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Epistemological issues concerning computer simulations in science and their implications for science education

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Abstract

Computers and simulations represent an undeniable aspect of daily scientific life, the use of simulations being comparable to the introduction of the microscope and the telescope, in the development of knowledge. In science education, simulations have been proposed for over three decades as useful tools to improve the conceptual understanding of students and the development of scientific capabilities. However, various epistemological aspects that relate to simulations have received little attention. Although the absence of this discussion is due to various factors, among which the relatively recent interest in the analysis of longstanding epistemological questions concerning the use of simulations, the inclusion of this discussion on the research agenda in science education appears relevant, if we wish to educate scientifically literate students in a vision of the nature of science closer to the work conducted by researchers today. In this paper we review some contemporary thoughts emerging from philosophy of science about simulations in science and set out questions that we consider of relevance for discussion in science education, in particular related with model-based learning and experimental work.

Keywords: simulations in science; epistemology; simulations in science education

1. Introduction

Computers represent an undeniable aspect of daily scientific life (Kauffmann & Smarr 1993). They are applied to all areas of traditional natural sciences, whether theoretical or experimental, and have generated specific scientific disciplines. Not only have they increased the speed and changed the way in which calculations are done, but they have also changed the way in which the data are inspected (Lenhard 2010), the type of questions that may be asked –very often, the subject of the investigation is conditional upon whether it is computationally possible-, and even the way in which the data are presented, with dynamic and highly visual presentations. Although this connection between computers and scientific practice began at the start of the 1940s, it has been further strengthened and has reorganized scientific practice as digital computer and its availability has developed, with the consequent affordability of personal computers, as well as the standardization of hardware and software (Johnson & Lenhard 2011).

Thus, computational techniques have introduced new tools into science. Within the broad spectrum of techniques and methods that fall under the loose heading of computational science, we will focus on computer simulations[1], which form a special and very important sub-domain of computational science. The use of simulations in the development of knowledge has been compared to the introduction of the microscope and the telescope, constituting "a significant and permanent addition to the methods of science" (Humphrey 2004). This has attracted the attention of some epistemologists who have pointed out that computer simulations not only constitute a new tool, but a new form of scientific production (Galison 1996; Winsberg 1999). This new form of scientific production would also present epistemological problems that are also new, such as the modification of the role of differential equations as the principal tool of physics (Fox Keller 2003; Johnson & Lenhard 2011); the nature of modeling and its relation with existing theories (Winsberg 2010); the classic division between scientific theory and empirical methods (Humphreys 2004) and the meaning and the objective of explanations (Johnson & Lenhard 2011).

Since the 1980s simulations have been proposed in the area of science education as a useful tool for improving the conceptual understanding of students and in general the development of scientific capabilities, (e.g. de Jong & Njoo 1992; Hsu & Thomas 2002; Huppert & Lazarowitz 2002; Kaput 1995; Tao & Gunstone 1999; Zacharia 2003; Zacharia & Anderson 2003 and a recent critical review on the topic by Smetana & Bell 2012). Moreover, some researchers support the idea that they are one of the most powerful applications of the new technologies: as not only can they simulate real processes in all areas (movement, photosynthesis, atomic configurations, etc.), but they can also simulate the performance of "virtual experiments", which are too hazardous and costly to perform in school laboratories (Hsu & Thomas 2002; Henessy 2006).

Besides, if we wish to train students in a vision of the nature of science that is closer to the research work that is now prevalent, it would appear necessary to include simulations in science teaching practices because of their centrality to the daily tasks of contemporary science. However, epistemological aspects that relate to simulations have received little attention in science education. The absence of this discussion is due to various factors, among which the relatively recent interest in the analysis of longstanding epistemological questions concerning the use of simulations, which only began to attract attention in the philosophy of science towards the end of the 1990s, and the differences between simulations used in the science classroom and those that are specifically scientific (Doerr 1997), which is an important point that we will address later on.

[1] As in the literature, we shall also use the following terms interchangeably, throughout the text: simulations, computer simulations, computational models and computational modeling (that is, a model running on a digital computer, with special characteristics that differentiate it from more traditional modeling, a point discussed in section 2. 3).

Nevertheless, the inclusion of some key aspects of the current epistemological debate on the research agenda in the area of science education, at least for secondary and university educational levels, appears relevant. On the one hand, the new epistemological questions that are raised by simulations affect various points that are considered fundamental for the understanding of the nature of science (e.g. Osborne, Collins, Ratcliffe, Millar, and Duschl 2003; McComas and Olson 1998; Lederman et al. 2002): particularly, data analysis and interpretation, the construction of hypotheses and predictions, and the diversity of scientific methods. As an example, one of the research results of Wong & Hodson (2009), in which scientists were interviewed about various aspects of the scientific enterprise and its nature, showed that recent technological advances are making it possible, in some areas, to generate knowledge without the need to generate prior hypotheses.

In addition, there is another significant reason to give serious consideration to epistemological aspects of simulations for the training of scientifically literate citizens. Over recent years, simulations in the area of climate science and the knowledge gained from them have had a profound impact on public policy (Winsberg 2010). Arguments for and against the reasons and effects of global warming are usually centered on the results of climate simulations (Guillemot 2010). However, the layman has no clear conception of what those simulations are and the validity of their results, especially if we take into account the difference between the use of the word simulation in everyday language and in the sciences (Fox Keller 2002). Moreover, it would appear that we run into some difficulties when we try to separate simulation and reality, as simulations appear to be "obviously true" because of their apparent capability to "imitate" reality, in such a way that some educational researchers (for example, Lunnetta et al. 2007) suggest that a new objective for students in the 21st c. would be to learn to discriminate between reality and virtual reality.

The main objective of this paper is to review epistemological issues concerning simulations and to discuss their possible implications for research and teaching in science education. We have organized it into four sections, as follows: in section two, after a brief introduction of the principal historical steps in the development of computational modeling, we try to explain, in very general terms, how simulations, despite their great diversity, are constructed in science, in order to highlight where their specific features may appear that made them so peculiar. This section ends by addressing certain epistemological issues, which we think are significant for science teaching and that emerge from their use. In section three, we revise the different kinds of simulations used in science education and the main results of the research in this area. This section ends by positing the relevance and benefit of approaching epistemic issues concerning simulations in two areas of science education, experimentation and model-based learning, that frequently use them in their didactic strategies. In the fourth and final section, we set out our concluding remarks.

2. Simulations in the sciences

According to the dictionary of the *Real Academia Española* [Royal Spanish Academy], to simulate is to represent something, by pretending or imitating what is not. This definition, common to several different languages, denotes the negative nature that the term simulation has in colloquial use. However, as Fox Keller (2003, p. 198) has pointed out, the Oxford Dictionary has, since the Second World War, when computer simulations first began to appear, incorporated a definition that is not only of a positive character, but reflects its scientific meaning: "*The technique of imitating the behaviour* *of some situation or process . . . by means of a suitably analogous situation or apparatus, especially for the purpose of study or personnel training."*

This is certainly a very wide definition that covers all of the different types of simulations currently used in different areas: Ören (2011 a, b) has listed more than 100 definitions on simulations and about 400 different types of modeling and simulations are currently in use. As a working definition, for the purposes of this study, simulations are the representation of the dynamic behavior of a system that moves it from state to state in accordance with an approximate (mathematical) model that is used to implement it on a computer. It would be of interest to learn about the origins and evolution of simulations, in order to arrive at a more precise definition of what today we understand as computer simulations, which is nevertheless sufficiently broad to include the majority of their different types.

