Cellular Automata in Complex Matter

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Complex matter may take various forms from granular matter, soft matter, fluid-fluid, or solid-fluid mixtures to compact heterogeneous material. Cellular automata models make a suitable and powerful tool for catching the influence of the microscopic scale in the macroscopic behavior of these complex systems. Rather than a survey, this paper attempts to bring out the main concepts underlying these models. A taxonomy is presented with four general types proposed: sandpile, lattice-gas, lattice-grain, and hybrid models. A discussion follows with general questions; namely, grain-size, synchronization, topology and scalability, and consistency of the models.

1. Introduction

Complex matter may take various forms from granular matter, soft matter, fluid-fluid, or solid-fluid mixtures to compact heterogeneous material. Complex matter involves a diversity of dynamical processes including sandpile equilibrium or avalanches, mixing, stratification or segregation, various flow patterns in silos, emulsion or sedimentation in multiphase suspensions, miscible or immiscible flows in porous media, and so forth. Long-range propagative phenomena may include the void propagation in a porous medium, the force transmission in a granular packing, the progression of wave fronts in active media, or the evolution of a fissuration at the onset of a defect in a compact material. Various aspects of critical phenomena are encountered in the behavior of complex matter. Some transition examples are liquid/solid transitions, from free flow to arching effects in hoppers, mixed/unmixed transitions of bidisperse mixtures, laminar to turbulent evolution in fluid flows, or instabilities near percolation thresholds. It stands to reason that a thorough investigation of the behavior of complex matter is therefore of major importance for industrial and scientific applications.

The theoretical methods currently used to tackle these problems can be split into the three distinct levels of continuum models, particle

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dynamics, and cellular automata (CAs). CAs make suitable and powerful tools for catching the influence of the microscopic scale in the macroscopic behavior of complex systems. In short, a cellular automaton (CA) network is a spacetime discretization of time into steps and space into interconnected cells. The cells take on integer values and the time evolution is governed by a transition function that updates the new state of the cells synchronously from the current state of their local neighborhood. A CA can be one- or multi-dimensional. In the simplest case, one-dimensional elementary cellular automata (ECAs) are constructed from the binary-valued ($k = 2$) transition rule acting from nearest-neighbors ($r = 1$). Following Wolfram, there exist 256 possible transitions denoted by their rule number [1]. Even with this minimal definition, very complex dynamics may be revealed in the spacetime diagram, depending on the random initial configuration. Starting from the fact that complex matter may behave like a *particulate* system, a CA for complex matter (CACM) can be viewed as an extreme simplification of particle dynamics. A frequent misreading about CACM tells that they would be nothing more than ersatz or succedanea used as a substitute for unduly time-consuming computational methods and that they will be dumped soon because of the future generation teraflops computers. But, observing that primitive CA rules are able to capture the essence of complex behaviors readily leads to refuting this erroneous statement. According to Toffoli's "*rather than*" paradigm, CAs are the outstanding alternative to finding the ordinary (ODE) or partial (PDE) differential equation of a phenomenon in complex matter [2].

Rather than a survey, this paper will attempt to bring out the main concepts underlying CACM models and give insights for future work. None whatsoever of our own outcomes are presented herein, but a taxonomy as a proposal intended to tidy up the broad world of CACM. The paper is organized as follows. The CACM set is divided into four sections. The first is the sandpile models underlying the universal concept of self-organized criticality. The second section consists of the lattice-gas models and why they evolved from pure lattice-gas, to lattice-Boltzmann, and then to extended lattice-Boltzmann models. The third section is the lattice-grain models in their miscellaneous aspects, including the related traffic flow model that is beyond our scope of study. The final section is a unified subset of hybrid models including a neural approach in reaction/diffusion, an environment dealing with the rheology of composite pastes, and movable CAs. A discussion is proposed about general questions related to CAs; namely, grain-size, synchronization, topology and scalability, and consistency of the models. We focus on models and applications, not on CACM architectures. For this reason and except in specific cases, such names as von Neumann, Ulam, Burks, Margolus, Vichniac, Clouqueur, Adamatsky, Latkin, Yepez, and other pioneers not forgot-

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ten will neither be referenced nor mentioned. This work is an extension of a previous study related to parallel computing technologies and presented elsewhere [3].

2. Sandpile Models

This section may show how a universal concept of self-organized criticality (SOC) can arise from a simple sandpile model when a flow of grains is poured on the top.

2.1 Self-Organized Criticality in the Sandpile

The primary sandpile model is the "BTW" CA of Bak, Tang, and Wiesenfeld [4], where a one-dimensional CA simulates a two-dimensional heap. At each time step, a cell n contains an integer z_n that denotes the height difference (or local slope) between two neighboring sites. The process is symmetric so only the right-hand side is considered. Adding a grain is accomplished by an elementary operation. Whenever a critical state $z_n > z_c$ is reached, where z_c is a user-defined local critical slope, then grains fall. As a matter of fact, the transition that yields the new state of cell n from its current state and the current state of its left and right neighbors follows a simple but nonlinear (because of the threshold condition) discretized diffusion equation. Although this rule is really plain, the model exhibits complex phenomena at the macroscopic level, introducing the concept of SOC [5]: the angle of equilibrium of the heap is noised by multiscale fluctuations, which can lead to avalanches of various intensities. Rules of two-dimensional CAs for three-dimensional heaps acting on square cells were also defined by the authors.

