.105] emphasize that there are various computational explanations. The *objective computational landscape* (how intrinsically difficult problems are, how frequent easy problems are) probably influences how science develops, even if knowing exactly what it looks like and how it constrains scientific activity is of the utmost difficulty. However, the *epistemic computational landscape* (scientists' beliefs about the objective computational landscape) may just be as important since it frames modeling choices made by scientists.

Other potentially influential factors may also include how difficult it is to explore the objective landscape (and the corresponding beliefs regarding the easiness of this exploration), how much scientists, who try to avoid failure, are prone to resort to tractable models, or which techniques are used to select such tractable models (since some specific techniques, like polynomial approximations, may repeatedly select the same models within the pool of tractable models). Finally, modeling conservativeness may also stem from the computational and result pressure experienced by scientists, that is, how scarce computational resources are in their scientific environment and how much scientists need to publish results regularly.

Universality, Minimality, and Multiple Realizability

Other explanations may be offered in terms of how weak the hypotheses are to satisfy a model or a distribution. For example, the Poisson distribution is often met because various types of stochastic processes satisfy the few conditions that are required to derive it [34.41, pp. 88–89]. Relationships between models and how models approximate to each other may also be important. Typically, the Gaussian distribution is the limit of various other distributions (see however, *Lyon* [34.109] for a more refined analysis and the claim that in Nature Gaussian distributions are common, but not pervasive). More generally, models that capture universal features of physical systems and are rooted in basic properties, such as their topology, can be expected to be met more often. Therefore, for reasons having to do with the mathematics of coarse-grain descriptions, and the explanation of multiple realizability, many systems fall into the same class and have similar descriptions [34.110–112] when minimal, macro-level, or simply qualitative models are built and explored.

Importantly, all the above explanations are not exclusive. Typically, the emphasis on tractability may be a general one in the sense that models always need to be tractable if they are to be used by scientists.

34.3.4 The Production of 'New' Knowledge: In What Sense?

Be Careful of Red Herrings!

It is commonly agreed that computer simulations produce *new knowledge*, *new data*, *new results*, or *new information* about physical systems (*Humphreys* [34.41], *Winsberg* [34.113, pp. 578–579], *Norton* and *Suppe* [34.114, p. 88], *Barberousse* et al. [34.91, p. 557], *Beisbart* [34.115]). This can be considered as a factual statement, since contemporary science, which is considered to produce knowledge, relies more and more heavily on computer simulations.

At the same time, the notion of knowledge should not be a red herring. It is commonly considered that experiments, inferences, thought experiments, representations, or models can bring knowledge, which then generates the puzzle that widely different activities have similar powers. The puzzle may be seen as somewhat artificial since knowledge, especially scientific, can be of different types [34.81], and when *new* knowledge is produced, the novelty can also be of different types. In this perspective, it may be that what is produced by each of these activities falls under a general identical concept but is significantly different. From this point of view, the real question concerning computer simulations is not whether they produce *knowledge*, but in which particular sense they produce knowledge, what kind of knowledge they produce, what is specific to the knowledge produced by computer simulations, and what type of novelty is involved.

A comparison can be made with thought experiments, for which the question of how they can produce new knowledge has also been debated. Both activities correspond to the exploration of virtual situations, and do not involve direct interactions with the systems investigated. From this point of view, computer simulations and thought experiments can be seen as platonic investigation of ideas, with this difference that, for computer simulations, the mind is assisted by computers [34.41, p. 115–116]. Overall, computer simulations have been claimed to sometimes play the same role of unfolding as thought experiments [34.87], have sometimes been equated with some types of thought experiments [34.116], and it has been suggested that computational modeling might bring the end of thought experiments [34.117]. Importantly, even if thought experiments are perhaps less used in science than formerly, this latter claim seems implausible. The reason is that there are different kinds of thought experiments, and many reveal conceptual possibilities that have little to do with computational explorations. Arguably, the possibility to set up computer simulations would have added nothing to famous thought experiments such as those made by Galileo, Einstein, Podolsky and Rosen, or Schrödinger. (I am grateful to Paul Humphreys for emphasizing this point.) In any case, a satisfactory account of these activities should account for both similarities and differences in how they work epistemologically and how they are used.

In any case, the question of how and what we can learn about reality by using these methods arises, even if the sources of puzzlement do not exactly touch the same points in each case. Indeed, how mental thought experiments work is more opaque than how computer simulations do. For this reason, their rational reconstruction as logical arguments [34.118, p. 354] is more controversial than that of computer simulations [34.115], and it is less clear whether their positive or negative epistemic credentials are those of the corresponding reconstructed argument [34.119]. (For example, if certain thought experiments are reliable because mental reasoning capacities about physical situations have been molded by evolution, development, or daily experiments, it is not clear that their logical reconstruction will more vividly make clear why they are reliable.) The situation is clearer for computer simulations since the process is externalized and is based on more transparent mechanisms (see however Sect. 34.3.2). Then, if computer simulations are nothing else than (computationally assisted) thinking corresponding to the application of formal rules, and their output is somewhat contained in the description of the computational model, how knowledge is generated is clearer but the charge of the lack of novelty is heavier.

The Need for an Adequate Notion of Content

Suppose that a physical system S is in a state s at time t and obeys deterministic dynamics D. Then, the description of D and s characterizes a mathematical structure M, which is the trajectory of S in its phase space and is known as such. If a computer simulation unfolds this trajectory, then it explicitly shows which states S will be in. At the same time, any joint description of one of these states and of the dynamics denotes the same structure M, which is known to characterize the evolution of S. So, from a logical point of view, no new content has been unraveled by the computer simulation, which can at best be seen as a means of producing new *descriptions* of identical contents. In brief, if knowledge is equated with that of logical content, computer simulations do not seem to be necessarily producing new knowledge. We may even be tempted to describe computer simulations as somewhat infertile and thereby perpetuate a tradition according to which formal or mechanical procedures to draw inferences, and rules of logic in particular, are sterile, as far as discovery is concerned, and can at best be used to present pieces of knowledge that have already been found – a position defended by *Descartes* in 1637 in the *Discours de la Méthode* [34.120]. This kind of puzzle, though particularly acute for computer simulations, is not specific to them and is nothing new for philosophers of language – Frege and Russell already analyzed similar ones. However, this shows that, *pace* the neglect for linguistic issues in the present philosophy of science, without an adequate theory of reference and notion of content that would make clear what exactly we know and do not know when we make a scientific statement, we are ill-equipped to precisely analyze the knowledge generated by computer simulations [34.41, 121].

Computational science may also remain somewhat mysterious if one reasons with the idealizations usually made by philosophers of science. As emphasized in Sect. 34.1.4, idealizing away the practical constraints faced by users is characteristic of much traditional philosophy of science and theories of rationality. In the present case, it is true that "*in principle*, there is nothing in a simulation that could not be worked out without computers" [34.122, p. 368]. Nevertheless, adopting this in principle position is unlikely to be fruitful here since, when it comes to actual computational science, which scientific content can be reached *in practice* is a crucial issue if one wants to understand how computational knowledge develops and pushes back the boundaries of science (see *Humphreys* [34.41, p. 154] and *Imbert* [34.102, §6]).

Overall, it is clear that present computational procedures and computer simulations do contribute to the development of scientific knowledge. Thus, it is incumbent on epistemologists and philosophers of sciences to develop conceptual frameworks to understand how and in what sense computer simulations extend our science and what type of novelty is involved.

Computer Simulations and Conceptual Emergence

Computer simulations unfold the content of computational models. How to characterize the novelty of the knowledge that they bring us? Since the notion of novelty is also involved in discussions about emergence, the literature about this latter notion can be profitably put to work here.

Just as emergence may concern property instances and not types [34.123, 124, p. 589], the notion of novelty needed here should apply to tokens of properties instantiated in distinctive systems and circumstances, or to specific regularities the scope of which covers such tokens and circumstances. For example, the apparition of vortices in fluids is in a sense nothing new, since the behavior of fluids is covered by existing theories in fluid dynamics, no new concept is involved, and other phenomena of this type are already understood for some well-studied configurations. At the same time, finding out that patterns of vortices emerge in configurations of a new type is a scientific achievement and the discovery of some new piece of knowledge.

Importantly, as emphasized by *Barberousse* and *Vorms* [34.125, p. 41], the notion of novelty should be separated from that of surprise. When the exact value of a variable is precisely learnt and lies within the range that is enabled by some physical hypothesis or principle, we have a kind of *unsurprising novelty*. Barberousse and Vorms give an example from experimental science, but computer simulations may also provide exact values for quantities, which agree with general laws (e.g., laws of thermodynamics) and are therefore partly expected.

In addition, computer simulations can provide cases of *surprising novelty*, concerning behaviors that are covered by existing theories like chaotic behavior for classical mechanics. Indeed, Lorenz attractor and behaviors of a similar type were discovered by means of computer simulations of a simplified mathematical model initially designed to analyze atmospheric convection, and this stimulated the development of chaos theory [34.125, p. 42].

This leads us to a type of novelty, related to what Humphreys calls conceptual emergence. Something is conceptually emergent relative to a theoretical framework F when it requires a conceptual apparatus that is not in F to be effectively represented [34.41, p. 131], [34.123, p. 585]. The conceptual apparatus may require new predicates, new laws and sometimes the introduction of a new theory. Importantly, conceptual emergence is not merely an epistemic notion. It does not depend on the concepts we already possess and the conceptual irreducibility is between two conceptual frameworks. Further, even if instances of the target pattern can be described at the microlevel without the conceptually emergent concepts, the description of the pattern itself, if it is made without these novel concepts, is bound to be a massive disjunction of microproperties, which misrepresents the macro-pattern qua pattern. Also, the same conceptually emergent phenomena may arise in different situations and its description may therefore require an independent conceptual framework, just like the regularities of special science require new concepts, unless one is prepared to describe their content in terms of a massive disjunction of all the cases they cover [34.126].

Interestingly, various phenomena investigated by computational science are conceptually emergent. Even if computer simulations are sufficient to generate them, identifying, presenting, and understanding them may require further analyses of the simulated data, redescriptions at higher scales and the development of new theoretical tools. For example, traffic stop-and-go patterns in CA models of car traffic, emergent phenomena in agent-based simulations, and much of the knowledge acquired in classical fluid dynamics seem to correspond to the identification and analysis of conceptually emergent phenomena. Effectively, it is by conceptually representing these phenomena in different frameworks that one manages to gain novel information about these systems, above and beyond our blind knowledge of the microdynamics that generates them.

It is important to emphasize that different types of novelty described above are also met in experiments exploring the behavior of systems for which the fundamental physics is known. In other words, the potential novelty of experimental results should not be overemphasized. Even if only experiments can *confound* us [34.127, pp. 220–221] through results which are not covered by our theories or models, many of the new empirical data that these experiments provide us with are no more novel than those produced by computer simulations. The statements describing these results are not *strongly referential*, in the sense that no unknown aspects of the deep nature of the corresponding systems would be unveiled by a radically new act of reference [34.87, pp. 3463–3464]. These statements derive from what we already know about the physical systems investigated, and the experimental systems unravel them for us. In this sense, they are merely *weakly referential*.

34.4 Computer Simulations, Explanation, and Understanding

Can scientists provide explanations by simulating phenomena? If the answer is based on the explanatory requirements corresponding to the existing accounts of explanation, it is hard to see why some computer simulations could not be explanatory (Sect. 34.4.1). Why the specificities of computer simulations should necessarily deprive them for their explanatory potential is also unclear (Sect. 34.4.2), which is compatible with the claim that computer simulations are used for inquiries whose results are, on average, less explanatory (Sect. 34.4.3). Be this as it may, because they heavily rely on informational and computational resources, computer simulations challenge our intuitions about explanatoriness, and in particular the expectation that good explanations should enable scientists to enjoy first-person objective understanding of the systems they investigate (Sect. 34.4.4). Even if computer simulations fail to meet these expectations because of their epistemic opacity, understanding may sometimes be regained by appropriately visualizing the results or studying phenomena at a coarser level (Sect. 34.4.5). In any case, scientific judgments about such issues are influenced by disciplinary norms, which may sometimes evolve with the development of computational science (Sect. 34.4.6).

34.4.1 Traditional Accounts of Explanation

Philosophers of science have discussed intensively the issue of scientific explanation over the last decades. The seminal works of Hempel were published in the 1940s, when computational science started to develop. However, until recently, discussions about computer simulations and explanations did not interfere with each other – which could suggest that for theorists of explanation, *how* explanations are produced does not in fact matter. While it is true that many of the examples of explanatory inquiries analyzed in the literature are simple and, at least in their most elementary versions, do not belong to computational science, it is hard to see why computer simulations could not in some cases satisfy the requirements corresponding to major accounts of explanations. According to the deductive-nomological (hereafter DN) model, one explains a phenomenon when a sentence describing it is logically deduced from true premises essentially containing a scientific law [34.128, pp. 247–248]. For example, the explanation of the trajectory of a comet, by means of a computer simulation of its trajectory based on the laws of classical (or relativistic) mechanics together with the initial positions of all bodies significantly influencing its trajectory, seems to qualify as a perfect example of DN explanation – provided that computer simulations can be seen as deductions [34.91, 115].

