#### 1 Authors Response to Refereed Comments for gmd-2021-66

2 Dear GMD Referees,

I can not thank you enough for taking the time to do a thorough review of my paper 'Spatial Agents for Geological Surface Modelling'. Especially, since there are, as noted in your review intro's, aspects that you may not have been familiar with either from the agent side, or from the structural geology perspective. To be sure, the programing that was done in Netlogo is also not familiar to many researchers. It is an interesting proto-typing environment that is easy to learn and accessible to the public, so perhaps that may help in reaching the masses. Your comments are both appreciated, and I hope all dealt with, as outlined below, with an aim to increasing readability and clarity for a wider audience. I tried to do my best to address your concerns through re-organizing, adding definitions of terms, making key points early and adding some relevant references should someone pick up this research in the future. I also added a new figure (Fig. 5) summarizing agent communications that shows, in a basic way, how the main components of the system work.

- 12 I have not seen any other comments or concerns come in through the GMD discussion site, but perhaps there may be a need 13 to address things after reading this version and posting it on the GMD site.
- 14 Regards,

trick. Idep

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- 16 Eric A. de Kemp
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- 18 Ottawa, Canada
- 19
- 20 Note Author Responses in (Arial Font) Dark Red (with Review Simple Markup)
- 21 Page and Line numbers from new document Spatial\_Agents\_GMD\_r5.pdf (Markup on).
- 22

#### 23 Comment on gmd-2021-66

- 24 Anonymous Referee #1
- 25 Referee comment on "Spatial Agents for Geological Surface Modelling" by Eric A. de Kemp,
- 26 Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2021-66-RC1, 2021
- 27 General comments:
- 28 I'll start with a caveat: in retrospect, I am probably not be an ideal reviewer for this
- 29 paper, as I have no experience in the application of solid modeling techniques to infer and
- 30 visualize subsurface geological structures. However, a silver lining maybe is that I can
- provide a general geoscience perspective on this paper.
- This is probably a good thing as, I believe, it forced me to make things more understandable for the nonspecialist.
- 35
- 36 (One terminology note: the phrase 'geological modelling' is used here to mean creating
- 37 digital representations of 3D sub-surface geological structures, but the same term also

refers to the use of numerical models to study the dynamics of geological and geophysical
systems. These are very different things, so a definition early in the paper would be
helpful.)
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I have included a line in the abstract "...approaches to creating 3D geological models involves development of
surface components that represent spatial geological features, horizons, faults and folds, and then assembling
them into a framework model as context for down-stream property modelling applications (geophysical inversions,
thermo-mechanical simulations, fracture density models etc.)." to clarify this modelling definition.

10 11 In addition ....

P.2, L.24 ... Introduction "Herein we focus on the starting framework model, the stratigraphic and structural
 surface model that provides the initial context for these more down-stream property embedded modelling efforts."

This paper makes two valuable contributions. First, it evaluates the use of agent-based
modeling techniques, which are widely used to study system dynamics in fields like
ecology and sociology, for inferring and graphically representing 3D geological structures
from sparse data.

- 19
- 20 That is a good characterization of what I was trying to do.21
- Second, it presents a new open-source software package to carry outthis kind of modeling, using the NetLogo package.
- 24
- Yes, for sure and hopefully initiate future research with other agent environments.
- 27 To the best of my (admittedly limited)
- knowledge, both of these represent novel, interesting, and valuable contributions. And
  clearly a tremendous amount of effort has gone into developing the ideas and the
  accompanying software implementation.
- 32 Excellent, thank you for that!
- 33

- 34 For these reasons, I feel that the manuscript is
- appropriate for Geoscientific Model Development, and should find an audience among
   geologists who are interested in inferring subsurface geological structures from limited
- 37 observations.
- 38
- 39 Great!
- 40
- 41 One of the challenges with this manuscript is that it assumes a lot of background
- knowledge on the part of the reader, which risks limiting its impact. One recommendationtherefore is to do some fairly thorough editing to make it more widely accessible.
- 44
- I fully agree. Without pointing out all changes, the mark-up document in word is maybe the best
  way to go to check these changes. The Spatial\_Agents\_GMD\_r5.pdf content is also loaded, below, to
  see the extensive changes that have been made.
- 49 One thing that I believe would help is some re-ordering of the information presented,
- 50 especially in the introduction. Such re-ordering could make this manuscript accessible to a
- 51 wider audience, and therefore draw more attention to this important work. Here's one
- 52 potential re-organization of the introductory material:

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The intro (P.2,L.15 to P.9,L5) has been expanded, with more sections and completely re-organized with lots of re-writing to make things clearer. I spell out more clearly what the problem is and the challenges we face in modelling, and importantly why the agents may be helpful in dealing with this. An early reference to Fig. 1 should help as it visually states the problem with standard models looking like nothing seen in geology.

9 "The *major challenge* that this paper is trying to address is the breakdown in achieving geologically realistic model results 10 from sparse data in more complicated geological scenarios when using the existing methods and algorithms. This is no doubt 11 a problem in other modelling domains as well, but is acute in geological applications, where access to data in the subsurface 12 is often extremely expensive, terrain access prohibitive, or the depth of investigation too extreme for direct sampling and 13 must rely on coarser geophysical methods that often do not adequately image the features being modelled. This paper 14 explorers the use of extension, propagation and cohesion methods, which can be considered part of 'swarm' technology, 15 using spatial agents in an attempt to deal with this challenge.

Geological modelling covers a wide range of applications and domains from thermo-mechanical modelling (Cloetingh et al., 2013) to basin analysis (Barrett et al., 2018), mineral potential estimation (Skirrow et al., 2019) in 3D (Hu et al., 2020;
Sprague et al., 2006) and even 4D applications (Parquer et al., 2020; White, 2013). *Herein we focus on the starting framework model*, the stratigraphic and structural surface model that provides the initial context for these more down-stream property embedded modelling efforts. "

a - Explain briefly what is meant by geological modelling in this paper, and why it matters
(a few sentences or a paragraph, with general references for those unfamiliar with the
field/area).

26 See above comments.

b - Explain the major challenges that this paper and the techniques and software it
describes are meant to address (e.g., sparse information about the subsurface,
uncertainty in 3D location and/or properties, long computation times using standard
algorithms, or whatever)

33 again, see above comments.

c - Explain why current methods are limited (i.e., why do we need a new and different
approach?), and thus why it's worth trying an alternative approach.

In P.3, L.7, I add an explanation as to why we need a new approach and agents may be theanswer...

This is dealt with also in a new titled section 1.1 Agent Challenge and later in (P.5, L.8) 1.4 Role of *Interpretation*, (P.8 L.10) which is really what we do now to deal with sparse data; we use our
knowledge either instead of algorithms, or to supplement them.