According to Kadanoff et al. [6], the process is shown to be self-similar with scale invariance. Since the sandpile algorithm acts on systems of finite size, and in order to understand how this fact affects the system behavior, the techniques of finite-size scaling (borrowed from Wilson's renormalization procedure) and of multifractal analysis are used to extract the power-laws and critical exponents that govern the sizes and frequencies of avalanches.

2.2 Stratification and Segregation in a Binary Sandpile

The sandpile paradigm is applied by Makse et al. [7, 8] to granular mixtures of two different species where four different generalized angles of repose can coexist. The angle of repose depends on the size of (small or large) rolling grains and on the aspect of their (rough or smooth) surface. At each time step, a set of grains of two different species is poured onto the top of the pile. Two macroscopic phenomena are observed: either a stratification of a mixture of large rough grains and small smooth grains, or a complete segregation of a mix-

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ture of small rough grains and large smooth grains. Moreover, the stratification displays the formation of a two-layered kink moving uphill at constant velocity whereas the segregation shows a clear bipartition separated by a thin mixed barrier.

The twofold dynamics are confirmed experimentally, and theoretically, using the recent "BCRE" continuum formalism introduced first by Mehta, and by Bouchaud et al. for a single species sandpile, then extended by Boutreux and de Gennes (BdG) to bidisperse mixtures. The resulting set of "convective/diffusion" equations that governs the interface between the "fluid" surface and the underlying "solid" bulk is argued to include the essential features of the physics of granular flow (see [8] and references therein).

2.3 Self-Organization and Stratigraphy in Aerolian Sand Ripples

A well-known self-organized process derived from sandpile dynamics and commonly found in sand deserts, atop dunes, or sandy beaches is the metamorphosis of a flat sandy surface into a periodic rippled pattern due to the action of an external force, from wind or water. This process can be explained by the combination of two types of sand grain movement: saltation and reptation. If we restrict ourselves to the aerolian case, saltating grains fly above the bed and strike the surface while reptating grains are ejected out of their bed under the impact, and creep forward. Similar artifacts are also observed during surface erosion via ion-sputtering in amorphous materials.

The first self-organized CA approach for the analysis of sand ripples is the "worm" model (whose creeping metaphor is easy to imagine on a rippled surface) of Haff and others [9–11]: the time evolution is governed by the advancement of a worm's head incrementing its size and simultaneously decrementing the size of the worm in front. Since short worms run faster than long ones, a merging of two successive worms should occur. Werner and Gillespie focus on average size and standard deviation resulting from random fluctuations of the worm's size: the evolution of the system is a Markov process whose analysis follows a mean-field approximation.

A quite different approach is the "NO" CA of Nishimori and Ouchi [12] that maps an explicit linear, continuous saltation/reptation process onto a two-dimensional lattice wherein the saltation length depends on the local slope and the reptation follows a two-dimensional diffusion equation. Whenever the wind force exceeds a critical value, ripple patterns spontaneously appear. Besides, Barchan dune-like patterns are yielded by a large-scale model that affects the saltation procedure. The drawback of the NO CA is that the growth of a ripple's height is unbounded since it is linear in time. Hence, it is not self-organized and ripples may become infinitely high. The approach was recently improved by the saltation-creep-avalanche (SCA) model of Caps and Vandewalle [13] who reintroduced the angle of repose into the system.

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Anderson and Bunas [11] focus on the stratigraphy carried out by a binary mixture but the relevant result of Makse [14], whose BCRE-BdG formalism again takes into account the interactions within the fluid-solid interface, leads to realistic morphologies of either inverse-graded or normal-graded lamination or cross-stratification depending on the size and shape of the grains.

2.4 Self-Organized Criticality in Natural Hazards

The unified concept of SOC was applied to earthquakes by Bak and Tang [15] as a consequence of Earth's crust being in a self-organized critical state. A simple CA "stick-slip" model yields two- and three-dimensional exponents as a prediction for the Gutenberg–Richter power-law distribution for energy released at earthquakes. Their pioneering work gave rise to a broad research field in geophysics. A simplification of the so-called stick-slip motion of the Burridge–Knopoff slider-block is the one-dimensional CA of Nakanishi [16], which shows behavior similar to the Carlson–Langer formalism describing the Newtonian equations of motion by coupled ODEs. In the two-dimensional "OFC" CA of Olami et al. [17], a nonconservative, quasistatic rule yields a dynamical phase transition from localized to nonlocalized effects. By observing that a short-range interaction, where energy is only transferred to the nearest-neighbors of a triggered cell, may lead to nonphysical stress distributions, Weatherley et al. [18] defined a new type of CA with long-range energy transfer. In the same way, the CA of Castellaro and Mulargia [19] includes effects due to the transient loads of elastic waves. They observed that a loading rate acts on a larger time scale than that of fracture propagation, which is assumed to be comparatively instantaneous.

