

A real-space cellular automaton laboratory

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ABSTRACT: Geomorphic investigations may benefit from computer modelling approaches that rely entirely on self-organization principles. In the vast majority of numerical models, instead, points in space are characterized by a variety of physical variables (e.g. sediment transport rate, velocity, temperature) recalculated over time according to some predetermined set of laws. However, there is not always a satisfactory theoretical framework from which we can quantify the overall dynamics of the system. For these reasons, we prefer to concentrate on interaction patterns using a basic cellular automaton modelling framework. Here we present the Real-Space Cellular Automaton Laboratory (ReSCAL), a powerful and versatile generator of 3D stochastic models. The objective of this software suite, released under a GNU licence, is to develop interdisciplinary research collaboration to investigate the dynamics of complex systems. The models in ReSCAL are essentially constructed from a small number of discrete states distributed on a cellular grid. An elementary cell is a real-space representation of the physical environment and pairs of nearest-neighbour cells are called doublets. Each individual physical process is associated with a set of doublet transitions and characteristic transition rates. Using a modular approach, we can simulate and combine a wide range of physical processes. We then describe different ingredients of ReSCAL leading to applications in geomorphology: dune morphodynamics and landscape evolution. We also discuss how ReSCAL can be applied and developed across many disciplines in natural and human sciences. Copyright © 2013 John Wiley & Sons, Ltd.

KEYWORDS: computer modelling; cellular automaton; stochastic process; dune morphodynamics; landscape evolution

Introduction

A number of challenges remain to be addressed in the growing field of computational geomorphology (Coulthard, 2001; Willgoose, 2005). Most of them are related to the origin of the available theoretical formalisms and their accuracy to be exploited and combined for predictability purposes (Dietrich *et al.*, 2003). Although the traditional top-down strategy may lead to some success (Tucker and Hancock, 2010), there is definitely room for alternative methods based on finite state systems, small-scale interactions and stochastic processes (Turcotte, 2007; Werner and Gillespie, 1993). This is particularly true if these approaches can be implemented in a very efficient way, and if a large diversity of new patterns can arise spontaneously.

Elementary structures with primitive individual behaviours can produce sophisticated collective patterns when they interact with each other within systems. Now recognized as complex systems in many branches of knowledge (Axelrod, 1997; Bonabeau, 2002; Epstein and Axtell, 1997; Innes and Booher, 1999; Jensen, 1998; Werner, 1999), the interdisciplinary field of complexity science offers a general framework for the analysis of their underlying mechanisms of emergence (Goldenfeld and Kadanoff, 1999). In practice, the challenge is to relate micro and macro levels of description, not with direct cause/effect relationships, but in a manner that involves patterns of in-

teractions between the constituent parts of the system over time. With this purpose in mind, the cellular automaton approach provides generic numerical methods for the simulation of complex systems (Toffoli, 1984; Wolfram, 1986).

Among the class of reduced complexity models, cellular automata (CA) are systems that iteratively evolve on a grid according to local interaction rules. As reviewed by Chopard and Droz (1998), CA models have been used with success to study different phenomena in both natural (e.g. biology, ecology, chemistry, physics) and human sciences (e.g. history, sociology, anthropology, and economics). Following the precursory work of Von Neumann (1966), a conventional cellular automaton consists of a lattice of individual elements, each of which can be assigned a scalar property. This scalar property may change as the result of external forcing affecting all of the elements and internal interactions between elements. External forcing is often assumed to occur at a constant rate, and the internal interactions are usually simplified to include only next-neighbour interactions. The CA generator presented here retains the simplicity of such conventional cellular automata, while also proposing a modular approach for the modelling of diverse combinations of physical processes.

The most important feature of CA models is that they are constructed from a set of discrete structures starting from an elementary length scale which integrates all the diversity of the smaller-scale properties. In this case, a major disadvantage

is that the local interaction rules cannot be defined independently from an exact determination of the value of this elementary length scale. Hence the parametrization of CA models cannot be derived from first principles only, but needs to be determined a posteriori from the output of the numerical simulations. Nevertheless, this apparent weakness related to the discontinuous nature of the CA model is also the main strength of this discrete approach. Indeed, the dynamics are governed by small-scale interactions, which are known to produce collective behaviours as a result of both negative (damping) and positive (amplifying) feedbacks. Basically, the interactions between the constituent parts of the systems are associated with exchanges of information and communication that may in turn favour the emergence of a new level of organization. In this case, the feedback mechanisms are just the means by which action is organized and expressed with respect to the internal sources of information.

For all these reasons, CA models can be described as a complementary approach for the modelling of natural systems with an infinite number of degrees of freedom and/or for which the role of discontinuities and heterogeneities cannot be neglected (e.g. Bak *et al.*, 1988; Blanter *et al.*, 1999; Nagel and Schreckenberg, 1992; Narteau, 2007a, 2007b; Narteau *et al.*, 2000a, 2000b, 2003; Olami *et al.*, 1992). Simultaneously, these discrete models offer the opportunity to explore new mathematical objects which cannot be studied analytically or from the behaviours of individual structures alone. Then, keeping in mind that the ultimate objective is to forecast the occurrence of large-scale phenomena, alternative methods may be developed from direct comparisons between observations and model outputs. Therefore, the simplest CA approach still provides one of the best and most efficient sources of comparison by means of numerical simulations (Wolfram, 1983).

Here, we present a Real-Space Cellular Automaton Laboratory (ReSCAL), a class of algorithm that can be used to analyse a wide variety of natural systems using the same level of conceptualization (Narteau *et al.*, 2001). As described in the next section, the basic principle of ReSCAL is to replace the continuous physical variables by a discrete set of state variables representing the different phases of a natural system at any point in space. Thus transitions from one state to another may be associated with individual physical processes using only nearest-neighbour interactions and a limited number of control parameters. Various applications presented in the third section demonstrate the feasibility and potential benefits of the proposed method in geophysics.

The Real-Space Cellular Automaton Laboratory

As a complete software suite written in C language, ReSCAL includes a number of tools for the creation of the initial cellular space and conversion of the output data files to various formats. Based on a generic iteration scheme, the main program is dedicated to numerical simulations. Most of the parameters can be edited in a text file by using a comprehensive syntax. Generally, the simulations are displayed within a graphical user interface. In the case of a 3D space, surfaces may be rendered with standard light-source shading, so that the images are often very detailed.

Main iteration scheme

A model generated by ReSCAL consists of a cellular space that simulates small-scale interactions between elements regularly distributed over a 1D, 2D or 3D rectangular grid. Hence a physical environment is fully described by a lattice of discrete values

encoding the state of the cells (Figure 1a). At the elementary length scale of the lattice, each cell has a characteristic length l_0 .

The evolution of our system is governed by a finite set of interactions corresponding to individual physical processes. Formally, interactions are defined in terms of transitions within pairs of nearest neighbour cells (doublets). Therefore, we will consider a set of transitions characterized by:

- the initial states (S_1^i, S_2^i) of the doublet;
- the final states (S_1^f, S_2^f) of the doublet;
- the orientation of the doublet;
- a transition rate.

Once the cellular space is initialized, an iterative scheme takes place (Algorithm 1). At each iteration step, we randomly select a transition with respect to the cellular space and the transition rates. Then, we apply the transition on a doublet. Our implementation of this scheme is based on structured data organized as cross-referenced arrays of cells and doublets. Before going into more detail, let us define some convenient notions that may prove useful to describe the organization of data structures.