Analog statements can be made concerning the causal and unificationist models of explanations. The computer simulation of the comet's trajectory is a way to trace the corresponding causal processes, described in terms of mark transmission [34.129] or of conserved quantities such as energy and momentum [34.130]. Other causal theorists of explanation like Railton have claimed that explanatory progress is made by detailing the various causal mechanisms of the world and all the nomological information relevant to the investigated phenomenon; the corresponding "ideal explanatory text" is thereby slowly unveiled [34.131]. But, one should note that, because such ideal explanatory texts are necessarily complex, their investigation is almost inevitably made by computational means.

Similarly, computer simulations can sometimes be instantiations of argument patterns that are part of what *Kitcher* describes as the explanatory store unifying our beliefs [34.107]. For example, the computation of the comet's trajectory can be seen as an instantiation of "the Newtonian schema for giving explanations of motions in terms of underlying forces" [34.132, p. 121, p. 179].

Be this as it may, computer simulations have often been claimed, both by scientists and philosophers, to be somewhat problematic concerning explanatoriness and lacking some of the features that are expected to go with the fulfillment of explanatory requirements. This reproach of unexplanatoriness can be understood in several senses.

34.4.2 Computer Simulations: Intrinsically Unexplanatory?

One may first claim that computer simulations in general, or some specific types of them, do not meet one's favorite explanatory requirements. For example, agent-based simulations may be described as not usually involving covering laws nor providing explanatory causal mechanisms or histories [34.75, 133]. However, one should not ascribe to computer simulations reproaches that should be made to the field itself. If a field does not offer well-entrenched causal laws and one is convinced that explanations should be based on such laws, then the computer simulations made in such fields are not explanatory, but this has nothing to do with computer simulations in general. Also, some computer simulations are built with scientific material like phenomenological regularities, which potentially makes them unexplanatory, but this material could also be used in the context of explanatory inquiries involving arguments or closed form solutions to models. Thus, the problem comes from the use of this material and not from the reliance on one or another mode of demonstration – and claiming that computer simulations are unexplanatory is like blaming the hammer for the hardness of the rock.

For this reproach to be meaningful (and specific to computer simulations), it should be the case that other inquiries based on the same material are indeed explanatory, but that the corresponding explanations based on computer simulation are not, because of specific features of computer simulations or some types of them. It is not completely clear how this can be so. Computer simulations are simply means of exploring scientific models and hypotheses by implementing algorithms, which provide information about tractable versions of these models or hypotheses. Therefore, their explanatory peculiarity, if any, should be an effect of specific features like the use of algorithms, coding languages, or external computational processes.

There is no denying that the need to format scientific models and hypotheses into representations that are suitable for computational treatment comes with constraints. For example, a recent challenge has been to adapt coupled circulation models and their algorithms to the architecture of modern massively parallel supercomputers. Similarly, when one uses CA models for fluid dynamics, the physical hypotheses must be expressed in the straightjacket of up-to-date rules between neighboring cells on a grid. Beyond these genuine constraints on computational practices, one should remember that, computational languages, provided they are rich enough, are content neutral in the sense that any content that can be expressed with some language can also be expressed with them. Similarly, computational devices like the computers we use daily are universal machines in the sense that any solution to a computational problem (or inference) that can be produced by other machines can also be produced by them. For these reasons, it is hard to see why, *in principle*, computer simulations should be explanatorily limited, since the theoretical content and inferences related to other means of inquiries can also be processed by them.

The case of CA models abovementioned exemplifies nicely this point. For several decades, CA models have been used under various names in various fields; from Schelling's investigations about spatial segregation in neighborhoods, analysis of shock waves in models of car traffic, models of galaxies, investigations of the Ising model, to fluid dynamics (see *Ilachinski* [34.134] for a survey). Because existing theories and scientific laws are not expressed in terms of CA, some philosophers have claimed that CA-based simulations were merely phenomenological [34.135, pp. 208–209], [34.9, p. 516]. Nevertheless, *Barberousse* and *Imbert* [34.100] have argued that such bold *general* statements do not resist close scrutiny. They present the case of lattice gas models of fluids and argue that, beyond their unusual logical nature, from a physical point of view, such mesoscopic models and computer simulations make use of the same underlying physics of conserved quantities as more classical models, and can be seen as no less theoretical than concurrent computer simulations of fluids based on macroscopic Navier–Stokes equations. Therefore, there is no reason why such computer simulations could not be usable for similar explanatory purposes.

Overall, there is no denying that *some* (and possibly many) computer simulations are not explanatory. Providing various examples of unexplanatory computer simulations is scientifically valuable, but it says nothing general about their general lack of explanatory power, unless one shows why unexplanatoriness stems from specific features of (some types of) computer simulations qua simulations. In the absence of such conceptual analyses, one can simply conclude that some scientific uses of computer simulations, or some computational practices, turn out to be unexplanatory.

34.4.3 Computer Simulations: More Frequently Unexplanatory?

A different claim is that, given the current uses of computer simulations in science, they are more often unexplanatory than other scientific items or activities, even if this is partly a contingent matter of fact. The explanatoriness of computer simulations can be threatened in various ways. Computational models may be built on false descriptions of target systems or may lack theoretical support and simply encapsulate phenomenological regularities; they may have been spoiled by the approximations, idealizations, and modeling tricks used to simplify models and make them tractable; they may depart from the well-entrenched explanatory norms in a field or may not correspond to accepted explanatory methods. Clearly, none of these features is specific to computer simulations. However, it may be the case that because of their current uses in science, computer simulations more frequently instantiate them.

The Lure of Computational Explorations

Because they are powerful heuristic tools, and because other means of exploration are often not available, computer simulations are more often used to toy and tinker with hypotheses, models, or mechanisms and, more generally, to *experiment on theories* [34.135, 136]. This may especially be the case in fields where there is no well-established theory to justify (or invalidate) the construction of models, or where collected evidence is not sufficient to check that the simulated mechanisms correspond to actual mechanisms in target systems. For example, in cognitive science, competing theories of the mind and its architecture coexisted for decades, and even modern techniques of imaging like fMRI (functional magnetic resonance imaging), though empirically informative, do not provide sufficient evidence to determine how the brain works precisely in terms of causal mechanisms. Accordingly, in this field, developing a model that is able to simulate the cognitive performances of an agent does not imply that one has understood and explained how her brain works, and more refined strategies that constrain the functional architecture must be developed if one wants to make explanatory claims [34.4, Chap. 5]. The issue is all the more complex in this specific field since the inquiry may also involve determining (verses assuming) whether neural processes are computations [34.137]. Similarly, in the social sciences, empirically validating a simulation is far from being straightforward and as a result the epistemic and, in particular, explanatory value of computer simulations is often questionable [34.138].

Overall, since computer simulations offer powerful tools to investigate hypotheses and match phenomena, it is a temptation for scientists to take a step further and claim that their computer simulations have explanatory value. In brief, computer simulations offer a somewhat natural environment for such undue explanatory claims.

The Worries of Under-Determination

In the case of computer simulations, the higher frequency of inappropriate explanatory claims may be reinforced by the combination of several factors.

When toying with hypotheses, scientists are often interested in trying to reproduce some target phenomenology, so they often do not tinker in a neutral way. The specific problem with computer simulations is that, in many cases, getting the phenomenology right is somewhat too easy, and the general problem of underdetermination of theoretical claims by the evidence is particularly acute.

First, computer simulations are often used in cases where data are scarce, incomplete, or of low quality (see, e.g., [34.78, Chap. 10] for the case of climate data and how making data global was a long and difficult process). The scarcity of data can also be a primary motivation to use computer simulations to inquire about a system for which experiments are difficult or impossible to carry out, like in astrophysics [34.139]. Furthermore, knowledge of the initial and boundary conditions out of which the computer simulations should be fed may also be incomplete, which leaves more latitude for scientists to fill in the blanks and possibly match data. As a result, confidence in the result of computer simulations like the Millennium Run and in their representational and explanatory success is in part undermined [34.139].

Second, computer simulations usually involve more variables and parameters than theories. For example, for a 10×10 grid with cells characterized by three variables, the total number of variables is already 300. This raises the legitimate suspicion that, by tuning variables in an appropriate way, there is always a means to obtain the right phenomenology. (Ad hoc tuning is of course not completely straightforward, since the many variables involved in a computer simulation are usually jointly constrained. Typically, in a fluid simulation, all cells of the grid obey the same update rule and are correlated.) This possibility of tuning variables and parameters is indeed used in fields like machine learning, which can be based, for example, on the use of artificial neurons. In such fields, one first combines a limited number of elementary mathematical functions (e.g., artificial neurons) that, when adequately parameterized, reproduce potentially complex behaviors found in databases (the learning phase). In a second step, one uses the parameterized functions (e.g., the trained neural network) on new cases in the hope that extrapolation and prediction are possible. In such cases, even if the right phenomenology is reproduced, and extrapolation partly works, it is clear that the trained neural network and the corresponding mathematical functions do not explain the phenomena. Overall, this means that the ability to reproduce some potentially complex phenomenon is far from being sufficient to claim that the corresponding computer simulation has explanatory power (see also [34.140] for the issue of the over-fitting of computer simulations to data).

Third, when scientists do succeed, they may be subject, as other human creatures, to confirmation biases, overweigh their success and tend to ignore the fact that various mechanisms or laws can produce the same data (or that other aspects of their computer simulations do not fit). While such biases are not specific to computational inquiries, they are all the more epistemologically dangerous since matching phenomena is easy.

Complex Systems Resist Explanation

Because they are very powerful tools, computer simulations are specifically used for difficult investigations, which usually have features that may spoil their explanatory character [34.141, 142]. Typically, in the natural sciences, computer simulations and computational methods are centrally used for the study of so-called complex systems [34.143, 144], see also Chap. 35. Realistically investigating complex systems would imply taking into account many interrelated nonlinear aspects of their dynamics including long-distance interactions and, in spite of the power of modern computers, the corresponding models are usually intractable. Therefore, drastic simplifications need to be made in both the construction of the model and its mathematical treatment, which often threatens the epistemic value of the results.

Importantly, for the above reasons, the problem of the explanatory value of computer simulations can arise even in fields like fluid dynamics where the underlying theories are well known. It is no surprise that this problem is more acute in fields, such as the human and social sciences, in which no such theories are available, the investigated objects are even more complex, sound data are more difficult to collect and interpret, and the very nature of what counts as a sound explanation and genuine understanding is more debated [34.145, 146] especially in relation to computer simulations [34.133].

For these reasons, even if there are good arguments for claiming that computer simulations do not fare worse than other methods like analytic models or experiments (see [34.40] for the case of economics), it is not surprising that their potential explanatory power is undervalued.

Overall, it is plausible that often computer simulations have less explanatory power than other methods, and that this does not stem from their nature but from the type of uses they usually have in science. If this is the case, the question of the explanatory power of computer simulations is to be treated on a case-by-case basis by using the same criteria as for assessing the explanatory power of other scientific activities, *pace* the distrust that shrouds the use of computer simulations.

34.4.4 Too Replete to Be Explanatory? The Era of Lurking Suspicion

Theories of explanation should capture our intuitions about what is explanatory. From this point of view, it is interesting to see whether computer simulations meet these intuitions, especially when they fulfill the explanatory requirements described by theories of explanations.

Computer Simulations and Explanatory Relevance

Good explanations should not include explanatorily irrelevant material. While determining whether some piece of information is explanatorily relevant to explain some target fact is a scientific task, finding a satisfactory notion of explanatory relevance is a task for philosophers. Despite progresses concerning this problem, current accounts of explanation still fall short of capturing this notion [34.147, 148]. At the same time, existing results are sufficient to understand why computer simulations raise concerns regarding explanatory relevance.

Scientific information, in particular causal laws, accounts for the behavior of phenomena. Thus, it is legitimate, when trying to explain some phenomenon, to show that its occurrence can be derived from a scientific description of the corresponding system. Nevertheless, even then, one may fall short of satisfying the requirement of explanatory relevance. This is clearly explained by *Salmon* in his 1989 review of theories of explanation, where he asks "Why are irrelevancies harmless to arguments but fatal to explanations?" and further states that "irrelevant premises are pointless, but they have no effect whatever on the validity of the argument" [34.149, p. 102]. While philosophers have mainly focused on the discussion of irrelevant unscientific premises, the problem actually lies deeper. Parts of the content of laws or mechanisms, essentially involved in explanatory arguments, can be irrelevant to the explanation of aspects of phenomena that are covered by these laws or mechanisms [34.148]. So the problem is not simply to discard inessential (unscientific or scientific) premises, but also to determine, within the content of the scientific premises that are essentially used in explanatory derivations, what is relevant and what is not [34.102, 148, 150].

This problem is especially acute for computer simulations. Take a computer simulation that unfolds the detailed evolution of a system based on the description of its initial state and the laws governing it. Then all aspects of the computational model are actually used in the computational derivation. At the same time, all such aspects are not necessarily explanatorily relevant with respect to all facets of the computed behavior. Typically, some aspects of the computed behavior may simply depend on the topology of the system, on symmetries in its dynamics or initial conditions, on the fact that some initial quantity is above some threshold, etc.

