New Mathematics for Old Physics:
The Case of Lattice Fluids

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·Abstract

We analyze the effects on modeling of the introduction of new mathematical tools on an old branch of physics by focusing on lattice fluids, which are cellular automata (CA)-based hydrodynamical models. We examine the nature of these discrete models, the type of novelty they bring about within scientific practice and the role they play in the field of fluid dynamics. We critically analyze Rohrlich', Keller's and Hughes' claims about CA-based models. We distinguish between different senses of the predicates "phenomenological" and "theoretical" for scientific models and argue that it is erroneous to conclude, as they do, that CA-based models are necessarily phenomenological in any sense of the term. We conversely claim that CA-based models of fluids, though at first sight blatantly misrepresenting fluids, are in fact conservative as far as the basic laws of statistical physics are concerned and not less theoretical than more traditional models in the field. Based on our case-study, we propose a general discussion of the prospect of CA for modeling in physics. We finally emphasize that lattice fluids are not just exotic oddities but do bring about new advantages in the investigation of fluids' behavior.

·Keywords

cellular automata, computer simulation, fluid dynamics, lattice fluids, theoretical model, discrete model, phenomenological model, micro-macro relations, Navier-Stokes equations, Boltzmann equation, mathematical formalism, scientific languages, scientific practices

1. Introduction

It is by now a common view in philosophy of science that theories are too large units for the analysis of scientific development and that we should turn to finer-grained description of scientific activity. In this paper, we focus on modeling practices and ways of representing phenomena and drawing inferences about them. We investigate a case in which an old representing practice (based on the use of differential equations) has suddenly been paralleled by an entirely different one (based on the use of discrete mathematics). Our main focus is on the nature of such a shift and its impact on fluid modeling and theorizing.

Two decades ago, fluid dynamics went lattice: besides computer simulation based on the discretization of Navier-Stokes equations, which remains an active field of research, simulations of a novel type flourished, some of them based on cellular automata, others on finer kinds of lattices. The main feature of this new way of studying fluids is that it is based on an apparently irrealistic representation of fluid molecules as cells on lattices that can only move along a few allowed directions. In spite of their apparent simplicity, these models have many applications, like the study of porous media or the decreasing of air-noise in cars, and are thus intensively investigated. Lattice hydrodynamics now has its own summer schools and textbooks (Boon et alii 2001, Succi 2001).

From a philosophical point of view, lattice hydrodynamics is intriguing: What kind of models are lattice fluids? How are they to be analyzed? Does their emergence indicate that a "new kind of science" is developing? Or are they on a par with more traditional models? In order to answer these questions, we first present in section 2 what lattice fluids are. We then discuss the nature of lattice fluid models and the role they play in the field of fluid dynamics. We do that by critically analyzing Rohrlich', Keller's and Hughes's claims about the phenomenological nature of CA-based models (section 3): we distinguish different senses of the predicates "phenomenological" and "theoretical" and emphasize that lattice-gas models, far from introducing any revolution, are rather conservative and no less theoretical or fundamental than more traditional models in the field. In section 4, we give more general arguments about the prospect of CA for modeling in physics. We finally emphasize in section 5 that in practice, CA-based models are not superfluous oddities but bring about scientific benefits that cannot be drawn from other models.

2. Lattice Hydrodynamics

In this section, we give a brief presentation of these models called "lattice fluids". We present their historical origin as well as their main characteristics as physical models.

2.1 What Is a Lattice Fluid?

Lattice fluids are models of fluids that are made up of lattices composed of cells that can be in various, discrete states. In the simplest models, on which we shall focus in this paper, the cells can only be in one of two states: occupied or vacuous. From a computer science and mathematical point of view, lattice fluids can be viewed as cellular automata (hereafter CA)[1],

[1] A cellular automaton is a discrete dynamical system on a regular spatial lattice, each point in which is called a cell. A cell can only have a finite number of states. The states of the cells in the lattice are updated according to a local rule: the

that is, discrete non linear dynamical systems with many degrees of freedom. From a modeling point of view, they can simply be viewed as entirely discrete models of fluids in which combinations of black cells represent molecules and the rule of the automaton represents the possible moves and collisions of molecules: “intuitively, a *lattice gas* is a system of particles that move in discrete directions at discrete speeds, and undergo discrete interactions” (Toffoli and Margolus 1996, 10). The first lattice models of fluids were developed by physicists entertaining no connections with computer science or IA and working in the tradition of semi-discrete models originally studied by Maxwell and later by Broadwell (Maxwell, 1890, Broadwell, 1969, Hardi et alii, 1973, 1976). In this perspective, the simplest models of lattice fluids are just physically interpreted CA, which computational simplicity makes it easier to investigate the behavior of highly-idealized if not fictional fluids. Figure 1 illustrates how particles hop from vertex to vertex on a square (resp. on a hexagonal) lattice. In both pictures, the particle is in the middle of the lattice and the arrows represent the 4 (resp. 6) possible moves that the particle can make in one time unit.

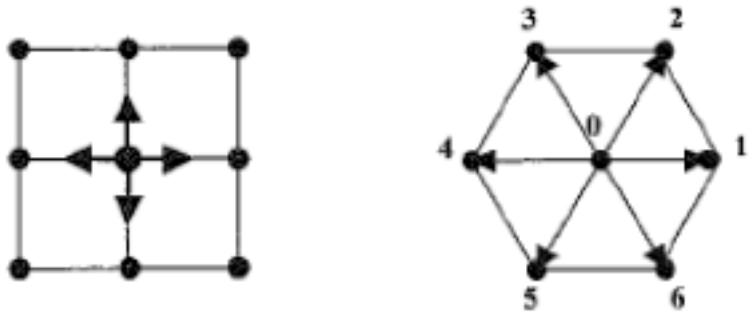

Figure 1. The square and hexagonal grids of the HPP and FHP automata.

In their 1990 review paper on the use of CA in physics[2], Toffoli and Margolus recall that:

> “The [reaction] that we most often [hear] about CA is the following: ‘I’ve been shown CA that make surprisingly good models of, say, hydrodynamics, heat conduction, wave

state of any cell at a given time only depends on its own state and of the states of its nearby neighbors. All cells in the lattice are updated synchronously.

[2] CA have been and are used in two different ways in physics. First, CA are used to study empirical phenomena, like the formation of galaxies, the properties or crystals, or the behavior of fluids. This first use belongs to “normal science” in Kuhn’s sense: it is about applying, and adapting, mathematical tools to empirical problems, not about challenging underlying theories. The second way is more speculative. It is based on the tentative claim that “nature, at some extremely microscopic scale, operates exactly like discrete computer-logic”, to quote Feynman, who himself toyed with this idea (Feynman 1982). This hypothesis has been further developed by Fredkin (1992), Vichniac (1984), Margolus (1984) and Wolfram (1992). It had previously been discussed by Konrad Zuse (see Fredkin 1992 for a review). It is so far a purely conjectural hypothesis about what our universe is like at its most fundamental level; the aim of such investigations is to discover a new fundamental physical theory and to formulate it with the help of CA.

These two ways of using CA have not always been clearly separated, be it in scientists’ or in philosophers’ writings. Nevertheless, for the sake of philosophical analysis, it is important to be aware that these are two different enterprises, which raise different philosophical questions. As will be obvious, we are dealing in this paper with the first enterprise, namely the “ordinary” study of empirical phenomena with the help of CA, by contrast to the search for a fundamental theory of a supposedly discrete universe.

scattering, flow through porous media, nucleation, dendritic growth, phase separation, etc. But I'm left with the impression that these are all *ad hoc* models, arrived by some sort of magic. I'm a scientist, not a magician'."

