Geoscientific
Model Development
Discussions

Interactive comment on "CellLab-CTS 2015: a Python library for continuous-time stochastic cellular automaton modeling using Landlab" *by* G. E. Tucker et al.

C. NARTEAU (Referee)

narteau@ipgp.fr

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This paper presents a flexible Python library for creating continuous-time cellular automaton models. I think this an interesting paper, which presents important and innovative advances for the discrete modeling of natural systems.

From my point of view, the main novelty is the treatment and the tracking of individual cells. The addition of metadata into cells (i.e., the accumulation of information about the current state of a cell) provides a decisive improvement in the direct determination of an entire range of properties that depend on the space-time trajectory of a particle within a system. There are applications in all domains of science for which the current

physical and/or chemical states of an element depend on its past history.

With the development of computing power, there was a diversification of the types of continuous models from the resolution of nonlinear partial differential equations to discrete elements methods. I consider that the type of models proposed here by *Tucker et al.* transpose such a diversification strategy into the cellular automaton formalism. As far as I can judge, the GMD journal seems perfectly appropriate for this kind of theoretical developments.

The paper is well organized, and all the most interesting properties of this new python library are solidly illustrated and supported by the results of the selected models. The more detailed comments on the manuscript listed below are purely editorial, and I enthusiastically recommend publishing with minor revision.

Detailed comments

- I would suggest a less technical title such as
    "Continuous-time stochastic cellular automata modeling using Landlab"

- Check *"pair-wise"* or *"pairwise"*.

- 9509-Line 6: *"bedforms"* instead of *"dunes"*, to enclose both ripples and dunes.

- Sections 3 and 4.3: please specify that each pairwise transition is associated with a time-independent stationary Poisson process.

- Section 4.3: the choice of the python language has benefits (multi-platform, object-oriented) and some disadvantages (slower than C, and it is not easy to make multi-threading). Concerning the algorithm itself, the event queue method is a practical approach, which may have a high memory cost. In addition, this

method cannot be implemented for (externally controlled) time-dependent transition rates. In this case, all the transition times should be recalculated and sorted again.

- Section 4.6: this is a new and valuable contribution to research, which is perfectly illustrated by the model of the luminescence signal. I have the feeling that realistic signals can be easily obtained using macroscopic properties as arguments of the callback function, for example some information about the sediment concentration with depth.

How do you plan to track the position of individual cells (see for example Zhang et al., 2014) ?

- Section 5.1: from Fig. 9, I understand that you only consider isotropic transitions from *rock→saprolite* to *saprolite→saprolite* states. Could you check it in the text (9524-Line 24) ?

Considering saturation, a major challenge in studying weathering is to couple a dissolution-crystallisation model with the modeling of the flow in a fracture network.

- Section 5.2: nice example of an epidemic-type model that could be analyzed using the different grid types, an advantage of the proposed library.

Roughly, I imagine that the disease propagates if an infected cell can at least infect another cell before it recovers. In a next-neighbor approach, such as the one proposed here, the threshold-values of the rate parameters for death or recovery should depend on the grid type.

- Section 5.3: it is quite a rather unconventional lattice gas model, essentially because it is not synchronous and deterministic. Then, it takes advantage of pairwise transition to deal with multiple-choice transitions. Such a new and provocative model is therefore a perfect illustration of the richness of the approach and I

understand why it is presented here. In the future, this model needs to be developed in a dedicated manuscript, for example studying more closely the hourglass problem (Fig. 15).

At this stage, it is a nice example of what can be done with pairwise transitions and, for the cohesion of the manuscript, I recommend to add a discussion about the time scales in this model and how the continuous time approach may contribute to some classical problems in modeling granular flows.

From Fig. 11, I am not sure to be able to reproduce all the motion and collision rules. For example, I have the feeling that two oblique transition are missing. There are 9 different states. For the considered pair orientation, is it possible to see all the 9^2 transitions in a single table ? I think it will be really useful, at least in supplementary material. Then, anyone can take it and obtain all the possible transitions by rotation.

In Fig. 11, check that a probability is assigned to all multiple-choice transitions. Note that I would prefer no probability as soon as the (new part of the) method is based on asynchronous transitions and independent transition rates for each of them. You can just specify in the caption that, when there is more than one transition for a doublet, all transition rates are equal such that all transitions have the same occurrence probability. It can be generalized to all transition rates for all doublets.

How the number of particles affect the result shown in Fig. 12 ? It is not important at this stage, but it is clear that the density of particle in lattice gas model is a critical parameter.

Could you clarify what are f and e, and why you use a relation such as $f = 1 - e$. e is a coefficient of restitution in the text (9527-Line 29), while it is a rate in caption of Fig. 13.

- First paragraph of the Discussion: It is right that this approach can be used to

mimic micro-scale processes. However, it can also be used to investigate systems starting from an intermediate length scale which integrates information from smaller scales. In other word, the elementary length scale of this type of model (i.e, the characteristic size of an individual cell in the model) does not have to be associated with a single discrete element in nature. It can also be a representation of the physical environment at a given length scale.

As soon as the elementary length and time scales of the model are assimilated as internal units of the numerical model, the time-implementation scheme gives the opportunity to analyze large-scale phenomena using only these quantities. Then, in the natural environment under consideration, the exact values of these units may be derived a-posteriori from observations or another theoretical framework. Such a rescaling strategy has shown to be efficient and robust in the modeling of dunes.

To account for these comments, I can propose to:
(9529-Line7) replace *"micro-physics"* by *"relevant length scale"*.
(9529-Line 10) remove *"such as sediment grains"*.
(9529-Line 11) replace
"This approach can shed light on the relationship between micro-scale and macro-scale behavior, rather than simply having to assume a particular relationship."
by
"Starting from an elementary length scale, this approach can shed light on collective behaviors which may be difficult to simulate when assuming a particular relationship."

- Second paragraph of the Discussion: With respect to the previous comment, I think that it is possible to model heterogeneous granular systems. In this case, it is necessary to work at a length scale that incorporate more than a single grain. From my point of view, the main challenge with cell-pair transition is to incorpo-

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rate long-range processes such as potential fields or elastic stresses. A solution may be to consider multiscale cellular automaton (see for example *Blanter et al. (1999)* or *Narteau (2007)*), but this is another story.

Bibliography

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