Accordingly, the following methodological maxim may be proposed: *the more an explanation (resp. an argument) contains independent pieces of scientific information, the more we are entitled to suspect that it contains irrelevancies (regarding the target behavior).*

At the same time, one should remain aware that explaining some target phenomenon may sometimes irreducibly require that all the massive gory details involved in the simulation of the corresponding system are included. For example, as chaos theory shows it, explaining the emergence and evolution of a hurricane may essentially require describing the flapping of a butterfly's wings weeks earlier.

An additional problem is that there is no general scientific method to tell whether a premise, or some part of the information it conveys, is relevant. Contrarily to what the hexed salt example [34.151] may perhaps suggest, irrelevant pieces of information within an explanation do not wear this irrelevance on their sleeves and are by no means easy to identify. This is the *problem of the lack of transparency, or of opacity, of irrelevant information*.

Overall, since they are based on informationally replete descriptions of their target systems, computer simulations legitimately raise the suspicion of being computational arguments that contain many irrelevancies, and therefore of being poor explanations – even when they are not.

Computer Simulations, Understanding, and Inferential Immediacy

Mutatis mutandis, similar conclusions can be reached regarding the issue of computational resources. Since this issue is closely related to the question of how much computer simulations can bring about understanding, things shall be presented through the lens of this latter notion.

It is usually expected that explanations bring understanding. Theorists of understanding, while disagreeing on the precise nature of this notion, have explored its various dimensions, which provides a good toolkit to analyze how computer simulations fare on this issue.

Hempel cashes in the notion of understanding in terms of nomic expectability. From this point of view, taken as explanatory arguments, computer simulations seem able to provide understanding since, like other scientific representations, they can rely on nomological regularities. Further, in contrast to sketchy explanations, they make the nomic dependence of events explicit. Consider the explanation analyzed by *Scriven* that "the impact of my knee on the desk caused the tipping over of the inkwell" [34.152]. The *hidden strategy* described by *Woodward* [34.153] is to claim that the value of this latter nonnomological explanation is to be measured against an *ideal* explanation, which is fully deductive and nomological and describes the detailed succession of events that led to the stain on the carpet, even if this complete explanation is often inaccessible. From this point of view, a computer simulation can offer a way to approach such an ideal explanation, by providing an explicit deduction of the lawful succession of events that brought about the explanandum. However, an epistemic problem is that, once such a computer simulation has been carried out (and properly stored), it is possible to explicitly highlight any part of it, but it is not possible to scrutinize all parts because there are too many of them. This is one of the reasons why computer simulations are intrinsically opaque to human minds [34.41, §5.3], see also Sect. 34.3.2.

Be this as it may, causal theorists of explanation should agree that computer simulations often contribute significantly to developing our understanding by reducing uncertainty about the content of causal ideal explanatory texts, as requested in [34.131].

Computer simulations also seem to be able to provide unificatory understanding. For unificationists like *Kitcher*, understanding is a matter of "deriving descriptions of many phenomena using the same pattern of derivation again and again" [34.107, p. 423]. Since computer simulations offer more ways of deriving phenomena, by providing new patterns of derivation or instantiating existing patterns in more complex cases, at least some of them contribute to unification.

Things are less straightforward with Woodward's account of explanation and understanding. *Woodward* argues that a good explanation provides "understanding by exhibiting a pattern of counterfactual dependence between explanans and explanandum" [34.154, p. 13]. From this point of view, computer simulations fare well since, if one does not go beyond their domain of validity, they provide general patterns of counterfactual dependence between their inputs I and outputs O, which are obtained by applying t times their update algorithms (UA), that is, more formally, $O(t, l) = UA^t(I)$.

Is there a philosophical catch? Woodward also requires that the pattern of counterfactual dependence be described in terms of a functional relation. But what is to count as a *function* in this context? Functions can be defined explicitly (by means of algorithms) or implicitly (by means of equations). The advantage of computer simulations is that they provide algorithmic formulations based on elementary operations of how the explanandum varies with the explanans. From this point of view, computer simulations are more explicit than models, which simply provide equations linking the explanans and the explanandum. However, the problem is that with computer simulations any kind of functional immediacy is lost, since it is computationally costly to carry out the algorithm. Indeed, Woodward usually describes straightforward examples of functional dependence like $Y = 3X_1 + 4X_2$. With such functions, we may feel that the description of the counterfactual dependence is *just there*, since, by *simply instantiating* the variables and carrying out the few operations involved, specific numerical relations are accessible. In such simple cases, a human mind can do the work by itself and answer the corresponding what-if-things-had-been-different (what-if) questions. In contrast, with a computer simulation, computing the output takes much computational power. So the tentative conclusion is that computer simulations provide understanding in Woodward's sense, but this understanding is not immediately accessible, the degree of (non)-immediacy being described by the computational resources it takes to answer each what-if question. Importantly, an equation-based model may give the illusion of immediacy, since the equation presents a short description of how the variables are correlated. However, one should watch out that short equations can be unsolvable, and short descriptions of algorithms (like $O(t, l) = UA^t(I)$) with simple inputs can yield complex behaviors that are computationally costly to predict [34.155].

Similar conclusions can be reached if one focuses on analyses of understanding proper. *De Regt* and *Dieks* propose to analyze understanding in terms of intelligibility, where this latter notion implies the ability to recognize qualitative characteristic consequences without performing exact calculations [34.156]. In this sense, understanding seems to be a matter of immediacy, as was already suggested by *Feynman*, who described it as the ability to foresee the behavior of a system, at least qualitatively, or the consequences of a theory, without solving exactly the equations or performing exact calculations [34.157, Vol. 2, 2–1].

Depending on the cases, foreseeing consequences requires logical and cognitive operations to a greater or lesser extent. Thus, the above ideas may be rephrased in a more gradualist way, by saying that the less inferential or computational steps one needs to go through to foresee the behavior of a system or the consequences of a theory, the better we understand it. In this perspective, computer simulations fare terribly badly, since they involve going through many gory computational steps and, even once these have been carried out, scientists usually end up with no simple picture of the results and no inferential shortcuts that could exempt them from this computational stodginess for future similar investigations.

Understanding: What Do We Lose with Computer Simulations?

Before the advent of computational science, explanatory advances in science were always the direct product of human minds and pen-and-rubber methods. Therefore, any actual scientific explanation that satisfied the requirements for explanatoriness was also human sized, and the epistemic benefits logically contained within such explanations could actually be enjoyed by competent and informed epistemic agents. In [34.158, p. 299], *Hempel* states that an explanatory argument shows that "the occurrence [of an event] was to be expected" and he adds "in a purely logical sense." This addition emphasizes that expectation should not be understood as a psychological notion nor refer to the psychological aspects of the activity of explaining. In the case of computer simulations, this addition is somewhat superfluous. Nomic expectability remains for scientists, since, based on computer simulations, they may know that they can entertain the belief that an event should happen. However, this belief is completely *cold*. Since the activity of reasoning is externalized in computers, it is no longer part of the proper cognition of scientists and does not come with the psychological side-effects associated with first-person epistemic activities, such as emotions or feelings of expectation, impressions of certainty and clarity, or the oft-mentioned aha or eureka feeling which usually comes with first-person experiences of understanding. In other words, with computer simulations, the mind is no longer the carrier of the activity of explanation, and simply records what it should believe. Unfortunately, epistemic benefits associated with the individual ability to carry out this activity are also lost. Since the explanatory argument can no longer be surveyed by a human mind, the details of the relations between the premises of the explanatory argument and its conclusion are opaque. Therefore, scientists are no longer able to encompass *uno intuitu* all aspects of the explanation and how they are related, to develop expectations about counterfactual situations (in which similar hypotheses are met), and the unificatory knowledge that only global insights can provide is also lost. Overall, with computer simulations the objective intelligibility that is enclosed in explanations and can be accessed by first-person epistemic appropriation of the explanatory arguments can no longer be completely enjoyed by scientists (see also [34.159] for further analyses about epistemic opacity in this context). In this perspective, the problem of computer simulations is not that they have less explanatory value but that *we cannot have epistemic access to* this explanatory value. In brief, this problem would not pertain to the logic of computer-simulation-based explanations but to their epistemology.

New Standards for Understanding?

The gradualist description regarding the need of cognitive and logical operations to foresee consequences (see Sect. 34.4.4 Computer Simulations, Understanding, and Inferential Immediacy) suggests that the boundary between cases where intelligibility is present or is lost is not completely sharp. Importantly, the ability to foresee consequences depends on various factors such as the knowledge of physical or mathematical theorems to facilitate deductions, the knowledge of powerful formalisms to facilitate inferences, how much the intuition of scientists has been trained to anticipate consequences of a certain type and has somewhat internalized inferential routines, etc., [34.102, §6.4]. In other words, at least in some cases, the frontiers of what has a computational explanation, but remains unintelligible to a human mind, can be pushed back to some extent.

This raises the question of how much the frontiers of intelligibility can be extended and whether the ideal of inferential or computational briefness for explanations should be considered as a normative standard. Two positions are possible. One may claim that genuine explanations should *always* yield the possibility for human subjects to access the corresponding understanding. Or one may claim that, as shown by computational science, we have gone beyond human-sized science, not all good explanations can be comprehended by human minds, and this is not a defect of *our* science, even if it is clearly an epistemic inconvenience.

A motivation for endorsing the former claim is that the lack of intelligibility of explanations often stems from epistemic flaws of the agents producing them and can be corrected. Typically, in science, results are often laboriously proved and, with the advance of scientific understanding, shorter and clearer proofs, or quicker algorithms, are found.

Overall, it seems sound to adopt the following methodological maxim: *the more resources we need to produce (or check) an explanation (resp. an argument, a proof), the more we are entitled to suspect, in the absence of contrary evidence, that the explanation is unduly complex*. From this point of view, computer simulations do not seem flawless, since they make abundant use of computational and inferential resources. Accordingly, it is legitimate to suspect computer simulations of providing unduly complex explanations, which have simpler versions yielding the expected accessible understanding.

Nevertheless, this philosophical stance may be inappropriate in many cases. There is a strong suspicion that explaining phenomena often requires using an irreducible amount of resources. This idea of computational irreducibility has been vocally advanced, though not clearly defined, by *Wolfram* [34.155], and philosophers have toyed with close intuitions in recent discussions about emergence [34.74, 123, 124, 160–162]. Capturing the idea in a clear, robust and fruitful definition is a difficult on-going task [34.163]. However, there seems to be an agreement that this intuitive notion is not empty, which is what matters for the purpose of the present discussion. Overall, this means that in all such cases, asking for computationally simple explanations does not make sense, since such explanations do not exist. In this perspective, tailoring our explanatory ideals to our human capacities is wishful thinking, since in many cases, the inaccessibility of the usual epistemic benefits of explanations does not stem from our epistemic shortcomings.

This suggests that we may have to bite the bullet and say that, sometimes, computer simulations do bring full-fledged explanation and objective understanding, even if, because of our limited cognitive capacities, we cannot enjoy this understanding and the epistemic benefits harbored by such explanations. In other words, both of the above philosophical options are correct, though in different cases.

Ideally, one would like to be able to know when each of these two options should be adopted. Unfortunately, determining whether a computational process can be shortcut or a computational problem solved by quicker algorithms, seems to be in practice opaque (*problem of the lack of transparency of the optimality of the computational process*). This means that in most cases, when facing a computational explanation of a phenomenon, one does not know whether there are computationally or inferentially shorter versions of this explanation (and we are to be epistemically blamed for being so explanatorily laborious), or whether one cannot do better (and the process is intrinsically complex).

Overall, because determining whether explanations are informationally minimal (regarding the use of relevant information) and whether arguments or computations are optimal is opaque, computer simulations are doomed to remain shrouded in suspicion about their explanatoriness, *even in cases in which there is no better (that is, shorter or less informationally replete) explanation*. In brief, the era of suspicion regarding the explanatoriness of computer simulations will not end soon.

34.4.5 Bypassing the Opacity of Simulations

Even when computer simulations are epistemically opaque, some strategies can be tried to regain predictive power, control, and potentially understanding regarding the corresponding inquiries.

Understanding, Control and Higher Level Patterns

As emphasized by *Lenhard* [34.159], by *manipulating* computational models and observing which behavior patterns are obtained, scientists can try to control the processes involved and develop "a feeling for the consequences." Lenhard suggests that this *understanding by control*, which is oriented toward design rules and predictions, corresponds to a pragmatic account of understanding, which is also involved in the building of reliable technological artifacts.