2.1. Brief history of simulations

Since the end of the 19th c., various analogical models were proposed that imitated the behaviours of real systems, such as the tide-predicting machine of Lord Kelvin (1872), or those that resolved specific classes of mathematical problems, such as the differential analyzer of Vannevar Bush (1927) (Mindell 2002). However, we had to wait for the appearance of programs that functioned in digital computers for calculus and the imitation of systems to acquire a new dimension. The origin of these programs is found in the development of techniques to determine the reliability of various nuclear weapons, at the Los Alamos research laboratory, between 1946 and 1952. The assessment of these proposals implied finding the solutions to equations to predict highly non-linear phenomena, such as neutron diffusion, for example. To do so, various approaches to the computational procedures of that time were prepared, the most famous of which was the Monte Carlo method (Galison 1996).

So, computer simulations opened the door to the study of complex systems, which, because of their characteristics, could not be covered in an exact analytic manner. This was its first contribution: to provide work plans to find approximated solutions (not the exact ones of analytical methods) with sufficient precision and speed. However, according to Fox Keller, although they "*started out as little more than a mechanical extension of conventional methods of numerical analysis, where what was being "simulated" were the pre-computer, handwritten equations … such methods rapidly grew so effective that they began to challenge the status of the original, soon threatening to displace the very equations they were designed to simulate.*" (op. cit., p. 210).

Following the historical development of simulations outlined by Fox Keller, three stages may be identified, in which successful developments gradually developed and were accumulated, generating new effects, and progressively undermining the traditional notions of theory, experimentation and data. However, the basic concepts and techniques of simulations that may be highlighted at each stage all emerged in the initial stage: Monte Carlo methods, finite element methods, cellular automatism, and artificial neuronal networks (Lenhart 2010). Moreover, Fox Keller insists that the novelty that epistemologists now see in simulations was neither found at one instantaneous moment, nor was it a pattern at that initial stage. It came instead from an accumulative process of small perturbations, based on what had already been achieved, in which the simulations gradually gained more ground and were converted into an indispensable tool in all scientific areas. It is worth mentioning that the uses that these three stages characterize are still valid in research into various scientific areas, particularly in physics.

The first of the stages identified by Fox Keller is the use of the computer to find solutions to pre-established mathematical models, which are analytically unsolvable, in terms of numeric analysis. The consolidation of this way of using the simulations began to raise questions, fundamentally, over the role of differential equations as a principal tool in theoretical physics.

A second stage, which started in the mid-1950s in the area of fluid dynamics and plasmas may be characterized by the emergence of the use of simulations to determine the standard features required in realistic approximations to physical models of complex systems. A general theory exists for these systems, but their application to specific cases, in other words, to the preparation of models is extremely complex. So, first of all, a simplified system replaces the real system and then the equations that support the theory of this simplified system are transformed for subsequent treatment by numeric analysis, and for input into the computer; the resultant simulations are compared to the “true” behavior of the system, in order to evaluate the simplifications. Rather than the evaluation or resolution of the mathematical expressions, the priority in this method is the simulation that the computer produces of this simplified version of the physical system. As a result are obtained models (equations) that are physically more realistic and computationally treatable. This type of simulation, of great use in various branches of the experimental sciences, gives rise to the so-called “computational experiments” or “virtual experiments”. They have emerged as an alternative somewhere between theoretical and laboratory-based experiments, thereby establishing new relations between the nature of modeling and its relation with theory and experimentation.

Finally, Fox Keller highlights a third use, or stage: the construction of (theoretical and/or experimental) models of phenomena for which there is neither a theory, nor are there exact nor approximate equations, but only a rudimentary idea of the underlying dynamic; for example, in the case of the modeling biological phenomena. The objective in this case is the simulation of the phenomena in itself, questioning, both the meaning and the objectives of a scientific explanation. The agent-based models used in biology fit into this group, as do the works developed in the 1980s in the area of artificial life.

Thus, the original use of simulations as tools for the resolution of unsolvable scientific equations[2] has gone far further, such that they are now used for practical reasons (for example, experimental costs or impracticable experiments, such as the formation of black holes) and ethics (for example, the diffusion of a new virus in the population). They are more appropriate than experiments when it is necessary to optimize any given experiment or when there is no theory that can directly explain a phenomenon and an effort is made to reproduce it and to understand the factors that might influence it (such as in the social sciences) (Humphreys 2004). None of these applications share a theory or have common laws, but instead a set of skills, “a new mode of producing scientific knowledge that was rich enough to coordinate highly diverse subject matter.” (Galison 1996, p. 119), which is how scientists working with simulations understand them.

[2] Although this, as Humphreys (2004) has highlighted, is no slight matter: a great part of the success of physics is due to the development of better methods of calculation.

Therefore, simulations can not simply be reduced to numerical methods broadly improved by the use of rapid calculation processes on computers. Fundamentally, this new mode of producing scientific knowledge has increased the number of phenomenon that can be modeled and has enormously increased our capability to apply theories to the world. Although we may think that "in principle", if the equations that describe a phenomenon exist, they can be solved, it would be ingenuous to suppose that, even if we had an infinite amount of time, a group of "human calculators"[3] could, for example, find the solutions to forecast European weather trends one week in advance (Humpreys 2004).

It is worth remembering that when Newton introduced the fundamental equation of mechanical dynamics, he affirmed its (almost) universal application, even though (almost) nowhere was it analytically solvable: the analytic solutions that might have been achieved, would only apply within a range of idealized conditions. In fact, almost all of the many classes of differential equations are analytically unsolvable, as far as we are currently aware; the number of models that may be resolved using solely analytical techniques being very limited. So, our current understanding of all complex and most especially all non-linear systems that characterize the vast majority of phenomena in the universe, have in fact been made possible by the use of simulations.

2.2. How to simulate a phenomenon

Computer simulations, for Humphreys (2004, p. 110), may be defined as follows:

"System S provides a core simulation of an object or a 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 represents the structure of the real system R, then S provides a core simulation of system R with respect to B."[4]

However, this definition alone is not enough to understand the epistemological particularities introduced by simulations. To do so, it is necessary to gain a better understanding of how they function. Although, as stressed in the brief history of the development of simulations presented in the previous section, simulations vary in many forms, from the closed ended ones that were first developed to the more open as agent-based simulations, all of them may be characterized as transformations of mathematical models in discrete algorithms that imitate the behavior of systems, for which different methods exist to transform the equations into computationally treatable algorithms (among which, Monte Carlo, finite differences,[5] etc.). This would appear to imply a

[3] We recall that the term "computer" referred to people whose job it was to make calculations, in general women; it was only later that it came to refer to an electronic device (Galison 1996).

[4] This definition includes the simulation of mathematical objects, because B is not required to be real.

[5] In the Monte Carlo method, a formal isomorphism is established between differential equations with certain equations in probabilistic theory, using the probabilistic relations to resolve the differential equations and replacing the calculation of all combinatorial possibilities for an entire sequence of events, by an estimation of the results obtained for a "sample" of attempts. The general idea of the finite-element method is the division of a continuum by a series of points known as nodes into a set of small interconnected elements, based on the idea that the equations that govern the behaviour of the continuum will also govern that of the

relatively simple process in areas with well-established theories: given the phenomena and having selected one part of its behavior for simulation, the physical principles are chosen that are the most appropriate for its description, the mathematical model (or set of differential equations emerging from the theory that describe the phenomena) is determined, the parameters and the initial values of the variables are established, the type of computational method is chosen to transform the differential equations into algorithms that the computer can solve, and the algorithm is then fed into the computer to obtain the results.