Landslides are commonly caused by a trigger such as an earthquake, a downpour, or a sudden snow melt. Their study also gave rise to various approaches of sandpile-type CAs in order to extract the critical exponents of their power-law behavior. Most of the authors have calibrated their theoretical results from thorough inventories of topographic databases to forecast the risk conditions of real events: debris-flows [20–22] or snow avalanches [23]. More theoretically, the SOC of the landslide model of Hergarten and Neugebauer [24] is implicitly based on a set of PDEs that includes the aspects of slope stability and mass movement. Recently, the CA of Piegari et al. [25], which is claimed to be at the edge of the SOC limit, is a dissipative, anisotropic version of the OFC CA including a space-time dependent factor of safety derived from the stability criterion of Terzaghi.

It should be noted that an earthquake has nothing to do with a pile of sand, except for its self-organized behavior, which emphasizes the universal character of SOC. Turcotte and Malamud [26] propose an inverse-cascade model of metastable clusters as a general explanation for the power-law frequency-size statistics produced by these self-organized CA and their associated natural hazards which may lie far beyond our scope of complex matter.

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3. Lattice-Gas Models

Owing to the copious amount of literature about lattice-gas models and to the wide diversity of their application fields spreading from hydrodynamics of homogeneous or multicomponent fluid flows, thermohydrodynamics, magnetohydrodynamics to particle suspensions, soft matter, reaction/diffusion processes, crystallization or growth processes, and even to other areas observed in some granular systems which may be related to other types of CACM that are tackled in subsequent sections of this paper, we refer the reader for more general questions to the monographs of Rothman and Zaleski [27], Chopard and Droz [28], Wolf-Gladrow [29], and to some recent reviews on the subject (Boghosian [30], Luo [31], and Chopard et al. [32]).

3.1 Historicity of Lattice-Gas Cellular Automata

An important class of CACM includes all lattice-gas automata (LGAs), applied first to hydrodynamics. A fluid "particle" is a large group of molecules. The first discrete velocity model comes from Broadwell [33] nearly 10 years before the "HPP" gas of Hardy, Pomeau, and de Pazzis [34], wherein a two-stage transition follows a collision-propagation scheme (the term "collision-advection" is now preferred to avoid confusion with long-range propagative interactions). In the input step of the collision, two particles can collide on a site of a square lattice. The output step starts the advection, where density (namely the number of particles), momentum, and energy are conserved at each site. Upon completion of the advection stage, particles have moved to their nearest-neighbor site. According to the now popular DnQm terminology where n denotes the dimension of the lattice and m the number of velocity directions incident to a site, the HPP gas will be said to follow a D2Q4 scheme.

Some analogy is often observed between the Ising spin model [35] (seldom called Lenz–Ising [36]) and the LGA. Whereas a lattice-gas site may be either occupied or empty, a spin in the Ising lattice may be either up or down. The Ising model applies to various phenomena wherein collective effects are produced by local interactions between two-state particles. Ferromagnetism is a typical case, and so are binary alloys or liquid/gas transitions. The correspondence between density ($n = 0, 1$) in lattice-gas and spin direction ($s = \pm 1$) in the Ising lattice is simply given by the variable transformation $n = (s + 1)/2$.

3.2 Pure Lattice-Gas Models

After the HPP, the "FHP" model of Frisch, Hasslacher, and Pomeau [37] deals with a D2Q6 hexagonal lattice where up to three particles can collide. It was shown by the authors that the HPP LGA could not be consistent with the Navier–Stokes equation while the FHP symmetries ensure consistency. The evolution equation of the FHP can be av-

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eraged from Boltzmann's molecular chaos approximation and expanded in a Taylor series up to the second order. The equilibrium state follows a Fermi–Dirac distribution from which a Chapman–Enskog analysis yields the hydrodynamic equations of the FHP, but under the condition of a low Mach number, that is, small velocities. For more details, the reader is also referred to Wolfram, who produced at the same time a LGA for fluids [38], and Doolen [39].

An extended FHP model [40] includes all possible conservative collisions, with up to a seven-velocity D2Q7 template (one particle may stay at rest). From this model, a three-dimensional gas may handle three-dimensional problems on a cubic grid with a D3Q15 template (six neighboring nodes sharing a surface, eight neighbors sharing a corner) or with up to a D3Q27 template (by adding the 12 neighbors sharing an edge).