An ordered pair of states (S_1, S_2) associated with an orientation is called a generic doublet and can be regarded as a template for the real doublets (Figure 1b). Among all possible generic doublets, some are said to be active if the pair (S_1, S_2) matches exactly the initial states (S_1^i, S_2^i) of at least one transition with the same orientation. Analogously, a doublet in the cellular space is an active doublet if the respective states of its cells and its orientation correspond to an active generic doublet. It is obvious that only active doublets may undergo a transition.

For every active generic doublet, we generate a doublet array whose elements are the set of positions of the corresponding active doublets that are present in the cellular space. Thus we achieve direct access in the cellular space each time an active doublet is randomly chosen from the elements of a doublet array. Conversely, as the active doublet undergoes transition, the two states of the doublet may change. This implies an update of the doublet arrays impacted by the modification of the cellular space. Therefore, each element of the cellular space contains a maximum of three references to the doublet arrays, one for each orientation. When a doublet has operated a transition, we update the references contained in the first cell of all active doublets that have been modified and the corresponding elements of the doublet arrays. Finally, we obtain a set of cross-referenced data structures between the cellular space and the doublet arrays.

Algorithm 1: Main iteration scheme of ReSCAL. The general process may be described as a Markov chain; an iteration is associated with a single transition of an active doublet.

```

Creation of the cellular space
Initialization of the transitions
Initialization of the doublet arrays
while number of active doublets > 0 do
    Weighted random choice of a transition  $T$ 
    Random choice of an active doublet  $D$ 
    Transition  $T$  applied on  $D$ 
    Cross references updated for all impacted doublets near  $D$ 
    if condition then
        | Additional functions and modules
    end
    Time evolution
end

```

The search for algorithmic efficiency is a major issue in ReSCAL, considering the large number of doublets in a 3D

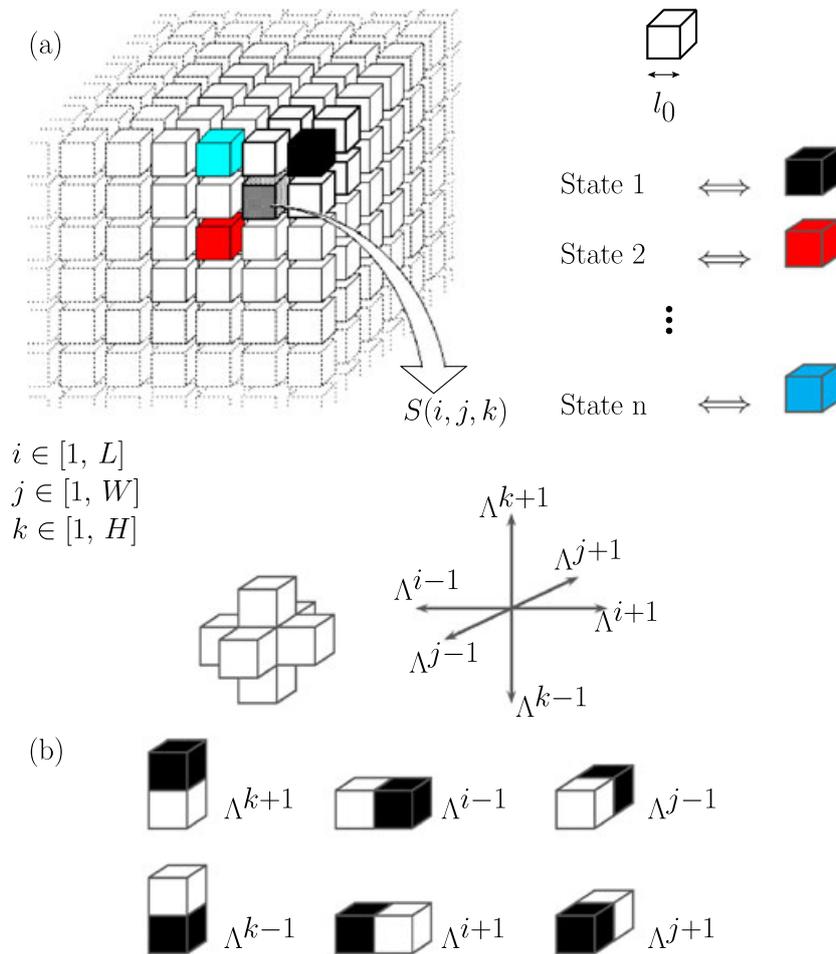


Figure 1. The Real-Space Cellular Automaton Laboratory. (a) A 3D square lattice is a real-space representation of the physical environment under consideration. At the elementary length scale l_0 , each cell can be in a finite number of states and interact with next-neighbour cells along the lattice directions. All transitions acting on a doublet are given a specific transition rate for each orientation. (b) Generic doublets with different orientations for a two-state model. Once considered as initial doublet of a transition, they become active generic doublets. Within the cellular space, a high number of doublets belonging to these generic classes may coexist. This figure is available in colour online at wileyonlinelibrary.com/journal/espl

space. It led us to implement dynamic defragmentation of the doublet arrays. Indeed, the random choice of an active doublet is straightforward and fast if each doublet array remains a contiguous pool in memory. As a result, ReSCAL application can reach execution speeds up to 10^6 transitions per second in a $10^3 \times 10^3 \times 10^3$ cellular space.

A continuous time stochastic process

The main iteration scheme behaves like a dynamical system, whose evolution is entirely defined as a stationary stochastic process based only on the knowledge of the cellular space and the transition rate values. Practically, this can be regarded as a generalized Poisson process or a specific type of continuous-time Markov process. Most importantly, in such a memoryless random process, low-probability events may occur at each iteration. Here, the transition rates are expressed in units of t_0^{-1} , where t_0 is the characteristic time scale of the model.

Let us consider a set of n transitions T_1, \dots, T_n with respective rates $\Lambda_1, \dots, \Lambda_n$. If we take into account the cellular space, the overall rate at time t of the set of transitions is

$$\Lambda(t) = \sum_{i=1}^n N_i(t)\Lambda_i \tag{1}$$

where $N_i(t)$ is the number of active doublets for the transition T_i . It follows that, considering a generalized Poisson

process, the probability for a transition to occur between t and $t + \Delta t$ is

$$P(t, \Delta t) = 1 - \exp(-\Lambda(t)\Delta t) \tag{2}$$

Thus we can set the waiting time before the next transition to the value

$$\Delta t = -\frac{1}{\Lambda(t)} \ln(1 - p) \tag{3}$$

where p is a random variable drawn from a uniform distribution between 0 and 1. The time interval from one transition to another is therefore a random variable which is entirely determined by the configuration of active doublets.

Determination of the transition requires the computation of a weighted random choice. Indeed, the statistical weight $w_i(t)$ of a transition T_i at time t is given by

$$w_i(t) = \frac{N_i(t)\Lambda_i}{\Lambda(t)} \tag{4}$$

Drawing at random on the cumulative distribution function of all these weights, it is therefore possible to choose the generic doublet that operates a transition at time $t + \Delta t$. Finally, we can directly select at random an element in the corresponding doublet array.