Other authors have emphasized that, even if the details of computer simulations cannot be followed by human minds, one may sometimes still obtain valuable insights by building coarse-grained representations of the corresponding target systems and analyzing whether macro-dynamics emerge when microinformation is thrown away [34.164]. Surprisingly, the existence of coarse-grained dynamics seems to be compatible with complex, potentially computationally irreducible, dynamics at the microlevel [34.165, 166], even if this by no means warrants that control or understanding can always be regained at the macro-level. Thus, the question arises as to when and how much epistemic virtues like predictive power, control, and potentially understanding, which are somewhat lost at the microlevel, can be partly recovered at the macro-level, and how the corresponding patterns can be detected. The treatment of such questions requires the analysis of logical and mathematical relations between descriptions of systems at different scales and, for this reason, it should gain from ongoing debates and research in the philosophical and scientific literature about the emergence of simple behavior in complex systems.

Visualization and Understanding

Another important issue is how to exploit macro-level patterns that are present in computer simulations to restore partial cognitive grasp of the simulated systems by humans. Given the type of creatures that we are, and in particular the high visual performance of the brain, using visual interfaces can be part of the answer. Indeed, the format of scientific representations partly determines what scientists can do with them – whereas, as emphasized by [34.41, p. 95], philosophers have often considered the logical content of a representation to be the only important element to analyze them. To go further into these issues, sharp analyses of representational systems and their properties are required. Tools and concepts developed in the Goodmanian tradition prove to be extremely useful [34.167]. For example, *Kulvicki* [34.29] highlights how much graphs and images can present information more immediately than symbolic representations can. This notion of immediacy is cashed in in terms of semantic salience, syntactic salience or extractability. *Vorms* further shows how taking into account formats of representation in the analysis of scientific reasoning is crucial, since inferences have different cognitive costs depending on the format of representation [34.168]. *Jebeile* [34.169] applies similar concepts to computational models and argues that visualization tools can have a specific explanatory role since they do not merely present computational data in more accessible ways, but also suggest interpretations that are not contained in the original data, highlight relations between these data, and thereby point at elements of answers to what-if questions.

Overall, the issue of how much visualization can convey objective understanding remains debated. For example, *Kuorikoski* [34.164] acknowledges that visual representations are cognitive aids but emphasizes that they often merely bring about a *feeling* and *illusion* of understanding. So, there is the need of epistemological analyses which would make clear in which cases, and how, visual representations can be reliable guides and self-certifying vectors of knowledge, which partly enable their users to determine whether and how much they should trust them.

34.4.6 Understanding and Disciplinary Norms

All the above discussion has been based on general arguments about explanations and understanding. However, as already emphasized, explanatory norms sometimes differ from one field to another, economics being, at least in its mainstream branches, a paradigmatic case of a field in which simulation methods are shunned [34.37]. Similarly, the explanatory status of computer simulations and computational models varies across fields like cognitive sciences, artificial intelligence [34.137], artificial life [34.170] or within fields themselves (see, e.g., [34.171] for the case of computational chemistry and [34.79] for that of climate science).

This is not the place to discuss whether these variations regarding explanatory norms are deep, or whether they result from differences in theoretical contexts, in the degrees of complexity of the systems investigated, in the difficulties to collect evidence about them, in the scientific maturity and empirical success of these fields, etc. Such questions cannot be answered on the basis of armchair investigations. Field-specific studies of the explanatoriness of computer simulations, made by scholars who are in the same time acutely aware of present discussions about scientific explanation, are needed.

34.5 Comparing: Computer Simulations, Experiments and Thought Experiments

Computer simulations, experiments, and, to a lesser extent, thought experiments share various similarities, which calls for an explanation. Indeed, similarities between experimental activities and computational science are even found in mathematics, where some methods are claimed to be *experimental* (Sect. 34.5.1). Computer simulations, experiments and thought experiments can sometimes be seen as ways of carrying out similar activities, or activities having similar constraints (Sect. 34.5.2). Should an additional step be made, and computer simulations be considered as experiments? A close scrutiny of the existing arguments in favor of this claim shows that it meets insuperable difficulties, both regarding the analysis of computer simulations and experiments. Further, the claim does not even seem necessary to account for the importance of the material aspects of simulations (Sect. 34.5.3). Finally, even if computer simulations can yield knowledge, which can sometimes be more reliable than that produced by experiments, unless a strong case against empiricism is properly made, computer simulations do not seem to seriously threaten the unique foundational role of experiments as the source of primary evidence upon which science is built (Sect. 34.5.4). In any case, discussions about the relationships between experiments and computer simulations should remain compatible with the actual existence of hybrid (both computational and experimental) methods (Sect. 34.5.5).

When in the 1990s philosophers of science started investigating computer simulations, they soon realized that the object of their inquiry cross-cut traditional categories like those of theories, models, experiments or thought experiments. Similarities with experiments were particularly striking, since, among other things, computer simulations involved the treatment of massive data and statistical reasoning, required robustness analysis, and were claimed to yield new knowledge. As a result, computer simulations were suggestively dubbed by various authors as computer *experiments*, numerical *experimentation* or in-silico *thought experiments*, even though it was not always conceptually clear what these potentially metaphorical characterizations meant exactly.

All such similarities are worth analyzing and potentially call for explanations. They may be the sign of an identical nature between (some of) these activities, of common essential features, or may just be shallow or fortuitous. Clarifying this issue is also a way to analyze these activities more acutely by singling out what is specific to each or common to them and to determine to what extent epistemological insights can be transferred between them.

34.5.1 Computational Mathematics and the Experimental Stance

Experimental Proofs in Mathematics

Since aspects related to the representation of material systems are absent from mathematics, a comparison with this field can be hoped to be fruitful to *analyze* what exactly is experimental in computational science.

The mathematical legitimacy of computers for the production of proofs has been discussed for several decades. Computational proofs like that of the four-color theorem by *Appel* et al. [34.172, 173] were rapidly labeled *quasi-empirical* and discussions raged about how they should be interpreted [34.174, p. 244]. Such computational *proofs* can actually be seen as having roots in the older tradition of *quasi-empirical mathematics*, practiced for example by mathematicians like Euler, and philosophically defended by authors like *Lakatos* [34.175] or *Putnam* [34.176]. Interestingly, even in these contexts, the labels *empirical* or *experimental* were used to refer to various aspects of the activity of proving results.

Like experiments, computational proofs involve external processes, which are fallible. Their reliability can then be seen as being partly of a probable nature and needs to be assessed a posteriori by running these external processes several times and checking that the apparatus involved worked correctly. By contrast, proofs which can be *actively* and *directly* produced by humans minds, can provide a priori knowledge, the validity of which is assessed by (mentally) inspecting the proof itself, qua mathematical entity. Further, computational proofs, like experiments and empirical methods in mathematics, usually provide particular numerical results: as the computational physicist Keith Roberts writes it, "each individual calculation is [...] analogous to a single experiment or observation and provides only numerical or graphical results" (quoted in [34.70, p. 137]). Therefore, to obtain more general statements (and possibly theories), probabilistic inductive steps are needed. Overall, such debates illustrate the need to clarify the use in this context of labels like *experimental* or *empirical*.

The Experimental Stance

The case of computational mathematics also makes clear how scientists can adopt an experimental stance for inquiries where no physical process is investigated, and the nature of the object which is *experimented upon* is completely known.

Experimenting involves being able to trigger changes, or to intervene on material or symbolic dynamical processes, and to record how they vary accordingly. As noted by *Dowling* [34.136, p. 265] and *Jebeile* [34.169, II, §7.2], processes for which the dynamics is known can also work as black boxes, since the opacity of the process may stem either from our lack of knowledge about its dynamics, or from the mathematical unpredictability (or epistemic inaccessibility) of its known dynamics. In this perspective, contrarily to *Guala* [34.177], being a black box is not a specific feature of experiments.

Finally, when experimenting on a material or formal object, it is better that interactions with the object be made easy and the results be easily accessible to the experimenters (e.g., by means of visual interfaces) so that tinkering is made possible [34.136] and intuitions, familiarity, and possibly some form of understanding [34.159, 169, III] can be developed.

34.5.2 Common Basal Features

Some similarities of computer simulations and experiments (and thought experiments) may be accounted for by highlighting common basal features of these activities, which in turn account for the existence of their common epistemological features, such as the shared concerns of practitioners of experiments and computer simulations for "error tracking, locality, replicability, and stability" [34.70, p. 142]. In this perspective, one should characterize the nature and status of these common basal features.

Role or Functional Substitutability

Though computer simulations, thought experiments and experiments are activities of different types, they can sometimes be claimed to play identical roles. Typically, computer simulations are used to gain knowledge about how physical systems behave (hereafter *behavioral knowledge*) when experiments are unreliable, or making them is politically or ethically unacceptable [34.41, p. 107]. Importantly, acknowledging that computer simulations can sometimes be used as substitutes for experiments by no means implies that they can play *all the roles of experiments* (Sect. 34.5.4). Further, one should be aware that, at a high-level of abstraction, all activities may be described as doing similar things; therefore, these shared roles should be shown in addition to have nontrivial epistemological implications. For example, one may argue that *providing knowledge* or *producing data* are roles that are endorsed by computer simulations, thought experiments, or experiments. However, this may be seen as some partially sterile hand-waving. Indeed this points at a too abstract similarity if these activities produce items of knowledge of totally different types, and nothing epistemologically valuable can be inferred from this shared characterization (see [34.81] for a presentation of the different types of knowledge involved in science).

El Skaf and *Imbert* [34.87] make an additional step when they claim that these activities can in certain cases be *functionally substitutable*, that is, that we can sometimes use one instead of the other for the purpose of a common inquiry – which remains compatible with the fact that these activities do not play the roles in question in the same way, that they come with different epistemic credentials, provide different benefits, and therefore, as role holders, are not *epistemologically substitutable*. El Skaf and Imbert, in particular, claim that computer simulations, experiments, and thought experiments are sometimes used for the purpose of unfolding scenarios (see also Hughes' notion of demonstration in Sect. 34.6.1) and argue that investigations concerning the possibility of a physical Maxwellian demon were indeed pursued by experimental, computational and thought experimental means. The existence of such common roles then provides grounds for analyzing similarities in the epistemological structure of the corresponding inquiries.

Morrison [34.178] goes even further since she argues that some computer simulations are used *as* measuring instruments and therefore that they have the same epistemic status as experimental measurements. She first claims that models can serve as measuring instruments, and then shows that this role can be fulfilled in connection with both computer simulations and experiments, which are similarly model shaped. An important part of her strategy is to relax the conditions for something to count as an experiment, by discretely giving primacy, in the definitions of scientific activities, to the roles which are played (here measuring) and by downplaying the importance of physical interactions with the investigated target systems in the definition of experiments (which are simply seen as *a way* to perform this measuring role). *Giere*'s rejoinder denies the acceptability of this strategy, and follows the empiricist tradition, when he claims that "a substitute for a measurement is not a measurement, which traditionally requires causal interaction with the target system" [34.179, p. 60]. Indeed, the potential additional pay-offs of experiments, as primary sources of radically new evidence, come from these causal interactions. Accordingly, their specificity is not due to their roles, qua information sources (since thought experiments, models, or theories are also information sources), but from the type of epistemological credentials that come with the corresponding information, and grounds our ultimate scientific beliefs. A different nonempiricist epistemology might be developed, but the bait must then be swallowed explicitly, and it must be explained why such an epistemology, in which activities are exclusively individuated on the basis of their function and the importance of other differences is downplayed, should be preferred. In any case, an account of how to individuate these functions would be needed, since at a high level of abstraction, various activities can be seen as performing the same function.

Beyond Anthropocentric Empiricism

To practice science, humans need to collect observations and make inferences. Since human capacities are limited, various instruments have been developed to extend them and these instruments have been partly computational for decades. These parallel developments of observational and inferential capacities come with common epistemological features. In both cases, restricted empiricism, which gives a large and central role to *human* sensorial or inferential capacities in the description of how scientific activities are carried out, is no longer an appropriate paradigm to understand scientific practices. Indeed, the place of human capacities within modern science needs to be reconsidered [34.8, 41, 180]. Further, the externalization of observations and inferences comes at the price of some epistemic opacity and passivity for the practitioner, since, as humans, we no longer consciously carry out these activities. Instead we simply state the results of experimental or computational apparatus. However, this also comes with gains in objectivity since observational and informational procedures are now carried out by external, transparent and controlled apparatus, which no longer have hidden psychological biases nor commit fallacies.

The development of computational instruments and computer simulations also raises similar epistemological problems. For example, the apparently innocuous notion of data seems to raise new issues in the context of computational science. Computer simulations, like models, have been claimed to be useful to *probe* physical systems and to be used as *measuring instruments* [34.178]. Whatever the interpretation of such statements (Sect. 34.5.3), it is a fact that both computer simulations and computational instruments provide us with *data*, which raises transversal questions.

A datum is simply the value of a variable. It can be taken to describe a property of any object. In this simple sense, data coming from experiments and computer simulations can play a similar role by standing for the properties of some target system within some representational inquiries. Furthermore, in both cases, their interpretation usually involves heavy computational treatments. In particular, mathematical transforms of various types serve to separate information from noise, remove artifacts, or recover information about a system property out of intertwined causal signals, like in computed tomography imaging techniques [34.121]. From this point of view, as emphasized by *Humphreys* [34.181], here one departs from a principle frequently used by traditional empiricists, and according to which "the closer we stay to the raw data, the more likely those data are to be reliable sources of evidence."