43

44 "Existing methods applied to the combined sparse data and complex geology scenario, will tend to produce holes, gaps

45 and feature drop-outs, away from control data, as well as arbitrary horizon thickness changes that combine to give a

46 geologically unreasonable bubble gum look to these models (Fig. 1). Current methods in sparse data configurations tend to

bias for these unrealistic geometries using radial based kernel functions, optimized for local smoothness in order to achieve
a mathematical solution (Hillier et al., 2021; Hillier et al., 2014). This often comes at the price of geological realism (Hillier et al.)

a mathematical solution (miller et al., 2021; miller et al., 2014). This often comes at the price of geological fealism (Hiller et al., 2021; MacCormack and Eyles; 2012). Is it possible that, with a new approach, geological features could be more

- 50 realistically modelled by using spatial agents to 'fill-the-gaps' in the process?"
- 51 52

d - Give a quick background summary (2-3 sentences) on agent-based modeling that
gives readers a basic sense of what it is, e.g., that it's a technique used in simulation
modeling of complex systems in which individual entities such as animals or households
interact with an environment and with one another.

6 This has been dealt with in Intro Section 1.2 (P.6, L.3...) 7

8 "In general, an agent-based system is used to see the effects of autonomous individuals, groups or objects on the overall
9 system when solutions are onerous and/or computationally expensive. A global algorithm involving a single large multi10 parameter matrix inversion may take many days to compute with a single outcome, but an agent-based model may be able to
11 produce several outcomes in minutes or hours (Siegfried, 2014). Agent-based models have their roots in the development of
12 cellular automata and complexity theory, which has been able to model complex natural and artificial systems with simple
13 neighbourhood algorithms (Cervelle and Formenti, 2009; Wolfram, 1994; Von Neumann, 1966)...."

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e - wrap up the intro with a quick summary of what this paper does (maybe this is a good place to say you're doing this in the context of Loop 3D, and explain briefly what that is).
This way, by the end of your Intro section, readers will know what problem you are trying to solve, why it matters, why it is a problem, and what (basically) your proposed approach is. You have all of the pieces already, but they are currently presented in an order that risks leaving readers drowning in a sea of jargon before they have a chance to get to the cool new ideas and techniques.

Agreed, to much jargon. All the pieces have been re-ordered. It flows a bit better, in my opinion.
The end of the intro (P.3, L.7-24) is much improved and clearer for the general modeller.

The general Intro is followed by sections 1.1 to 1.5. More details and explanations were added in
these sections. I added two references from Brodaric on interpretation that will give some
background on geologic mapping practice. 3D modelling is just an extension of this 2D practice
that requires mental extension and propagation functions from experience of natural forms. We
want to capitalize on some of these functions with agents. (Cohesion, extension etc.)

- 3233 (P. 5, L.1) Section 1.1 Agent Challenge
- 34 (P. 6, L.3) Section 1.2 Agent Applications
- 35 (P.7, L.13) Section 1.3 Agent Characteristics
- 36 (P.8, L.10) Section 1.4 Role of Interpretation
- 37 (P.8, L.22) Section 1.5 Demonstration Codes38

These could all be wrapped into a section 2 and the rest of the sections incremented, but I felt each
of these sections was just an intro into the topics that do get more elaborated later in the paper.
This could be changed, perhaps it would flow better?

42

A related challenge is that the manuscript does not really articulate (at least not until deep
into the details) what is wrong with current modeling algorithms and why an agent-based
approach might offer a better alternative. A couple of sentences articulating this
somewhere in the introduction would help motivate the rest of the paper.

- 47
- 48 This is now up front in the intro ...
- 49 (P. 5, L.1) Section 1.1 Agent Challenge
- 50

51 One general grammatical note: the manuscript contains quite a few incomplete sentences,

52 which need to be fixed before final publication. I have flagged some of these below with

1 'inc'.

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3 Thanks for taking the time to look at these. These were all fixed. I do have some kind of mental
4 block with starting sentences with a conjunction; such as, for example ...

6 Specific comments (by page and line numbers):

7 1, 13-15 this opening statement of the abstract is a nice example of the challenge readers 8 face with this piece (but there is a potential fix). For a reader to care about the topic in this sentence, they have to know what is meant by 'spatial and property interrogation 9 functions' and 'estimations and construction operations'. It's only at the end of the 10 11 sentence that we get to the heart of the matter: 3D geological surfaces. You have an opportunity to invert this in a way that could make it more accessible. Start off with a 12 statement about how important it is build 3D-rendered models of geologic structures, and 13 how the sparsity of data makes this difficult. Then state that agent-based modeling 14 15 provides a potential solution, and that the contribution of this paper is to test it out. By laying out the ideas in this sequence, right away you have presented an interesting 16 research challenge, and followed up with a solution. Now the reader has a reason to care 17 18 about technical things like property interrogation functions.

Absolutely. I was too close to the trees on this. The abstract is re-written with a new paragraph
added, to focus on the problem that the Geological surveys face, in-fact my own work practice
faces this every day and a major reason I started going down this road. The abstract is still under
500 words.

P.1, L.13 "Increased availability and use of 3D rendered geological models has provided society with predictive
 capabilities, supporting natural resource assessments, hazards awareness and infrastructure development. The Geological
 Survey of Canada, along with other such institutions, have been trying to standardize and operationalize this modelling
 practice."

1, 18-19 geologic modelling has multiple meanings - please define what you mean by it inthis context.

33 See comments above. Dealt with.

2, 3-22 As noted above, the introduction is hard to follow. It could benefit from a clearer
articulation of the nature of the goal and the need for solutions. In particular, it sounds
like the core problem is one of limited data, so why does the answer lie in software
architecture? How do those two things relate?

40 Again, see comments above on the restructuring and enhancement to the intro with a new section 1.4 Role of Interpretation. The limited data and software architecture relationship is dealt with 41 42 (P.8,L.19) by showing the link between knowledge driven map interpretation (drawing lines on 2D surfaces with some trend geometry data points) in 2D, and ability of agents to links features 43 sampled with sparse data. I do not make an elaborate final application that does this, but I think 44 45 there is enough there to demonstrate that with all the pieces, in this agent framework, it could be 46 done. Down the road, I think especially the cohesion and eventually rheological (stiffness; response 47 to stress; fold characteristics etc.) properties of agents could help here.

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49 "Spatial agents have the potential to support this interpretive role, provided some of their key characteristics can be leveraged towards geological feature estimation and feature to feature relationship extension. This could be accomplished by more efficient exploration of the model solution space through extension of horizon contacts, fault networks and fabrics."

1 2 2, 23 - 3, 1: I have some familiarity with agent-based modelling but I worry that readers 3 who have never heard of it would struggle to get the basic idea from this somewhat abstract description. Maybe it would help to start off not by identifying different categories 4 of ABMs, but instead to convey the gist of the technique first and what fields it is used in 5 (which you address later in the MS; e.g., to simulate individual entities in computer 6 7 games, animals in ecological simulations, households or sectors in economic simulations, 8 etc.) I do like the carpenter example (examples are always helpful) but in that particular example it's not clear why 'single agent' applies (is the carpenter one agent, and the 9 house another? is there only one carpenter?) 10

12 Yes, agreed. I move the general agent introduction and explanation earlier in the paper. 13

3, 8 Surely ABMs can themselves be computationally expensive. It is not clear why they
would be expected to reduce computation time relative to whatever the alternatives might
be (presumably some kind of 'global' algorithm?).