Additional modules and functions

ReSCAL is also a software package constructed on a modular basis for simulating systems in which multiple physical phenomena are combined. Therefore, we present a few modules or functions that are used in the various models described subsequently.

Avalanches

The role of gravity is essential in most natural systems, especially in granular materials where avalanches occur when a static angle of repose is exceeded. To take into account this angle of repose in the model, we have to choose a specific state, obviously the denser one, and calculate the topography that the corresponding cells produce from the bottom of the system. Then, we can compute the gradient to get the direction and the magnitude of the steepest slope at any point of this interface.

The avalanche module is based on a diffusion with threshold mechanism. The threshold is simply the repose angle θ_c of the dense material under consideration. In practice, we activate the four horizontal transitions that are associated with the motion of the cells with the highest density. The corresponding transition rate Λ_θ is not constant over time and depends on the local slope θ as follows:

$$\Lambda_\theta = \Lambda_{ava} \delta_\theta \quad \text{with} \quad \delta_\theta = \begin{cases} 0 & \text{if } \theta \leq \theta_c \\ 1 & \text{if } \theta > \theta_c \end{cases} \quad (5)$$

where Λ_{ava} is a constant transition rate.

A lattice gas cellular automaton

ReSCAL offers the opportunity for flow computation using a lattice gas CA (Frisch *et al.*, 1986; Rothman and Zaleski, 2004). This numerical method converts discrete motions of a finite number of particles into physically meaningful quantities and is an alternative to the full resolution of the Navier–Stokes equations. Overall, it is based on next-neighbour interactions that can be mapped on the cellular space of the main CA model. In addition, this discrete model is particularly useful to analyse the complex interplay between an evolving topography and a flow. To this

end, a distinction is made between states where the fluid particles can propagate and states impermeable to the flow.

To reduce the computation time, we do not implement a 3D lattice gas CA. Instead, we consider a set of uniformly spaced vertical planes parallel to the direction of the flow (the spacing is a parameter of the model). Each plane is composed by the square lattice of the main CA model (Figure 2a). Fluid particles are confined to these 2D planes and they can fly from cell to cell along the direction specified by their velocity vectors. Within a square lattice, we use a multispeed model taking into account motions of particles between nearest and next-nearest neighbours (d’Humières *et al.*, 1986): slow-speed particles are moving between nearest neighbours; fast-speed particles are moving between next-nearest neighbours (Figure 2a). Two fluid particles with the same velocity vector cannot sit on the same site. Thus there is a maximum of eight particles at each site. The interactions between particles take the form of local instantaneous collisions on all sites with several particles (Figure 2b). The evolution of the whole system during one iteration (or motion cycle) consists of two successive stages: a propagation phase during which all particles move from their cells to their neighbours along the direction of their velocity vectors, and a collision phase during which particles on the same cell may exchange momentum according to the imposed collision rules (Figure 2b). These collision rules are chosen in order to conserve both mass and momentum.

Finally, using the output of the lattice-gas cellular automaton, we estimate both components of the local velocity field by averaging the velocity vectors of fluid particles over space and time. The velocity \vec{V} is expressed in terms of a number of fluid particles. In practice, given the size of the lattice and the physical environment, it takes a variable number of iterations to stabilize the flow (Figure 2c). The parallel computation of the vertical planes using a multiprocessing library (OpenMP) leads to higher numerical efficiency.

Rotation

In many physical environments, anisotropic phenomena may change of orientation due to a variable external forcing. Hence

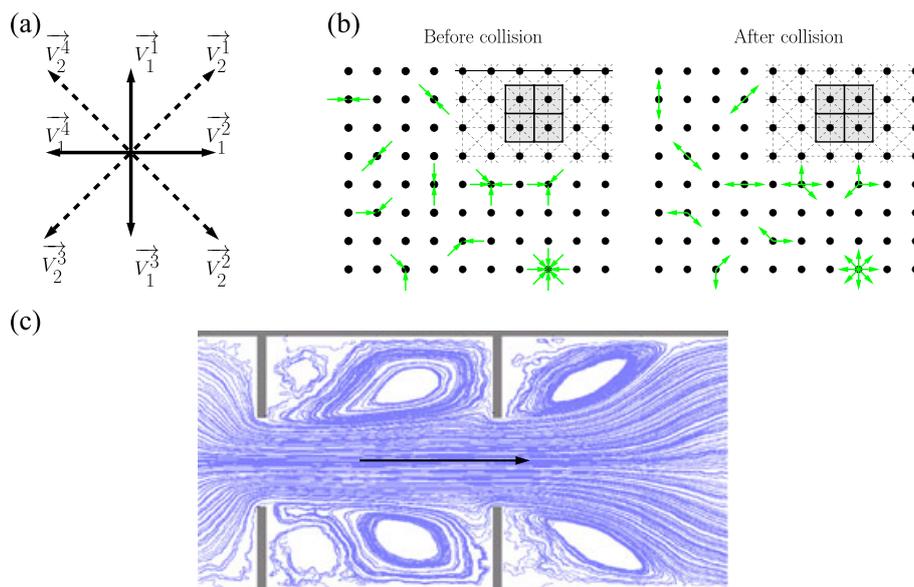


Figure 2. The lattice gas CA model in ReSCAL. (a) The different velocity vectors in the lattice gas cellular automaton. We have $\|\vec{V}_2^i\| = \sqrt{2}\|\vec{V}_1^i\|$. (b) Different examples of collisions between fluid particles (see the entire list in d’Humières *et al.*, 1986). Particles and their velocity vectors are represented by arrows. Each dot is a node of the lattice gas CA model as well as the centre of a cell of the main CA model. At the top right, we show four of these cells in light grey and the paths along which the fluid particles are moving (dashed lines). (c) Simulation of flow through a pipe with obstacles using ReSCAL. The black arrow indicates the direction of flow. This figure is available in colour online at wileyonlinelibrary.com/journal/esp

it may be convenient to use the same set of transitions and the same configuration of cells for different orientations of the lattice. For this particular reason, a rotation function in 2D or 3D space has been implemented in ReSCAL. This provides two different operating modes:

- A first mode simulates the action of a rotating table by applying a rotation inside a vertical cylinder centred in the middle of the cellular space. When the rotation angle is not a multiple of $\pi/2$, one may expect a number of defaults like the disappearance and duplication of cells, due to the rectangular and discrete geometry of the system. Such inevitable effects have been reduced by rounding functions, so that they remain relatively limited in space and time. Actually, for each cell of the new cellular space (i.e. after rotation), we apply an inverse rotation and select the state of the nearest cell in the old cellular space, thus preventing the appearance of empty cells.
- A second mode is addressing the case of periodic boundary conditions. In addition to the discretization issue previously mentioned, we are also facing some classical problems of symmetry for the rotation of a rectangular lattice. As long as no perfect solution exists for all angle values, we implement a rotation algorithm ensuring that all discontinuities remain at the boundaries of the system. In most practical cases, the boundary artefacts disappear by global averaging after a limited number of transitions if the frequency of rotations is low with respect to the overall transition rate Λ (Equation 1).

As described subsequently in the applications, the rotation function and the lattice gas CA can be used simultaneously to simulate multidirectional flow regimes. In this case, the fluid particles are still evolving on the same grid but the physical environment is rotated according to a given sequence of angles and time intervals. Numerically, it may have a cost because it is necessary to restabilize the flow with respect to the new configuration of cells after each rotation.