The examples Toffoli and Margolus give to answer this reaction are the Lattice Gas Cellular Automata (LGCA). We shall emphasize in this paper that LGCA are no magic of any sort and that their connection with physical theories is tight: when they are analyzed against the principles of classical mechanics and kinetic theory, it becomes clear that the difference with more traditional models is only apparent.

2.2 A Brief History

By forming a "loose analogy" (Hasslacher 1987, p. 186) with the structure of the Ising model, Hardy, de Pazzis and Pomeau (1973, 1976) created the first minimalist fluid model on a two-dimensional square lattice, known as the "HPP gas". In this model, physical space is represented by a square lattice and particles hop from one vertex to one of the neighboring vertexes in one time step. This implies that there is absolutely no notion of continuous motion between sites in this model.

This first model, however minimal, exhibits important macroscopic properties, like the emergence of scale separation and local equilibria. Nevertheless, the emerging macrodynamics is unsatisfactory since it does not obey Navier-Stokes equations and exhibits unphysical features. The main reason for this failure is that the lattice is only symmetric under $\pi/2$ rotations, which is insufficient to insure the isotropy of the usual tensors describing the fluid. Further, the HPP separately conserves the horizontal component of momentum on each horizontal row and the vertical component on each vertical column. These are spurious (unphysical) conservations. A solution to this problem is to change for a hexagonal lattice.

By 1985, Frisch, Hasslacher and Pomeau demonstrated that it is possible to approximate solutions to Navier-Stokes equations by using lattice gas methods. The proof was only valid, at the time, for low-velocity incompressible flows. The FHP lattice gas uses 6 particle directions and it obeys Navier-Stokes equations in the macroscopic limit. We describe it further in the following subsection.

2.3 The Main Model

The FHP Simple Hexagonal Model[3] is the minimal totally discrete model from which hydrodynamic behavior can be recovered in two dimensions[4]. In a typical lattice-gas simulation of a fluid, about 10^9 particles are involved. The coordinate system for a single-speed six-directional world is the set of unit vectors:

$$\hat{\mathbf{i}}_\beta = \left\{ \cos\left(\frac{2\pi\beta}{6}\right),\ \sin\left(\frac{2\pi\beta}{6}\right) \right\}, \quad \beta = 1, \cdots, 6.$$

[3] See Boon and Rivet (2001) for a pedagogical introduction to lattice gas hydrodynamics.

[4] Lattice gas hydrodynamics has also been developed for 3D models.

Here is a list of the "ingredients" that are needed to build up a minimal cellular-space with a dynamics that reproduces the collective behavior predicted both by the incompressible and the compressible Navier-Stokes equations, with about 10^9 molecules:

- a population of identical particles, each with unit mass and average speed *c*;
- a totally discrete phase space and discrete time;
- a minimal set of collision rules that define systematic binary and triple collisions such that momentum and particle number are conserved (see figure 2);
- an exclusion principle: two particles at the same site at the same time cannot move along the same direction.

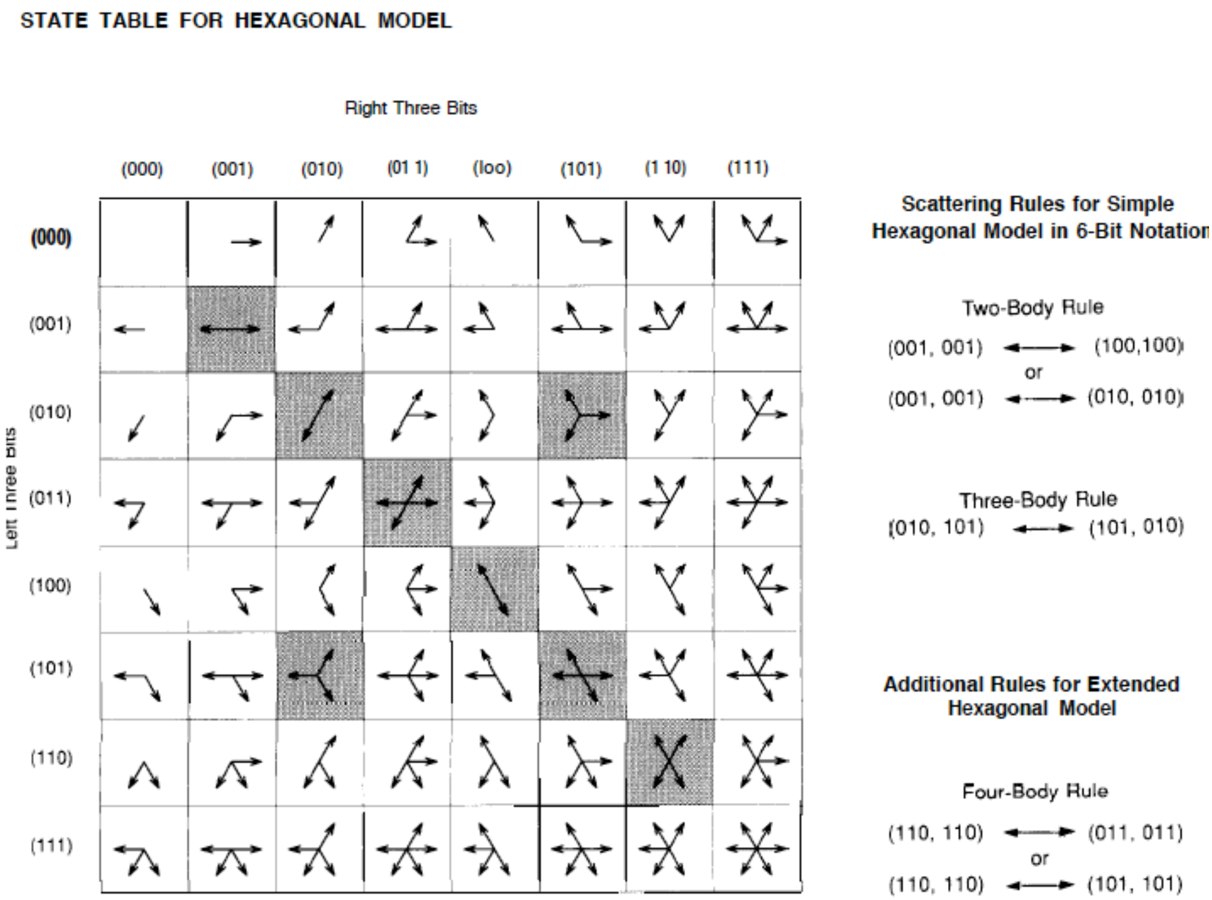

Figure 2. State table and collision rules for the original hexagonal model (taken from Hasslacher 1987).

Figure 2 shows all possible states of the hexagonal lattice gas. Each state can be expressed in a 6-bits notation, given on the left and on top of the table. For instance, the cell at the right of the upper line shows a state in which three particles are present, going in the three directions indicated by the arrows. This state is coded as (000, 111). Collision states are shaded in gray and the scattering rules are indicated at the right of the table. According to these rules, the state (001, 001), which is the first gray-shaded cell at the top-left of the table, either results in state (010, 010), which is represented in the gray-shaded cell next to it on the downward diagonal, or in state (100, 100), represented below on the same diagonal.

As surprising as it may be, this poor cartoon of molecular dynamics, in which the entire state of the N site lattice gas is specified by $6N$ bits (to be compared with the infinity of degrees of freedom in continuum kinetic theory), can display the main features of hydrodynamic phenomena[5] (we shall emphasize some differences in the next sections).