At the same time, there are different types of epistemological data, and the need for their common study should not introduce confusion in their understanding. In science, one seeks to determine how much data reliably stand for their target, and which properties exactly they refer to. Humphreys's remark above the computational treatment of data, reproduced above, highlights the fact that causal information concerning the source is crucial to treat and interpret data and to determine what empirical content they bring about this source (this is the *inverse inference problem*), given that data do not wear on their sleeves details of how they were produced. From this point of view, experimental and computational data have utterly different causal histories – so what gives its sense to the computational treatment is potentially of a different nature [34.91, 121]. Overall, more pointed comparative analyses of data obtained by computer simulations and computational instruments are still to be carried out, to understand their semantics and epistemology and highlight both their nonaccidental similarities and specific differences (see [34.182] for the case of computational instruments).

Computational science must also face the challenge of data management. While the steps of *traditional* mathematical proofs and arguments, once produced, can be verified by scientists, things are usually different for computer solutions, even if they are merely executions of computational programs [34.91], or arguments [34.72]. Details of computer simulations are in general not stored since this would require too large amounts of memory (even if, in some cases like the Millennium Run, scientists may decide to keep track of the evolution of the computer simulation). In other words, like experimental science, computational science involves choosing which data to keep track of, developing powerful devices to store them, finding appropriate ways to organize them, providing efficient interfaces to visualize, search, and process them, and, more generally, developing new methods to produce knowledge from them. This also raises questions about how these data can or should be accessed by the scientific community, and which economic model is appropriate for them [34.183]. In brief, the epistemology of computer simulations here meets that of big data [34.184, 185], even if it cannot be assumed that on-going debates and analysis about the latter, because they are mostly focused on questions raised by empirically collected data, will naturally apply to, or be insightful for, the corresponding problems raised by computer simulations.

Different Activities, Similar Patterns of Reasoning

As noted by *Parker* [34.186], strategies developed to build confidence in experimental results, and described in particular by Allan Franklin, seem to have close analogs for the justification of results generated by computer simulations. Indeed, the interpretation of the results of computer simulations as evidence for hypotheses about physical systems can sometimes be made through an error-statistical perspective [34.187] as in the case of experiments [34.188].

Similar patterns of reasoning are also used to argue in favor of the existence of specific mechanisms or entities on the basis of patterns within data, modes of visualizations of these patterns, or our ability to manipulate the actual or represented systems and find pattern regularities in their behavior (see [34.71] for a description of the *homomorphic tradition*, in which visual forms are given much importance, in contrast to the *homologic tradition*, which is more based on logical relationships). More generally, visualization techniques, aimed to facilitate the reasoning about results present in large databases, are crucial in the case of both experiments and computer simulations (Sect. 34.4.4).

Importantly, these similarities may have different explanations. For example, they may simply stem from the need to treat massive amount of data by efficient standard procedures, or be a consequence of features shared by experimental and computational data, independently of their quantity, like the presence of noise, or may correspond to the application of general types of evidential or explanatory arguments to data having different natures.

The Reproducibility of Results

Reproducibility is a typical requirement for experiments, though it is one that is sometimes difficult to achieve because of the tacit knowledge involved in the carrying out of experiments [34.189]. Similar problems may arise with computer simulations. Even if the latter are nothing more than computations and are in principle reproducible, in practice reproducibility may sometimes be difficult, especially in the context of big science. For example, computer simulations may be too big to be reproduced (all the more since scientists have in general little incentive to reproduce results). Numerical codes may not be public (because they are not published or shared), and many of the computational details may be left tacit. Finally, computer simulations involving stochastic processes may not be exactly reproducible because the random numbers came from external physical signals or because the details of the pseudorandom number generator are not made public.

Experimenters' and Simulationists' Regresses

Good scientific results are usually expected to be robust against various changes [34.190], in particular those related to implementation or material details, and this is why failure of exact reproducibility should not be a worry.

Still, when one faces an inability to reproduce a result, the problem may arise from a lack of robustness or flaw in the original experiment or computer simulation, or from a failure to reproduce it correctly. Accordingly, as emphasized by *Gelfert* [34.191], computer simulations are affected by a problem similar to that of the experimenter's regress [34.192], which is met when to determine whether an experimental apparatus is working properly scientists have no criterion other than the fact that it produces the expected results. As noted by *Godin* and *Gingras* [34.193], regresses like that highlighted by Collins are instances of well-known types of arguments already analyzed in the framework of ancient skepticism (more specifically, regresses or circular relations regarding justification). As such, they are specific neither to experiments nor to computer simulations – even if solutions to these problems, as those described by Godin and Gingras or *Franklin* [34.194], may be partly activity specific. In any case, adopting a general comparative perspective provides a way to analyze more acutely what is epistemologically specific or common to scientific activities.

34.5.3 Are Computer Simulations Experiments?

Some authors go as far as claiming that, at least in *some* cases, what we call computer simulations *are* in fact experiments. In this perspective, Monte Carlo methods, sometimes labeled *Monte Carlo experiments* or *Monte Carlo simulations*, seem to be a philosophical test case (like analog simulations, Sect. 34.2.2). Such methods are used to compute numbers (e.g., pi), sample target distributions or produce dynamical trajectories with adequate average properties. They rely crucially on the use of randomness [34.8, 72]. They may look closer to experiments because they sometimes use physical systems, like a Geiger counter, to generate random events.

Still, *Beisbart* and *Norton* claim that Monte Carlo methods are not experiments, since randomizers can be replaced by computer codes of pseudorandomizers [34.72, p. 412]. This shows that these computer simulations do not require contact with the randomizer as an external object; therefore no direct empirical discovery about the nature of physical systems can be made by them and they should not be seen as having an experimental nature. In brief, in Monte Carlo simulations, the physical systems involved are simply used as computers to generate mathematically random sequences.

Beyond the analysis of specific cases, some authors have defended the bolder claim that all computer simulations are experiments (what *Winsberg* calls the *identity thesis* [34.195, §5]). While this goes against inherited scientific common sense (computations are not experiments!), the claim should be carefully examined. Indeed, in principle there is no impossibility here: while computations, logically defined, are not experiments, we need physical machines to carry them out. Therefore, in the end, computers, instruments and experimental systems are physical systems that we use for the purpose of doing science – and it all boils down to how we conceptualize in a coherent and fruitful way these external worldly activities. In brief, perhaps, after all, we would be better off revising our epistemological notions so that computer simulations are seen as genuine examples of experiments – a revisionary position with regard to the empiricist tradition since it ignores the specificity of experiments as primary evidential sources of knowledge.

In what follows, I review existing arguments in favor of the claim that computer simulations are experiments, and how these arguments have been criticized. Overall, as we shall see, in contrast to what is claimed in [34.195, §5], it is very dubious that discussions about the *identity thesis* are simply a matter of perspective and where the emphasis is placed. A minute, conceptually rigorous, and sharp treatment of this question can be found in [34.53, 72, 91, 196] and [34.169, Chap. 7].

Problems with Analyses in Terms of Common Physical Structures

Some authors analyze computer simulations as manipulations of physical systems (the computers), which instantiate or realize models that are also instantiated or realized by the investigated physical systems.

Norton and *Suppe* [34.114] are good representatives of this tradition. They first try to describe formal relations between what they call a *lumped model*, the structure of the target system, and the programmed computer, which is supposed to embed the lumped model. They further argue that these relations account for the experiment-like character of computer simulations: instead of experimenting on real systems, computer simulations are used as physical stand-ins or analogs to probe real-world phenomena, and one thereby learns thing about the represented systems. This suggestive position has charmed various authors. It also has similarities with accounts of scientific representation made in terms of similarity [34.28], isomorphism, or weaker relationships between the representation and the target system [34.197, 198], even if the authors that defend the above view have not adopted so far this line of argument.

However, in the case of computer simulations, this view does not seem to resist close scrutiny, for reasons specific to computational activities. While in the case of analog simulations both the represented system and the analog computer instantiate a common mathematical structure (Sect. 34.2.2), such a claim cannot be made for digital computers. The general idea is that steps of computational processes are multiply realizable and that, conversely, how physical states of computers are to be interpreted is contextual and partly arbitrary [34.4]. It is true that for every step of a computation to be carried out in practice, one needs to use a physical machine that can be seen as instantiating the corresponding transition rule. However, physically different machines can be used to carry out different parts of a computation (for example when the computation is distributed). Furthermore, even if a single machine is used, different runs of the program will correspond to different physical processes, since the computer may process several tasks in the same time and contextually decide how its memories are organized, and even within the same computation, a single part of the memory may be used at different steps to code for different physical variables [34.91, pp. 564–566], [34.196, pp. 81–84]. Overall, in the general case, the relation between the physical states of the represented target system and the physical states of the computer(s) that may be used to simulate its behavior is a many-many one, and the idea that the phenomenon is recreated in the machine "is fundamentally flawed for it contradicts basic principles of computer architecture" [34.196, p. 84]: in the case of a successful computer simulation, one can simply say that every step of the computation has been carried out by some appropriate physical mechanism, but there is no such thing as a computer instantiating the structure of the model investigated. (Note that the argument based on multiple realizability is in the spirit of those originally developed by *Fodor* [34.126] in his discussion of the reduction of the special sciences).

Problems with Common Analyses in Terms of Intervention or Observation

Computer simulations have also been claimed to qualify as experiments "in which the system intervened on is a programmed digital computer" [34.199, p. 488], or to involve observations of the computer as a material system [34.114, p. 88]. *Winsberg* even goes as far as to claim that [34.195]

> "nothing but a debate about nomenclature [...] would prevent us from saying that the epistemic target of a storm simulation is the computer, and that the storm is merely the epistemic motivation for studying the computer."

Such claims can be answered along the same lines as the previous argument. There is of course no denying that when one runs a computer simulation one interacts with the interface of the computer, which triggers some physical change in the computer so that the right computation is carried out. Similarly, once the computation is finished, the physical state of the memory in which the result is stored, triggers a causal mechanism that produces changes in the interface so that the result can be read by the user. However, the definition of an intervention at the model level does not determine a specific intervention at the physical level of the computer. The reason is that, as emphasized above, even within the same computational process, the way that the intervened model variable is physically represented in the computer may vary, and how the computer, qua physical system, evolves precisely may depend on various parameters such as the other tasks that it carries out at the same time. In brief, the idea that actual computer simulations, defined at the model level, could be seen as the investigation of the computer, qua physical machine, which is used to carry them out, seems to be riddled with insuperable difficulties.

Finally, one should mention that epistemic access to the physical states of the computer corresponding to the successive steps of a computation is usually not possible in practice [34.196, p. 81].

Problems with General Analyses in Terms of Epistemological and Representational Structure

Some authors have also argued that computer simulations and experiments share an epistemological structure, or epistemological aspects, and have used this claim to justify the identity thesis.

For example, it has been claimed that in both cases one interacts with a system to gain knowledge about a target system, and the internal and external validity of the processes needs to be checked. This type of analysis stems from a 2002 paper by *Guala* [34.177] in which he presents a laboratory experiment in economics aimed at investigating behavioral decision making by giving decisional tasks to real human subjects in the laboratory. In this case, a hypothesis about how agents behave in the laboratory is investigated (internal validity hypotheses); then, based on similarities between the experimental situation and the real-life situation, an external hypothesis is made about the behavior of agents in real life situations (external validity hypothesis). The notion of internal validity comes from social science and corresponds to the (approximate) truth of inferences about causal relationships regarding the system that is experimented on. External validity corresponds to the (approximate) truth of the generalization of causal inferences from an initial system, for which internal validity has been demonstrated, to a larger class of systems. *Guala* further claims that both computer simulations and experiments fit this epistemological description in terms of internal and external validity arguments, but cautiously concludes that their "difference must lie elsewhere" [34.177]. According to him, computer simulations and experiments are different, since in the latter case there is a material similarity between the object and the target, whereas, in the former case, there is a formal similarity between the simulating and the simulated systems (a claim which seems to be falling under the above criticism directed at Norton and Suppe and their followers).

Guala's conceptual description is endorsed by most authors who try to picture computer simulations as some sort of experiment. For example, *Winsberg* accepts the description, but claims that the difference between experiments and computer simulations lies in the type of background knowledge that researchers use to justify the external validity hypothesis [34.113, p. 587], a position which is again revisionary with regard to the empiricist tradition if this is the only specificity ascribed to experiments.

A serious worry is that describing the investigation of the computational model in terms of internal validity is problematic and artificial, since, as can be seen above, computer simulations cannot be considered as investigations of the causal behavior of the computer, qua physical system. For the same reason, the use of the notion of external validity is inappropriate, since for computer simulations inferences about the target system do not involve the generalization of causal relations taking place in the computer to other systems by comparing their material properties but involve the *representational* validity of the computational model.

A final problem is that the characterization of the methodology of experimental studies in terms of internal and external validity, though useful in the social sciences, is not a general one. Using it as an accepted general framework to compare experiments and computer simulations looks like a hasty extrapolation of the case of laboratory experiments in experimental economics, not to mention the fact that economics may be seen as a bold pick to build a general conceptual framework for experimental studies.