Chains of transitions

Some phenomena are not associated to independent stationary processes, but rather to a dynamical sequence of time-dependent processes. To address such cases, an optional mechanism enabling chains of transitions have been added to the main iteration scheme. The system keeps the memory of the last transition together with the position of the doublet that was modified. Then, a neighbouring doublet may instantaneously operate a transition according to a given probability of occurrence (i.e. the magnitude of the coupling). A necessary condition in a chain of transitions is that the two neighbouring doublets have at least one cell in common.

A typical example for a chain of transition is bedload transport (see 'A landscape evolution model', below). It is clear that a significant part of erosion is caused by the transport of solid material due to the collisions of grains with the immobile sedimentary layer. In this case, it seems impossible to separate the transport and erosion mechanisms and a chain of transitions may be created between them.

Note that chains of transitions generate a new level of interaction between independent physical processes. In the future, they could be used as a generic tool to analyse systems with long-range interactions.

Variable transition rates

It is often difficult not to take into consideration functional dependencies between the magnitude of different processes. Indeed, non-stationary processes are commonly observed when an external forcing changes the overall intensity of a physical

mechanism. Transition rates may also vary with respect to a local threshold value. This has led us to integrate two additional classes of functions in the iteration scheme of ReSCAL:

- A regulation function may be called at each iteration of the main scheme. It updates the transition rates with respect to time.
- Secondly, some transitions may be associated to a callback function. When one of these transitions occurs, the callback function recalculates a probability for the transition to be aborted considering a local dependence on a given parameter. Note that, in this case, the method for the determination of the time step should integrate the probability distribution function of this parameter over the entire population of active doublets.

Applications for Complex Geomorphological Systems

To illustrate the capabilities of ReSCAL and the way it could be used in natural sciences, we present a 2D model for diffusion (Brown, 1828) and 3D models for dune morphodynamics (Narteau *et al.*, 2009; Zhang *et al.*, 2010, 2012) and for the evolution of landscapes. For all these CA models, special attention is given to scaling as a prerequisite to comparisons with natural observations and interpretation of the results. Basically, the example on diffusion serves to show that CA models may equally well reproduce the asymptotic behaviours of continuous models. Then, using as examples the numerical results obtained for the analysis of landscape patterns and populations of dunes, we explore new frontiers of complex geophysical systems to shed some light on the additional predictive power of CA models.

A 2D model of diffusion

Diffusion offers the simplest way of comparing the result obtained by continuous and discrete models. For example, Fick's second law predicts how diffusion modifies concentration with respect to time and distance:

$$\frac{\partial C(x, t)}{\partial t} = D \frac{\partial^2 C(x, t)}{\partial x^2} \quad (6)$$

where C is the concentration in dimensions, D the diffusion coefficient, x the position and t the time. This equation has for solution

$$C(x, t) = A \operatorname{erf}\left(\frac{x}{\sqrt{2Dt}}\right) + B \quad (7)$$

where A and B are two constants that depend on the boundary conditions. Then, starting with a step in density from 0 to 1 in a closed system, we can, for example, predict the evolution of concentration at any point in space (Figure 3a).

Using ReSCAL, we can produce an N -particle random walk CA model operating on a 2D grid (Figure 3b). Practically, we consider two states to mimic individual particles and their surrounding material (e.g. a gas). Then, we simulate a random walk by the four doublet transitions associated with the displacement of the centre of mass of the particles. Obviously, all the transition rates are equal in order to generate isotropic random motions. According to Equation 3, the time step is inversely proportional to the number of active doublets and, at each iteration, we can randomly select the doublet that operates a transition among the entire population of active

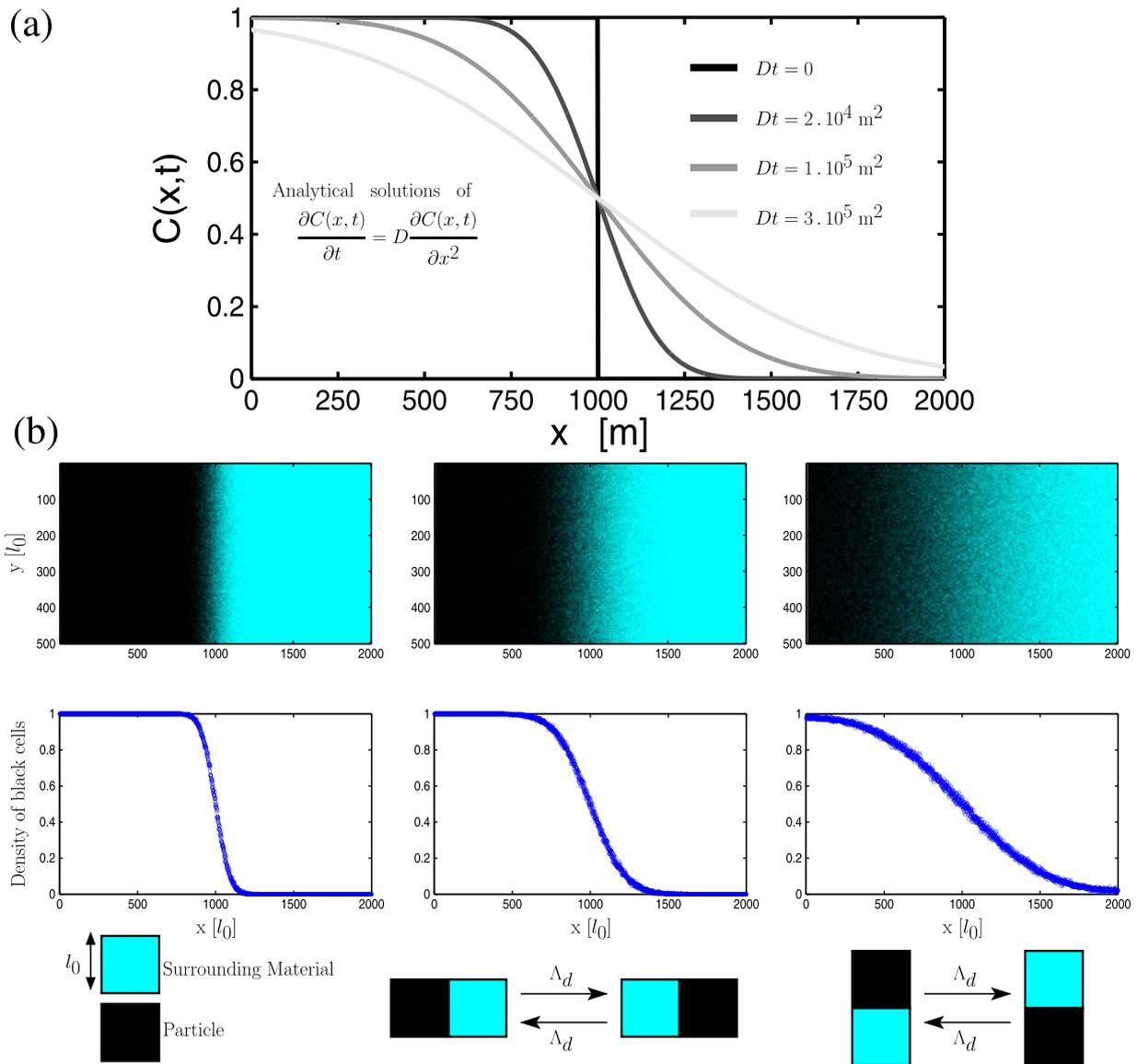


Figure 3. A CA model of diffusion using ReSCAL. (a) Analytical solutions of the Fick's second law at different times are used for comparison with the results of the CA model. (b) Evolution of a 2D N -particle random walk CA model using ReSCAL: $H = 500 l_0$, $L = 2000 l_0$. Two states and four transitions with the same rate Λ_d are used to reproduce random particle motions. Note the similarities between the results obtained by the discrete and the continuous methods. In both cases, the initial condition is a discrete step in density from 0 to 1 along the horizontal direction. This figure is available in colour online at wileyonlinelibrary.com/journal/espl

doublets. Starting with the same initial condition as in the continuous model, it is observed that the evolution of the concentration of particles is in perfect agreement with the analytical solutions of Equation 6 (Figure 3b).