Seen in this way, it would appear that simulations are nothing more than improved methods of solving equations. However, the situation is much more complex and from this complexity emerges great part of the epistemological issues that we will discuss in this paper and that apply to almost all kind of simulations, although the problems increase in areas that may be defined as theoretically poorer. In the first place, the transformation of the model with its initial parameters and values into an algorithm that may be implemented on the computer is neither an obvious nor a simple procedure. In line with Winsberg (2010, pp. 10-17), there are two aspects in the creation of a viable computer algorithm. The first aspect is related to the algorithm that results from the direct transformation of the continuous differential equations into discrete differential equations. This step can result in a very computationally costly algorithm or an algorithm that, as a consequence of the approximations used to move from continuous to discrete equations, is unstable, and produces errors and unreliable results. It is therefore necessary to set aside the algorithm, which would otherwise be the next step on the basis of the mathematical model, in order to simplify the model, by ignoring or by discarding some factors, by reducing the model's degrees of freedom and by adopting what are known as unrealistic assumptions of symmetry in the computational model.

The other point is the inclusion in the algorithm of mathematical relations to model factors of the physical model that are fundamental for an understanding of the behavior of the system, but would, if applied in the computer model with its precise mathematical formulae, be computationally untreatable. These relations are usually very simple and have no direct connection with the original differential equations. Their construction is sometimes guided by theory, at other times by physical "intuition", but also in response to the computational limitations observed by trial and error. They may be considered "rough-and-ready, theoretically unprincipled model-building tools" (Winsberg, ibid., p. 12) constructed to capture some natural important effect that has been left out of the computational model because of technical limitations. When these model-building tools are combined with the more theoretical equations, they produce more realistic results than those that would otherwise have been produced, had those tools not been taken into consideration. One of these tools is "eddy viscosity", widely used in the simulation of fluids with turbulent flows, in the dynamics of fluids and meteorology as well as in the study of the connective properties in giant dwarf stars (Winsberg, ibid.). Another example of these tools is the "Arawaka operator" used in the simulations of atmospheric dynamics (Küppers & Lenhard 2005).

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element. Thus, it is possible to pass from a continuous system (infinite degrees of freedom), governed by one or by a system of differential equations, to a system with finite degrees of freedom, the behaviour of which is modelled by a system of either linear or non-linear equations. Visually, it is like dividing the space into a reticular mesh, seeking the solution at the points that are determined by the mesh.

A further possibility in this same direction is the substitution of the real physics of a process that might be highly complex by phenomenological relations. For example, in the case of red dwarves, to account for surface energy loss, the real physical process was substituted by the standard formula for the radiation of a black hole, solely applied at the points at which it was considered that the star would radiate heat efficiently. In short, the parametric relations that appear in a simulation often have no direct counterpart –in a strictly realistic sense, from an ingenuously realistic point of view - in a real system.

Once the computer model has been implemented, the algorithm produces a data set that requires interpretation. A variety of complex visualization techniques are used to interpret the results, an effort is made to integrate the data cloud with other sources of knowledge, including observational data, and the credibility and reliability of some of the features of those data sets are determined. With all of this, a series of static or dynamic images are finally generated[6], to arrive at the end-result of the simulation, which Winsberg refers to as "models of phenomena", on which basis scientists can start to study the emergent patterns.

2.3. Epistemological problems relating to simulations

The methodological novelties introduced by simulations have challenged some relevant epistemological notions in science[7], some of which we shall discuss in this section.

a) New role of mathematics in research

The origin of physics coincided with the origin of differential calculus. Since Newton, who also invented methodological criteria for rationally testing mathematical models, unmatched even to this day (Harper 2011), this form of calculus has been considered its principle tool, as it would not otherwise have been possible to describe the continuum and therefore, to represent reality. In fact, ever since mathematics became a precise tool for prediction in the 18th c., mathematical models described by differential equations came to be considered as "true" representations, as their predictions were verified. However, the "experiments in theory", characteristic of the first and second stages in the development of simulations, started to gain their own life, questioning the primacy of the most conventional mathematical techniques, in particular differential equations (Fox Keller 2003; Johnson & Lenhard 2011).

Likewise, the success of simulations increased the legitimacy of the practice of numerical analysis among scientists, which was not, until the appearance of computing, anything more than an auxiliary calculus tool. During the second half of the 19th c. numerical methods were developed from the need to solve specific problems in astronomy, physics and engineering, but only during the 1940s did numerical analysis really became a bona fide mathematical discipline and not just a collection of recipes

[6] The series of dynamic images constitute the animations.

[7] It is important to highlight that we are focusing only on the debate surrounding the epistemology of science. The lively discussion among mathematicians concerning epistemological issues (among others, the notion of proof) relating to the use of computers is beyond the scope of this study.

(Benzi 2009). This change not only challenged the hegemony of a particular type of mathematical tool, but also fundamentally challenged the realism associated with the representations of continuous variables (Fox Keller 2003), even going so far as to call into doubt the very concept of space as a continuum. So, in the field of cellular automatism, it was proposed that space could be a discrete temporal spatial network of bits of information (Vichniac 1984; apud. Fox Keller 2003)[8].

In relation to the acceptance of this change in the scientific community, the empirical study conducted in the area of astro-physics by Sundberg (2010b) appeared to show that both postures coexist: on the one hand, the skeptics express doubts over the elevation of simulations to the level of analytical methods, and on the other, there are those that propose the analysis of simulations in themselves, without any need to return to underlying equations to justify the resulting simulation or to improve ease of computation for a relevant simulation feature.

b) Simulations as semi-autonomous models

A further question has to do with the status of simulations as models[9]. Over recent years, the traditional view of models, which gave them a secondary role in relation to theory, insofar as it considered that models were fundamentally nothing more than a representation that makes sense of mathematical formalism, has run into criticism from semanticists (Cartwright 1999; Sismondo 1999). In their view, models are something other than only theory plus data and, as they are partially independent from theory and from the world, they have an autonomous component that turns them into instruments of exploration in both domains (Morgan & Morrison 1999), into tools for intervention and for the manipulation of phenomena (Cartwright 1983; Hacking 1983), increasing the number of phenomena and processes that may be explained.

Simulations fit perfectly into this vision of models as instruments of mediation. For example, in the previously discussed case of the construction of simulations for complex systems in fluid dynamics, the real systems in themselves are not well understood, even if the theoretical elements for an understanding of their basic dynamics are known; the construction of the simulations are guided, but not determined by the theory and data from different sources has also to be used. Thus, emergent simulations can not be reduced to mere calculations. Moreover, simulations gradually and in an iterative way perfect the models with which the phenomena are described, as they allow the determination of their most relevant parameters for their description, producing new results in this way, which are beyond the reach of theories on the basis of which they were constructed, functioning more as mediators between theory and experimentation (Galison 1997).