It is true that in experiments, the measured properties are often not the ones that we are primarily interested in and the former are used as evidence about these latter target properties. Typically, vorticity in turbulent flows is difficult to measure directly, and is often assessed by measuring velocity, based on imaging techniques. In more complex cases, the properties measured can be seen as a way to *observe* different and potentially remote target systems, as is vividly analyzed by *Shapere* with his case study of the observation of the core of the sun by the counting of ^{37}Ar atoms in a tank within a mine on Earth [34.180]. Importantly, in all such cases, the measuring apparatus, the directly measured property, and the indirectly probed target system are related by causal processes. The uses of the collected empirical information then vary with the type of inquiry pursued. The evidence may be informational about the physics of a particular system, like the Sun. Or, it may be used to confirm or falsify theories (like in the case of the 1919 experiment by Eddington and the relativity theory). In some cases, *though by no means all*, it may be used to draw inferences about the nature or behavior of a larger class of similar systems – which are not related to the measured system by a causal relationships. If this latter case of reasoning about external validity is taken as paradigmatic for experiments, and the causal processes between the target experimented systems (the source) and the measuring apparatus (the receptors), which are present in all experiments, are considered as a secondary feature, experimental activities are misrepresented. As Peschard nicely puts it "the idea that the experiments conducted in the laboratory are aimed at understanding some system that is outside the laboratory is a source of confusion" [34.200]. General conceptual frameworks that do not introduce such confusion are however possible. For example, *Peschard* proposes [34.200]

> "to make a distinction between the *target system*, that is manipulated in the experiment or represented in the computer simulation, and the *epistemic motivation*, which in both cases may be different from the target system "

(see also the distinction between the result of the unfolding of a scenario and the final result of the inquiry in [34.87]).

Overall, the common description provided by Guala, and heavily relied upon in [34.113, 199] to support versions of the *identity thesis* can be defended only by squeezing experiments and computer simulations into a straightjacket which misrepresents these activities, is not specifically fruitful, and meets insuperable difficulties.

Materiality Matters

Clearly, for both experiments and computer simulations, materiality is crucial. However, it does matter differently, and one does not need to endorse a version of the identity thesis to acknowledge the importance of materiality when claiming for example that, to understand computational science, the emphasis should be on computer simulations which can be in practice, and therefore materially, carried out by actual systems [34.41, 91].

For experiments, material details are relevant throughout the whole inquiry when producing, discussing and interpreting results, their validity and their scope (especially if one tries to extrapolate from the investigated system to a larger class of materially similar ones). By contrast, for computer simulations, material details are important to establish the reliability of the computation, but not beyond: only the mathematical and physical details of the investigation matter when discussing and interpreting the results of the computer simulation and the reliability of the inquiry.

34.5.4 Knowledge Production, Superiority Claims, and Empiricism

The question of the epistemic superiority of experiments over simulations has also been discussed. *Parke* [34.201] takes it for granted that "experiments are commonly thought to have epistemic privilege over simulations" and claims that this is in fact a context-sensitive issue. As we shall see, if one puts aside the question of the specific role of experiments as the source of primary evidence about nature, it is not clear whether the general version of the superiority claim has actually been defended, or whether a straw man is attacked.

Computer Simulations, Experiments and the Production of Radically New Evidence

Let us try to specify what the general superiority claim could be and how it has really been defended.

The obvious sense in which experiments may be *superior* is that they can provide scientists with primary evidence about physical systems, which originate in interactions with these systems, and cannot be the product of our present theoretical beliefs. It is unlikely that computer simulation can endorse this role. As *Simon* pithily puts it, "a simulation is no better than the assumptions built into it, and a computer can do only what it is programmed to do" [34.12, p. 14]. From this perspective, experiments have the potential to surprise us in a unique way, in the sense that they can provide results contradictory to our most entrenched theories, whereas a computer simulation cannot be more fertile than the scientific model used to build it (even if computer simulations can surprise us and bring about novel results, see Sect. 34.3.4). This is what *Morgan* seems to have in mind when she emphasizes that "[N]ew behaviour patterns, ones that surprise and at first confound the profession, are only possible if experimental subjects are given the freedom to behave other than expected," whereas "however unexpected the model outcomes, they can be traced back to, and re-explained in terms of, the model" [34.202, pp. 324–5]. In brief, experiments are superior in the sense that, in the empirical sciences, they can serve a function which computer simulations cannot.

Roush [34.203] has highlighted another aspect regarding which experiments can be superior to simulations. She first insists that we should compare the two methods *other things being equal*, especially in terms of what is known about the target situation. Then, in any case in which there are elements in the experimenter's study system that affect the results and are unknown, we may still run the experiment and learn how the target system behaves; by contrast, in the same epistemic situation, the simulationist cannot build a reliable computer simulation that yields the same knowledge. However, when all the physical elements that affect the result are known, a simulation may be as good as an experiment, and it is a practical issue to determine which one can in practice be carried out in the most reliable way.

Thus, for a quantitative comparison to be meaningful it should be related to roles which can be shared by experiments and computer simulations, such as the production of *behavioral* knowledge about physical systems, the relevant dynamics of which is known (Sect. 34.5.2).

Grounds for Comparative Claims

Scientists and philosophers have emphasized over the last decades that computer simulations are often *mere simulations* [34.177], the results of which should be taken carefully. As seen above, economists *shun* simulation; similarly, *Peck* states that evolutionary biologists view simulations with suspicion and even contempt [34.204, p. 530]. Nevertheless, however well advised these judgments may be, they cannot by themselves support a *general* and *comparative* claim of superiority in favor of other methods, but at most the claim that, in fields where other methods are successful and computer simulations have little epistemic warrants or face serious problems, these other methods will usually or on average be more reliable (exceptions remaining possible).

Some authors have discussed the comparative claim by analyzing the power of the types of inferences made to justify knowledge claims in each case. In [34.199], *Parker* adopts Guala's description of experiments (resp. computer simulations) as having material (resp. formal) similarities with their target systems (see the discussion in Sect. 34.5.3) and studies the claim that inferences made on the basis of material similarities would have an epistemic privilege. (Guala does not seem to endorse a comparative claim. He argues that material similarities are a specific feature of experiments, implying that the prior knowledge needed to develop simulations is different from that needed to develop experiments.) Again, the common description in terms of internal and external validity regarding the inferences from one physical system to another gives the semblance of a new problem. However, if, as suggested above, the material properties of computers matter only in so far as they enable scientists to make logically sound computations, and no similarity between systems is involved, the grounds and rationale for this discussion between the properties of the computer and those of the target system collapse. A way to save the argument is to claim that the aforementioned formal similarities are simply those between the computational model and the target system, but then the question boils down to the much more familiar comparison between model-based knowledge (here extracted by computational means) and some type of experiment-based knowledge.

On what grounds could the general privilege of experiment-based behavioral knowledge then be defended? Since experiments and computer simulations are different activities, which are faced with specific difficulties, it is hard to see why computer simulations should always fare worse. Why could simulations based on reliable models not sometimes provide more reliable information than hazardous experiments? Indeed, it is commonly agreed that, when experiments cannot be carried out, are unreliable, or ethically unacceptable, computer simulations may be a preferable way to gain information [34.41, p. 107].

Justified Contextual Superiority Claims

Interestingly, superiority claims can sometimes be made in specific contexts. *Morgan* presents cases in economics in which a precise and contextual version of the superiority claim may be legitimate [34.202].

Like Guala, Morgan discusses laboratory experiments in economics, that is, purified, controlled, and constrained versions of real world systems, which are studied in artificial laboratory environments (in contrast with field experiments, which "follow economic behavior *in the wild*" [34.202, p. 325]) and are aimed at investigating what is or would be the case in actual (nonsimplified) economic situations. Mathematical models can also be used for such inquiries and, in each case, scientists run the risk of describing artificial behaviors. *Morgan* then makes the following contextual claim that "any comparison with the model experiment is still very much to the real experiment's advantage *here*" [34.202, p. 321] (my emphasis) on the grounds that, in this case, the problem of making ampliative analog inferences from laboratory system to real-world systems is nothing compared with the problem of the realism of assumptions for models exploring artificial models [34.202, pp. 321–322]. She does not justify this point further, but a plausible interpretation is that, in such cases, mathematical models necessarily abstract away essential parts of the dynamics of decision making, which arguably are preserved in experiments because of the material similarity between the laboratory and real agents. In brief, while material similarity plays a role in her argument she does not make the general claim in the core of her paper that material similarity will *always* provide more reliable grounds for external validity claims than other methods (even if her formulation is less cautious in her conclusion).

Overall, such sound contextual comparative judgments require two premises: first that in some context computer simulations are not reliable (or have reliability r) and second that in the same context material similarities provide reasonably reliable inferences (or have reliability $s > r$). (Indeed, analogical reasoning based on material similarities, in which one reasons based on systems that are representative of or for larger classes of systems [34.127], can sometimes be powerful ways to make sound – though not infallible! – contextual inferences. As emphasized by *Harré* and *Morgan*, "shared ontology [...] has epistemological implications" [34.202, p. 323], since "the apparatus is a version of the naturally occurring phenomenon and the material setup in which it occurs" [34.205, pp. 27–8]. After all, different samples of the same substance obey the same laws, even if contextual influences may change how they behave and any extrapolation is not possible.)

34.5.5 The Epistemological Challenge of Hybrid Methods

Whether computer simulations and experiments are ontologically, conceptually, and epistemologically distinct activities or not, it is a fact that jointly experimental and computational *mixed* activities have been developed by scientists. Their study was pioneered by *Morgan*, who presents various types of hybrid cases in economics [34.206] and biomechanics [34.127]. For example, she reports different mixed studies aimed at investigating the strength of bones and carried out by cutting slices of bone samples, photographing them, creating digital 3-D images, and applying the laws of mechanics to these experiment-based representations. Morgan further attempts to provide a principled typology of these activities. This proves difficult because "modern science is busy multiplying the number of hybrids on our epistemological map" and because the qualities of hybrids "run along several dimensions" [34.127, p. 233]. Overall, sciences illustrate "how difficult it is to cut cleanly, in any practical way, between the philosopher's categories of theory, experiment and evidence" [34.127, p. 232], and, we may add, computer simulations or thought experiments.

Should these hybrid methods lead philosophers to reconsider the conceptual frontiers between experiments and computer simulations? We can first note that their existence may be seen as a confirmation that the traditional picture of science, in which theoretical, representational or inferential methods on one hand and experimental activities on the other play completely different but complementary roles, is not satisfactory (Sect. 34.5.2). Then, if one grants that activities like experiments, thought experiments and computer simulations can sometimes play identical roles, it is no surprise that they can also be jointly used to fulfill them. Similarly, a group of four online players of queen of spades sometimes involve virtual players – but most people will be reluctant to see this as sufficient grounds for claiming that bots are human creatures.

In any case, these hybrid activities raise epistemological questions. What, if anything, distinguishes a computer simulation that makes heavy use of empirical data from a measurement involving the computational refinement of such data [34.53, 121]? How much should the results of these methods be considered as empirical? Overall, what type of knowledge and data is thereby generated (see [34.53] for incipient answers)?

34.6 The Definition of Computational Models and Simulations

The main definitions of computer simulations are critically presented: Humphreys's 1994 definition in terms of computer-implemented methods, Hartmann's 1996 definition in terms of imitation of one process by another process, Hughes's DDI (denotation, demonstration, interpretation) account of theoretical representation, and finally Humphreys's 2004 definition, with its emphasis on the notion of a computational template (Sect. 34.6.1). The questions that a satisfactory definition should answer are then discussed, in particular which notions should be primitive in the definition, whether computer simulations should be defined as logical or physical entities, whether they correspond to success terms, how the definition should accommodate the possibility of scientific failure and the pursuit of partly open inquiries, or to what extent computer simulations are social, intentional, or natural entities (Sect. 34.6.2).

I come back finally to the issue of the definition of computer simulations. Providing a definition may look at first sight to be easy, since what computers are is well-known and clear cases of computer simulations are well identified. However, a sound definition should also be helpful to analyze less straightforward cases and be fruitful regarding epistemological issues related to computer simulations, not least by forcing philosophers to clarify the various intuitions which are entertained across scientific fields about these methods.

It is not difficult to present definitions that accommodate *some* types of computer simulations or *some* particular (or field specific) uses of computer simulations. Nevertheless, failing to distinguish between what is typical of computer simulations in general and what is specific to particular cases can lead (and has led) to heedless generalizations (Sect. 34.5.3). Things are all the more tricky as the very same types of computer simulations, qua formal tools (e.g., agent-based, CA models, equation-based simulations, etc.,) can be used in different epistemic contexts for different purposes, and require totally different epistemological analyses. The case of CA-based computer simulations exemplifies the risk of too quick *essentialist* characterizations. While it was believed that these models were appropriate for phenomenological simulations only [34.9, 135], their use in fluid dynamics has shown that they could supply theoretical models based on the same underlying physics as traditional methods [34.100].

The following section is organized as follows. Existing definitions and the problems they raise are presented first, and then issues that a good definition of computer simulations should clarify are emphasized.