The results presented in Figure 3 show that, smoothing the fluctuations of the discrete model over a sufficiently large scale, it is capable of perfectly predicting the evolution of concentration. This demonstrates that CA models are physically based models that can provide the same amount of information as any other type of continuous model. Then, we infer that, despite a different level of conceptualization which makes them more difficult to understand, the CA models may also have high predictive skills in domains for which there is not yet a complete family of solutions derived from a set of differential equations (see 'Dune morphodynamics' and 'A landscape evolution model', below).

If the CA model for diffusion can be implemented in different types of environments, there is still the question of the determination of its elementary length and time scales $\{l_0, t_0\}$. Unfortunately, no pattern formation can occur in such a simple diffusive system and the only scaling parameter is given by

the dimensionless diffusion coefficient Dt/m^2 . This number can be directly compared to its counterpart in the model $t_0/(\Lambda_d l_0^2)$. However, there is still one ingredient missing for the determination of the $\{l_0, t_0\}$ -values which has to be determined arbitrarily. For example, the l_0 -value can be obtained from the direct comparison between the dimension of the system (in units of meters) and the size of the square lattice (in units of l_0). In this case, we get the t_0 -value by matching the dimensionless diffusion in the model to that in the material under consideration.

Dune morphodynamics

Dunes are bedform features which propagate downstream when the flow reactivates motion of particles that have been buried in the lee. In nature, changes in direction and intensity of the flow, variations in sediment supply, vegetation as well as dune-dune interactions may produce a wide range of dune field patterns. Hence the physics of sand dunes has often been used as a paradigm for understanding and investigating

self-organization and complex systems (Baas, 2002; Kocurek and Ewing, 2005; Nishimori and Ouchi, 1993; Werner, 1995; Werner and Gillespie, 1993). In a continuation of this effort, we use ReSCAL to couple a cellular automaton for sediment transport and a lattice gas cellular automaton for flow dynamics. The originality of the approach is to implement for the first time the permanent feedback mechanisms between flow and bedform dynamics using a set of discontinuous methods.

In the CA model of sediment transport, we consider three states (fluid, mobile and immobile sediment) and different sets of transitions to simulate erosion, transport, deposition, gravity and diffusion (Figure 4a). These anisotropic sets of transitions take into account the flow orientation, so that the model of sediment transport alone can produce bed form features. However, the main difference from classical models is that we also simulate the flow to calculate the bed shear stress.

As previously detailed, the flow is calculated in 2D vertical planes parallel to the direction of the wind and confined by two walls of neutral cells at the top and the bottom of the system. The fluid particles can only move within the fluid state of the CA of sediment transport. Other states are considered as solid boundaries on which the fluid particles are rebounding. In order to implement this feedback mechanism of the topography on the flow, we are continuously monitoring the evolution of the bed topography (see 'Avalanches', above). Thus we can evaluate the direction of the normal vector to this topography, and determine locally how a fluid particle rebounds on a sedimentary cell. In practice, we simply impose no-slip boundary conditions on the bed surface and free-slip boundary conditions along the

ceiling as a first approximation of a free surface. Then, motions of fluid particles adapt to changes in topography, and the flow field is strongly coupled to the bedform dynamics.

From the velocity \vec{V} expressed in terms of a number of fluid particles and the normal \vec{n} to the topography we calculate the bed shear stress:

$$\tau_s = \frac{\tau_0 \partial \vec{V}}{\partial \vec{n}} \quad (8)$$

where τ_0 is the stress scale of the model expressed in units of $l_0^{-1} t_0^{-2}$. We then consider that the erosion rate is not constant (see 'Variable transition rates', above), but linearly related to the bed shear stress τ_s according to

$$\Lambda_e = \begin{cases} 0 & \text{for } \tau_s \leq \tau_1 \\ \Lambda_0 \frac{\tau_s - \tau_1}{\tau_2 - \tau_1} & \text{for } \tau_1 \leq \tau_s \leq \tau_2 \\ \Lambda_0 & \text{else} \end{cases} \quad (9)$$

where Λ_0 is a constant rate, τ_1 is the threshold for motion inception and τ_2 is a parameter to adjust the linear relationship. By definition, $(\tau_s - \tau_1)$ is the excess shear stress from which we can account for the feedback mechanism of the bed shear stress on the topography.

Using this dune model, we can reproduce a huge variety of dune patterns according to specific wind regimes (Figures 4b and 5). Simultaneously, the bedform dynamics can explore a full hierarchy of length scales, from the elementary wavelength that perturbs the initial flat sand bed (λ_{\max}) to the size of the