I include a reference from Siegfried (2014) to support this, see his text intro on 1.1 Motivation
where he argues that for "Solving complex systems ... characterized by non-linear aggregate behavior (i.e. The
aggregate behavior of the individual components is not derivable from the summation of the activities of individual
components)" and he goes on to say that complex natural systems are essentially requiring a simulation approach
to model in a meaningful way. I think the structural agent framework is just that kind of solution.

24 I agree, for me it is more of an intuitive notion and yes, I am leaping a bit. I have seen firsthand what matrix 25 solvers (large multi-parameter inversions) for geoscience data (geophysical, structural inversion) can provide. It is 26 far from satisfactory, and is like trying to tie thousands of elastics with various strengths (weights) inside a multi-27 sided container with movable walls. You may eventually (after a very long time) get the container to be stable and 28 stand on its own, but it will look nothing like it was supposed to represent. With agents there is no balancing act, 29 to invert a large mathematically conditioned matrix, that may or may not be solvable. Instead, we allow the system 30 to do simpler calculations, with simple rules at the local level. Perhaps a solution, or similar but many solutions, 31 emerge depending on how well we have designed the system. It does seem intuitively more natural and more 32 efficient to do this. This has yet to be rigorously tested, which I have only scratched the surface of in this study. 33 That is why I wanted it to be a more concept paper.

35 3, 15-18 This is a useful statement of the paper's objective. It sets up readers to expect to
36 learn next what are these graphical tasks, and why agent-based techniques makes them
37 easier or more efficient or more effective, etc.
38

39 Good.

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41 3, 20 - 4, 2 This is a nice overview of ABM applications. Consider moving it before the
42 more abstract discussion of agent properties. It gives readers a sense for how and why
43 the technique is used.

45 Yes, the section was moved to an earlier part of the paper.

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47 4, 3-15 It is not totally clear what you mean by anisotropy and gradient-type information.
48 Consider leaving that bit for later, when the application examples will make it easier to
49 understand in context. More generally, there is a lot of jargon in this paragraph: to make
50 sense of it, a reader has to know what you mean by multi-scalar environment, model
51 element interactions, multi-source physical dependencies, non-centralized control
52 structures, global partitioned data structures, etc. Consider either adding text to define
53 these various terms, or deleting them, or replacing them with more accessible

1 descriptions. That said, the examples are great; in general, more examples and fewer 2 jargon terms would help. 3 Definitions for Anisotropy, gradient-type and jargon clarified. 4 5 See P.5, L.20 "better model the local structural trends or anisotropy, and extend features such as regional fold 6 plunges." 7 8 Intro rewording and added examples to help clarify terms along with multi-scalar use is brought 9 out in the example in the intro of molecular to galactic modelling. 10 (see P.6,L.20 to P.7,L1) 11 12 "These applications generally do not use trend information, or what structural geologists refer to as anisotropy, and gradient 13 type information such as horizon dip data, with polarity, or direction, which the structural agents do in this study, however 14 these diverse applications do have some common elements that software agents are well suited to. The problem domains have 15 multi-scalar environments; molecular to planet scale, with local or global model element interactions, and non-linear, multi-16 source physical dependencies. Agents could be interacting at molecular scale with quantum-mechanical, ionic and 17 thermodynamic influences, for example, for protein-folding (Semenchenko et al., 2016; Nelson et al., 2000), for a visual 18 demonstration of molecular agent simulation see: https://www.youtube.com/watch?v=4Z4KwuUfh0A or at galactic scale 19 http://www.gravitysim.net/index.html." 20 21 section 1.3 this is a good description of the problem of interpreting a 3D subsurface geologic structure given sparse data. Consider moving it, or a suitably edited version of it, 22 23 up near the beginning of the paper, where you are framing the fundamental problem to be 24 solved. 25 This was moved, now in the abstract and general introduction section. 26 27 section 1.4: It is great that there are example codes provided. 28 Actually, most of the work over the last few years was in developing these codes. 29 30 section 2, 2-5 This sentence or something like it would be helpful in the first paragraph of 31 the paper to educate the reader on what is meant in this context by 'geological modelling'. 32 33 Yes, agreed. See earlier comments, this was reworded and moved up. 34 35 6, 11-12 and fig 1: nice illustration of the challenge, and how different algorithms can 36 come up with very different solutions given the same data. Suggest moving this figure up 37 closer to the opening of the manuscript. 38 39 Indeed, Figure 1 is now earlier as part of the introduction. 40 41 8, 19 I'm not familiar with the terms 'line and fabric densification' or 'contact estimation' -42 some definitions would help here. 43 44 Section 2.1 Structural Agents, has a more information now and less jargon. Formlines are defined 45 and some jargon deleted. 46 47 (P.10,L.25) "Typically, structural trends are manually traced in 2D, on maps and cross sections, with what are referred to as 'form lines' 48 49 that match the local planar fabric observations." 50 51 section 2.1 This section says a bit about what tasks agents are used to achieve (e.g., interpolation) but so far one thing that is missing is an explanation of why agent-based 52

1 algorithms might be expected to do a better job than the more conventional alternatives. 2 For example, is the idea that a large number of agents, each implementing a fairly simple 3 set of rules, would be easier to program, or faster to run, or less costly in memory resources, than a running a single but presumably more complicated 'global' algorithm? Or 4 that an agent based approach makes it easier to adapt sampling density according to local 5 features in the data, because agents can 'signal' one another or spawn new agents in 6 7 response to finding something 'interesting' (by whatever criteria) in the data? Whatever 8 the case, this paper would really benefit from a concise statement about how and why agents might be expected to provide a better solution (and along the way, to tell us a bit 9 about what the standard, non-agent algorithms and methods look like, and why they are 10 11 problematic). 12 13 Yes, I agree a better explanation was needed. I added new text going into more detail.... 14 15 (P. 10, L.17-21) "The major benefit of spatial agents is that they can be programed to act as a swarm. That is, they can act 16 collectively, having cohesion with their local neighbours, thus providing the spatial continuity required to construct 17 continuous features. The swarm may also be given shape-based rules, such as, keep members on a local plane or within a

specified degree of curvature. This is difficult to achieve with a global algorithm; inverting a matrix containing all
 constraining data and properties."

With the re-organization of the paper and new text in the introduction, and better explanation of the structural
agents the issue of how and why the agents might provide a *'better and more efficient solution'* is partially
addressed. It is more explicitly dealt with in new text at (P.7,L.1-6)

"The ability to operate in a non-centralized control structure, being sensitive to other neighbours conditions and geometric
states as well as their ability to respond to local or globally changing conditions may give spatial agents an advantage. Their
independence allows them to operate as individual elements, for example a single point observation, or to work collectively
as a team or 'swarm'. This allows the application of agent rules that may determine local cohesion levels and shape
characteristics as well as changes of state depending on specific conditions such as moving in a direction, stopping, or
spawning other processes."