Besides, due to the construction process itself, it is very difficult to be certain about the causes of a successful simulation. For several authors, the objective of a simulation is the construction of instrumentally reliable models (Suarez 1999), which are

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[8] Similar ideas have been proposed by some theoreticians in the field of quantum information (Wheeler 1990; Brukner & Zeilinger 2005).

[9] The status of models in relation to theory and experimentation is not, in fact, an epistemological problem specific to simulations, but a general problem (Frigg & Reiss 2009); however the reappraisal of models in relation to theory coincided with the generalization of the use of simulations in all scientific areas, which may not be coincidental.

representative of a physical system, but without the aim of being a realistic representation of the physical system and its behavior. Therefore, there are authors that affirm that simulations will never equal the traditional notion of models, remaining a sort of second-order model (Küppers & Lenhard 2005). Computer simulations, for Winsberg, *"involve a complex chain of inferences that serve to transform theoretical structures into specific concrete knowledge of physical systems* ... [he argues that] *this process of transformation is also a process of knowledge creation, and that it has its own unique epistemology"* (Winsberg 1999, p. 275).

It is interesting to highlight that computer models in climate science are criticized by people who do not consider them "good science", because they are not founded on data and solid theories (Guillemot 2010) and who also question the possibility of verifying the projections of the models in relation to the data. The first of these criticisms relates more to the role of the models in general, and not only the computer models, in relation to theory. In response to these criticisms, in climate science, Edwards (1996, apud. Guillemot 2010) pointed out that the relation between models and data, even though interdependent, is symbiotic rather than circular. Norton & Suppe (2001) argued that that interdependence also exists between theory and experimentation and that the absence of certainty and the construction of simplified hypotheses are not inherent to computational models.

c) Simulations and experimentation

Scientists construct computational models and work on them, even though they are considered experimentalist or theoretical, understanding work on a model as the action of exploring the relations between data input and output, in order to produce verifiable predictions or better models, changing, adding and adapting parameters and repeatedly running the simulations (Winsberg 2003; Lenhard 2010). This double relation with theory and experimentation has disconcerted epistemologists of scientific disciplines who seek to understand *"how simulation can have methodological and epistemological features in common with experimentation, while still playing the role of a form of scientific theorizing*" (Winsberg 2003, p. 106).

The relation between simulation and experimentation is seen by epistemologists in different ways. The so-called "numerical experiments" that underlie simulations are likened to laboratory experiments, insofar as they can represent the system under study, with the possibility of varying parameters and testing theoretical hypotheses, as well as in the type of results that arise (data sets that have to be organized and interpreted). Indeed, some people see no difference between experiments and simulation (for ex., Hughes 1999; Humphreys 2004, Norton & Suppe 2001).*"Simulation modeling is just another form of experimentation, and simulations are nothing other than models of data"* (Norton & Suppe 2001, p. 92). According to these authors, simulations imitate the systems that are of interest, making it possible to perform experiments on them, in the same way as on any other experimental objectives. In this case, the physical object experimented upon is the computer.

Other authors, however, consider that simulations are not comparable to experiments, as they lack "materiality" (Guala 2005; Morgan 2003). Parker (2009), guided by Hacking's definition of an experiment as a research activity into a system to see how the interesting properties of that system change, considers that the problem is not materiality, given that what is relevant for the justification of certain inferences on systems is the similarity that may arguably exist between the system on which the experiment is based and the target system. In the case of simulations, the intervention is on the computer program the parameters of which are modified, and about which arguments are advanced in support of its similarity with the target system.

In fact, simulations and experiments have many points in common, one of which is error management. As previously discussed, errors in simulations arise from the transformation of continuous into discrete equations and from the conversion of the mathematical structure of the model into a computationally feasible structure[10]. Researchers working with simulations have to learn to appraise, in the same way as experimental scientists, the classes of error that can appear. *"Precision, accuracy, error analysis and calibration are concepts that we typically associate with experimentation and not with theorizing, but they are also very much a part of the vocabulary of the simulationist"* (Winsberg 2010, p. 43)[11]. In addition, simulations and instruments share similar calibration processes, such as their use in situations in which the result is known, or, the evaluation of their reliability, by reproducing the results with other instruments. In the case of simulations this evaluation is done by trying to achieve similar results from the algorithms constructed in a different way. The history of simulations for Winsberg (2010) is very similar to the history of scientific instruments: an evolving set of techniques, practices and circumstances that mature over time, which are refined when more precise and reliable techniques are needed, in a process that gives them further credibility that is not exclusively dependent on their theoretical grounding.

However, there is a fundamental difference: computer experiments are based on symbols and digits; there is no direct contact with the world. Like experimentation they also require manipulation, but not the fact that experiments constitute "the acid test" of the world over theories (Guillemot 2010). In other words, experiments, when performed, even when guided by theory, apply in systems over which we neither have any control nor know how they will function. And, in that sense, they allow us to test theories. However, simulations, when performed, apply in systems that we have purposely created, selecting some data or laws to the detriment of others. As Turkle stressed (2009, p. 40): "*An experiment, in ideal terms, turns to nature ready to be surprised. But if experiments are done "in simulation", then, by definition, nature is presumed to be "known in advance", for nature would need to be embedded in the program".*

In a more simplified way: in the experimental sciences, there is theory and then experimentation. The experimental results are confronted with theoretical calculations. Obviously, approximations or "calculations" (Hacking 1983) or models are necessary, in order to relate them, in the broadest sense discussed earlier (Cartwright 1999), but

[10] Durán (2013, p. 107-108) divides the systematic errors in simulations into three kinds: physical errors (related to the malfunctioning of any physical component of the computer), logical errors (related to coding errors or a part of a faulty compiler or a computer language, leading to instabilities in the behavior of the computer program) and representational errors (the most common ones, located at the level of the mathematical model or the specification, as, for example, a grid too big for precise results, bad approximations, unacceptable mean square errors, etc.)

[11] The preferential vocabulary among those that use simulations is full of experimental metaphors.

both processes are the result of two types of different yet interconnected practices, in two types of communities with specific objectives and techniques (Galison 1987).

In computer modeling, the hypothesis to be tested (for example, modifying a parameter) and the numerical experiments are in a continuum: in order to verify a hypothesis, it has to be transformed into algorithms and inserted in the computational model, which then performs the simulation. But it is a virtual experiment, which produces no objective facts, even though it increases the range of explorable domains (Guillemot 2010). Therefore, some authors point out that experiments have a superior epistemological status with regard to simulations, because of their greater potential for the validation of their results (Morgan 2003). Winsberg, however, argues that one may not speak of epistemological superiority, but rather of priority: the experiments have the crucial role of testing theories, hypotheses and models (Winsberg 2010, p. 71), which is not possible with simulations, as it is necessary to have both theoretical and experimental knowledge of system dynamics to construct them[12]. In other words, it is assumed that several characteristics of the system that one wants to learn are already known, in order to construct the computational models.

Accordingly, various sociologists and historians (e.g. Rohrlich 1991; Kauffmann & Smarr 1993; Galison 1996; Dowling 1999) have argued that simulations are a completely new scientific activity. Even though they share the manipulation of equations with theory and the way that algorithms are manipulated with experimentation, which produce long data sets that have to be interpreted, *"the resulting bricolage creates a marginalized nether land that was at once nowhere and everywhere on the usual methodological map"* (Galison 1996, p. 20).

d) Simulations and the objective of the explanations

Another relevant epistemological question has been put forward by people that suggest that the mass use of simulations has implied or is implying a change in the meaning and the objective of explanations (Johnson & Lenhard 2011).