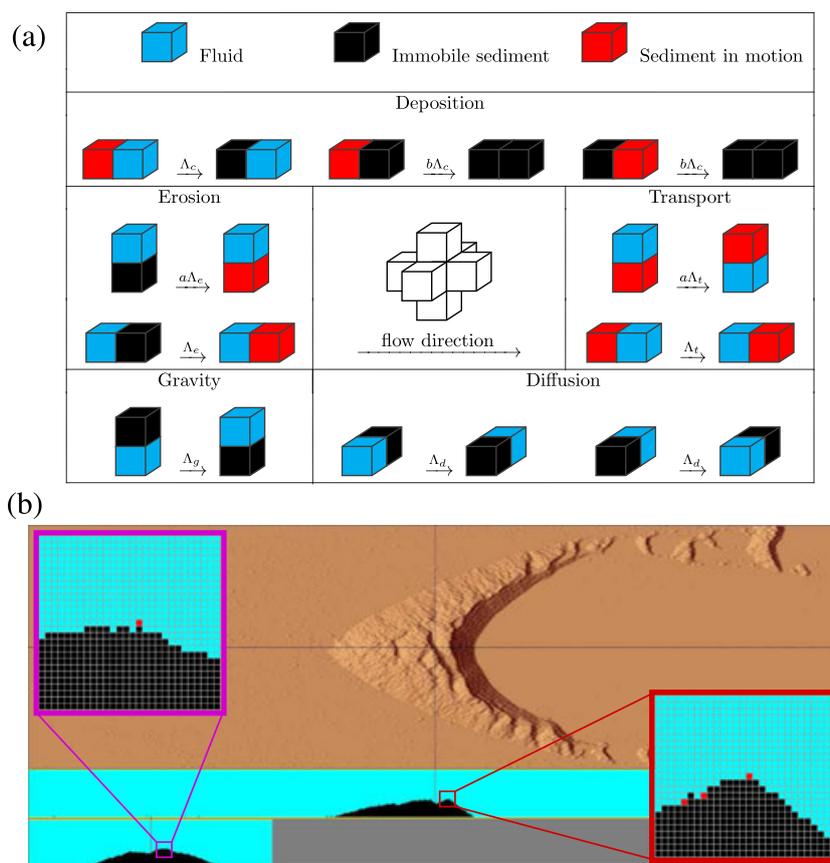


Figure 4. A CA dune model using ReSCAL. (a) In the CA model, three states are used to reproduce the fluid, mobile and immobile sediment. Transitions for erosion, deposition and transport ensure conservation of mass. The rates for erosion, deposition and transport are such that $\Lambda_c < \Lambda_0 < \Lambda_b$, where Λ_0 is the maximum value of Λ_e (see Equation 9). Gravity and diffusion are occurring over much shorter and longer periods of time, respectively. We chose $\Lambda_d \ll \Lambda_0 \ll \Lambda_g$, $a=0.1$ and $b=10$ (Zhang *et al.*, 2010). (b) Topography of a barchan dune in the CA dune model. The same instability is responsible for the formation of dunes on a flat sediment layer and for the development of superimposed bedforms. Dashed line corresponds to the longitudinal and the transverse vertical slices of cells shown below. Two insets zoom in on regions of high sediment transport. This figure is available in colour online at wileyonlinelibrary.com/journal/espl

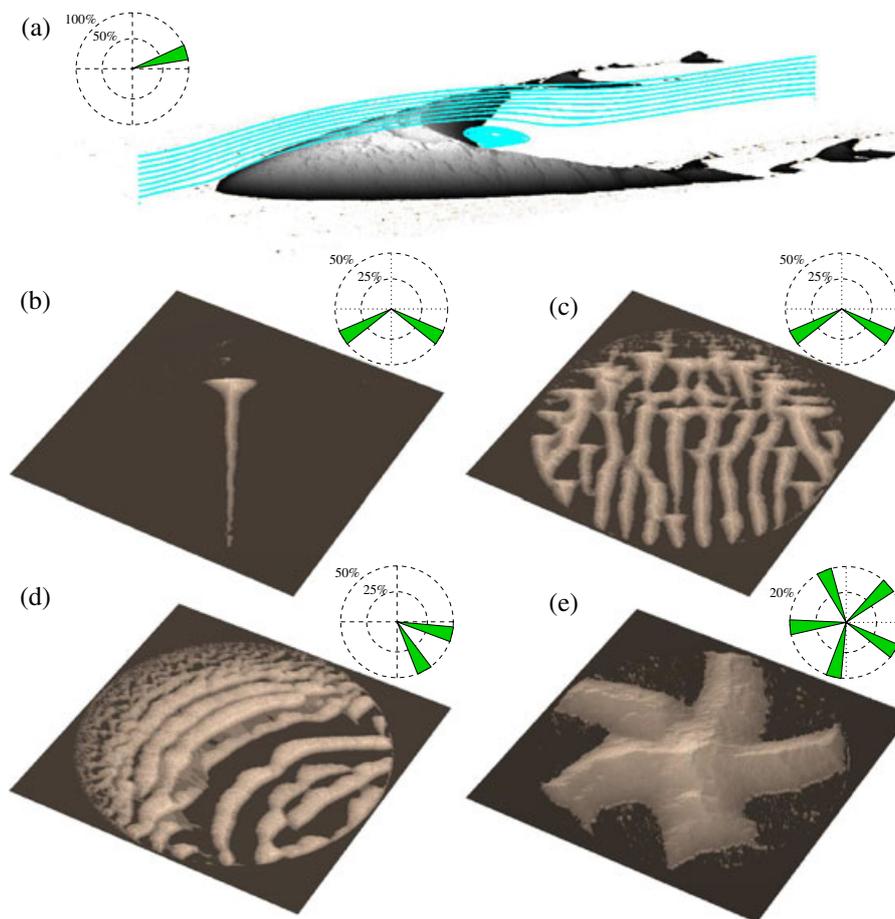


Figure 5. Dune patterns produced by the CA dune model using ReSCAL. (a) Barchan dune calving smaller barchans off its horns while superimposed dune patterns nucleate and propagate on the faces exposed to the flow. Velocity field lines show the recirculation zone on the lee side. (b) An isolated longitudinal dune produced by two winds of equal strength and duration with an angle $\Theta = 2\pi/3$. (c) Population of longitudinal dunes using the same wind regime. (d) A population of transverse dunes produced by two winds of equal strength and duration with an angle $\Theta = \pi/3$. (e) A star dune produced by five winds of equal strength and duration. The angle between two consecutive winds is always the same ($\Theta = 2\pi/5$), so that the total sediment flux is null. Insets show the wind roses. This figure is available in colour online at wileyonlinelibrary.com/journal/espl

giant dune that scales with the depth of the flow. On these giant dunes, superimposed dunes are likely to develop, favouring complex dune–dune interactions and the development of secondary dune features (Figure 4b).

In the framework of this paper, it is important to underline that the physical mechanisms responsible for the emergence of these dune patterns had not been numerically accessed so far. This is mainly because previous continuous and discrete models consider empirical laws that have been established according to specific conditions (Eastwood *et al.*, 2011; Werner, 1995). When these conditions are not met, the law is no longer valid and may limit pattern formation on more realistic dune features. This is not the case for our CA dune model, in which the dynamic equilibrium between flow and topography arises as an emergent property. Then, the instability responsible for the formation of dunes from a flat sand bed can also generate superimposed waveforms on the top of large dunes, as is commonly observed in dune fields (Elbelrhiti *et al.*, 2005). Confinement of the flow is also essential for the limitation of dune size and for the final shape of dune fields (Andreotti and Claudin, 2007). One more time, we do not impose any ad hoc retroaction mechanism in our CA dune model. Instead, the limitation in dune size is just the result of the acceleration of the flow induced by confinement and of consecutive changes in the distribution of the bed shear in the neighbourhood of dune crests. Then, we can show that, as in nature, the characteristic wavelength of giant dunes can be directly related to the average depth of flow (Zhang *et al.*, 2010).

However, the most important point for our present purpose is that the outputs of numerical simulations can be quantitatively compared to real bedforms to provide the scaling of the model and fully determine the $\{l_0, t_0\}$ -values. Indeed, our model spontaneously generates periodic dune patterns from a flat sand bed, so that the instability responsible for the formation of dunes in nature can be studied by a linear stability analysis (Narteau *et al.*, 2009). As a result, we can quantify the characteristic length scale for the formation of dunes in the model and compare the λ_{\max} -value in units of l_0 with its counterpart in nature in units of metres (Elbelrhiti *et al.*, 2005). Thus, we determine the characteristic length scale l_0 of the model. Using this value, we set the characteristic time scale t_0 by matching the average saturated flux in the model to that in the dune field. In this case, because the λ_{\max} -value may be directly related to the ratio between the sediment and the fluid density times the grain diameter (Hersen *et al.*, 2002), the $\{l_0, t_0\}$ -values can be entirely defined from the values of these physical parameters in all types of physical environments where the dune instability has been observed. There is no doubt that this rescaling strategy is a major step for a CA dune model and for reduced complexity models in general.