31 32

33 8, 21-23 The idea that agents construct triangular meshes from point data is alluded to 34 here, and shown in Fig 4, but the description is relegated to an appendix. Yet this actually 35 seems important enough to consider pulling into the main text. At this point in the 36 manuscript, the end of page 8, the text has not yet offered much description of what it is 37 these spatial agents actually do. It would help to have a description of at least one 38 example of a particular agent algorithm, to help readers picture how this is meant to work. For example, does an agent 'move' around the space at random until it finds a 39 40 point, and then create a triangular mesh element? A verbal description of the algorithm, 41 even if it is just one out of several algorithms that are used in the accompanying software, would really help a lot in understanding how this approach works. We learn later, in 42 section 3, about how some of these agents operate, but by giving an example earlier in 43 44 the manuscript you can give the reader a more intuitive sense of what this kind of agentbased 45 approach involves. 46

New explanations to give a simple procedure description of the meshing process as an example of
how agents can work, see (P.11,17 to P.12,L.6). A new pseudo-code is also provided in the
Appendix-B.

- 51 11, 6 what is a 'free' agent and how does it differ from any other type(s) of agent?
- 52

# A free agent is not yet part of a swarm. See section 2.2 Agent communication (p.14,L.5). A better definition was given.

P.11, 12-13 can you say more about how an agent would perform interpolation? Would it be
limited to a particular neighborhood of points, and if so how is that neighborhood defined?
Again, why would this be preferable to just doing a global IDW or SLERP?

# 8 New text added giving more details of how the swarm behaves

9 (P.15,L.4-8) "It is in this way that an agent can define a local neighbourhood as a local swarm, not just by proximity, but also with geometric properties such as orientation. An agent might be very close to its neighbour but may not be selected to be in the swarm because it is oriented at too high an angle thus promoting agents that are near co-planar to be working together. Agent interpolation is *not actually replacing more classical schemes*. SABM's are more of a framework in which interpolation and other spatial operators can be called from as needed."

- 14 15 The interpolator (IDW/SLERP) coupled with the cohesion functions produce swarms that try to have 16 their members match data orientation and/or position, but also keep the local swarm looking like a 17 surface, or close to co-planar. This happens with no gridding or mesh. It is however not a 18 completely data driven approach. Individual structural agents may not even see the data, but they may see their neighbours and become part of their swarm, that have some members who see the 19 20 data. Members who see the data can be influenced by it, and then transfer properties to the whole 21 swarm. This is a way of extending the data without producing a drop off weight value with 22 increased distance. The application will need to balance this data weighting versus swarm cohesion 23 effect. Currently the user balances this manually, by setting distance and attraction parameters 24 until a desired form is achieved, so there is a knowledge guided approach acting here. These parameters are described in the code comments. I did not discus this aspect in detail in the paper 25 26 because it opens the door to the knowledge versus data issue. How to decide what the relative 27 influence of knowledge versus data will be. I honestly would rather leave it for the next phase of 28 research. In the end what happens if we make a system that can deliver a nice version of what is 29 in your head while attempting to respect all the data? We want to go beyond this to making all the 30 end member models that at least make geological sense while coming close to respecting all the 31 data. Maybe, only a sub-set of these matches what is in your head. Maybe none of them do, which 32 is good to clear the head of bad ideas. So far, no system dealing with sparse data, that I am aware 33 of, can achieve this. 34
- Section 2.3: now we are finally getting a look at advantages of agent-based methods over
  traditional approaches. It would be really helpful to give a brief summary of this
  information in the introduction, so readers understand the motivation for this alternative
  approach.
- 39

# 40 Yes, for sure. This material was put earlier into the introduction.

41

42 13, 6 Would you not have issues with inter-agent communication in a parallel distributed 43 system? It certainly seems worth experimenting on, but I know that the somewhat similar 44 method of discrete-event simulation has challenges with parallel operation because you 45 can't predict in advance when initially independent operations on different parts of the 46 model space will end up triggering simultaneous or conflicting modifications to the same 47 data (still, the comment about 'yet to be tested' is fair enough, and I agree). 48

Yes, also I agree it is not a given. I do think separate swarms could be assigned separate GPU's,
but their members do change often, which has to be updated for that processor. If each search
agent had its own GPU perhaps that would work, but again lots of inter-agent communication is
needed. There are many other optimizations that could be made as well such as not processing

1 agents that have reached a stable configuration or have reached a stop-criteria. Each geometric 2 function could be assigned a processor (CPU/GPU) since most of them act like a black box. 3 Although not implemented herein, ultimately, the structural interrogator agents are supposed to be temporary. They would be there to act as control points for local meshing. Once the mesh is built, 4 they are not needed as all the geometry information (normals; eigenvectors; swarm membership 5 6 history), can be transferred the mesh nodes. Currently the codes *geoswarm* and *mesh* are 7 separate. This is all for potential future research. I have also not discussed implementation of 8 uncertainty handling but that could be a big part of the future developments. In my opinion, it was beyond the scope of this concept paper since uncertainty management would need a new set of 9 properties and functions beyond what the existing geometry engine provides currently. 10 11 12 13 13, 18 This is interesting - can you say more about 'interrogators or observation sets'? Does this mean for example that you use agents both to represent observational features 14 15 (such as a known dip at a particular (x,y,z) location) and to perform actions like 16 interpolation? 17 18 Yes, that is true agents can be data or interrogators (essentially search agents) but not at the same time. This is 19 clarified in 20 (P.17.L.15) "...spatial agents may represent control data, interrogators or estimated solutions. They could also morph from one type to another. For example, a data agent could extend itself by expanding incrementally along 21 the dip plane directions into estimation points. They may have properties for tracking local swarm or global 22 23 states, continuously checking..." Also, this is made clearer with an expanded description of section 2.1 Structural 24 Agents. 25 26 Section 3: it is great that there are codes provided for each of these examples. 27 28 Indeed. I wanted to show it is not just a hunch, but works in small ways. 29 30 15, 2-5 This specific example of an agent's behaviour is really helpful. Consider presenting this or another example much earlier in the manuscript, not as a comprehensive 31 32 description of the different agent types and their behaviours (you already have that material down here in section 3), but just to give the reader a general idea of what you 33 34 mean when you refer to 'spatial agents' in the paper's introduction. (Something like: 'For 35 example, to help interpolate the surface of a dipping geologic unit, one could define an agent that moves randomly through the data volume until it encounters a dip observation, 36 at which point it uses a local interpolation algorithm to spawn new dip markers in the area 37 around the observation'...or something along those lines, though actually Mesh agents 38 39 might be an easier example to understand). 40 41 This was fixed in an expanded step-by-step description of the mesh program (see P.11,L.15 to 42 P.12,L.6). Also, pseudo-code added to Appendix B. 43 44 Technical corrections: 45 2, 7 17 inc fixed (EdK) 46 4, 6 inc fixed (EdK) 47 5, 2 inc fixed (EdK) 48 12, 10 inc (also, not obvious what 'contributions from multi-scalar and deep multiproperty 49 data' means) 50 Line added with examples for clarification ... (P.16,L.7) "Preserving contributions from multi-scalar and deep 51 multi-property data, such as fold shape parameters, or geophysical rock properties." 52