34.6.1 Existing Definitions of Simulations

Computer-Implemented Methods

As emphasized by Humphreys, a crucial feature of simulations is that they enable scientists to go beyond what is possible for humans to do with their native inferential abilities and pen-and-paper methods. Accordingly, he offered in 1991 the following working definition [34.7]:

> "A computer simulation is any computer-implemented method for exploring the properties of mathematical models where analytic methods are unavailable."

This definition requires that we possess a clear definition of what counts as an analytic method, which is not a straightforward issue [34.60]. Further, as noted by *Hartmann* et al. [34.10, pp. 83–84], it is possible to simulate processes for which available models are analytically solvable. Finally, as acknowledged by Humphreys, the definition covers areas of computer-assisted science that one may be reluctant to call computer simulations. Indeed, this distinction does sometimes matter in scientific practice. Typically, economists are not reluctant to use computers to analyze models but shun computer simulations [34.37]. Since both computational methods and computer simulations involve computational processes, their difference must be either in the different types (or uses) of computations involved either at the mathematical and/or the representational level.

One Process Imitating Another Process

Hartmann proposes the following characterization, which gives the primacy to the representation of the temporal evolution of systems [34.10, p. 83]:

> "A model is called *dynamic*, if it [...] includes assumptions about the time-evolution of the system. [...] Simulations are closely related to dynamic models. More concretely, a simulation results when the equations of the underlying dynamic model are solved. This model is designed to imitate the time-evolution of a real system. To put it another way, a simulation imitates one process by another process. In this definition, the term process refers solely to some object or system whose state changes in time. If the simulation is run on a computer, it is called a computer simulation."

This definition has been criticized along the following lines. First, as noted by *Hughes* [34.13, p. 130], the definition rules out computer simulations that do not represent the time evolution of systems, whereas arguably one can simulate how the properties of models or systems vary in their phase space with other parameters, such as temperature. Accordingly, a justification for the privilege granted to the representation of temporal trajectories should be found, or the definition should be refined, for example, by saying that computer simulations represent successive aspects or states of a well-defined trajectory of a system *along a physical variable* through its state space. Second, the idea that a specific trajectory is meant to be represented may also have to be abandoned. For example, in Monte Carlo simulations, we learn something about *average values* of quantities along sets of target trajectories by generating a potential representative of these trajectories, but the computer simulations are not aimed at representing any trajectory in particular. One may also want a computer simulation to be simply informative about structural aspects of a system. Overall, the temporal dynamics of the simulating computer is a crucial aspect of computer simulations since it "enables us to draw conclusions about the behavior of the model" [34.13, p. 130] by unfolding these conclusions in the temporal dimension of our world, but the temporal dynamics of the target system may not have to be represented for something to count as a computer simulation.

Third, the definition is probably too centered on models and their solutions [34.207], since it equates computer simulations with the solving of a dynamic model that represents the target system. This is tantamount to ignoring the fact that describing computer simulations as mathematical solutions of dynamic models is not completely satisfactory. What is being solved is a computational model (as in *Humphreys*'s definition [34.41], see below), which can be significantly different from, and somewhat independent of, the initial dynamic model of the system, which usually derives from existing theories. Effectively, different layers of models, often justified empirically, can be needed in-between [34.13, 97, 208]. For this reason, the representational relation between the initial dynamic model and the target system, and between the computational system and the target system, are epistemologically distinct.

Finally, the definition may be reproached for entertaining a recurrent confusion about the role of materiality in computer simulations (Sect. 34.5.3), by describing the representational relation as being between two physical processes, and not between the computational model and succession of mathematical states which unfold it (*in whatever way they are physically implemented and computed*) and the target system.

Computer Simulations as Demonstrations

Hughes does not propose a specific definition of computer simulations since he believes that computer simulations naturally fit in the DDI account of scientific representation that he otherwise defends [34.13, p. 132]. According to the DDI, which involves denotation, demonstration, and interpretation as components [34.13, p. 125]:

> "Elements of the subject of the model (a physical system evincing a particular kind of behavior, like ferromagnetism) are *denoted* by elements of the model; the internal dynamic of the model then allows conclusions (answers to specific questions) to be *demonstrated* within the model; these conclusions can then be *interpreted* in terms of the subject of the model."

The demonstration can be carried out by a physical model (in the case of analog simulations) or by a logical or mathematical deduction, such as a traditional mathematical proof, or a computer simulation. Further, according to *Hughes*, in contrast to Hartmann's account, "the DDI account allows for more than one layer of representation" [34.209, p. 79]. Overall, a virtue of this account is that it emphasizes the common epistemological structures of different activities by pointing at a similar demonstrative step, which excavates the epistemic content and resources of the model (see also [34.210] for refinements, [34.87] for an analysis which extends the idea of demonstration, or *unfolding*, to thought experiments and some types of experiments, and [34.72] for the related idea that computer simulations are arguments). While as a definition of computer simulation, Hughes's sketchy proposal has somewhat been neglected (see however [34.208]) it is a legitimate contender and it remains to be seen how much a more developed version of is would provide a fruitful framework for philosophical discussions about computer simulations.

Computer Simulations as the Concrete Production of Solutions to Computational Models

In order to answer problems with the previous definitions, *Humphreys* proposed in 2004 another definition of computer simulations, which is built along the following lines [34.41]. He defines the notion of a theoretical template, which is implicitly defined as a general relation between quantities characterizing a physical system, like Newton's second law, Schrödinger's equation, or Maxwell's equations. A theoretical template can be made less general by specifying some of its variables. When the result is *computationally tractable*, we end up with a computational template. (Thus, what qualifies as a computational template seems to depend on our computational capacities at a given time.) When a computational template is given (among other things) an interpretation, construction assumptions, and an initial justification, it becomes a computational model. Finally, *Humphreys* offers the following characterization [34.41, pp. 110–111]:

> "System S provides a core simulation of an object or process B just in case S is a concrete computational device that produces, via a temporal process, solutions to a computational model [...] that correctly represents B, either dynamically or statically. If in addition the computational model used by S correctly represents the structure of the real system R, then S provides a core simulation of system R with respect to B."

Another important distinction lies between the computer simulation of the behavior of a system and that of its dynamics [34.41, p. 111] since, even when the computational model initially represents the structure and dynamics of the system, the way its solutions are computed may not follow the corresponding causal processes. Indeed, in a computer simulation, the purpose is not that the computational procedure exactly mimics the causal processes, but that it efficiently yields the target information from which an appropriate dynamic representation of the target causal processes can finally be built for the user. For reasons of computational efficiency, the representation may be temporally and spatially dismembered at the computational level (e.g., by computing the successive states in a different order), as may happen with the use of parallel processing, or of any procedure aimed at partially short cutting the actual physical dynamics.

The space here is insufficient to analyze all the aspects of the above definition and to do justice to their justification – all the more so since further complications may be required to accommodate even more complex cases [34.208]. Suffice it to say that this elaborate definition, which is aimed at providing a synthetic answer to the problems raised by previous definitions, is one of the most regularly referred to in the literature.

34.6.2 Pending Issues

Simulating or Computing

Giving a definition of computer simulations implies choosing which notions should be regarded as primitive and how to order them logically. Some authors first define the notion of simulation and present computer simulations as a specific type of simulations. For example, *Bunge* first defines the notion of analogy, then that of simulation, and finally that of representation, as subrelation of simulation. For him, an object x simulates another object y when (among other things) (1) there is a suitable analogy between x and y and (2) the analogy is valuable to x, or to another party z that controls x (see [34.11, p. 20] for more details).

A potential benefit of this strategy is that it becomes possible to unify in the same general framework various different types of analogous relations between systems such as organism versus society, organism versus automaton, scale ship versus its model, computer simulations of both molecular and biological evolution, etc. Similarly, *Winsberg* [34.195, §1.3] suggests that the hydraulic dynamic scale model of the San Francisco Bay model should be viewed as a case of simulation (see [34.211] for a recent presentation and philosophical discussion of this example in the context of modeling). While scale models can obey the same dimensionless equations as their target systems and be used to provide analog simulations of them, Winsberg's claim is not uncontroversial and may require an extension of the notion of simulation. Indeed the model and the Bay itself do not exactly obey the same mathematical equations. For example, distortions between the vertical and horizontal scales in the model increase the hydraulic efficiency, which implies adding copper strips and the need for empirical calibration. Therefore, this is not exactly a case of a bona fide analog simulation (Sect. 34.2.2) but of a complex dynamical representation between closely analogous systems. In any case, if one adopts such positions, it is then a small step to describe other cases of analogical reasoning between material systems (and possibly cases of experimental economics, in which the dynamics of the analogous target system is not precisely known and external validity is to be assessed by comparing the material systems involved) as cases of simulations (Sect. 34.5.3).

At the same time, unification is welcome only if it is really fruitful (and is, of course, not misleading). As seen above, the problem with such analyses is that they tend to describe computer simulations as involving a representational relationship between two material systems and to misconstrue how computers work (see again Sect. 34.5.3). They thereby tend to misrepresent the epistemological role of the physical properties of computers and the fact that computational science involves two distinct steps; one in which computer scientists warrant that the computer is reliable and another in which scientists use computations and do not need to know anything about computers qua physical systems. A way out of this deadlock may be to use a flexible notion of simulation, which can be applied to relations between physical *or* logical–mathematical simulating processes and the target simulated physical processes. Then, the question remains as to what exactly is gained (and lost) from an epistemological point of view by putting in the same category modes of reasoning of such different types – if one puts aside the emphasis on the obvious similarities with analog simulations, which are a *very specific* type of computer simulation (Sect. 34.2.2). Overall, it is currently far from clear whether this unificatory move should be philosophically praised.

Abstract Entities or Physical Processes

Arguably, computations are logical entities that can be carried out by physical computers. Then, the question arises should computer simulations also be seen as abstract logical entities, or should they be seen as material processes instantiating abstract computations? Hartmann's definitions present computer simulations as processes, whereas Humphreys's definition is more careful in the sense that the computing systems simply *produce* the solution or *provide* the computer simulation. Clearly, to analyze computational science, it is paramount to take into account material and practical constraints since a computer simulation is not really a part of *our* science and we have no access to its content unless a material system *carries* it out a for us. At the same time, just like the identity of a text is not at the material level, the identity of a computing simulation (and the corresponding equivalence relationship between runs of the same computer simulation) is defined at the logical (if not the mathematical) level and the physical computer simply presents a token of the computer simulation. From this point of view, the material existence of computer simulations and the in principle/in practice distinction emphasized by *Humphreys* [34.41] have epistemological, not ontological, significance, that is, they pertain to what we may learn by interacting with actual tokens of computer simulations [34.91, p. 573] but not to the nature of computer simulations. Similarly the identity of a proof seems to be at the logical level, even if a proof has no existence nor use for us unless some mathematician provides some token of it.

Success, Failure, and the Definition of Computer Simulations

A computer simulation is something that reproduces the behavior or dynamics of a target system. The problem with characterizations of this type is that they make computer simulation a success term and if a computer simulation mis-reproduces the target behavior, it is no longer a computer simulation. This problem is a general one for representations, but is specifically acute for scientific representations (*Frigg* and *Nguyen* Chap. 3, this volume). Indeed, while anything in art can be used to represent anything else, scientific representations are meant to be informative about the natural systems they represent. This is part of their essential specificities and, arguably, a definition according to which any process could be described as a scientific computer simulation of any other process is not satisfactory. At the same time, one does not want something to be a computer simulation, or a scientific representation, based on whether it is scientifically successful and exactly mirrors its target (remember that, for some scientific inquiries, representational faithfulness is not a goal and may even impede the success of the investigation [34.212] and [34.23, Chaps. 1 and 3].

An option is to say that something is a scientific representation if it correctly depicts what its user wants it to represent. However, this may raise a problem for computer simulations that were carried out and had subsequent nonintended uses, like the millennium simulation. It may also raise a problem for fictions, which strictly speaking seem to represent nothing [34.25, p. 770].

Finally, failed representations, which do not represent what their producers believe them to depict, are also a problem. Representational inquiries can fail in many ways, and failures are present on a daily basis in scientific activity, from theories and experiments to models and simulations. For this reason, descriptions of scientific activities should be compatible with failure, especially if they are to account for scientific progress and the development of more successful inquiries. Indeed, it would be weird to claim that many of the computer simulations that scientists perform and publish about are actually not computer simulations. Further, whether a genuine computer simulation is carried out should be in general transparent to the practitioner, and this cannot be the case if computer simulation is defined as a success term and scientific failure is frequent (see also [34.213, pp. 57–58]).

Overall, a question is to determine where the frontier should lie between unsuccessful or failed computer simulations, and potential cases in which something that was believed to be a computer simulation by scientists actually is not. This in turn requires knowing how computer simulations can fail specifically [34.92] and which failures are specific to them. In brief, one needs to be able to decide on a justified basis which failures disqualify something from being a computer simulation and which ones simply alter its scientific, epistemic, or semantic value. This analysis may also have to be coherent with analyses about how other types of scientific activities such as experiments and thought experiments can fail [34.214], especially when these activities play similar or identical roles.