A landscape evolution model

The development of Earth's surface topography is often the result of sediment transport in dilute phases and high water

discharges. Under these conditions, the characteristic time scales of fluid flows may be many orders of magnitude shorter than those of the erosional processes. In addition, the computational cost of multiphase flow simulation by a real-space CA may be too high to be manageable in practice. For these reasons, we neglect here the modelling of water flows to focus on the motion of a sediment phase with high concentration.

As for the dune model, the landscape evolution model needs at least three states (land, mobile sediment and atmosphere) to simulate erosional, depositional and transport processes (Figure 6a). However, in this case, erosion is related to different denudation mechanisms of weathering, surface splash and mass wasting, while deposition may be related to settling, cohesion or sedimentation. All these mechanisms are incorporated into two symmetric sets of transitions for the production (erosion) and stabilization (deposition) of mobile sedimentary cells (Figure 6a). The contrast in density between the two sedimentary states determines the number n of mobile cells that may be produced by a single land cell. Then, the mobile sedimentary cells may move through transport transitions, which are strongly anisotropic to take into account gravity. In this way, mass transport is driven by the slope and magnitude of

the erosion/deposition processes, which both control the distribution of mobile sedimentary cells. Nevertheless, with this simple set of transitions, there is not yet a retroaction of transport on the erosion rate.

In order to simulate the effect of mechanical incision resulting from sediment motion along slopes or channels, a fundamental characteristic of the real-space CA landscape model is to introduce a coupling between transport and erosion using only next-neighbour interactions. Practically, it takes the form of a chain of transitions: a horizontal transition of transport can trigger a vertical transition of erosion with the probability P_v (Figure 6a). Thus we generate a new microscopic level of interaction between two independent physical processes (see 'Chains of transitions', above) and we end up with a discrete model in which there is a complete feedback mechanism between sediment transport and topography (Figures 6b and 7).

Figure 6b shows the evolution of a flat slope in the absence of any tectonic uplift. We consider closed boundary conditions except at the downstream border where the sediment can escape the system above a certain limit, defined as the outlet height. From the numerical results, we identify different stages in the evolution of topography. First, random erosion and

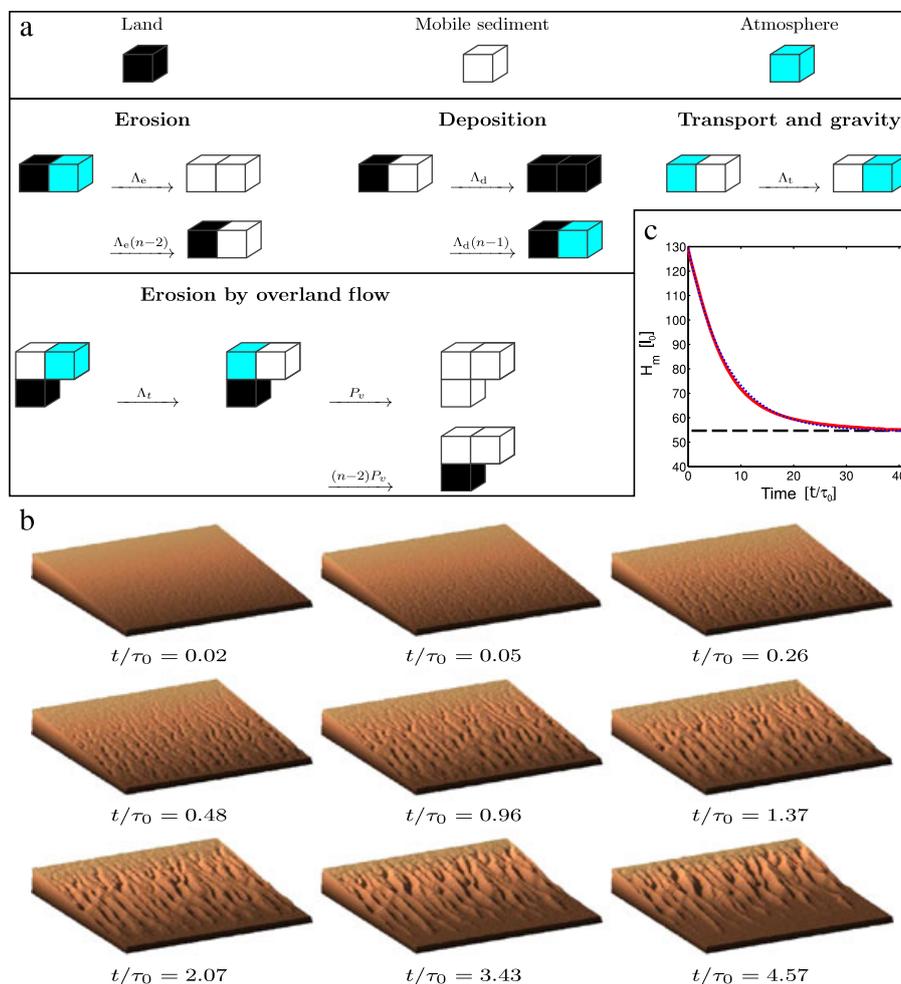


Figure 6. A landscape evolution model using ReSCAL. (a) In the CA model, three states are used to reproduce land, mobile sediment and the atmosphere. One land cell can produce n mobile sedimentary cells. Transitions for erosion, deposition and transport ensure conservation of mass. Here, we only show transitions along one specific direction, but there are six times more transitions in 3D (three doublet orientations and, for each of them, two symmetric doublets). For erosion and deposition, the transition rates are isotropic. To take into account gravity, this is not the case for transport transitions: vertical transition rates are set to 0 and $10^5 \Lambda_t$ for ascending and descending motions, respectively. Erosion by overland flow occurs through a chain of transitions that generates a new level of interaction from transport to erosion processes. (b) Evolution of the topography starting from a constant slope with a horizontal surface of $200 \times 200 l_0^2$. In this model, τ_0 is an arbitrary time scale. We set $\Lambda_e \tau_0 = 1$, $\Lambda_d \tau_0 = 5$, $\Lambda_t \tau_0 = 10$, $P_v = 10^{-2}$ and $n = 3$. (c) Evolution of the mean elevation. The solid line is the mean elevation over long times. The black dashed line shows the outlet height $h_e = 55 l_0$. The dotted line is the best fit of $h_e + (h_0 - h_e) \exp(-t/T)$ to the data with $h_0 = 130 l_0$ and $T/\tau_0 = 16.5$. This figure is available in colour online at wileyonlinelibrary.com/journal/esp