2.4 The Physics of Lattice Fluids

As can be inferred from figure 2, conservation of momentum and particle number is built from the start into *exactly computable* collision rules. In order to understand how LGCA reproduce the collective behavior predicted by the compressible and incompressible Navier-Stokes equations, we quickly review how this result is established for the FHP model. The first move is to switch from a deterministic to a probabilistic description, in order to apply the familiar tools from kinetic theory. The lattice form of the single-particle distribution function can be obtained via the following identifications:

$$f(\mathbf{r},\Gamma,t) \rightarrow f_\beta(\mathbf{r},t)$$
$$\int f(\mathbf{r},\Gamma,t)d\Gamma \rightarrow \Sigma_\beta f_\beta(\mathbf{r},t) \equiv \rho,$$
$$\rho\mathbf{v} \rightarrow \Sigma_\beta \hat{\mathbf{i}}_\beta f_\beta$$

where $\mathbf{r}$ stands for position, Γ for all other coordinates in phase space, such as momentum, ϱ for density, $\mathbf{v}$ for the velocity of a fluid element, t for time and f is the phase space distribution function in the usual continuous case. From this new, continuous writing, one can pass to the master equation for f_β in the absence of collisions (for a square lattice):

$$f_\beta(\mathbf{r}+h, t+k) - f_\beta(\mathbf{r},t) = 0, \text{ with } h = \hat{\mathbf{i}}_\beta d_x, k = d_t,$$

where d_t, $d_x << 1$, and the following convention is adopted: n_β ($\mathbf{r} + \hat{\mathbf{i}}_\beta$, t) is the number of particles in the direction β at the node $\mathbf{r} + \hat{\mathbf{i}}_\beta$ at time t. Using the Taylor series expansion, the master equation becomes

$$0 = d_t\partial_t f_\beta + d_x\hat{\mathbf{i}}_\beta\cdot\nabla f_\beta + \frac{1}{2}d_t^2\partial_t^2 f_\beta + \frac{1}{2}d_x^2(\hat{\mathbf{i}}_\beta\cdot\nabla)^2 f_\beta + d_x d_t(\hat{\mathbf{i}}_\beta\cdot\nabla)\partial_t f_\beta$$

To the lowest order in h and k, this gives

$$\partial_t f_\beta + \hat{\mathbf{i}}_\beta\cdot\nabla f_\beta = 0,$$

[5] A set of more recent tools, called Lattice Boltzmann Methods (LBM), enables physicists to obtain even better results. LBM are slightly different from LGCA but keep the same spirit. The basic idea is that the Boolean occupation numbers n_i are replaced with the corresponding ensemble-averaged populations $f_i = \langle n_i \rangle$. "Instead of tracking single Boolean molecules we content ourselves with the time history of a collective representing a 'cloud' of microscopic degrees of freedom". See (Succi, 2001, pp. 40-65).

which is the standard form of the transport equation in the absence of collisions. One may add a collision operator $C_\beta(f)$ in order to obtain the full Boltzmann transport equation

$$\partial_t f_\beta + \hat{\mathbf{i}}_\beta \cdot \nabla f_\beta = C_\beta(f)$$

which describes how the probability distribution of the microscopic states evolves in phase space. The next step is to use appropriate approximations and Chapman-Enskog expansion to compute the integrals corresponding to the different conserved quantities. This is how Euler and Navier-Stokes equations are recovered, as well as tensors describing the fluid.

The best example of how the macroscopic behavior of the fluid depends on the microscopic behavior of particles is the derivation of the momentum stress tensor Π_{ij} describing and controlling the convective and viscous terms in the Euler and Navier-Stokes equations. This tensor must be isotropic (since fluid motions are isotropic). However, as alluded above, a square lattice does not contain enough symmetries for Π_{ij} to be isotropic; in two dimensions, only a hexagonal lattice does. By using considerations on tensor structure for polygons and polyhedra in *d*-dimensional space, one can also arrive at satisfactory (but not always tractable) models in any dimension.

2.5 Some Questions About Lattice Fluids

At first view, there is a sharp contrast between CA-based fluids and traditional models of fluids. Fluids have been studied for two centuries first by the analytical exploration of PDEs and after 1945 by simulations computing numerical solutions of (discrete approximations of) Navier-Stokes equations. Lattice fluids only emerged after 1986; the mathematical theory of CA, which mostly began after 1980, is still under-developed. It seems hard to see how the rich body of knowledge about fluid qua continuous media built within classical mechanics could translate into a CA-based picture of physical systems, all the more because the discrete and anisotropic nature of these models stands in blatant violation of what our present theories say about the world.

At the very least, fluid dynamics is a field that is *prima facie* not favorable if not orthogonal to CA-modeling (in contrast with other cases like the Ising model, of which we say a few words below) because PDEs seem to play a crucial role in it since its target systems are described at the microscopic level by classical mechanics laws, which are usually formulated in terms of continuous differential equations, and at the meso- and macroscopic level by Boltzmann and Navier-Stokes differential equations. In the remaining of the paper, we try to assess to what extent these prima facie views about the use and place of CA models in fluid dynamics can be sustained or should be modified.

3. Epistemology of CA-Based Models, Through the Lens of Lattice Fluids

We start by scrutinizing whether lattice fluids are the result of a radically new way of modelling. In order to do so, we first discuss the views of the philosophers of science who have analyzed CA-based models, mainly Fred Rohrlich and Evelyn Fox Keller. This discussion leads us to distinguish two senses of the word "theoretical", which we explore in section 3.2. We further discuss the epistemology of CA-based models by assessing their potential relationships to physical theories in section 3.3.

3.1 Views About the Specificity of CA-Based Models

A common view about the study of empirical phenomena with the help of CA-based models is that these models have little to do with physical theories. We now analyze this view, as expressed by Keller and Rohrlich. This allows us to shed light in the next subsection on the type of philosophical work that is required in order to better understand in what sense lattice fluids are *new* hydrodynamic models.

Let us start our inquiry into philosophers' views about CA-based empirical models with a quote from Evelyn Fox Keller (2003, pp. 208-209), who, embracing under the same heading cellular automata and artificial life, declares:

> "The third class of computer simulation I want to discuss departs from the first two in at least one crucial respect: It is employed to model phenomena which lack a theoretical underpinning in any sense of the term familiar to physicists – phenomena for which no equations, either exact or approximate, exist (as for example in biological development), or for which the equations that do exist simply fall short (as for example in turbulence). Here, what is to be simulated is neither a well-established set of differential equations […] nor the fundamental physical constituents (or particles) of the system […], but rather the phenomenon itself. In contrast to conventional modeling practices, it might be described as modeling from above."

This claim is consonant with Rohrlich's views about CA, which he exemplifies in his 1990 paper by the case of CA-based simulations of galaxy formation (pp. 512-514). According to Rohrlich, a theory-based approach to this problem would involve, at least, Newtonian gravitational theory. "Since this approach is not possible, an option is to turn to a phenomenological statistical model based on CA". Rohrlich defines "phenomenological theories" (p. 508) as (*i*) "involv[ing] a large amount of empirical input", (*ii*) being "competent only over a relatively narrow domain of phenomena", (*iii*) "typically almost devoid of 'unobservable' constructs", (*iv*) "and thus appeal[ing] to the instrumentalist". "Fundamental" theories are to be understood as "non-phenomenological", the opposition between "fundamental" and "phenomenological" being a matter of degree. Rohrlich claims that the CA-based model of galaxy formation is phenomenological "because it uses various adjustable parameters taken from observation, such as the rotational speed or the radius of a galaxy" but says nothing about the other criteria of his own definition. A final assertion of his may be mentioned, that "physically, CA type models are necessarily of a phenomenological nature rather than of a fundamental one" (p. 516).