An important feature of LGAs is their capability of handling complicated geometries and boundary conditions: slip, no-slip, or partial slip conditions are easily carried out by reflection, bounce-back, or by a combination of both schemes for particle/wall as well as particle/particle interactions. Therefore, LGAs have proved their efficiency with various applications in hydrodynamics: miscible or immiscible fluids or flow through porous media (as in Rothman [41], Rothman and Keller [42], Stockman et al. [43, 44]) are some relevant examples where classical computational methods may fail or involve extra difficulty to model.

3.3 Lattice-Boltzmann Models

Nevertheless, pure LGAs have some shortcomings that appear through the mentioned analytical transformation of the evolution equation. That is, statistical noise, lack of Galilean invariance, spurious nonphysical quantities resulting from the symmetries of the network and, at least in the three-dimensional case, huge collision matrices or look up tables. Indeed, some of them can be overcome: for example, the noisy effect may be shortened by averaging the results of simulation in space and time or by running a lot of samples with different seeds for their random sequence. But the best way seems to average the microdynamics before rather than after a simulation, whence the intrinsic specificity of lattice-Boltzmann (LB) models.

In LB models, the evolution equation no longer contains the Boolean motion of actual particles. It does contain a real-valued probability of presence, namely, the single distribution function. McNamara and Zanetti [45] introduced the Bhatnagar–Gross–Krook (BGK) approximation [46], an ODE that equalizes the Lagrangian derivative of the distribution along the local velocities with the difference between the Maxwell–Boltzmann equilibrium distribution and a single distribution, normalized by a relaxation time due to collisions. The moments should ensure the conservation of density, momentum, and energy. The BGK equation yields the evolution equation, again

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expanded in a Taylor series up to the second order, from which a Gaussian-type quadrature yields the hydrodynamic Navier–Stokes equation. It should be pointed out that the collision operator is now linearized [47–49].

To prevent inconsistency due to insufficient symmetries in the HPP grid, the given development dealt with a D2Q9 template. Similar developments may be derived from the FHP templates D2Q7, D3Q15, or D3Q27 [50] depending on the symmetry required. More details about the theoretical aspects of LB models can be found in Lallemand and Luo [51].

Typical applications of LB models to hydrodynamics show relevant phenomena in fluid flow [52], complex fluids [53], or multicomponent fluids in complicated geometries [54]. We should also mention the problem of particle suspensions, which is difficult to tackle by classical computational methods [55, 56].

3.4 Extended Lattice-Boltzmann Models

The "pure" LB model may suffer from some limitations depending on particular situations. For instance, although LB simulations show a good behavior for laminar flow or slightly turbulent flow, new extensions are needed for turbulent flow at a high Reynolds number. However, knowing that momentum and configuration spaces can be freely discretized from the BGK construction, this property was explored to redefine arbitrary mesh grids for a significant increase of the Reynolds number [57–60]. The LB equation turns into a discretized Boltzmann equation and the collision-advection into a three-stage collision-advection-interpolation process.

Another weakness of the LB model appears in the situation of compressible flow. Presently, a quite different approach leading to a "gas kinetic scheme" is proposed to simulate shocks of interfaces and high Mach number flows [61]. Besides, a generalized LB model has been carried out to prevent a risk of numerical instability of the constrained BGK approximation and to release the Prandtl number, fixed to unity because of the uniform relaxation time [51, 62].

New extensions of the LB model are likely to appear and will continue to evolve from fine- to coarse-grain in order to tackle new or still unsolved problems, or problems that remain up to now the private area of classical computational fluid dynamics [63, 64].

4. Lattice-Grain Models

The fact that granular media are neither a gas nor a liquid nor a solid or that they can encompass the three phases as a whole likely induced the concept of "lattice-grain" or "granular media lattice-gas" owing to the lack of terminology about this kind of complex matter.

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4.1 Historicity of Lattice-Grain Cellular Automata

Historicity of discrete models of granular flow under gravity may cover a period of 40 years, from the pioneering work of Litwiniszyn about random walk stochastic processes [65, 66] to the emergence of the first "granular" CAs in the 1990s. The Litwiniszyn model is a two-dimensional random walk within a brickwork pattern of "cages" with a stepwise grain/cavity exchange rule acting under gravity and wherein a trough pattern is induced by an output of dry sand through a bottom slot (in short, a silo-like emptying process). In addition, a memory effect that could be likened to an inertial effect allows the cavity to "remember" its left or right direction at the previous step. Later on and in related works, Müllins [67] claims that these problems of granular flow under gravity may be converted to boundary value problems in ordinary diffusion theory. It is also observed that by reversing the emptying process into a memoryless filling process, the Galton picture is recovered, with a simple Gaussian distribution of the heap. Following Litwiniszyn and Müllins, Caram and Hong [68] reintroduce a similar, so-called "diffusing void model" that deals with free surfaces and obstacles.

4.2 Cellular Automata for Granular Flow

Constructed from the preceding terminology, prototypes of CAs or CA-like models applied to granular flow were brought out by Savage [69] and Osinov [70]. The underlying process is proved to follow a Fokker–Planck equation, reducible into a simple diffusion equation in the memoryless case. Furthermore, it is observed that while the model is embedded onto an orthogonal lattice that does not exactly reflect the Litwiniszyn brickwork, this discrepancy only affects the coefficients and not the form in the equation.

