Geosci. Model Dev. Discuss., 8, C3905–C3914, 2016
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Geoscientific Model Development Discussions
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8, C3905–C3914, 2016

Interactive Comment

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

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Received and published: 31 January 2016

In the following, reviewer comments are shown in *italics*, and our responses are shown in plain text.

1 Comments by C. Narteau

This paper presents a flexible Python library for creating continuous-time cellular automaton models. I think this an interesting paper, which presents important and inno-

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vative 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.

We appreciate Prof. Narteau's comments, and are grateful for the time he has taken to review the manuscript.

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

Good idea. The facts that the software is a programming library and that it is written in Python both appear in the first sentence of the abstract, so it is reasonable to remove them from the title. However, in keeping with GMD format, we have kept the name and version number of the software.

Check "pair-wise" or"pairwise".

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"Pairwise" seems to be in common use, so changed to this usage throughout.

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

Changed as suggested.

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

Changed text in Section 3 to read "Using Poisson process theory, we can describe each pairwise transition with a time-independent stationary Poisson process. The probability distribution of time to the next transition at a particular pair is...". Inserted sentence at the beginning of 4.3, which now reads "Unlike a traditional discrete-time CA, CellLab-CTS does not use time steps. Instead, we iterate through a sequence of pair transitions, or *events*. As noted earlier, each pairwise transition is associated with a time-independent stationary Poisson process. Thus, the time intervals between successive transition events at a particular location are stochastic, with an exponential probability distribution."

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.

This is a fair summary of strengths and weaknesses of the algorithmic implementation. Because these issues are addressed in the Discussion section, and the reviewer seems to be simply making some observations rather than suggesting particu-

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lar changes in the manuscript, we have not made any modifications in response to this comment.

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 argu- ments 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) ?

To answer this question for readers, the text in what is now the 3rd paragraph in Section 4.6 has been expanded to: "For each transition involving such an exchange, the simulation keeps track of the location of the properties in question, thereby allowing the positions of individual particles to be tracked. Each node location is assigned a *property ID* that points to the array element in which property data for that particle are stored. This array element also corresponds to the original starting location of the particle in question. For example, suppose that property data for node 5 are stored at array location 19. This would indicate that the particle represented by node 5 began at node 19 and subsequently moved to node 5."

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 net- work.

The confusion is understandable. Yes, the transitions are isotropic. To make this clearer, we added the following text: "These transitions represent isotropic transformation of rock-saprolite pairs to rock-rock pairs (two transitions are necessary because

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ordering matters: 0-1 is a different pairing than 1-0, and so both must be included in order to implement isotropic transitions)."

Regarding dissolution-crystallization, yes, this is what we were getting at. Now added sentence "An interesting future challenge would be to couple a dissolution-crystallisation model with a model of aqueous flow in the 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.

Yes, exactly. We now mention this in the discussion section: "The ability to switch between grid types makes it possible to test whether grid type has any influence on the solutions, and if so, to correct for it."

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 con- tribute to some classical problems in modeling granular flows.

In fact, the lattice-grain example is part of an application of the model that we are working on, and we plan future paper(s) on this topic. We added a comment on the

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time scale: “This parameter [g] sets the time-scale for the model; $1/g$ is intended to represent the time required for an initially stationary grain to fall a distance of one cell.”

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 92 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.

We have added a second table listing all pairs and their transitions (if any) for one of the three orientations. Note that this is labeled as Table 2, but it would serve well as an appendix or supplement rather than appearing in the main text.

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.

We have added text to the caption to address this issue.

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.

Yes, particle density is a critical parameter in lattice-gas models. In this case, the average density is conserved as indicated in the figure. We feel that further discussion of this point would detract from the focus of the paper, and is best left for later work.

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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.

We have added text in this section to clarify that e is a rate that is related to a coefficient of restitution.

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."

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"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."

Great point and suggested modifications, which we have adopted in the revised text (with some modification to the above).

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 incorporate 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.

We appreciate the suggestion and references. We expanded on the relevant sentence to hint that there may be hope of a solution to the multi-size problem.

2 Comments by T. Coulthard

This is an interesting description of a set of Python libraries/routines for implement- ing a different way of treating CA. It is well written, easy to follow and very well described. I have but a few minor comments below - and would also draw to the authors attention that if there are any movies/video's of the model operation (there are graphics/screen grabs) then these can now be DOI'd and citable via GMD... http:// www.copernicus.org/ news_and_press/ 2015-10-29_cooperation-tib-av.html

We appreciate learning about this capability, and are thinking seriously of taking advantage of it with a set of papers related to Landlab that are planned for the near future.

9509: 15: "These models are especially attractive for geoscience applications because

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their parameters represent rates that can be directly related to field and laboratory measurements, and because they avoid the need for a discrete-time approximation (Narteau et al., 2001, 2009; Rozier and Narteau, 2014)." - can this statement be expanded/fleshed out a little? I think its critical to the readers understanding of why this method may be better than traditional CA.

Right. The notion is indeed a bit hard to grasp at first. We have added a sentence to help clarify. We could go into greater depth here, but in this part of the manuscript we want to get the reader quickly to the statement of summary and objectives of the paper; therefore, we do not elaborate further here but instead rely on the examples later, as well as the references given.

9510 - only Wolfram referenced in the first paragraph (1-17). - maybe a reference or two to back up these statements?

We added a reference to the excellent book on CA by Chopard and Droz.

section 3 9511-9522. A good clear description and example - but what is the advantage - or clear reason for using this method over other ways? Possibly compare to how this might be carried out with a regular CA (or could not if that is the case..)? There is some discussion of this in the - discussion - but I wonder if some arguments might be better explained with the example here?

We have added a paragraph toward the end of section 3 that comments on the value of a stochastic CA approach: “The suspended-sediment model illustrates the advantage of a stochastic, as opposed to deterministic, approach: we are dealing with a system that is in fact inherently stochastic and unpredictable, because the grain motions arise from turbulent velocity fluctuations. It is of interest to know how this inherent variability leads to emergent pattern formation, such as the diffusion-like time evolution of average concentration (without settling) or the development of a Rouse-like concentration profile (with settling).”

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Interactive comment on Geosci. Model Dev. Discuss., 8, 9507, 2015.

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