We first note that Keller and Rohrlich conflate several theses that we think should be kept distinct, namely that

(*a*) The building up of CA-based models is mainly *guided* by the consideration of phenomenological regularities.

(*b*) CA-based models do not *describe fundamental properties* of the systems of interest ("fundamental properties" being those properties that, according to the prevailing theories in the corresponding fields, should be used to give a sound theoretical account of the target phenomena).

(*c*) CA-based models do not *have any theory-based justification*. Instead, their success is due to their incorporating elements that are known to be instrumental to match phenomena (typically, adjustable parameters).

Thesis (*a*) is about the process of discovery and implies nothing about justification. We shall not discuss it. By contrast, theses (*b*) and (*c*) are about the sense in which CA-based models are not theoretical.

3.2 Some conceptual distinctions

We now offer a conceptual toolbox for analyzing models and modeling in their relationships with theories, which we exploit throughout the remaining of the paper. The first distinction we propose is between two senses in which a model can be said "theoretical": with respect to the relationships of its content to the current theories, or with respect to the justification these relationships bear to its success. According to the first sense, a model is "theoretical-*c*" when the fact that its content relies on the prevailing theories in the relevant field is the reason why it accounts for the target phenomena. According to the second, a model is "theoretical-*j*" when it is known that the justification of its success can be grounded in the relevant theories. The latter predicate is relative to a state of scientific knowledge about the connections between theories, models and phenomena. Calling a model "theoretical-*j*" is therefore a claim about the way the model is known to be related to available theoretical knowledge about the investigated phenomenon. Note that a model can be theoretical-*c* without being theoretical-*j* when no justification of its success in terms of its theoretical content is available yet. Thesis (*b*) says that CA-based models are not theoretical-*c* whereas thesis (*c*) says that they are not theoretical-*j*: their potential success is not justified on the basis of otherwise available theoretical knowledge. A further distinction is needed to account for the fact that some models are theoretical-*j* (according to available background theories) without being known to be theoretical-*c*: the success of these models is theoretically justified, but they do not capture, as far as we know, what is actually the case. We call these models "weakly theoretical-*j*" (and illustrate this distinction below)[6]. Accordingly, Keller's and Rohrlich's claim that CA-based models are not theoretical admit a weak and a strong versions:

(*Weak version*) CA-based models are not theoretical-*j* since they "lack a theoretical underpinning" (Keller) and use "adjustable parameters" taken from observation (Rohrlich) to catch the target phenomenology.

(*Strong version*) CA-based models are not theoretical-*c* because they do not simulate "the fundamental physical constituents (or particles)" (Keller) and they do not use any "unobservable constructs" corresponding to theoretical descriptions (Rohrlich).

In the same way as different senses of the word "theoretical" need to be distinguished, two senses of the word "phenomenological" seem to us important to keep apart:

(*i*) In the first sense, a model is called "phenomenological" when it is not theoretical (in any sense of the term). This is the sense Rohrlich seems to have in mind when he states that a CA-model of a galaxy is phenomenological because it does not rely upon Newtonian mechanics. The point here is the ability for a model to encapsulate (some of) the content of bona fide physical theories or to be backed up by theoretical justifications.

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[6] For sure, there exist clearly phenomenological CA-models, models lacking any theoretical content or theoretical justification, as the Schelling model of segregation effects (1969, 1971), forest fires models (Bak et al. 1990, Grassberger 2002) or traffic flow models (Nagel and Schreckenberg 1992) apparently are. The last two examples belong to fields where any theoretical account is simply missing and the Schelling model has been built up independently of traditional sociological theorizing. In all these cases, theoretical justifications are hardly available.

It may be argued that, even if there is no general theory covering a domain of phenomena, other theoretical justifications may still be cooked up. For example, a justification based both upon theoretical hypotheses that are not unified within a single theory and mathematical arguments may also be viewed as theoretical. For instance, when one assumes that basic events in a given domain are independent and uses probability theory, one may in certain cases give a theoretical explanation based on a Poisson law, even if no theory is involved. We will not push this point further.

(*ii*) The second sense of "phenomenological" is relative to fundamentality. Some theories are more fundamental than others, which are then called "phenomenological", in a different sense from (*i*). Strictly speaking, "fundamental" and "phenomenological" in this second sense only apply to theories, but "phenomenological" may nevertheless be applied in a derivative sense to the models of the theory.
In brief, "phenomenological" can either mean "non-theoretical" (in any sense of the term) or "theoretical-but-not-fundamental".

Because Rohrlich and Keller, in the quotes we recalled in section 3.1, do not pay enough attention to these different meanings of "phenomenological", their claims are susceptible of divergent reconstructions[7]. As for Rohrlich, his claim that "physically, CA type models are necessarily of a phenomenological nature rather than of a fundamental one" could first be construed as saying that they cannot be theoretical in any of the above distinguished senses –and consequently, they can even less be fundamental, since this would mean that they are theoretical *and in addition* that the theory on which they rely is at the bottom of the fundamentality scale. Alternatively, it could be interpreted as saying that CA-based model can be theoretical but that the underlying theories are necessarily close to the phenomenological top of the fundamentality scale (even if this view does not fit with his description of the galaxy model), but Rohrlich does not give any evidence in favor of the latter interpretation (and it is difficult to see which evidence he could give in favor of such a bald negative general claim).

Finally, as "fundamental", "theoretical" and "phenomenological", when applied to models, are gradual predicates, a third interpretation of Rohrlich' claim is that within a given field, CA-based models are more phenomenological than traditional models, which rely more stringently upon available theories within this field. This version of the claim makes sense even in fields, like fluid dynamics, in which the available theory is not fundamental. Fluid dynamics is therefore an appropriate field to focus on when investigating the issue of relative phenomenologicality, because it provides us with examples of physical systems for which both traditional, PDE-based, and CA-based models have been and still are currently investigated in order to study the same type of phenomena. The third interpretation of Rohrlich' claim then implies that CA-based models of fluids are less theoretical than models derived from Navier-Stokes equations (even if the latter models are themselves phenomenological in the sense that they are built out of a phenomenological theory).

3.3 About Lattice Fluids Being Theoretical Models

We can now discuss the above claims and show that lattice fluids are theoretical models in the senses that we described above. The distinctions we have introduced first allow us to maintain that Keller's ambiguous claim that CA-based computer simulation "is employed to model phenomena which lack a theoretical underpinning in any sense of the term familiar to physicists" (2003, pp. 208-209) clearly misinterprets the field of lattice hydrodynamics (one of Keller's own examples). If it is read as saying that CA can be used in a non-theoretical way, it is almost trivially true, poorly informative about CA, and highly non-specific. The same can be said of most formalisms or models. If it is to be understood as saying that CA are or must be used in a non-theoretical way, it does not apply to lattice hydrodynamics. As we have shown in section 2, the construction of lattice fluids is guided by well-known physical principles. It heavily relies upon application of kinetic theory and it follows the same theoretical route and the same steps as can be found in the usual

[7] We thank an anonymous reviewer for helping us clarifying this point and encouraging us to explore further these interpretations.

theory-guided derivation of Navier-Stokes equations. As this derivation goes from the micro-scale to macroscopic phenomena, describing lattice fluids as "modeling from above" is also misleading. Overall, lattice fluids are clearly theoretical-*j*: the above-described derivation of Navier-Stokes equations from these models, which mirrors the usual theoretical pathway to Navier-Stokes equations, makes clear that the success of the FHP model does have a theoretical justification. For the same reason, it cannot be described as simply warranted by the "adjustment of empirical parameters" (Rohrlich).