- 1 12, 12 inc fixed (EdK)
- 2 12, 17 inc fixed (EdK)
- 3 13, 7 inc fixed (EdK)
- 4 15, 13 criterion fixed (EdK)
- 5 19, 7 inc fixed (EdK)
- 6 20, 3 inc fixed (EdK)
- 7 20, 9 was fixed (EdK)
- 8 20, 19 inc fixed (EdK)
- 9 21, 3 inc fixed (EdK)
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#### 12 **Comment on gmd-2021-66**

13 Guillaume Duclaux (Referee)

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Referee comment on "Spatial Agents for Geological Surface Modelling" by Eric A. de Kemp,
Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2021-66-RC2, 2021

17 Review of "Spatial Agents for Geological Surface Modelling", by Eric de Kemp.

18

19 This manuscript presents an innovative contribution to the challenging task of generating 20 3D surface model of complex geological terrains. The generation of 3D models (in the 21 sense of 3D maps and not 3D thermo-mechanical models) is of considerable interest to 22 the broad structural geology and tectonics research community studying the geometry of 23 geological units/objects and contacts in deformed regions, and is also of economic 24 significance for the ressource industry. The author presents here a new surface modelling/meshing method based on spatial agents which has the potential to overcome 25 26 some of the limitations inherent to the more classical implicit methods used in 3D 27 geological modelling. The spatial agent methods have been used now for about a decade for modelling features in a wide range of fields outside of Earth sciences, but such 28 29 methods, here involving structural agents, have never been used specifically for resolving 30 complex geological geometries in 3D by satisfying contacts and structural observations. 31 The paper first introduce the agent method and briefly reviews published literature on agent applications in various fields. The second section of this contribution presents the 32 33 challenges faced when applying current geological surface modelling techniques to 34 complex geological structures with sparse control points. Section 3 presents spatial agents example and how they can be used for solving surface modelling problems in structural 35 geology in order to insure that surface topology is sound and verifies fabrics observations. 36 37 The 6 main structural agents programs presented by the author represent building blocks that could be combined to eventually generate complex surface geology models. Section 4 38 39 discuss the future of such methods. This work doesn't claim that spatial agents are the 40 ultimate solution for resolving complex surface models, but it provides solid evidence that 41 used in conjunction with other Loop 3D tools it could definitely improve the surface model 42 building workflow and insure structural observations are respected. 43 44 The limitations of the current implementation are explicitly presented in the conclusions, which 45 keeps this contribution honest.

46

Thank you for seeing that I don't claim to create a whole new system solution, just enough to get
the conversation going and hopefully get someone interested to work on this more intensely,
perhaps as a graduate or post-doc study.

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51 The manuscript is well written and articulated. It contains 7 figures and 3 appendices.

1 some figures should be better called in the text. I do not have any major concern with 2 respect to this contribution that seems to represent a solid proof of concept and tile the 3 path for future applications of spatial agents for 3D geological modelling. This work is of broad interest to the community, and especially relevant to the those interested in 3D 4 structural mapping, tectonic interpretation of complex terrains, and the community 5 6 involved in 3D surface modelling in general. As such it seems worth publication in GMD 7 and well suited for this special issue on Loop 3D modelling. I recommend accepting the 8 manuscript with minor revisions and a few technical corrections (see minor comments 9 below). 10 11 Super! Thanks for all your work to check the manuscript. 12 13 I think many of the concerns of Reviewer 2 (Guillaume Duclaux) are dealt with in my response to 14 reviewer 1 so please check my responses there as well. 15 16 Minor comments: 17 18 + NetLogo-3D: this seems to be the correct spelling. It changes throughout the manuscript (starting in the abstract). Could you please insure spelling is correct and 19 20 consistent? (p5, p13, p17, p27, p28) 21 22 Fixed (EdK), and changed to NetLogo 3D throughout. 23 + p2, line 13: there is a typographical error for "conductivity" 24 25 Fixed (EdK). 26 + p4, line 24-25: I would suggest the author edit slightly the last sentence of the page. I 27 believe a model never reconciles all the data... Remembering Box famous aphorism "All 28 models are wrong, but some are useful" we can safely say that no model will reconcile and 29 respect all data. I would possible write down : "[...] explanatory model that aims to 30 reconcile and respect all the available data". 31 Fixed (EdK), re-worded (P.8,L.18) "that aims to reconcile and respect all the available data...". 32 33 I would say that an exact fitting model is exactly matching the data, that could be just 1 data point, that was used 34 to make it BUT that the model is still wrong because where the model is estimating away from data it can have 35 high degree of various errors... spatial, gradient, conceptual ... 36 37 + p5, line 4: section 1.4 title could be revised a bit... in fact it rather presents the outline 38 of the paper. Maybe something like "Outline and demonstration code" ? 39 I re-organized so the paper outline comes at the end of the general introduction and before section 40 1.1. 41 + p7, Figure 1: I would love to see what surface model spatial agents would generate 42 using the data provided in a). Could the structural agents programs presented here 43 resolve this surface in a way that satisfies the control structure in b)? 44 45 I dream about this! So far, I have run several experiments, on that data, that produce local 46 swarms wrapping around the on-contact control points, but they conflict with the stratigraphic 47 levels as there is no multi-level code yet. If I use a single level, it gets close to a reasonable 48 solution, coaxial structures are preserved but the spatial continuity is not very good. I need better 49 cohesion algorithms to glue the agents, or start to mesh them and freeze the local solution before 50 moving on. Basically, it needs the next phase of research to get a good result. It would need a 51 dedicated effort I think, and perhaps a more industrial strength agent environment that can handle

| 1<br>2<br>3                | larger coordinates than NetLogo (such as <i>Massive</i> , or <i>Repast Symphony</i> https://repast.github.io/screenshots.html).   |
|----------------------------|---|
| 5<br>4<br>5                | + p8, line 23: the notion of continuity for spatial agents is not very to me, even when looking at Fig 4. I believe the author should explain what is meant in more details.  |
| 7<br>8<br>9                | New text was added (P.11,L.17 to P.12, L.6) to better explain the meshing, and continuity clarified with "overall continuity, meaning the surface has no holes or branches."  |
| 10<br>11<br>12<br>13<br>14 | + p11, lines 3-4: I reckon an UML diagram or some schematics illustrating agents interaction would be helpful to those like me who are not familiar with such functions.  |
|                            | Yes, agreed, I created a new general agent communication diagram, see Figure 5. The caption and connection labels should made things clearer.   |
| 15<br>16<br>17             | + p12, lines 11-12: a reference to Figure 1 would be great here.  |
| 17<br>18<br>19             | + p12, line 12-14: I totally agree! Geophysics alone is definitely not designed to assess   |
| 20<br>21                   | What is good is that we can get gradient information and feed that to the agent system.   |
| 22                         | + p14, line 4: please add the missing "." in the caption between "data" and "Depending"   |
| 24<br>25                   | + p14, line 15: please add some comas : [] the program, its intended behavior, and the main []  |
| 26                         | Done (EdK).   |
| 27<br>28                   | + p15, line 2: a reference to Figure 2 should be added here.  |
| 29                         | + p16, line 2: a reference to Figure 3 should be added here.  |
| 30<br>31<br>32             | + p29, line 21: What is the polarity of the rock unit is unknown? High grade metamorphic  |
| 33<br>34<br>35             | rocks generally have no evident markers for polarity. Is it set to 0? NaN?<br>Done, herein we set unknown to 0, but in other applications (e.g. Gocad SPARSE plugin) the local<br>orientation label is 'overturned' and set to 1 (logical) for upright, 0 for overturned and -1 for |
| 36<br>37                   | unknown (EdK).  |
| 38                         | + references formatting in the text need to be formatted according to the journal   |
| 39<br>40                   | Done, many fixes (EdK).   |
| 41<br>42                   | Comas are missing between author names or et al. and the year. Some   |
| 43<br>44<br>45<br>46       | references have typos (i.e. p3 line 22 "Motieyan. and Mesgari", or p13 line 14 "from dekemp").<br>Done, many fixes (EdK).   |
| 47                         |   |
| 48<br>49<br>50<br>51       | Guillaume Duclaux<br>Nice, 05/08/2021   |
| 71                         |   |