Although this model is able to display some realistic patterns like funnel or Couette flows depending on the boundary conditions, it clearly suffers from insufficiency due to the physical limitations in the local interaction law. Some correlative attempts, sometimes with somewhat sophisticated transition rules, were applied to hopper and Couette flows [71] and to the free surface segregation of a binary mixture [72]. In the first case, Gutt and Haff mimic Newton's law of particle dynamics where the gravitational acceleration is simulated by an integer "position offset" and the time evolution undergoes a periodic partial scanning of the cells. In the second case, Fitt and Wilmott adopt a mesoscopic approach where a cell stands for a box containing a volume of small and large particles and with a bottom-up driven time evolution.

A conclusive contribution to lattice-grain CAs is the energetic model of Baxter and Behringer [73] that deals with a hexagonal lattice where an anisotropy of (long) grains is considered. The two-stage transition follows an interaction/collision rule using a criterion of energy minimization. Applied to hoppers, the process displays realistic

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patterns of grain segregation as well as density waves in the flow. The main contribution of our model is the use of crystal-like exclusion rules in a multiphase context [74]. The time evolution in the hexagonal lattice follows a two-stage request/exchange transition rule using a criterion of kinematic exclusion. Realistic patterns may appear in various configurations: mass or funnel flow, density waves, arching effect in hopper processes, and mixing or segregation of a bidisperse medium in rotating drum processes are some examples. It would be fruitful to study both types of granular CAs to find whether there exists an underlying differential scheme to be consistent with the time evolution induced by their transition rule and to try to unify other kinetic, CA-based approaches of granular behavior that are not driven by the Boltzmann equation (see the recent work of Jasti and Higgs [75] and references therein).

4.3 Lattice-Gas Related Models

Modified versions of LGAs are introduced by Peng and Herrmann [76] to reveal the phenomena of density waves formation in granular flow through a vertical pipe under gravity. A power-law distribution of the power spectrum of the density fluctuations shows that interparticle dissipation and roughness of the pipe walls are responsible for the generation of waves, similar to the kinetic waves observed in traffic jams. The basic model is a FHP-gas, but the dissipation (a specific feature of granular media) is simulated in a simple way by additional collision rules. While the FHP-gas must satisfy the principle of single-occupancy, here an off-site collision mechanism is created, where colliding particles may be driven back to their source site during a transient state until equilibrium.

A similar approach is the granular media "GMLG" LGA proposed by Károlyi et al. [77], applied to the study of the friction-induced segregation observed during a silo filling process with a mixture of grains, and which is again an extended FHP-gas. Extra rules are created in order to include energy dissipation through particle collisions and friction: a neat scheme defines one restitution coefficient as the probability of energy conservation and four friction coefficients (since we are in a binary mixture) for moving particles as probabilities of either to scatter or to stop upon advection. Although this model uses the same BdG formalism as in the Makse sandpile [8], it should be emphasized that we deal here with a right FHP extended model [78] and not with a sandpile model.

4.4 Force Chains in Granular Packing

Another model that is in no way related to the BTW sandpile would be a first attempt to tackle the process of force chains forming in a granular packing. As noted by Liu et al. [79], no confusion should be made with the primary BTW sandpile, which is more a concept than a

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bead pack. In all cases, a two-dimensional CA simulates a two-dimensional heap. Liu et al. introduce a probabilistic "q" model, acting on a layered two-dimensional lattice, and assume that the dominant physical mechanism leading to force chains is the inhomogeneity of the packing. It is a random walk process where each particle transmits its weight to exactly one neighbor in the layer below. The network of force distribution is carried out by a mean-field theory approach. The "HHR" sandpile of Hemmingsson, Herrmann, and Roux [80] gives a description of static forces in a granular system. The time evolution, based on a downward row-by-row computation of the force distribution in the triangular lattice, appears to be not fully synchronous. But, the relevant fact is the dip observed under the heap, where the force network displays a depression underneath the apex. The related model of Goles et al. [81] seems to reproduce a variant of the time evolution in the "sandpile" paradigm, while provided with an additional parameter of inertia. Finally, the introduction of force transmission into our kinetic version [74] by a top-down scheme allows the model to take into account the influence of the initial stress state and of the wall roughness in silo flow modeling [82].

This new field focusing on the formation of force networks in granular packing seems to be somewhat immature and would likely open gates for further research. Moreover, as noted by the authors in the HHR CA [80], the downward sequential approach of these models suffers from a lack of Galilean invariance that should somehow be restored.