Since the scientific revolution of the 18th c., knowledge of a system came to be practically equivalent to knowledge of what might happen next, that is predicting unknown events and objects. When those events and objects were observed, the mathematical model was considered valid and its future predictions were taken seriously (Johnson & Lenhard 2011). So, many natural philosophers came to consider that the mathematical models were true representations of the mechanisms of physical systems. In this sense, nobody maintains that simulations have an ontological similarity to the systems that they imitate (Johnson & Lenhard 2011), given that simulations depend on computer mechanisms that have no real counterpart, as previously discussed. What computational models do is to produce a predictive response, not a mimetic model of the causal mechanisms of the real phenomenon. In addition, while traditional mathematical models had the objective of producing transparent causal explanations, computer models are opaque: what happens inside the computational model is not clear and, in some cases, the reason for the coherence between the resulting simulation and reality is not wholly explainable.

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[12] Theoretical knowledge to which we refer does not necessarily imply having a well-established theory of the phenomenological dynamics of the system of interest, but having some knowledge about its dynamics, as in the case of simulations in the area of social sciences.

Johnson & Lenhard (op. cit., p. 194) point out that given the epistemic opacity and the lack of ontological references, it is not possible to apply the argument of the "non-miracle" of scientific realism –if there were a coincidence between the results of the mathematical model and the experimental results, it would be miraculous if there were not some sort of truth in the model - to the predictions of simulations. In the case of simulations, it is possible to implement a variety of different models in the computer that "fit" the experimental data, as there are multiple possible routes towards coherence. These authors therefore speak about the emergence of a "culture of prediction" based on the mass use of simulation in scientific practice, where simulations would privilege recurrent experimentation on computational models and the evaluation of visual results, instead of the slower and more laborious work on mathematical models more "in tune" with real systems. The scientific strategy would, in comparison with traditional practice, be more exploratory, evolutionary, adaptive, provisional and highly visual. Turkle (1995, 2009) noted the different cultures that may be defined among scientists that use computers, which she classified as a culture of calculation and a culture of simulation. The first is modern for this author and is characterized by linearity, logic and depth, with the aim of explaining, unpacking, reducing and clarifying its outcomes. In opposition, the postmodern culture of simulation is fluid, decentered, and opaque and the search for mechanisms and depth is seen as futile.

Nevertheless, it is important to discuss why, in many areas of research, a prediction is sufficient in itself as a scientific goal. Let us remember our previous discussion about the limited analytical access we have to the vast majority of natural phenomena, although knowing, in cases, the differential equations that underlie them. In the case of complex systems, the introduction of finite element simulations provided a vast expansion for exploring dynamically sensitive regions. However, this access comes at a cost, in so far as it is only local regions, larger than any finite element of the whole vector field flow, that can be explored at any one time. We are not certain whether all significant non-linear features have been caught or, even, whether non-linear features are in fact hidden inside these finite elements; an uncertainty which forces us to conduct an exhaustive search. As Hooker (2011, p. 892) stressed, these searches produce immense data sets of multiple dimensions, often sparsely distributed and expressing subtle interrelations across data dimensions, space and time.

This situation makes it necessary to use methods to search into the data. Today, there are many global stochastic simulations capable of revealing important patterns. Many of these methods, known as model-free pattern extraction methods (among which, neural networks), do not rely on dynamical approximation or model interpretation at all; they are in fact methods for data-driven prediction without model- focused explanation. The interesting point here is that these non-parametric simulations provide more accurate predictions than others "more classical" simulations provide. And in the case of poor goodness-of-fit tests for the selection of one among a variety of computational models, which is quite a common situation in complex systems, prediction is underlined as a scientific goal that is in itself sufficient.

e) The validity of knowledge generated by simulations

Among various epistemologists, historians and sociologists investigating the use of simulations encounter a recurrent theme: the problem of how to validate the knowledge that they generate. Given the way of constructing the simulations, which are not exclusively derived from theory, how is it possible to evaluate the veracity of their results? The problem of validation is even more important if we consider that in relation to climate change, a theme that ranks high on the international political and diplomatic agenda, the majority of the results that drive these agendas emerge from climate modeling and from simulations of future climate change. However, both in climate science as in other areas, there are few studies on the validation[13] and the evaluation of simulations through comparison with observational data (Guillemot 2010).

Küppers & Lenhard (2005, p. 1) set out the problem of validation based on the example of Félix Krull, a character from a book of Thomas Mann, who so perfectly simulates the symptoms of a neuronal illness that he deceives the doctors and is released from military service. As pointed out earlier, the mathematical models described by differential equations are considered "true" representations, when their predictions are verified. In that sense, simulations are not "true" representations, as they depend on their capability to "imitate" the operation of a real system. How, therefore, to evaluate the knowledge produced by a simulation, even though it imitates or even perfectly reproduces the results of the real world? The problem resides in this difference between representation and appropriate imitation.

Scientists working with simulations employ different strategies, in order to argue the reliability of their results (Winsberg 2010): they argue the theoretical foundation of the model, the robustness of mathematical techniques used to transform the equations of the model into algorithms, the "calibration" of the simulation compared with what is known of the phenomenon (directly with experimental results, or indirectly, on the basis of the analysis or by comparison with other simulations), and they argue that the system responds as expected when the parameters are modified, or that it can reproduce some basic relations that are predicted by more phenomenological laws or theories.

In relation to the first two strategies, the simulations, even in the majority of the practices of the natural sciences, are not exclusively drawn from theory, for which reason they can not be validated by theoretical arguments (Küppers & Lenhard 2005). On the other hand, the translation of the mathematical model into algorithms, which can be run on a computer, often implies introducing artificial, non-realistic effects, in order to overcome numerical instabilities that emerge from the particular methods that are used. So, the validity of a simulation can not be assessed in relation to the validity of the mathematical model on which it is based. In addition, particular numerical methods can fail under strongly non-linear conditions that are of interest to simulate (Winsberg 2010).The other strategies are also used in experimental science, however as simulation and experimentation can not be equated, it is not very clear that the procedural aspects of these strategies are sufficient for their validation.

The early simulations of atmospheric dynamics represent one example that clearly shows how a simulation can behave in an appropriate way and be considered reliable by the scientific community, even though it is not structurally precise (Küppers & Lenhard 2005, pp. 3-5). The first atmospheric simulation was developed by Norman Phillips in 1955, on the basis of six fundamental equations, which reproduced atmospheric circulation quite well. However, it had a problem of instability: the simulation was

[13] In a recent work, Durán (2013) points that, although neither software nor hardware can be fully verified nor validated, researchers are developing methods for reducing the possibility of errors in order to increase the credibility of the model.

stable for only a few weeks. This problem was overcome in 1966s, by Akio Arawaka, for whom imitation was more important than a precise calculation of the solution. Arawaka used the same basic equations, but also a computational trick: he replaced the Jacobi operator, resulting from the fundamental equations that described the temporal variation, by another that he had purposely constructed, in order to support effective imitation. In addition, he introduced other assumptions, in order to guarantee the stability of the solution, which contradicted experience and physical laws, such as for example that kinetic energy in the atmosphere is conserved.