#### 1 Spatial Agents for Geological Surface Modelling

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#### 12 Abstract

11

13 Increased availability and use of 3D rendered geological models has provided society with predictive capabilities, supporting 14 natural resource assessments, hazards awareness and infrastructure development. The Geological Survey of Canada, along 15 with other such institutions, have been trying to standardize and operationalize this modelling practice. Knowing what is in 16 the subsurface, however is not an easy exercise, especially when it is difficult or impossible to sample at greater depths. 17 Existing approaches to creating 3D geological models involves development of surface components that represent spatial 18 geological features, horizons, faults and folds, and then assembling them into a framework model as context for down-stream 19 property modelling applications (geophysical inversions, thermo-mechanical simulations, fracture density models etc.). The 20 current challenge is to develop reasonable starting framework geological models from sparser data regions, when we have 21 more complicated geology. This study explores this problem of geological data sparsity and presents a new approach that 22 may be useful to open up the log jam in modelling the more challenging terrains using an agent-based approach. 23 Semi-autonomous software entities called spatial agents can be programmed to perform spatial and property interrogation 24 functions, estimations and construction operations for simple graphical objects, that may be usable in building three-25 dimensional geological surfaces. These surfaces form the building blocks from which full geological and topological models 26 are built and may be useful in sparse data environments, where ancillary or a-priori information is available. Critical in 27 developing natural domain models is the use of gradient information. Increasing the density of spatial gradient information 28 (fabric dips, fold plunges, local or regional trends) from geologic feature orientations (planar and linear) is key to more 29 accurate geologic modelling, and core to the functions of spatial agents presented herein. This study, for the first time, 30 examines the potential use of spatial agents to increase gradient constraints in the context of the Loop project 31 (https://loop3d.github.io/) in which new complementary methods are being developed for modelling complex geology for 32 regional applications. The Spatial Agent codes presented may act to densify and supplement gradient, and on-contact control

1 points, used in *LoopStructural* (<u>www.github.com/Loop3d/LoopStructural</u>) and *Map2Loop* 

#### 2 (<u>https://doi.org/10.5281/zenodo.4288476</u>).

3 Spatial agents are used to represent common geological data constraints such as interface locations and gradient geometry, 4 and simple but topologically consistent triangulated meshes. Spatial agents can potentially be used to develop surfaces that 5 conform to reasonable geological patterns of interest, provided they are embedded with behaviors that are reflective of the 6 knowledge of their geological environment. Initially this would involve detecting simple geological constraints; locations, 7 trajectories and trends of geological interfaces. Local and global eigenvectors enable spatial continuity estimates, which can 8 reflect geological trends, with rotational bias, using a quaternion implementation. Spatial interpolation of structural geology 9 orientation data with spatial agents employs a range of simple nearest neighbour to inverse distance weighted (IDW) and 10 quaternion based spherical linear interpolation (SLERP) schemes. This simulation environment implemented in NetLogo 3D is potentially useful for complex geology - sparse data environments where extension, projection and propagation functions 11 12 are needed to create more realistic geological forms.

13 Keywords – spatial agents, three-dimensional geological model, simulation, surfaces

#### 14 1 Introduction

The major challenge that this paper is trying to address is the breakdown in achieving geologically realistic model results from sparse data in more complicated geological scenarios when using the existing methods and algorithms. This is no doubt a problem in other modelling domains as well, but is acute in geological applications, where access to data in the subsurface is often extremely expensive, terrain access prohibitive, or the depth of investigation too extreme for direct sampling and must rely on coarser geophysical methods that often do not adequately image the features being modelled. This paper explorers the use of extension, propagation and cohesion methods, which can be considered part of 'swarm' technology, using spatial agents in an attempt to deal with this challenge.

22 Geological modelling covers a wide range of applications and domains from thermo-mechanical modelling (Cloetingh et al.,

- 23 2013) to basin analysis (Barrett et al., 2018), mineral potential estimation (Skirrow et al., 2019) in 3D (Hu et al., 2020;
- 24 Sprague et al., 2006) and even 4D applications (Parquer et al., 2020; White, 2013). Herein we focus on the starting
- 25 framework model, the stratigraphic and structural surface model that provides the initial context for these more down-stream
- 26 property embedded modelling efforts. Generally, these geological models can be represented as BREP (Boundary

Representation) models (Pellerin et al., 2017; Caumon et al. 2009) but recently many of these are defined through implicit
derived surfaces with topologically encoded volumes (Grose et al., 2021; de la Varga et al., 2019; Wellmann et al., 2019;
Grose et al., 2017; Laurent et al. 2016; Hillier et al. 2014, Frank et al. 2007; Courrioux et al., 2001; Lajaunie et al., 1997). In
each case the accuracy of the BREP and/or implicit surface model features such as horizons, folds or faults, are dependent on
the quality of the geological input data that is available, but also importantly, on the algorithms and methods used to build
them (Wellmann and Caumon, 2018; MacCormack and Eyles, 2012).

Existing methods applied to the combined sparse data and complex geology scenario, will tend to produce holes, gaps and
feature drop-outs, away from control data, as well as arbitrary horizon thickness changes that combine to give a geologically
unreasonable bubble gum look to these models (Fig. 1). Current methods in sparse data configurations tend to bias for these
unrealistic geometries using radial based kernel functions, optimized for local smoothness in order to achieve a mathematical
solution (Hillier et al., 2021; Hillier et al., 2014). This often comes at the price of geological realism (Hillier et al., 2021;
MacCormack and Eyles; 2012). Is it possible that, with a new approach, geological features could be more realistically
modelled by using spatial agents to 'fill-the-gaps' in the process?