4.5 Traffic Flow Related Models

A somewhat surprising observation is that granular flow may in some cases behave the same as road traffic flow. Therefore, considering that Bak's sandpile is more a paradigm than a pile of sand, traffic flow theory may help clarify our understanding of the complex behavior of granular matter. Whence this emergence of works with Leibig [83], Kurtze and Hong [84], or Helbing [85] and from [86] to [87] to bridge the gap. The study of road traffic flow is not a recent deal: one-dimensional models fit into single or multilane traffic, whereas two-dimensional models fit into urban traffic. The theory of traffic flow arose with the "car-following" model of Lighthill and Whitham, who state some analogy with the pressure in compressible flow in fluid-dynamics. Although the first single-bit CA was due to Gerlough some decades ago, it was only recently that a lot of "particle hopping models" (including [88–93]) were carried out. See the theory now unified with the "ASEP" and "STCA" models, simple enough to be outlined hereafter, in Nagel [94] and references therein.

Let v ($0 \le v \le v_{\max}$) and $g \ge 0$ be two integers that denote the particle velocity and the gap or number of empty sites ahead. The asymmetric stochastic exclusion process (ASEP) is defined by rules: (r_1)

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pick one particle randomly; (r_2) if $g > 0$ move one site ahead. The one-dimensional synchronous, two-stage, stochastic traffic cellular automaton (STCA) is defined as follows. Interaction: (r_1) $v > g$ (too fast) $\Rightarrow v \leftarrow g$ (slow down); (r_2) $v < g$ (enough headway) $\Rightarrow v \leftarrow v + 1$ (speedup); (r_3) $v > 0 \Rightarrow v \leftarrow v - 1$ (slow down) with probability p. Advection: (r_4) move v sites ahead.

Let us now consider Wolfram's ECA 184 constructed from rule 184 [1]. Observing that ECA 184 is the deterministic limit ($p \to 0$) of the STCA / 1 (where $v_{\max} = 1$) is straightforward. The spacetime diagrams of ECA 184 from single site seeds show a car moving alone with constant velocity. But, from an initial disordered state, the diagrams exhibit complex phenomena with critical points in phase transitions from jams to congestion depending on the flow density. Related works focus on the formation of kink solitons that appear in the physics of traffic jams [84, 95, 96]. The particle hopping models are consistent with the nonlinear diffusion Burgers equation (ECA 184) or the noisy Burgers equation (STCA, ASEP) whereas the density waves are described by the associated Korteweg–de Vries (KdV) equation.

The well-stated similarities between traffic flow and granular flow should then provide a suitable framework to unify the phenomena of density waves produced by the various lattice-grain model approaches [73, 74, 76]. Note also that similar problems exist in computer science, such as when internet traffic is likened to fluid models, or the deadlock event in distributed computing for resource allocation that can readily be likened to a kink front.

5. Hybrid Models

The three following CACM that are related to different species of matter and were not placed in any previous category are gathered here into a unified set of hybrid models.

5.1 Cellular-Neural Models of Reaction/Diffusion

Reaction/diffusion processes, often referred to as "autowave" phenomena [97], arise in various types of active media in complex matter. The first CA approaches to display realistic patterns of crystal-growth forms [98], stripes and streaks [99], Belouzov–Zhabotinski (BZ) or BZ-like rings, spirals [100], turbulence [101], or Liesegang fronts [102] highlight such physical, biological, or chemical examples. More recently, lattice-gas and lattice-Boltzmann theories were successfully applied to those reactive systems in a more unified way: see Boon et al. and Weimar [103, 104] and Chopard et al. [32].

The outcome of Bandman and Pudov's works is a hybrid, special-purpose "CA-CNN" system devoted to the study of reaction/diffusion

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phenomena [105]. It is a novel, fine-grain application of the "parallel substitution algorithm," which compounds the discrete character of the CA with the intelligency of neural networks (NNs) [106], lying within a range between extended CA with real numbers and restricted NNs with local connections. During the simulation of active media, the time evolution follows a stepwise, two-stage transition until equilibrium: the cell performs the diffusion rules and a neural function performs the reaction explicitly from a given PDE. Note that this model departs distinctly from Toffoli's paradigm [2] wherein the task of PDE solving is implicit. The system is intended to avoid the shortcoming of redundant discrete-continuous-discrete transformations that often cause problems of inaccuracy or instability in numerical computation. Simulations in the square lattice are carried out with promising issues [107].

5.2 Cellular Automata for Hydration of Cement-Based Materials

Correctly predicting the hydration and microstructure development of cement-based materials is not an easy task. Cement paste is probably one of the most complex materials, containing up to 15 different phases arranged into a complex microstructure. This complexity further increases in mortar where cement powder and medium grains coexist, and even more so in concrete as coarse aggregates are added in the mixture. A hybrid virtual cement and concrete testing laboratory (VCCTL) environment is provided at the National Institute of Standards and Technology (NIST) for simulating the hydration of cement-based materials and predicting their physical properties by virtual testing [108].