Another objection to the claim that LGCA are *bona fide* theoretical models of fluids might come to mind. Let us consider again traditional fluid dynamics. Once it has been shown how Navier-Stokes equations obtain from underlying microscopic features, the game is to call up mathematics to find out exact or approximate solutions to these equations in various situations, laminar or turbulent, in two or three dimensions, with high or low Reynold number, with or without rotation, etc. This game is a tricky one and it often takes a long time to bring about small improvements via mathematical methods, analytical or numerical. For this reason, fluid dynamics is a hospitable land for applied mathematicians and numericists. Could not then LGCA be viewed as new computational methods in applied mathematics, designed to explore Navier-Stokes equations, rather than as alternative models of fluids or, in short, as numerical recipes or "computational instruments" born from theoretical tinkering? From this perspective, their purpose would be to simulate "a well-established set of differential equations" (Keller), and they would meet this purpose because they are calibrated in a theoretically well-grounded fashion. This objection echoes the option we considered above, that some models are "weakly theoretical-*j*", that is, theoretically justified even if devoid of any theoretical content.

This objection is erroneous for the following reasons. First, as we have seen, LGCA do not arise from the numerical study of Navier-Stokes equations. They are obtained independently by taking into account conservation laws and symmetries. Since Navier-Stokes equations have been extensively studied in various situations for more than one hundred and fifty years and their empirical adequacy is established for a large domain of phenomena, it is no surprise that they come into the picture for the purpose of cross-checking against existing methods and results. This should not be interpreted, however, as a sign that LGCA depend in any way on these equations. Second, the use of LGCA and LBM in fluid dynamics requires much more understanding of the involved physical theories than pure numerical methods do[8]. Traditional fluid dynamics is a fruitful field for applied mathematics and numerical studies because much of the physics is built from the start into Navier-Stokes equations. It is thus less necessary to make use of deep insight into the physics in order to get meaningful physical results than in LGCA or LBM, because drawing purely mathematical consequences from Navier-Stokes equations is enough to achieve this aim. On the contrary, in lattice gas methods, it is necessary to be clear-headed about which physical effects depend on which microscopic properties at each step in order to see why exactly one asymptotically recovers the right meso- or macro-behavior for such or such lattice gas. This does not yet imply, however, that lattice fluids are theoretical-*c* (i.e. that their content is theoretically well-grounded) only that they are theoretical-*j* (i.e., we know that their success is theoretically well-justified). We shall now argue that they are *also* theoretical-*c*.

As the derivation presented in section 2.4 shows, some crucial properties are instantiated both by the FHP model and the models that, according to classical mechanics, exactly describe fluids: both possess a rotationally invariant dynamics, in which energy and momentum are conserved by contact processes. And all the symmetries associated with the hexagonal lattice are also possessed by the models that, according to classical mechanics, exactly represent molecular

[8] However, there also exists a branch of applied mathematics dealing with LBM with the aim of solving PDEs.

dynamics of fluids. Further – and this is the crucial point that was shown by Frisch, Hasslacher and Pomeau in their seminal 1986 paper – the possession of some symmetries at the micro level in collision models is sufficient to recover Navier-Stokes equations. In other words, in spite of their discrete character and all their missing symmetries, the properties these models share with exact models of fluids are sufficient to account for the target behavior. Wolfram, in his 1986 paper, provides in addition a general treatment of symmetries within lattice gas models and shows how possession of a certain number of symmetries makes it possible to get the right balances and therefore to recover the right macroscopic tensors describing the fluid. This general treatment thereby shows that the symmetries possessed by the hexagonal model is the minimal group of symmetries, and the FHP the minimal model, to recover Navier-Stokes behavior. For this reason, the FHP model can be described as both theoretical-*c* and theoretical-*j*, even though many of its other properties are not shared by the models that, according to classical mechanics, describe fluids.

At this step, we are in a position to assess the comparative claim that, for a given field, lattice models are doomed to be less fundamental or theoretical than traditional models. Comparative claims are a delicate matter because the fundamental or theoretical character of a model, even within a single field, is by no means one-dimensional: a model may be more phenomenological according to one aspect, although less so according to other aspects. For this reason, we do not have any definite claim to make here. The following remarks can nevertheless be made. It is true that lattice methods do not simulate "fundamental physical constituents" (since the particles in lattice fluids are pseudo-particles and do not purport to faithfully represent real particles). Nevertheless, as we have just shown, the fundamental ingredients that account for the right behavior are not the fundamental objects described by fundamental theories (here particles) but instead more general basic properties, such as symmetries.

It may be further noticed that the traditional, Navier-Stokes-based models are rather high on the fundamentality scale since they describe fluids as homogeneous media characterized by macro-properties. Lattice methods are somewhat below on this scale, as they illustrate a more fundamental perspective in which Boltzmann equation, which is an intermediate "meso-level" step on the way to Navier-Stokes equations, is the focus of theoretical questions[9]. As a consequence, lattice gas methods are more difficult to master[10] because they require physicists to fully understand much of recent statistical mechanics and to develop insights into the significance of basic symmetries (as we noted above) and their consequences at the meso-scale and beyond. This is especially necessary when spurious invariants have to be detected and destroyed (e.g., conservation of the horizontal component of momentum on each horizontal row in FHP) or when consequences of missing symmetries have to be scaled away (e.g., violations of Galilean invariance).

Relying on a careful examination of the senses in which the words "theoretical" and "phenomenological" are used when talking about models, as well as on a detailed comparison between traditional fluid models and lattice fluids, we can now conclude that on the whole, lattice fluids appear to be on the theoretical side, be it absolutely, or comparatively. Equipped with these preliminary conclusions, we now turn to a more general investigation of CA-based models in physics.

4. CA-Based Models in Physics: General Discussion

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[9] This feature of lattice methods undermines Rohrlich' claim that CA-based models are "typically almost devoid of 'unobservable' constructs".

[10] Wolf-Gladrow (2000, p. 245) observes that, whereas one can teach to a beginner how to use the simplest schemes of finite-difference or spectral methods to PDE within a few hours, this seems not possible for LGCA and LBM.

So far, we have focused our discussion of the epistemology of CA-based models on the case of lattice fluids. The question may arise whether lattice fluids are exceptional, or whether they are but one representative example of the potential fruitfulness of the use of CA in physics, despite their apparent oddity. In this section, we further discuss the supposed specificity of CA-based model by examining general objections to the use of CA-based theoretical models in domains of physics that are otherwise investigated by means of well-established theories.

A *prima facie* general (informal) objection against the existence of theoretical CA-based models in physics is the following:

> General Objection (GO): CA do not seem to be appropriate for the kind of physics we are used to, with all its differential equations, real and complex numbers, vector-spaces with infinitely-many dimensions, and above all symbolic calculus.

In order to assess the value of (GO), we first need to give it a more precise form. We discuss different, more precise versions of it in the following subsections.

4.1 About Theories, Models, and How They Are Formulated

(GO) can first be understood as a claim based on the main features of the current practices in the theoretical parts of physics:

> (GO_1) When considering the formal systems and modeling tools that are commonly used in the theoretical parts of physics, it seems hardly possible that CA-based models be able to perform the same tasks.