There is still one further question related to validation. As happens with the other computer programs, the public availability of simulation codes has increased over recent years, as well as the availability of commercial codes. This availability allows researchers to use computational models that "stem from", or have the structure of others already accepted by the scientific community, nevertheless, their validity has neither been corroborated, nor analyzed, nor studied (Turkle, 2009; Sundberg 2010a). It is interesting to note that, even if up until a few years ago the development of computer codes had a certain status within the academic field, given their current availability, this activity is now, in general, considered a waste of time. Sundberg (2010b) has studied this question with astrophysicists and meteorologists that work with simulations. In her case study, it is standard practice among doctoral students from important research institutes in both disciplines to "fine tune" an existing code, rather than a careful and detailed examination of it all.

In summary, there are various factors that can affect the reliability of the results of a simulation, at least insofar as we have, up until now, understood the validity of a physical model. It may be possible to imitate a phenomenon when errors of a different sign are cancelled. At times, it is necessary to incorporate contradictory hypotheses to imitate the real behavior of the systems; the commercial software convert the code into "black boxes" and at times a software and its simulations are validated in the absence of empirical verification, by sharing methods with other verified computational models.

Does this mean that the simulations and emergent knowledge of them are unreliable? If scientific realism is adopted as a point of view, the simulations would have to be true and correct representations of the phenomenon or system that they simulate and this, as we have seen, is not possible to do. However, the problem may be overcome by assuming a pragmatic position in relation to reliability, a position that separates reliability from truth, reducing the fundamental arguments of scientific realism, that success implies truth. A simulation can be, in the terms as defined here, highly reliable without even approaching the truth. On this point, Winsberg (2010, p. 133) has made it clear that a simulation is reliable when results are obtained that fit in well with the network of knowledge that is held on the system (theoretical knowledge of the system, previously accepted experimental or observational data, analytical results with paper and pencil and intuitive physics) and, in addition, it is able to produce successful predictions. This is what Suárez (1999) refers to as instrumentally reliable models. Along the same lines, Humphreys talks about "selective realism"—the aim of the simulation is to represent the real system only up to a predetermined degree of realism; an increase in that reality is almost always sacrificed, so that it may be mathematically and computationally manipulated. In fact, scientists tend to think in this way when working with simulations (Humphreys 2004).

3. Simulations in science education

3.1 The uses of simulations in science education

Simulations that facilitate the learning of sciences in schools are considered one of the most effective modes of computer-assisted instruction for science subject areas and have been studied for over three decades (Bayraktar 2002). According to a recent comprehensive and critical review of their usefulness in science education (Smetana & Bell 2012), simulation appears to be as efficient, if not more so, than other more traditional practices to promote learning about concepts, conceptual change and the development of procedural abilities. Like any other educational tool, they are of course dependent on the ways in which they may be used. In this sense, the importance of the teacher in providing guidance and support (Smetana & Bell 2012) is continually stressed in the literature. Teachers, however, do not appear to be sufficiently well prepared, it being helpful to provide them with opportunities to unpack to unpack how these new approaches and learning tools would benefit their teaching (Waight et al. 2013).

Many of the simulations that are used in science education are related to experimentation. Thus various authors maintain that simulations can replace real experiments, in those cases where the latter are very costly, dangerous, rapid and complex (Doerr 1997; Hsu 2002; Henessy 2006). In these simulations, the students manipulate variables, observe results and analyze tables, graphs and equations to identify and to describe the data (e.g. Confrey & Doerr 1994; Thornton 1987). In addition, in the case of more complex phenomena, simulations allow students to simplify them through the isolation and manipulation of one variable at a time, which helps their understanding of causal relations (Doerr 1997; de Jong & van Joolingen 1998).

However, the benefits of simulations are increasingly prescribed for the development of inquirer-based and learner–centered instruction as they appear to assist students in their understanding of the various phenomena and natural processes through the construction and evaluation of different hypotheses, obtaining rapid feedback, which involves them in active problem-solving process (White & Frederiksen 1998; Hargrave & Kenton 2000). Moreover, simulations make it possible to work with multiple representations, at the same time, and on the same screen, allowing the integration of various forms of scientific representation. Related to this representational characteristic, simulations allow the “visualization” of processes at a microscopic level, such as for example in chemistry, enabling the development of molecular-level thinking and at the same time allowing their visualization at a microscopic level and the establishment of relations with macroscopic observations (Özmen et al. 2009; Liu et al. 2008).

We should, however, distinguish between scientific simulations, which we have discussed in earlier sections, and what is understood by simulations in science education. Unlike simulations for scientific study, educational simulations may be defined as “*interactive learning environments in which a model simulates characteristics of a system, depending on actions made by the student*” (de Vries & Huisman in Kirschner & Huisman 1998). The fundamental difference is that, whereas scientific simulations seek a better understanding of complex phenomena and processes based on the construction of computational models, using well known theories (or theoretical considerations) as well as other sources of information, educational simulations aim to develop an understanding of the underlying model and from it, the theoretical principles among the students. Education simulations therefore require some type of guidance to be effective (de Jong & van Joolingen 1998). In a comprehensive review of the literature on virtual lab and simulation software for grades 6–12, Scalise et al. (2011) considered that the simulations used in science education can be grouped into two main categories: virtual laboratories and simulations of phenomena, the first used for on-screen simulation of the experiments that are traditionally performed in real school laboratories as part of the science curriculum and the second used to model a system or a process.

Two different forms of working may be distinguished in educational simulations (Doerr 1997) related to the agent that designs the simulation. On the one hand, exploration, in which students explore the consequences of their actions within the boundaries of a simulation created by the teacher or an expert to represent the knowledge of a specific content of an ideal model. The model is, therefore, already constructed. Used in this way, it allows the exploration of questions such as "what happens if . . .", by modifying parameters (Doerr 1997). The majority of applications available through Internet are designed for exploration and this was, in fact, the most common method in the investigations that were reviewed by Smetana & Bell (2012) and Scalise et al (2011).

Another form of working with simulations that is closer to the scientific paradigm is called 'modeling' in the literature on science education. To do so, programs are used that allow students to create their own simulations. In the construction of the model that must underlie the simulation, students should identify the relevant variables, quantify the relations between them, and evaluate their validity; exercises which allow them to express their own concepts and to learn from the processes used to represent them. There are two types of programs that allow this kind of work. On the one hand, programs such as STELLA[14] (e.g., Mandinach 1989; Steed 1992) enable students to model systems and automatically generate the mathematical relations from the qualitative relations that the students establish in graphic form. The modeling system of STELLA is relatively simple and it has powerful options for visualization and for the creation of graphic interfaces, as it is principally visual, although this may mean that certain models may become "tiresome". One of its advantages is the facility with which the students may modify the structure of the model that is generated and its parameters, after examining its output (Doerr 1996).

Other programs such as Modellus and Easy Java Simulator allow students to model phenomena, through the use of equations with ordinary derivatives, and to combine the representation of mathematical objects with analytical, analogic, and graphic representations (Teodoro 2002). These types of programs require a relatively high level of mathematical knowledge, appropriate only for the final years of secondary education. Programs such as Interactive Physics and Physlets (Christian & Belloni 2001), which are somewhere between the two types of uses, allow students to generate simulations in which they can select and measure different variables. These simulations are not completely straightforward; the student selects the physical situation to be studied – for example, in a collision between two bodies, the student can choose the shape of the bodies, the values of the relevant variables, etc. –but once the initial conditions are set,

[14] Other programs that allow modelling in K12 science teaching are LOGO (Papert 1980); Model-It (Jackson, Stratford, Krajcik, & Soloway 1996); ThinkerTools (White 1984); and BioLogicaTM (Buckley et al. 2004).

the objects are governed by Newton's laws, so the student will neither write down the equations, nor the relations that govern the movement of the objects.