The hydration code of VCCTL is a CA whose input is a three-dimensional microstructure of a mixture of cement grains and water. This microstructure is obtained using a two-dimensional digital image of the cement powder, its particle-size distribution, and a given water-to-cement ratio. The output is the cement paste microstructure after hydration [109]. The simulation runs during a user-defined number of hydration cycles. The hydration cycle is split into three steps: dissolution, random walk diffusion of the mobile agents, and reaction between colliding pixels. The result serves as the input for finite-element or finite-difference methods to extract macroscopic properties from the microstructure, that is, elastic Young's modulus and Poisson ratio [110].

Besides its use for a normal hydration process, VCCTL can also simulate degradations such as leaching, a dissolution of one or more phases that causes harmful effects to quality and durability of the material. The leaching simulation consists of replacing the pixels representing the leached phases by water-pixels. The influence of dissolution on the porous network percolation [111] as well as on the global capillary porosity of the paste is highlighted and serves again, as in the unleached case, as input data to evaluate the effect on the de-

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graded elastic moduli [112]. Multiscale simulations of leaching on mortar are also carried out and representative elementary volumes are defined for both micro and meso different scales by a homogenization procedure in [113].

5.3 Movable Cellular Automata

The movable cellular automata (MCAs) method of Psakhie, Horie, and their coworkers [114, 115], which may also be referred to as "movable lattice particles" according to Popov's terminology [116], provides a novel, alternative approach to the conventional finite-element method applied to the elastoplastic behavior of materials under the action of small or large deformations. This hybrid model combines the advantages of CAs and molecular dynamics within a mesoscopic representation of the material.

Like the fictitious "fluid" particles in the hexagonal symmetry of the FHP lattice-gas, "solid" particles are created, but the basic concept is a pairwise switching parameter that defines a linked state as a "chemical bond" whenever two neighboring particles overlap. The distance between centers is considered and, during a local deformation, the time evolution of their linked or unlinked state acts as in a bistable medium. As well as in molecular dynamics, the particle's motion is governed by a set of translational and rotational equations following the Newton–Euler interaction law. In this sense, the dynamics may be related to the Cundall–Strack distinct element method for granular media except that particles are here fictitious and constrained by the lattice structure (thus the term "movable" in the MCA concept). As a matter of fact, a (micropolar) Cosserat continuum is provided by additional degrees of freedom for each material point [117].

Although it is argued that if the MCA method, except for its novelty as an alternative approach, does not bring actual advantages over usual computational methods in elasticity, it may on the contrary appear as the only practicable approach in areas of large plastic deformation or in ultimate states of the matter where those methods may fail or undergo highly time-consuming remeshing schemes. The effectiveness of MCAs are revealed in various situations: behavior of steel under load at the onset of fracture, response of heterogeneous structures like concrete under static or dynamic loads, strength properties of anisotropic material like lignite, fracture energy absorption, roughness at surface interface, friction and melting in rail-wheel contact, wear phenomena in combustion engines, or crash tests (see [115, 118] and references therein).

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6. Discussion

This attempted CACM taxonomy will identify several relevant questions and problems; a few are pointed out in the following. Where is the border between fine- and coarse-grain CACM? Should the time evolution be synchronous? What about topology and scalability of the network? How can we validate the consistency of a model? We focus on and limit ourselves to this short list of often unsolved questions, issued from our local experience and knowledge.

6.1 From Fine-Grain to Coarse-Grain

From Wolfram's bit-scale ECAs to more sophisticated models, the range of complexity in CACM may be extremely wide. The increasing complexity in lattice-gas models from pure lattice-gas, to lattice-Boltzmann, until the extended lattice-Boltzmann as described in Section 3 is a relevant example. While a monophase fluid particle is encoded with a 4-bit (resp. 6-bit) word in the HPP (resp. FHP) cell, a real-valued distribution function is encoded in the lattice-Boltzman cell, whereas arbitrary meshes are redefined to encode the discretized Boltzmann equation in the extended models. Some models are essentially coarse-grained; the MCAs give typical examples in nature.

As a coarse paradigm in parallel computing, consider the subdivision of a spatial problem into cells according to a given tessellation. This is done in the framework of a cell-processor allocation strategy, whatever the computational method of the solver might be. Each cell solves its own subproblem at mesoscale and should exchange data with its near-neighbors at each time step according to a predefined neighborhood template. Why is this grid-based network not a CA? This odd question should raise a frequently claimed assertion that CAs would have lost their attractiveness over the growing computational power of today's computers. Observing that a simple HPP gas is able to reveal realistic phenomena, though possibly inconsistent, is sufficient to take this assertion as wrong. CAs will remain a genuine approach per se and the finer the grain, the better the model. Anyhow, the model-to-architecture correspondence from fine-grain to special-purpose and from coarse-grain to general-purpose is straightforward.