14 Section 1 provides an overview, context and review for the current study, surveying various application domains with an eye 15 toward natural and more specific earth sciences agent applications. Section 2 outlines the use of spatial agents for structural 16 geology. A summary of current geological surface modelling approaches is given, with some argumentation that highlights 17 the need for new approaches particularly when data is sparse, and geology is more complex. The mechanisms for using 18 constraints, inter-agent communication and characterization of required behaviors. A summary is given of the critical 19 intrinsic properties of spatial agents that may aid in future research in this area. In section 3 several spatial agent demos are 20 used to represent simple contact surfaces as agent constructed triangular meshes, fold closures and simulations of unmeshed 21 structural swarms from sparse points. There are 6 main programs, each highlighting critical functionality that will be required 22 should structural agents be developed into a more complete geomodelling system in the future. Lastly, section 4 provides a 23 discussion for how structural agents could be applied and some final conclusions from the study.



data. (a) Uniaxial dip data, with local opposing tops, represented on equal-angle Wulf plot (<u>https://app.visiblegeology.com/stereonet.html</u>). (b) Control
model developed with SPARSE (de Kemp et al., 2004), with F1-F2 horizontal, north trending hinges, (c) implicit surface models with Gocad/SKUA (Jayr et al., 2008) and (d) SURFE (Hillier et al., 2104).

#### 1 1.1 Agent Challenge

Spatial Agents are virtual spatial entities that have freedom to interact with each other and their environment, which can
include various domain data, in order to solve a well-defined problem, for example to predict the growth of an urban centre,
an ant hill or the course of a meandering river system under variable rain fall and soil conditions. Some of the core
characteristics of spatial agents could potentially be used to essentially 'grow' features away from the control data, keeping
them intact while extending and respecting regional gradient information. In a sense similar to how the human mind might
fill-in through geological interpretation of a map or cross-section.

8 The Loop effort is attempting to address this ongoing challenge (Ailleres et al., 2019) that tends to present itself when 9 geology becomes more complicated, with more elaborate geo-histories, for example, geo-histories with early cryptic 10 sedimentary and volcanic depositional cycles, and a spectrum of brittle to deeper crustal deformation events, and through 11 masking metamorphic processes. Geo-histories with overprinting intrusive events, from thin dyke swarms to consuming 12 batholithic intrusions can also completely erase all macroscopic evidence of earlier processes. The challenge is most acute 13 when the data required to accurately model these scenarios is quite limited. It is in these in-land frontier zones, where most of 14 our data is only at ground surface, interpreted from remote sensing images, or sparingly at depth, with clustered spatially 15 biased drill holes near mineralized zones. These regions may have been surveyed with geophysical instruments, and the data 16 used to derive models representing at depth rock property distributions for density and magnetic susceptibility, conductivity 17 and resistivity. However, in almost all cases there is a lack of high-resolution geophysics, as 2D or 3D seismic data, from 18 these surveys, which is more commonly available and used in the practice of hydrocarbon reservoir modelling workflows. 19 The suggestion, presented in this study, is that we may be able to better face some of the sparse data conditions, characteristic 20 of more complex geological terrains, by taking advantage of the properties that spatial agents posses. Primarily for spatial 21 agents to densify input constraints for horizon dips, better model the local structural trends or anisotropy, and extend features 22 such as regional fold plunges. These derived constraints could be useful as supplemental input to LoopStructural (Grose et 23 al., 2021) and Map2Loop (Jessell et al., 2021) to increase the accuracy and geological reasonableness of those downstream 24 models.

This study highlights the potential use of Spatial Agents in the context of the Loop project (Ailleres et al., 2019) that is
developing new methods supporting the modelling of more complex geological terrains. With this initial study, which is a

first to highlight their potential use for sparsely constrained complex geology, we may inspire more development in this area
 and complement the various new methods that emerge from Loop, and hopefully other initiatives in the future.

#### 3 1.2 Agent Applications

4 In general, an agent-based system is used to see the effects of autonomous individuals, groups or objects on the overall system 5 when solutions are onerous and/or computationally expensive. A global algorithm involving a single large multi-parameter 6 matrix inversion may take many days to compute with a single outcome, but an agent-based model may be able to produce 7 several outcomes in minutes or hours (Siegfried, 2014). Agent-based models have their roots in the development of cellular 8 automata and complexity theory, which has been able to model complex natural and artificial systems with simple 9 neighbourhood algorithms (Cervelle and Formenti, 2009; Wolfram, 1994; Von Neumann, 1966). Agent applications are 10 extensively used in the entertainment industry (Damiano et al., 2013); computer games for sports and battle simulation (Zuparic 11 et al., 2017; Guo and Sprague, 2016), landscape and land use design, management and visualization (Tieskens et al., 2017; 12 Valbuena et al., 2010); urban planning (Motieyan and Mesgari, 2018; Levy et al., 2016); crowd modelling for public transport 13 and community infrastructure design (Dickinson et al., 2019; Hoy and Shalaby, 2016); climate change and adaptation modelling 14 (Amadou et al., 2018); Architecture and Engineering design (Guo and Li, 2017; Van Dyke Parunak et al., 2001) as well as 15 hazard response and real-time three-dimensional mapping (Schlögl et al., 2019; Bürkle 2009); transportation and surveillance 16 using semi-automated or fully-autonomous vehicles such as drones and automobiles (Fagnant and Kockelman, 2014; de Swarte 17 et al., 2019). Agent-based modelling has been used in the Earth Sciences for spatial-temporal more process-oriented modelling 18 such as solar storm and flare activity (Schatten, 2013), Groundwater modelling (Jaxa-Rozen et al., 2019) and Earthquake 19 prediction (Azam et al., 2015) to name a few examples.

These applications generally do not use trend information, or what structural geologists refer to as anisotropy, and gradient type information such as horizon dip data, with polarity, or direction, which the structural agents do in this study, however these diverse applications do have some common elements that software agents are well suited to. The problem domains have multiscalar environments; molecular to planet scale, with local or global model element interactions, and non-linear, multi-source physical dependencies. Agents could be interacting at molecular scale with quantum-mechanical, ionic and thermodynamic influences, for example, for protein-folding (Semenchenko et al., 2016; Nelson et al., 2000), for a visual demonstration of molecular agent simulation see: https://www.youtube.com/watch?v=4Z4KwuUfh0A or at galactic scale

1 http://www.gravitysim.net/index.html. The ability to operate in a non-centralized control structure, being sensitive to other 2 neighbours conditions and geometric states as well as their ability to respond to local or globally changing conditions may give 3 spatial agents an advantage. Their independence allows them to operate as individual elements, for example a single point 4 observation, or to work collectively as a team or 'swarm'. This allows the application of agent rules that may determine local 5 cohesion levels and shape characteristics as well as changes of state depending on specific conditions such as moving in a 6 direction, stopping, or spawning other processes. This allows them to behave in a flexible and efficient manner, without the need 7 for global partitioned data structures or tightly coupled deterministic algorithms. Many agent examples are biologically based 8 such as the classic flock of birds examples; 'murmurings' and geese in V-formation, beehive and anthill construction examples 9 (Mnasri et al., 2019; Carrillo et al., 2014; Johnson and Hoe, 2013). These examples highlight the potential to capture multi-scaler 10 and complex interaction that has enhanced the uptake of this technology for medical and biology fields (An et al., 2017; Rigotti 11 and Wallace, 2015).