In general, research on educational simulations have fundamentally centered on cognitive aspects associated with its usage, while epistemological questions have received little attention. For example, looking in depth at all the articles analyzed in the review by Smetana & Bell (2012), only two of them (Hennesy et al. 2006; Marshall & Young 2006) point, in a roundabout way, to an aspect with epistemological implications relating to the authority that students project onto the computer, which may lead to misconceptions if they understand animations and images of abstract concepts in a literal way. Beyond this review, Kirschner & Huisman (1998) looked at the importance of discussing with students the restricted validity of simulations that were generated when working with a program that used some 500 input variables. Depending on the values assigned to those same variables, the simulation could, therefore, generate models that did not represent real processes. A further work that discusses this question is the review by Doerr (1996) on various investigations using the STELLA program. Doerr pointed out that the program can run a simulation regardless of the significance of the data inputs, although validation of the model with experimental data is fundamental. However, in relation to this point, Doerr recognized that there have been no investigations that examine the systematic evaluation of the models by students or how students understand that some features are intentionally excluded from a model or modified in a significant way, while others are artifacts of the simulation program or are invalid assumptions.

It could be argued that the dearth of investigations on the epistemological aspects of simulations is related to the aforementioned differences between scientific simulations and those used for didactic purposes. However, as we shall see next, some relevant epistemological points should still be discussed with the simulations designed by experts. If they have not been discussed, it is probably because up until now, in the field of investigation in science education, and for some time in epistemology, they have only been considered a tool, and not a specific scientific method.

3.2. Model-based learning and experimental work can be enriched with epistemological discussions about simulations.

As simulations are today a fundamental part of daily scientific tasks, working with simulations in science classes at all educational levels is seen to be as important as experimental work and problem solving (Scalise et al. 2011) and the discussion of some epistemological questions associated with them should certainly be introduced into any didactic approach In this section, arguments will be advanced to support the contribution of the epistemological notions, debated in earlier sections, in two areas in which simulations are already used as a training tool.

a) Model-Based Learning (MBL)

The central role claimed by models in science education has been widely debated over recent years, and is probably the area with the greatest discussion of epistemological questions (among others, Gilbert et al. 2000; Nola 2004; Izquierdo & Adúriz Bravo 2003; Halloun 2007). Among the different epistemological approaches, the semantic vision of models (van Fraassen 1980; Giere 1999) has reached a certain preeminence in science education, as it would appear to be the best adapted to teaching in this area, because it highlights the role of models as an active element in the process of knowledge generation and construction (Sensevy et al. 2008; Koponen 2007). In this area, many investigations and didactic proposals based on MBL use simulations, whether using tools for the creation of models (e.g. Stratford, Krajcik, & Soloway 1998; White & Frederiksen 1998, Sins et al. 2009) or simulations developed by experts for scaffolding scientific understanding (e.g. de Jong et al. 1999, Monaghan & Clement 1999; Windschitl 2001). When we think of models as vehicles for the generation of new ideas, the role of simulations, as used by scientists, is fundamental. However, a close analysis of the research that use simulations in MBL shows that the characteristics within the modeling that relate to the role of simulations are not emphasized and simulations are, in general, only used as a tool that can facilitate learning about modeling (e.g., Windschitl 2001, Sins et al. 2009, Waight et al. 2013) and not as a particular form of modeling in itself.

Considering simulations as a peculiar form of modeling implies approaching with students the way in which computational models emerge and their intricate form of relating theory, experimental data, intuition and tricks, to give the mathematical models a computationally viable form. As indicated earlier, students should manage to understand that some features are intentionally excluded from a model or modified in a significant way, in as much as they are either artifacts of the simulation program or non-valid assumptions (Doerr 1996). This necessarily leads to the problem of the validation of simulations; a much more complex problem, as we have seen, than the validation of traditional models in science. This is especially relevant, as it is precisely the notions that students acquire about this point, which will permit them to evaluate the results of scientific simulations.

Perhaps one way to implement these insights into the classroom could be through the use of the history of science, for example, related with the origins of simulations and also with the development of some paradigmatic computational models, such as those used in climate science, that are well documented. These examples can show students how scientists try to understand complex phenomena and the different ways they use to obtain computational tractable models and useful simulations that enable good predictions.

Another way may be to introduce the epistemological questions through students' reflection on what they think the simulation is doing, and how it is executed, and implemented. Certainly, the use of simulations that allow students to design the models themselves, to determine the relations between their respective elements, to generate the dynamic of these relations, and to understand their consequences, is the most appropriate way of integrating this discussion, as many programs are available at present, even for students that have mastered neither mathematical techniques nor programming skills. However, even in the case of closed simulations, prepared by experts, students have to be able to understand that mode of scientific production. Without this discussion, it may happen that students eventually consider that when they use simulations, the model is only for "*playing with values and formulas on the computer model so that they match the measured values*" (quoted from a student of Sins et al. 2009, p. 1219).

On another point, the discussion of the veracity or reliability of computational models inevitably leads us to revise the realist notion that both students and teachers tend to adopt in science education. As discussed earlier, it would appear necessary, in the case of simulations, to adopt more restricted stances, such as, for example, the selective realism of Humphreys (2004) or the notion of instrumental reliability proposed by Suárez (1999). Koponen (2007, p. 765) also discussed this point, although it was not directly related to simulations, but to the semantic view of models. He suggested that if we accept this viewpoint, which implies changing our point of view on models from only a mere representation of phenomena to the use of models as matchmaking tools, then realism in relation to the truth of the theories is challenged. This does not mean abandoning the positions of a realist, but of its discussion in parallel with other complementary views (Koponen 2007, Wong & Hodson 2009).

According to the results of the investigation by Wong & Hodson (2009), scientists are used to playing with both realism and instrumentalism, depending on their immediate proposals. For this reason, these authors argue that students should be taught to be realistic critics, capable of evaluating the status of a particular piece of knowledge and using it either in a realistic or in an instrumental way, in accordance with the demands of each situation. Doing otherwise, would not give an authentic vision of science. Simulations, in this sense, have a lot to contribute in a specific way to this discussion.

b) Experimental work

Much of the research into simulations refers to its use as a complement or substitution of experimental work. Simulations are used in relation to experimentation in two different ways: the majority use them as a substitute for real experiments (e.g., Hsu & Thomas 2002; Huppert & Lazarowitz 2002; Kaput 1995; Tao & Gunstone 1999; Zacharia 2003), but also as "dry laboratories" (Kirschner & Huisman 1998), to achieve specific cognitive skills, such as analysis, synthesis and evaluation (e.g., de Jong & van Joolingen 1998; Plass et al. 2011; Kukkonen et al. 2013).