An option to consider is that something is a computer simulation based on criteria that do not involve empirical success, and that it qualifies as an empirical success depending on additional semantic properties and on whether it correctly represents the relevant aspects of its (real or fictional) target system(s). This option is potentially encompassing enough (the scientifically short-sighted student can be said to perform a computer simulation), but discriminating between good and bad computer simulations is still possible. It is compatible with the fact that research inquiries are often open and scientists need not know in advance what in their results will have representational value in the end. Finally, it is also compatible with a different treatment of representational and implementation failures. Indeed, the possibility of being unsuccessful at the representational level is consubstantial to empirical inquiries and is in this sense *normal*. By contrast, an implementation failure is simply something that should be fixed. It corresponds to a case in which we did not manage to carry out the intended computation, whereas computing is not supposed to be a scientific obstacle, and we learn nothing by fixing the failure.

Natural, Intentional, or Social Entities?

A similar but distinct issue is to determine which type of objects computer simulations are, *qua token physical processes carried out by computing devices* – a question which is close to that of the nature of physical computers and is also related to that of the ontology of model (*Gelfert* Chap. 1, this volume).

Arguably, they are not simply natural objects which are defined by some set of physical properties and exist independently of the existence of the agents using them. Indeed, because computations can be multirealized and some runs of computations built by patching different bits of computation on physically different machines, it is unlikely that all computations can be described in terms of natural kind predicates (massively disjunctive descriptions not being allowed here) [34.126].

Further, for both computations and computer simulations, pragmatic conditions of use seem to matter. To quote *Guala* commenting on the *anthropomorphism* of Bunge's definition (see above), [34.177, p. 61]

> "it makes no sense to say that a natural geyser *simulates* a volcano, as no one controls the simulating process and the process itself is not useful to anyone in particular."

Indeed, even if any physical system can be seen as computing some (potentially trivial) functions (see below), any physical object cannot be *used* as a (general) computer, and we may have to endorse a position along the lines of Searle's notion of social objects [34.215], or of any analysis doing the same work: a physical object X counts as Y in virtue of certain cognitive acts or states out of which they acquire certain sorts of functions (here computing), given that these objects need to demonstrate appropriate physical properties so that they may serve these functions for us. A specificity of computer simulations is that, unlike entrenched social objects, such as cars or wedding rings, a small group of users may actually be enough for a physical system to be seen as carrying out a computer simulation. Thus, the evolution of a physical system (like a fluid) may count for some users as an analog computer, which performs a computer simulation, and for other users as an experiment, even if experiments and computer simulations are in general objects of different types, and this case is unlikely to be met in practice (Sect. 34.5.3).

In any case, what is needed for something to be used as a computer or a computer simulation is not completely clear. The physical process must clearly be recognized as instantiating a computer model. Control is useful but not necessarily mandatory (e.g., we may use the geyser to simulate a similar physical system, even if the geyser would not count as a controlled *versatile* analog computer). The possibility to extract the computed information is clearly useful – an issue that matters for discussions about analog and quantum computer simulations, and of course cryptography.

An alternative position is not to mention users in the definition and to claim that, pace the peculiar case of man-made computations (which may make use heavily of the possibility offered by multiple realizability, see Sect. 34.5.3), physical processes are the one-piece physical instantiations of running computer models (resp. computer simulations) and, as such, are computations (even if, sometimes, trivial ones). See [34.216] for a sober assessment of this pancomputationialist position. In this perspective, one may say that it is a practical problem to create artificial human-friendly computers which can *in addition* be controlled and the information of which can be extracted. While such positions may be palatable for those, like *Konrad Zuse*, *Edward Fredkin* and their followers [34.64, 217, 218], who want to see nature as a computer, it is not clear that such pancomputationalist theses, whatever their intrinsic merits for discussing foundational issues like the computational power of nature or which types of computers are physically possible, serve the purpose of understanding science as it is actually practiced.

An important distinct question is whether intentional or pragmatic analyses should also be endorsed regarding computational models and computer simulations, *qua representational mathematical entities*, that is, how much the intentions of users and conditions detailing how their use by scientists is possible, should be part and parcel of their definitions. Arguably, a scientific model is not simply a piece of syntax or an entity which inherently and by itself represents, completely or partially, a target system in virtue of the mathematical similarities it intrinsically possesses with this system. In order to understand how scientific representations and computer simulations work and actually play their scientific role, their description may have to include captions, legends, argumentative contexts, intentions of users, etc., since these elements are part of what makes them scientifically meaningful units. Indeed, how one and the same mathematical model represents significantly varies depending on the inquiry, subject matter and knowledge of the modelers. This is particularly clear in the case of computational templates, which are used across fields of research for different representational and epistemological purposes [34.41, §3.7], and which are scientific units at the level of which different types of theoretical and conceptual exchanges take place within and across disciplines [34.45]. Overall, this issue is not specific to computer simulations but can be raised for other scientific representations [34.23, 168, 219–221]. Thus, this point shall not be developed further.

Computer Simulations and Computational Inquiries

How should computer simulations be delineated? Computer simulations do not wear on their sleeves how they were built, contribute to scientific inquiries, should be interpreted and how their results should be analyzed. Accordingly, authors like Frigg and Reiss distinguish between computer simulations in the narrow sense (corresponding to the use of the computer), and in the broad sense (corresponding to the "entire process of constructing, using and justifying a model that involves analytically intractable mathematics" [34.30, p. 596]). See also the distinction between the unfolding of a scenario and the computational inquiry involving this unfolding at its core [34.87], or the description of how the demonstration activity is encapsulated in other activities in the DDI account of representation [34.13].

Whatever the choice which is made, there is tension here. As underlined above, an analysis of the identity of scientific representations cannot rest on the logical and mathematical properties of scientific models and their similarities with their physical targets, and indications about how these representations are to be interpreted cannot be discarded as irrelevant to the analysis of their nature and uses. At the same time, computer simulation, qua computational process, and the arguments that are developed by humans about it, are activities of different natures and play different roles. Therefore an encompassing definition should not lead to blur the specificities of the different components of computational inquiries (just like a good account of thought experiments should not blur that they crucially involve mental activities at their core and are part of inquiries also involving scientific arguments).

34.6.3 When Epistemology Cross-Cuts Ontology

Whatever the exact definition of computer simulations, it is clear that they are of a computational nature, involve representations of their target systems and that their dynamics is aimed at investigating the content of these representations.

Importantly, whereas the investigation of scientific representations is traditionally associated with the production of theoretical knowledge, the nature of computer simulations does not seem to determine the type of knowledge they produce.

Clearly, computer simulations can yield theoretical knowledge when they are used to investigate theoretical models. At the same time, even if computer simulations are not experiments (Sect. 34.5.3), they produce knowledge, which may qualify as empirical in different and important senses. As we have seen, computer simulations provide information about natural systems, the validity of which may be justified by empirical credentials rooted in interactions with physical systems for aspects as various as the origin of their inputs, the flesh of their representations of systems (see in Sect. 34.5.5 the examples by Morgan about the studies of the strength of bones), the calibration or choice of their parameters, or their global validation by comparison with experiments (Sect. 34.3.2). However, information about the dynamics represented cannot completely be of empirical origin, since it involves the description of general relations between physical states, and general relations cannot be observed.

From this point of view, computer simulations may be seen as a mathematical mode of demonstrating the content of scientific representations that is in a sense neutral regarding the type of content that is processed: empirically (resp. theoretically) justified representations in, empirically (resp. theoretically) justified information (or knowledge) out. This suggests that when analyzing and classifying types of scientific data and knowledge, the ways that they are produced and processed (experimentally or computationally) and where their reliability comes from (e.g., theoretical credentials or experimental warrants) are, at least in part, independent questions.

34.7 Conclusion: Human-Centered, but no Longer Human-Tailored Science

Computer simulations and computational science keep developing and partly change scientific practices (Sect. 34.7.1). Human capacities no longer play the role they had in traditional science, hence the need to analyze the articulation of computational and mental activities within computational science (Sect. 34.7.2). This requires in particular studying computational science for its own sake, which however should not be seen as implying that computer simulations always correspond to scientific activities of radically new types (Sect. 34.7.3). In any case, whatever the exact relations between computer simulations and traditional activities like theorizing, experimenting or modeling, it is a fact that recent investigations about computer simulations have shed light on epistemological issues which were de facto not treated in the framework of previous philosophical studies of science (Sect. 34.7.4).

Before the development of computers, humans were involved at every step of scientific inquiries. Various types of devices, tools, or instruments were invented to assist human senses and inferential abilities, and they were tailored to fit human capacities and organs. In brief, science was for the most anthropocentric science, that is to paraphrase *Humphreys* [34.41, §1.1] "science by the people for the people," and analysts of science, from Locke, Descartes, Kant to Kuhn, or Quine offered a human-centered epistemology [34.123, 124, p. 616]. Similarly, theories and models needed to be couched in formalisms which made their symbolic manipulation possible for humans (hence the success of differential calculus), problems were selected in such a way that they could be solved by humans, results were retrieved in ways such that humans could survey or browse them, etc.

34.7.1 The Partial Mutation of Scientific Practices

The use of computers within representational inquiries has modified, and keeps modifying, scientific practices. Theorizing is easier and therefore less academically risky, even in the absence of well-entrenched backing-up theories; solutions to new problems become tractable and how scientific problems are selected evolves; the models which are investigated no longer need to be easily manipulated by human minds (e.g., CA are well adapted for computations, but ill-suited to carry out mental inferences [34.43]; the exploration of models is primarily done by computers, making mental explorations and traditional activities like thought experiments are somewhat more dispensable [34.117] and [34.41, pp. 115–116]; the treatment of computational results, as well as their verification, is made by computational procedures; the storage of data, but also their exploration by expected or additional inquirers, are also computer based. Finally, the human, material, and social structure of science is also modified by computers, with a different organization of scientific labor, the emergence in the empirical sciences of computer-oriented scientists, like numerical physicists and computational biologists or chemists, or the development of big computational pieces of equipment and centers, the access to which is scientifically controlled by the scientific community (like for big experimental pieces of equipment).

34.7.2 The New Place of Humans in Science

Overall, the place and role of humans in science has been modified by computational science. Arguably, human minds are still at the center of (computational) science, like spiders in their webs or pilots in their spacecrafts, since science is still led, controlled, and used by people. Thus, we are in a hybrid scenario in which we face what *Humphreys* calls the anthropocentric predicament of how, we, as humans, can "understand and evaluate computationally based scientific methods that transcend our own abilities" [34.42, p. 134]. In other words, interfaces and interplays between humans and computers are the core loci from which computational science is controlled and its results skimmed by its human beneficiaries. More concretely, scientific problems still need to be selected; computational models, even if designed for computers, need to be scientifically chosen (e.g., CA-based models of fluids were first demonstrated to yield the right Navier–Stokes-like behavior by means of traditional analytic methods [34.43]; results of computer simulations, even if produced and processed by computers, need to be analyzed relative to the goals of our inquiries; and ultimately scientific human-sized understanding needs to be developed for new fundamental or applied scientific orientations to be taken.

34.7.3 Analyzing Computational Practices for Their Own Sake

Over the last three decades, philosophers of science have emphasized that in most cases computer simulations cannot simply be viewed as extensions of our *theoretical* activities. However, as discussed above, the assimilation of computer simulations with experimental studies is still not satisfactory. A temptation has been to describe the situation as one in which computer studies lay in-between theories and experiments. While this description captures the inadequacy of traditional characterizations based on a sharp and exclusive dichotomy between scientific activities, it is at best a metaphor. Further, this one-dimensional picture does little justice to, let alone help one understand, the intricate and multidimensional web of complex and context-sensitive relations between these activities.

An alternative is to analyze computational models, computer simulations, and computational science for their own sake. Indeed, computer simulations clearly provide a variety of new types of scientific practices, the analysis of which is a problem in its own right. Importantly, this by no means implies that these practices require a radically new or autonomous epistemology or methodology. Similarly mathematical and scientific problems can be genuinely independent, even when *in the end* they can be reduced by complex procedures to a set of known or solved problems. Indeed, the epistemology of computer simulations often overlaps piecewise with that of existing activities like theorizing, experimenting, or thought experimenting. Disentangling these threads, clarifying similarities, highlighting specific features of computational methods, and analyzing how the results of computer simulations are justified in actual cases is an independent task for naturalistic philosophers, even if one believes that, in principle, computer simulations boil down to specific mixes of already existing, more basic activities.

34.7.4 The Epistemological Treatment of New Issues

In practice, the analysis of computer simulations has raised philosophical issues, which were not treated by philosophers before computational studies were taken as an independent object of inquiry, either because they were ignored or unnoticed in the framework of previous descriptions of science, or because they are genuinely novel [34.96, 124, 207]. This a posteriori justifies making the epistemological analysis of computational models and computer simulations a specific field of the philosophy of science. How much computer simulations will keep modifying scientific practices and how much their philosophical analysis will finally bring about further changes in the treatment of important issues like realism, empiricism, confirmation, explanation, or emergence, to quote just a few, remains an open question.

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