(GO_1) is based on the current inability to guess how CA could be used in the future. Therefore, it is poorly grounded, for it is easier to assess the capacities of a tool once it has already been used than beforehand. There is an interesting precedent in the history of physics when for a few years, physicists were as puzzled in the face of a new formalism as some are today in the face of CA. When Schrödinger proposed a wave formulation for quantum mechanics using differential equations, it was obvious for no one that his theory was logically equivalent to the matrix mechanics that Heisenberg, Born and Jordan were developing since 1925 and that was a source of puzzlement. Schrödinger's formulation was favored because, among other reasons, it was based on familiar wave equations. By contrast, Heisenberg's formulation was couched in a strange new mathematical language, matrixes, which was at the time seldom used by physicists and considered to belong to the realm of pure mathematics. Not until 1932 was a sound proof of equivalence between the two formulations provided by John von Neumann.

The matrix mechanics example is a good reminder that the content of a physical theory or of a model is not bound to be attached to any particular formulation or formal tool. It can sometimes be expressed and explored by using different mathematical symbolisms, weird though some may look. The example also illustrates that mathematical tools do not wear their potential for physics on their sleeves. Their usefulness usually remains hidden unless they are tamed, their capacities explored, and corresponding know-how skills are developed by theoreticians or modelers. Therefore, CA being unusual mathematical objects, departing from traditional physical models, is little evidence about their theoretical potential.

4.2 About Languages and Formalisms

Let us go into a further stage of our discussion about the specificity of CA-based models and consider their syntactic and structural properties. CA can be viewed in at least three different ways: as language generators[11], as computational devices, and as mathematical structures. As a result, the above objection (GO) may be construed in further different ways, for languages, computational devices and mathematical structures do not play the same roles in scientific practice:

> (GO_2) CA and their associated languages are *in principle* too poor to represent or investigate theoretical features of phenomena either as language generators or as computational devices.

Under this construal, (GO) can be given *in principle* answers that are supported by computer science results. As a matter of fact, some CA rules have considerable computational capacities[12]. Some of them are Turing complete, *i.e.,* capable of universal computation, meaning that they can simulate any Turing machine and therefore generate and recognize all recursively enumerable languages[13]. For instance, particular Turing machines have been built up within the Game of Life (an intensively investigated CA) as well as, subsequently, universal Turing machines (Rendell, 2001). In the latter case, given the description of a Turing machine and its initial input, both appropriately coded within the initial configuration, the Game of Life can simulate the corresponding computation[14].

The fact that some CA can be Turing complete testifies that they can provide us with symbolic systems (resp. computational devices) that may be syntactically as rich as the richest symbolic systems (resp. computational systems) that can be created. Therefore, CA-languages can be syntactically as rich as those that are used in mathematical physics (*e.g.*, the languages of

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[11] CA, like other automata, can be viewed as formal language generating devices. Starting from an initial state, a CA evolves into new states. For a one-dimensional CA, each state is a string of 1 and 0. Each sub-string can be seen as a word and the succession of states can therefore be seen as the generation of a language (see Ilachinsky, 2001, 291-323 for an introduction).

[12] A usual strategy to demonstrate the computational power of a model *A* is to show that it can simulate another model *B* (e.g., a Boolean circuit, another CA, etc.) whose computational power is already known. For example, it can be shown that the Circuit Value Problem (given a description of a Boolean circuit having AND, OR and NOT gates as nodes and given the truth-values of the circuit input, find whether its output is true) can be reduced to such or such particular CA model (Squier and Steiglitz, 1993, Moore and Nordhal, 1997). A straightforward way to prove the reduction is to show that the basic logical components (wires, gates, clocks, etc.) and signals within *B* can be embedded within *A* by starting the automaton in an appropriate state so that the future state of a chosen site corresponds to the output of the target circuit. Therefore, for each finite Boolean circuit, it is possible to find a corresponding CA that does the same computation. As a consequence, these CA, fed with the appropriate configurations, can compute the values of the functions that are otherwise computed by Boolean circuits. And as is well-known, Boolean circuits are powerful computational tools since any deterministic Turing machine computation of length t can be converted into a Boolean circuit of depth $O(t)$.

[13] For the sake of precision, we emphasize that in order to describe the computational power of Boolean circuits or CA, it is required to refer to infinite collections or *families* of particular Boolean circuits and CA. A circuit transforming n inputs into m outputs is a finite object, which can only compute a function from binary strings of length n to binary strings of length m. The notion of a circuit can however be generalized so that families of circuits can be said to compute functions on strings of arbitrary length. In the simple case in which the output for function f: $\{0,1\}^* \rightarrow \{0,1\}^*$ has the same length $m(n)$ for all inputs of size n, one circuit α_n can compute f for all inputs of size n, that is to say the partial function f_n: $\{0,1\}^n \rightarrow \{0,1\}^{m(n)}$. Consequently, the function f can be said to be computed by the sequence $\{\alpha_n\}$ of circuits α_n. See (Greenlaw et al., 1995, §2.3) for more details.

[14] Note that there are still slight differences between universal Turing machine and these Game of Life constructs. For example, CA, by definition, do not have halting states. Second, in Turing machines, all but finite portions of the tape are blank at the beginning of a computation, whereas a CA may require an infinite pattern as initial condition.

matrixes or differential equations); in the same way, any computation that can be made within mathematical physics can in principle be made by means of CA. Briefly said, all that can be expressed or computed by means of the usual mathematical formalisms can *in principle* be expressed or computed by CA, even if this may involve intricate constructions.

The rebuttal we just gave to (GO_2) calls for several remarks:

(*i*) It does not imply, of course, that any aspect of the behavior of any physical system can be described and explained by means of a CA. In point of fact, it has been shown that, within the class of models that are described by current physical theories, some have a temporal evolution that cannot be computed by a Turing machine. For instance, Smith (2006) establishes that it is possible to describe a classical system by means of differential equations that cannot be simulated by a Turing machine. As a consequence, Turing completeness is perhaps not the right kind of expressive power to consider in order to describe the richness of the behavior of all physical systems. But the computational equivalence between CA and Turing machines shows that even if some physical systems are more powerful than universal computing systems (like CA), then they will also be too powerful to be studied by means of more traditional mathematical formalisms - in particular, the ones used in standard theories and models.

(*ii*) Computational constraints, measuring the easiness with which some goals are reached, are not taken into account in what we have just said, whereas, in practice, they usually turn out to be crucial. So the above equivalences do not imply that actual, efficient CA-based models can be built up in every case. Still, our purpose is not to make such a radical claim, but more modestly to rebut the general, in-principle objection (GO_2) about the capacities of CA.

(*iii*) Syntactic richness, on which we base our rebuttal, is not all what there is to the usefulness of scientific languages, which may possess additional properties (*e.g*., semantic or heuristic) that facilitate scientific investigation. CA may not possess these additional properties; in particular, they may receive a poor score with respect to easiness of interpretation and of inter-theoretical comparison with results couched in different formalisms.

Overall, what we have said above about the syntactic and computational richness of CA does not imply that there exists any practical way to turn CA into a human-friendly, versatile and tractable scientific formalism. However, it would be unreasonable to claim beforehand that no CA-rule will be found in the future that is practically appropriate for answering *some* types of questions or study some types of situations in physics. In short, even though syntactic richness does not imply practical usefulness per se, it nevertheless shows the absence of an important limiting factor. In the same way, Turing machines, lambda-calculus and recursive function theory are syntactically, but not practically, equivalent: depending on the investigated question, recursive function theory, say, is usable, whereas lambda-calculus is not.

We shall not discuss at length the possible pragmatic virtues of CA in this paper but wish to emphasize the following points. First, in order to assess the theoretical potential of CA as a usable mathematical formalism for physics, we need to recall that scientific theorizing is by no means limited to the formal exploration of the content of theories, taken as wholes, but also covers the development of particular models, or of particular aspects of some models. Even though CA do not seem appropriate for the first task (for instance, they are hardly suitable to derive Heisenberg relations from the principles of quantum mechanics), they may be efficient in fulfilling the second. At least, nothing precludes them to be so.