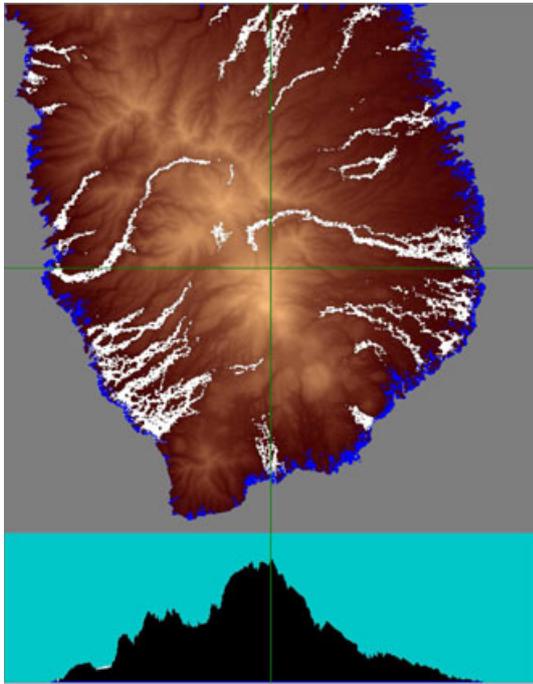


Figure 7. Sediment transport in a natural landscape using ReSCAL. The model applied on the actual topography of the Guadeloupe island, French West Indies. Mobile sedimentary cells are shown in white above the topography to highlight zones of sediment transport (top). The central vertical layer of cells going from left to right (bottom). This figure is available in colour online at wileyonlinelibrary.com/journal/espl

deposition events produce a small-scale roughness. Near the outlet, these small-scale topographic features grow to length scales that can eventually impact the motions of mobile sedimentary cells. The localization of the flow promotes incision and results in the formation of gullies. These gullies are unstable because of the positive feedback from transport to erosion. They are rapidly becoming channels that propagate upstream due to regressive erosion. On each side of these channels a new generation of gullies may appear. Thus the transport of mobile sedimentary cells form a drainage network that exhibits different levels of hierarchy and basins of different sizes. Upstream, as the slope is increasing, gravitational effects compensate for channel incision rate. On the eroded part downstream, a floodplain forms from the accumulation of mobile sedimentary cells. Finally, Figure 6c shows that the overall evolution of the landscape can be characterized by a single exponential decay (Granjon, 1996; Lague, 2001) with a characteristic time scale that could be related to the magnitude of the physical mechanisms implemented at the elementary length scale of the model.

All the landscape features produced by the model are macroscopic expressions of local patterns of interaction. As for the outcomes of laboratory experiments and *in situ* observations, these numerical results may be used to derive empirical laws statistically representative of the evolution of the topography. However, it is first necessary to determine precisely the length and time scales of the model. Different strategies may be suitable to set up these dimensions but, given the systematic occurrence of evenly spaced ridges and valleys in nature, the most promising lies in the mechanism of channel incision. By comparison with natural observations and solutions of nonlinear advection–diffusion equations (Perron *et al.*, 2009), the characteristic wavelength for channel inception in the model may be used to evaluate the elementary length scale of the cubic lattice. The time scale may then be derived from sediment flux in active channels.

Using this preliminary version of the real-space CA landscape model, we have observed that it is difficult to reproduce

large-scale depositional features like alluvial fans. For this purpose, the model can certainly be improved by including more realistic dependence of the transport capacity on the local configuration of mobile sedimentary cells. Nevertheless, this version of the model has already raised an important issue. Using only a single set of nearest-neighbour transitions, it is possible to reproduce a wide range of structures and dynamical behaviours that may be directly compared to the development of topography in nature. Overall, this indicates that, from steep unchannelled valleys to zones of deposition, a simple set of transitions may play the same role as a large number of geomorphological laws (see Table 1 of Dietrich and Perron, 2006). This opens new perspectives for the future of reduced-complexity models in geomorphology.

Concluding Remarks

ReSCAL is a scientific computing tool dedicated to the development of CA models in natural sciences. In geomorphology in particular, there are still a lack of theoretical formalisms and a limited understanding of the role of structural and compositional heterogeneities (Dietrich *et al.*, 2003). The CA approach can then be described as an alternative which focuses more on organization and pattern formation than on an exact description of small-scale physical and chemical processes. The basic assumption is that it is possible to work at another level of description on the basis of a collection of interacting elements. Therefore, it is necessary to develop new methods that take into account discontinuities and patterns of interaction between the various components of a system over time. Ultimately, the objective is to identify collective behaviours that depend only on a limited number of control parameters. Thus we may describe in greater detail the feedback mechanisms that may be encountered in natural sciences using comparisons between observations and the outputs of numerical simulations.

ReSCAL can be applied and developed to address challenging issues in the interdisciplinary field of complexity science. Traditionally, different methods have been used for the analysis of complex systems. The most popular method is based on the theory of dynamical systems (Manneville, 1991). It uses sets of coupled differential equations to reproduce a large variety of highly nonlinear behaviours. Nevertheless, as the number of degrees of freedom increases, it is generally impossible to find analytical solutions and all the results rely on the accuracy of the underlying numerical methods. In addition, as the solutions strongly depend on a predefined set of parametrized equations, this approach requires a deep understanding of all the microscopic couplings that may play a role in the dynamics of the system. Statistical physics is another method which focuses on systems with an infinite number of degrees of freedom (e.g. an ideal gas) and uses different techniques of averaging to describe the global equilibrium states of these systems. However, this approach does not adequately account for pattern formation and organization in open systems (Nicolis and Prigogine, 1977).

Dealing with a finite, but large, number of elements interacting with one another, the complex system science lies at the interface between dynamical systems and statistical physics. In this line of research, it is admitted that each complex system is different and that there is not a unique framework based on a comprehensive and codified set of laws. Then, the CA approach exploits computing power to study pattern formation by means of numerical simulations. Using ReSCAL, the general idea is not to address complex system analysis as an abstract modelling approach reserved to a small community of specialists, but to develop new collaborative efforts based first on observation. Indeed, CA models should not only be used to

reproduce known phenomena but also to identify new observables that will provide additional information on the global dynamics of complex systems. Then, numerical outputs can be used as a predictive tool to isolate precursory phenomena that would otherwise remain invisible (Shebalin *et al.*, 2011, 2012).

We do not only propose here a CA method, but also a strategy to determine the arbitrary length scales which are always involved in this type of discrete modelling approach. As shown by Narteau *et al.* (2009) with a CA dune model, the method consists of directly comparing, with the same techniques (e.g. linear stability analysis), the collective behaviours of the model with large-scale phenomena in nature. Thus we work at a macroscopic level of description to identify similar mechanisms of emergence and derive from them the elementary length and time scales of the model. Using this scaling, we can try to establish new links between CA methods and continuum mechanics to constrain the expression of complexity by a set of well-defined physical quantities. In all cases, we may learn lessons from the most distinctive features of the numerical objects under investigation (Le Mouél *et al.*, 2005).

ReSCAL has been shown to be effective in reproducing patterns that have never been accessible to numerical simulations before (Zhang *et al.*, 2010, 2012). We infer that it is because we focus first on nearest-neighbour interactions instead of predetermined sets of laws, which are assumed to be true for all time and places. This is also due to the stochastic nature of the model. Indeed, even if they are extremely rare, low-probability events may occur and trigger an instability which can develop at all scales.

Using a real-space representation, the cellular spaces of the different models may also be compared to analogue laboratory experiments and should be constructed following the same standards (e.g. physical environment, boundary conditions). An advantage of the CA models is that the entire configuration of the system can be easily adapted by changing the states of well-identified cells. In addition, as in all agent-based models, individual cells can be tracked in order to quantitatively estimate their migration history.

Finally, we conclude that ReSCAL provides a useful method to further explore complex systems in natural and human sciences with reasonable numerical efficiency. Obviously, it has to be done through the collaborative development of models that may be applied by various scientific communities.

Data and Resources

The Real-Space Cellular Automaton Laboratory (ReSCAL) is free software under the GNU general public licence. The source codes can be downloaded from <http://www.ipgp.fr/~rozier/rescal>.

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