However, many professors and researchers consider that experimentation with physical manipulatives is the only real, "hands-on" experimental activity, excluding from this categorization, virtual laboratories, which simulate experiments (Zacharia et al. 2008; Klahr et al. 2007). In fact, the absence or the low frequencies of some typical activities of real laboratories have been noted – peer participation, the analysis of sources of error and the comprehension of the complexity and the ambiguity of experimental work – among professors using simulations as experimental activity (Crippen et al. 2012). It is interesting to note that the America's Lab Report (National Research Council, 2006) concluded that the lack of available studies on these points left the review committee unable to draw conclusions on the benefit of using virtual labs. Nevertheless , the results of the investigations into virtual laboratories would appear to contradict this view, because the cognitive gains of students with either one or the other form of experimentation seem to be equal (for two well documented reviews on this topic see Triona & Klahr 2003 and de Jong et al., 2013). Some researchers consider that they could even be better than the laboratories with physical manipulatives, because they are easier and students can work with the data in a controlled environment and can exercise control over their variables, which is not generally achieved in standard laboratories (Klahr et al. 2007; Baser 2006).

De Jong et al. (2013, pp. 305-306) stressed that although physical and virtual laboratories can achieve similar student-related objectives, related to stimulating their interest in science, their conceptual understanding, and their inquiry skills, each of these different kinds of laboratories also have certain specific traits. Physical laboratories allow students to develop specific laboratory skills, such as practical skills or the ones related with a carefully planning of experiments. Virtual laboratories, moreover, are not only less time consuming, both in the setup as in their output results, but they also allow to adapt reality in the sense of making unobservable phenomena visible and of removing confusing details. Along similar lines, Chinn & Malhotra (2002, pp. 207-8), in their discussion of epistemologically authentic lines of inquiry, suggest that the advantages of a simulated experiment, in addition to cases in which hands-on activities can not be carried out, is that it allows the realization of: a) experiments at the theoretical level of the mechanism, in other words, the study of theoretical entities that could not otherwise be "visualized"(for example, simulations at a molecular or genetic-molecular level); b) different types of experiments on one single case; c) relatively complex scientific designs. Despite these advantages, Chinn & Malhotra (2002) highlighted that simulations demystify, in an artificial way, a large part of the disorder in the natural world and, moreover, students can not evaluate different models or variables other than those that are programmed, a point also discussed by Scheckler (2003). Addressing these issues, several authors have began to propose the benefits of combining both, physical and virtual experiments (for example, Zacharia et al., 2008; Jaakkola et al. 2011; de Jong et al. 2013).

Thus, the research in science education points to different features of simulations and experimentation, mainly related with the acquisition or improvement of different skills. But, as pointed out in the second section, experimentation and simulations are not considered equivalent in the epistemological discussion that has developed around simulations. As we have seen, experimental work cannot be substituted by simulations, as experiments continue to be the acid test of all theories relating to the world, having in this sense an epistemological priority, as they are the only mode of scientific production that allows us to evaluate hypotheses, models, and theories. Of course, this will never mean that students should not test hypotheses or models in a virtual lab, a methodology that appears to be successful at achieving several cognitive goals, or that they should not use simulations in science labs, given its ubiquity in science. But, although this discussion is yet to arise in science education literature, it appears relevant that students should be aware of the epistemological differences and similarities between simulations and experimentation.

Perhaps one way of informing students about the epistemological questions relating to experimentation and simulation might be through the development of research projects that blend both, in a similar way as scientists do, in which the experimental work serves, on the one hand, as a database for the generation of computational models and, in turn, as a means for their validation and as a source of new experiments. This echoes recent discussions on investigation into modeling in science education as an activity that can not be separated from experimentation (Sensevy et al. 2008; Koponen 2007). As suggested by Sensevy et al. (2008, p. 432) "*On the one hand, theory translates Nature itself into semiotic systems registering the observations (power of the abstract) and, on the other hand, the phenomena produced by the instruments reach some sort of autonomy that gives feedback on the theory (power of the concrete)*". In experimental work, combining hands –on activities and simulations we could help students achieve not only a more accurate notion of current scientific practice but also that semi-autonomous vision of models that allow them to connect with the measurable properties of the phenomena, something which has yet to be fully discussed in science education.

So, more frequent use of the computer in the science laboratory should take place, in order to provide a more authentic image of contemporary research in sciences, both for the purposes of data collection, manipulation, control and presentation as discussed by Wong & Hodson, 2009, and for the analysis of these data through the development or manipulation of certain sorts of simulations.

5. Final remarks

Certainly, simulations have not impacted on science in a "conceptual" form to the same extent as certain theories –consider the impact of relativity or quantum mechanics -, which is one of the reasons noted by epistemologists for the scant attention paid to them. However, they have impacted and in a strident manner, on the scientific practice and its application in all scientific areas. They have allowed scientists to greatly expand the knowledge about the world in such a way that our current understandings of all complex and above all non-linear systems that characterize the vast majority of phenomena in the universe have in fact been made possible only by the use of simulations.

However, simulations, as recent epistemological studies have shown, have proven to be much more than a fantastic tool for calculus, but a new form of scientific production.. Simulations therefore stir up classical epistemological notions, such as the ones presented in this paper: the modification of the role of differential equations as the principal tool of physics; the nature of modeling and its relation with existing theories; the classic division between scientific theory and empirical methods; the prediction as a self-sufficient goal in some areas of science to the detriment of explanation; and the need to assume a more pragmatic position in relation to reliability. Although we have discussed these issues in very general terms, the areas that are denominated complex systems, which spread to every branch of science, constitute a privileged arena in which to study these special features provided by simulations in scientific method.

In this paper we have tried to review these issues, arising from a large, diverse and quite recent literature, highlighting them for research in science education, where we have quite a good body of knowledge on the use of simulations for cognitive and motivational goals (although not yet used as widely in teaching as would be desirable), but that have not yet addressed them from an epistemological point of view. And, although there is today a wide ranging literature in science education on experimentation and models, which urges researchers and teachers to address their most relevant epistemological features, as they support the training of scientifically literate citizens, the same has not yet happened with simulations. If we are to take the recommendations of the various curricular reforms seriously that urge us to provide students with an opportunity for authentic inquiry, which *"refers to the research that scientist actually carry out"* (Chinn & Malhotra 2002, p. 177), we must include simulations in science education, but not, as seems to happen, uncritically and only as a tool.

Nevertheless, the way to introduce the epistemological problems discussed throughout this paper in the secondary and university education and in teacher training is an open question. We have only addressed, very generally, some possibilities in two research areas, experimental work and model based learning, that we think are key points to approach them. As stated above, research into these issues is at a primitive stage and more research is needed to offer specific suggestions. In fact, these questions form part of an ongoing research project in which one of the authors of this paper is currently engaged.

Recently, it has been argued that science education should not center exclusively on the teaching scientific concepts, but also on metaconcepts. Snir et al. (2003) defend the idea that the notion of model should be applied in this way, so that students know what it is and how it is used in science, as by *"doing so we are letting students take part in the process of scientific developments the way scientist do, even though it is in a structured and limited environment designed by us specifically for these purposes"* (Snir et al. 2003, p. 803). We consider that the same should apply to the case of simulations. So, in the same way as scientific theories and skills associated with scientific development are proposed as indispensable elements for the general training of students, we should include simulations not only as a tool to motivate students and to facilitate their learning, but with a similar status to the inclusion of experiments or modeling in the content of natural sciences. The training of scientifically literate citizens today requires them to know about the potential and the limitations of simulations, because simulations are connected to a large part of our emergent knowledge of the world – i.e. the practical application of theories to the world that is, as citizens, what interests us most.

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