More generally, mathematical formalisms, even when they are appropriate to present a theory, never give full access to its whole content: usually, multiple formalisms are used to investigate its different aspects and its different models. Therefore, even if CA are unlikely to provide physicists with an easy access to the whole content of any physical theory, they may still be used, as languages or computational devices, to investigate some aspects of some theoretical models. Lattice fluids are a nice example of the second point. Let us briefly give another, complementary example. Classical Billiard Ball Models (BBM) correspond to a class of models of classical mechanics. Some of them (or, better, series of snapshots of BBM taken at regular intervals) can be given a CA-based description and become "BBMCA" (Margolus, 1984). Due to this new formalization, these classical-mechanical models enter the realm of theoretical computer science, and by this means, entirely new theoretical results can be proved about them (when BBMCA are embedded in BBM): for instance, undecidability properties (Wolfram, 1985) or the complexity of the answer to some questions (Vatan, 1988) can be proven.

Be it enough to acknowledge that CA do not presently compete with the traditional, versatile, and human-friendly formalisms currently used in physics, like PDEs, and that they will perhaps never will. However, even though they are not as versatile and efficient as PDEs, they do not play in physics the limited, purely phenomenological role that Rohrlich and Keller ascribe to them. In section 5, we come back to these themes and emphasize that CA may present some advantages as formal tools that more traditional methods do not possess.

4.3 CA as Models of Their Own and the Relationship Between Models and Theories

In section 4.2, we have described potential (and actual) uses of CA as language generators and computational devices. CA can also be used as mathematical structures providing models (this was the very perspective of our case-study). As such, they can represent target physical systems and be studied for themselves as any other mathematical structure used in the same way. For example, the evolution of a CA can be sampled, averaged, submitted to statistical analysis, etc.

Nevertheless, as CA are discrete mathematical objects, legitimate doubts can be raised about their capacity to provide sufficiently rich mathematical structures to represent and study all aspects of all the systems described by currently available physical theories. Hughes thus writes: "I have no doubt that physical systems exist that decline to be squeezed into straight jackets, systems for example, whose dynamics depend crucially on the continuity, or at least the density, of the time series. For such a system a cellular automaton would not offer a reliable representation" (1999, 136). Hughes's general pessimism is comforted by his description of the failure of CA-based investigations of the Ising model. In his paper, Hughes makes a detailed analysis of this failure. In the following, we propose our own analysis of the Ising-model-case in order to assess the potential of CA to provide models for physics.

The Ising model is perhaps the best-known example of a discrete model of a set of continuous phenomena, enjoying a prominent place in statistical physics. Expectedly, at the beginning of the 1980s, great hopes were placed in CA as heuristic tools for the investigation of Ising-like models. Indeed, CA seemed particularly appropriate to develop models already involving a regular lattice structure and local dynamic rules, such as models of percolation, nucleation, condensation, etc., as well as the Ising model. For these reasons, ongoing attempts to use CA for studying Ising-like models were considered as a test-case for the fruitfulness of CA in physics. Unfortunately, it turned out that the task was not so simple: in spite of a striking resemblance between CA and the Ising model, it was shown that there is no obvious (topology conserving) simulation of the wandering of Ising configurations through the canonical ensemble with a simultaneous updating of all the spins at each interaction (Vichniac 1984, p. 101).

Hughes, relying on the failure of CA in a test-case that seemed favorable, concludes his 1999 paper with the following skeptical note about the representational capacities of CA: "Amidst all this enthusiasm, far be it from me to play the role of the designated mourner. But, as the example of the Ising models shows, a word of caution is called for. […] The constraints that prepared descriptions of physical system must conform to before they become eligible for modeling by cellular automata are severe " (the end of the passage is quoted above; 1999, p. 136). Hughes is certainly right in emphasizing that the use of CA as modeling tools is submitted to severe constraints – however, this is usually true for other modeling tools as well. Nevertheless, the story does not end here. After further and deeper investigations, the existence of a fundamental non-topology-conserving relationship between *d*-dimensional probabilistic CA (PCA) and (*d*+1)-dimensional Ising spin models was demonstrated (see Ilachinsky 2001, p. 343-369 for a review; Domany and Kinzel 1984; Georges and Doussal 1989 for the original articles). So the apparent failure of CA relative to the Ising case, which nurtures Hughes' 1999 skepticism, was in fact, as early as 1989, a *success* for CA-based investigations. When considered carefully, the Ising case does not turn out to be a philosophically decisive negative example.

If this precedent teaches anything, it is probably that CA can be usefully connected with some physical models, even if these connections are not as straightforward as physicists hoped them to be in the 1980s. In the Ising case, we do indeed possess a mathematical justification of the phenomenological success of the CA-based model, which is much more than an informal piece of evidence based on an apparent similarity of behavior: Ising-CA-models are weakly theoretical-*j*, even though they do not seem to be theoretical-*c*[15], contrary to lattice fluids, because they cannot provide any theory-based explanation of how Ising systems behave.

Overall, the Ising example and the lattice-fluid conjointly make up a less pessimistic and more balanced picture of the potential role of CA as possible (but not all-purpose) modeling tools in physics than appears in Hughes' paper. Further, both the Ising-CA-model and lattice fluids illustrate the claim that the theoretical potential of any mathematical model (or a formalism) is usually hidden. In both cases (Ising-CA-model and lattice fluids), the apparent properties of CA (as mathematical structures) and of the target systems do not match, but relying on deeper properties (like symmetries) allows one to exhibit common behaviors and provide physicists with theoretical understanding. From this perspective, far from exemplifying any revolutionary modeling practice, lattice fluids are rather representative of theory-induced modeling as it is usually practiced in physics. Basic theoretical properties of the investigated system are selected (namely, local conservation laws and symmetries); a representational strategy is designed to put these properties into a coherent representational framework and the results of the computational process are checked against what is already known about the system from the available theories (namely, that it obeys Navier-Stokes equations). In particular, it is not required, in order to achieve a good theory-induced model, to exactly represent *every* aspect of the studied system. In lattice fluids, one deliberately neglects microscopic features that play an important role in other modeling strategies, like continuity of motion of the particles. Neglecting properties or deliberately including some inexact properties can be instrumental in bringing about understanding because it provides clues about which original properties of the exact model are crucial to obtain some target behavior. From this point of view, the use of lattice fluids enhances our understanding of out-of-equilibrium fluids

[15] It cannot be excluded that further investigations show that Ising models and these CA-models share some more abstract properties in virtue of which they exhibit the same Ising-like behavior. It is for lack of such results that these CA-models can only be said to be weakly theoretical-*j*.

because they clearly indicate which microproperties of fluids are decisive to obtain the correct out-of-equilibrium dynamics[16].

5. LGCA (and LBM) Improve Our Scientific Performance

In section 3, we have argued that lattice fluids, far from being always purely phenomenological, are theoretical-*j*: the justification of their success is known to be grounded in the relevant theories. In section 4, we have given some general arguments explaining why it is hasty to conclude that CA cannot be used in physics for theoretical purposes. All the arguments given so far were "in principle" in the sense that we paid no attention to the practical advantages that CA could bring about or to the cognitive or computational cost of their use.