6.2 Synchronous or Asynchronous Time Evolution

In several CACM, the time evolution is sometimes governed by asynchronous rules. The principle of simultaneity of a transition rule is not respected in the asynchronous case, when some models adopt a bottom-up or top-down scanning of the cells in the case of gravity flows [69, 72], or a partial scanning in order to avoid coupling between a moving particle and its vicinity [71]. During the force network generation in granular systems, the time evolution is based on a

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downward row-by-row computation of the force distribution in the triangular lattice [79–82]. Our idea, which can be denied, is that "there is always something happening at a complex medium" and that top-down, bottom-up (gravity-based), or partial (implementation-based) asynchronous modes should be avoided. A sequential, asynchronous mode breaks the capability for an effective parallel implementation of the model. Moreover, and more physically, it may break the Galilean invariance of the physical process [51, 80]. So, the question is: how do we get a pure, synchronous transition rule?

Let us focus on a particular case, namely, our crystal-like granular CA [74]. The basic two-stage transition is unable to move two contiguous particles when one sends a request to the site of the other. Therefore, it does not allow a void to propagate and solid grains to tumble down simultaneously. Other similar observations arise in the situation of long-range interactions [18, 19]. Including a synchronous propagative mode leads to considering the transition and the time evolution at two different scales and to considering the process as instantaneous within one time step. This condition needs to set up a mechanism to stop this transitional sequence, namely, a criterion of termination for the current time step. This criterion is carried out by a global all-to-all communication over the whole network.

In the general case, synchronizing a transition using CAs is relevant to Myhill's "firing squad" problem (see Mazoyer [119] and references therein).

6.3 Topology and Scalability of the Network

The *local* topology of a CA, that is, the neighborhood template of the cell that governs the local computation in the transition rule, may have an important impact on the behavior of the model. In general, nearest-neighbor interactions are considered. For the one-dimensional case, that means that the individual computation works upon Wolfram's triplet ($r = 1$) centered on the cell [1]. The two-dimensional case allows several nearest-neighbor templates, the usual ones being either the (4-valent) von Neumann or the (8-valent) Moore neighborhood in the square tiling and, on the other hand, either the (3-valent) star or the (6-valent) honeycomb neighborhood in the hexagonal tiling. As an example, lattice-grain flow simulations act on the Moore template [69, 72] or on the honeycomb template [71, 73, 74], whereas the brickwork Litwiniszyn template [66] is homeomorphic to the honeycomb. As in [107], the Margolus split-swap seesaw in the Moore template is sometimes encountered in CA rules. The good properties of the hexavalent grid are important to notify: more symmetries, isotropy with maximal number of degrees of freedom, and maximal coordinence. A relevant observation upon the lattice-gas models is the inconsistency of the (von Neumann) HPP gas and the consistency of the (honeycomb) FHP gas with the Navier–Stokes equation. In the three-dimensional case, the face-centered hypercubic

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lattice, although non-isotropic, is unfortunately the least frustrating solution, since no isotropic tessellation of the three-dimensional space exists.

At the *global* level, the question of scalability should be pointed out: is a recursive network needed for scaling laws? Scaling laws are concerned with the choice of the model size, power-laws, renormalization or homogenization and/or localization procedures, critical phenomena, and critical exponents. For illustration, consider the case of a composite material. At the microscopic scale the material is inhomogeneous, whereas at the macroscopic scale it appears as homogeneous. A common procedure, acting at intermediate, mesoscopic scale, should evaluate a representative elementary volume (REV) that defines the minimal size of a homogeneous sample. The property of scalability for the underlying CA network is able to facilitate this kind of procedure. For the one-dimensional case, it is easy to choose a periodic ring of length 2^n in ergodic conditions. For the two-dimensional chessboard, one can refer to the recursive framework of Kadanoff for the ferromagnetic Ising model when four spins in a cell are condensed into one single spin in the renormalization procedure [120]. For the hexagonal case, the underlying graph is a hierarchical Cayley graph with periodic boundaries and maximal symmetries compared with the skewed framework of Niemeijer and van Leeuwen [121].

6.4 Consistency of the Models

Although difficult, the question of proving whether a CA model is consistent with mathematical equations involves the most challenging problems that depend upon a diversity of factors. Proofs of consistency are never easy even for simple cases and the deal may often be worse. To demonstrate this, we need to use the renormalization/homogenization procedures and comparative studies with other non-CA models such as particle dynamics, finite-difference, and finite-element, or volume methods, at least when these continuum methods are practicable. In several cases, the useful information of power-laws and critical exponents can yet be somehow extracted, the context of SOC being a meaningful example.

It is worthwhile keeping track of the diversity of PDEs that occurred throughout our enumeration of simple CACM models: the simple diffusion equation, the Fokker–Planck equation, the Navier–Stokes equation, the Burgers one with its correlated Korteweg–de Vries equation and the recent outcome of, say, the Boutreux–de Gennes equation. Incidentally, the CA-neural hybrid environment [105] that might be extended beyond the area of active media jointly with the "programmable matter" methods [2, 122] provide, by their respective explicit and implicit approaches, an idealized laboratory of prospective studies and investigations upon the CA/PDE relationship.

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