However, from the physicists' point of view, these in principle arguments may not be enough for accepting CA-based models as *bona fide* models, to work with on an everyday basis. For instance, as we emphasized in section 3.2, their physical interpretation is sometimes difficult, and it is hard to conceive how they could turn into a human friendly formalism that could be appropriate for the presentation and exploration of theories, in the same way as PDEs are. As they lack some of these general practical properties, they have to meet other requirements in order to be qualified as usable models. For example, their computational cost has to remain reasonable. Besides, they should not introduce superfluous intricacies because of their peculiar geometry. Do they meet these requirements? In other words, do they bring about scientific benefits that cannot be drawn from other models and that are accessible *in practice*? YES, as we shall argue in this section.

It is true that LGCA turned out to be hard to tame, and unpleasant surprises are still not uncommon when investigating their properties. Nevertheless, the study of lattice models is still expanding. They have been both calibrated by reference to many already known situations (Hasslacher, 1987) and progressively used independently in new situations (Doolen, ed. 1991; Rothman and Zaleski 1997; Succi 2001; Wolf-Gladrow 2000). Further, lattice methods are often more successful in modeling complex situations for which traditional computing techniques are not applicable: flows in porous media, immiscible flows and instabilities, microemulsion erosion and transport problems. Lattice methods also happen to be advantageous when complex boundary conditions are present. Due to the microscopic interpretation of the dynamics, these conditions can be taken into account in a much more natural way than in a continuous description (Choppard and Droz 1998, p. 7).

A closer look at some of the advantages of LGCA over finite difference methods helps understand why fluid dynamic studies based on LGCA have developed in the last two decades.

(1) A lattice gas is computationally stable, contrary to classical simulating programs, in which the code may stop running because the algorithm becomes unstable.

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[16] This point has already been emphasized by Batterman (2000, 2002a, 2002b) with respect to the understanding of well-known examples in universal physics such as critical exponents or properties of self-similarity of asymptotic states. Our example is another illustration of the fact that details may not matter in the very micro dynamics of a system. However, the reasons why details do not matter may be different in different situations. Therefore, a careful analysis of the physics involved is needed in each case. In our example, it would be nice to have a general theorem indicating that if such and such symmetries and invariances obtain, then the macrodynamics will converge towards Navier-Stokes equations. Such a theorem is not available yet; consequently, the physical analysis has to be made anew and the asymptotics calculated in each case. An analysis of LGCA in terms of renormalization group methods (RGM) would also be welcome. But in spite of scientists' efforts, RGM have not proved very useful so far on the way from LGCA to Navier-Stokes equations, even if they are used here and there, just like in fluid dynamics studies, to derive (or re-derive) such or such coefficients in an equation.

(2) In a lattice gas, momentum and energy are *exactly* conserved since no round off operations of any kind are carried out. (This is true only for LGCA, not for LBM in which some averages are computed). This eliminates a usual worry related to finite-difference simulations, in which, when integrating over long-time scales, “a small leakage would transform an ocean into an empty basin” after some time (Wolf-Gladrow, 2000, p. 11).

(3) Memory is used more efficiently than in classical computer simulation, since every single bit of memory is used equally effectively and codes for the presence or absence of a particle in a cell of the lattice (this is called “bit-democracy”). Only six bits of information are necessary to completely specify the state of a cell. On the other hand, in classical computer simulations, every number requires 64 bits.

(4) Boundary conditions are easy to implement (see above); this is an important aspect of these models' flexibility.

(5) As the required spatial and/or temporal averaging produces unavoidable noise, it is likely that emerging similarities are fairly robust.

(6) LGCA are well-adapted to parallel computation.

Overall, CA based models turn out to meet scientific success and fare better than PDEs in certain cases both from a theoretical point of view and from a practical point of view (present section). Presently, the choice between lattice fluids and more traditional types of investigation depends on the advantages attributed to either possibilities and is relative to one's scientific aim. In some cases, lattice fluids are assessed to fare better than other methods even if in other cases, they do not. In other words, they do improve our scientific performance and can compete with more traditional methods, although it is unlikely that they will outcompete them in the future (Succi, 2001, pp. 40-65). It also has to be recalled that the intensive investigation of finite-difference methods and computational schemes are only a few decades old and are themselves still under development. As noted by Wolf-Gladrow (2000, p. 246), the joint application of a wide variety of methods to find out numerical solutions to PDEs or explore the dynamics of physical systems indicates that for the moment, there does not exist a best scheme for this general task. The situation of coexistence of lattice fluids and finite difference methods is one of (mathematically justifiable) complementary pluralism, in which different methods have their own niches, and which allows for a highly desirable possibility, namely that of cross-comparisons.

It should finally be noted that these practical successes have not always been the expected ones: CA-based models for fluids became famous in the mid 1980s when it was predicted that they would be so much faster and simpler than other methods and this is why this new method was considered for classification because of its supposed decisive advantage in hydrodynamic simulation capability and therefore in military power (Pomeau, 2007). We indicated above that the theoretical potential of models or formalisms is usually hidden. The present case also illustrates that their *practical* potential is also far from being transparent.

5. Conclusion

Our aim in this paper was to critically assess the scientific novelty of CA-based models and analyze by this means how the invention and introduction of new mathematical tools may or may not be connected with radically new aspects of modeling. We have grounded our investigation into the lattice fluid case, which we have briefly presented in section 2. We have then critically discussed Rohrlich' and Keller's views about CA-based models in section 3 and emphasized that their claims about the phenomenological character of CA-based models and about the relationships between these models and physical theories are ill-grounded. We have distinguished different senses of the predicates "phenomenological" and "theoretical" and have argued that, at least in fluid dynamics, CA-based models can be theoretically well-grounded; from this perspective, they are not so different from more traditional and theory-based models relying on differential equations and finite difference methods. In section 4, we have further presented some general insights about the potential fecundity of CA-based models in physics. We have tried to separate aspects of modeling that are usually not sufficiently distinguished: theoretical language and formalism, mathematical properties of the models, and the relationship between theories and models. In order to make clearer how CA-based models of fluids can be just as theoretical as traditional PDE-based models, we have confronted this case to specific episodes in the history of physics: the emergence of matrix mechanics and the CA-based investigation of the Ising model. Finally, in section 5, we have emphasized that the development of lattice fluids as a subfield of fluid dynamics confirms that CA, both as models, languages providers and computational devices are *in practice* scientifically useful: the development of these new methods, even if theoretically conservative from the point of view of physics, gave birth to new questions and insights in theoretical physics, independent practices and domains of application. Overall, the conclusions we draw from these comparisons disagree with Rohrlich', Keller's, and Hughes' claims. When evaluating the nature of scientific practices, their specificity and novelty and the relations between them, philosophers should be careful that modeling practices are multi-dimensional entities and that practices that are radically different if not weird in terms of the formalisms and mathematical structures employed may share with more traditional ones a common theoretical core. Theoretical practices are not tied with some unique types of models and conversely mathematical structures do not wear their theoretical potential on their sleeves.

This does not amount to saying that the differences between CA-based models and more traditional models should be cut down or even neglected; nor does it imply that they can compete with other more traditional models on all scientific respects. However, claiming that lattice fluids are of a different kind (or purely phenomenological) is a way to miss much of their philosophical interest. It is precisely because they are at the same time so different and so conservative while fulfilling the traditional functions ascribed to other theoretical models like representing, predicting, or exploring aspects of theories, that, from a philosophical point of view, they are worth analyzing and can be informative about what is involved in theoretical modeling.

We finally emphasized that the theoretical character and practical potential of CA were not anticipated beforehand. CA, probably like most untamed mathematical formalisms usable in physics, are rather opaque tools both with respect to their theoretical uses and to their practical advantages. From this point of view, it is not surprising that they were for a great part mistakenly received and described both by physicists and philosophers.

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