12

#### 13 1.3 Agent Characteristics

14 Agents operate as semi-autonomous software entities that are not directly controlled by any centralized command structure 15 and can operate with a great deal of independence from each other. They are programed with roles, beliefs and behaviors that 16 can be triggered by the state of their local or regional environment. They can interact with other similar or different agents to 17 collectively achieve a goal, acting like a swarm. For example, considering a construction simulation game, a carpenter would 18 be considered a single agent that could be assigned the framing role to construct a house. The house in this case would be an 19 example of a single Agent-based Model (ABM). If there are many agents with different tasks but working collectively, 20 perhaps a team of framers with a foreman, an architect and a designer, working on a larger more complex building, this 21 would be a Multi-ABM (MABM). When two, three or four dimensional maps or entities with spatial properties critical in the 22 modelling process are involved, this is characteristic of Spatial Agent-Based Models (SABM). Spatial agents and spatial 23 multi-agent-based modelling systems (SABS and SMABS), or the non-spatial agent-based models (ABM) form a family of 24 approaches which have been used in a wide range of applications that take advantage of the efficiencies and freedoms that 25 these systems possess (Torrens, 2010).

1 SABM are not confined to operate within a regularized data structure such as an indexed space partitioned grid, although they 2 could still be programed to do that. These two characteristics, freedom from central command and a good degree of 3 independence, combine to make a powerful modelling combination that has been successful in many domains to solve 4 complex problems. Generally, applications have been successful when spatial agents are designed to perform environmental 5 tasks such as map their surroundings or interrogate a complex space, monitor the state of things that may change over time or 6 simulate complex self-organizing systems such as anthills, bee's nests and traffic jams. For the purpose of this study, the 7 objective is to determine if agents can perform the initial three-dimensional graphical tasks that will be important for future 8 geological applications. The focus will be on visualizing and modelling local and regional anisotropy, and manipulation of 9 structural agents representing classic geology strike-dip and horizon-contact data.

#### 10 1.4 Role of Interpretation

11 Earth Science in general, and geology in particular, is a domain characterized by the use of interpretation skills which are 12 fundamental to achieving successful practice. For problem representation, mapping applications and advancement of 13 knowledge in this field, experience and specific expertise is required to be able to solve complex spatial and temporal 14 relationships with limited observations (Brodaric, 2012; 2004). Knowledge of the processes that cumulatively produced the 15 resultant geometric forms, cross-cutting and overprinting relations and expectant natural patterns will drive an interpreter's 16 heuristic and narrow the solution space in which maps and cross-sections are developed. Ultimately for a reasonable three-17 dimensional and four-dimensional model of the subsurface these interpretive skills are utilized to come up with a cohesive, 18 explanatory model that aims to reconcile and respect all the available data.

Spatial agents have the potential to support this interpretive role, provided some of their key characteristics can be leveraged towards geological feature estimation and feature to feature relationship extension. This could be accomplished by more efficient exploration of the model solution space through extension of horizon contacts, fault networks and fabrics.

#### 22 1.5 Demonstration Codes

23 The properties and general behavior of spatial agents is demonstrated for the simplest of geological data, through several

24 agent demonstration programs. These codes and data can be freely downloaded (See

25 <u>https://github.com/Loop3D/GeoSwarm.git</u> or <u>https://doi.org/10.5281/zenodo.4634021</u>). The code implementation was done

26 in NetLogo 3D agent-based modelling software (Wilensky, 1999), taking inspiration from some earlier model examples such

as wave-3D (Wilensky, 1996) and flocking codes (Reynolds, 1987; Wilensky, 1998). The reader should download the
NetLogo 3D software and try some simple examples to gain a better appreciation of the agent environment (see Appendix A
for agent resources). Each code example provided will have a NetLogo 3D implementation version that can run the code (see
Appendix B). Additional information to access the codes and a summary of the quaternion math specific for rotation and
interpolation of structural geology data used in this study is provided in Appendix C.

6 2

# Current Geological Surface Modelling

7 Geological models are currently constructed through an iterative process of automated interpolation combined with 8 interpretation from data constraints (Caumon et al., 2009; Groshong, 2006). Computer methods and workflows are applied to 9 data and output a collection of essential geological features, generally faults and horizons, which combine to form a 10 framework structural and stratigraphic model. When data is relatively abundant such as from three-dimensional seismic 11 surveys, common for hydrocarbon exploration and reservoir modelling, standardized methods do an excellent job at 12 representing sub-surface geological scenarios. However, when data become limited and geology more complex, precisely in 13 areas with high potential mineral, things can break down. In these circumstances existing implicit interpolation algorithms, 14 that are considered state-of-the-art for geology, may precisely fit the data but have much reduced global geologic accuracy. 15 See for example, figure 1 in which c) and d) are implicit geological surface models developed respectively with 16 Gocad/SKUA (see https://www.pdgm.com/products/skua-gocad/) and SURFE radial basis function approaches (Hillier et al.; 17 2014). Note the missing representation of horizon C in the centre model c), and lack of through going spatial continuity of all 18 horizons in d). Both c) and d) would not be considered reasonable geological models by subject matter experts given the data.

19

1 Geological modelling is becoming a much more integrative, complex and computationally intensive undertaking (de 2 Kemp et al., 2017). There is a wealth of existing approaches for estimating geological surfaces with various data 3 types (geophysical, structural, stratigraphic) in a range of settings (Caumon et al., 2009). A common theme 4 emerging from the development of the arsenal of tools for this work, is that it is more and more difficult to come up 5 with a range of solutions that can both respect all the data inputs and the known complexity of features being 6 modelled (Jessell et al., 2014). In this under-determined problem domain, the move to leverage knowledge and data 7 to solve complex geology problems highlights the need to explore model spaces more efficiently for outcomes that 8 meet our minimum reasonableness criteria (Caumon et al., 2014, Jessell et al., 2014). Are agents a way to efficiently 9 tackle this problem, by providing a framework from which our existing tools can be embedded? This remains to be 10 seen, but at a minimum an exercise is needed to investigate if simple spatial agent operations can be used to model 11 structural geology data.

#### 12 2.1 Structural Agents

13 This study focuses on the use of spatial agents for enhancing knowledge driven estimation, projections and extension methods (Torrens, 2010; de kemp and Jessell, 2013) using sparse data, for regional geological domains. 14 15 Geoscience applications employing spatial agent-based modelling (SABM) have largely been focused on solving 16 time series problems, like land use change due to climate, urbanization and hazards (Torrens, 2010). Herein 17 however, the focus is on spatial variability, and distribution, rather than temporally changing environments. The 18 major benefit of spatial agents is that they can be programed to act as a swarm. That is, they can act collectively, 19 having cohesion with their local neighbours, thus providing the spatial continuity required to construct continuous 20 features. The swarm may also be given shape-based rules, such as, keep members on a local plane or within a 21 specified degree of curvature. This is difficult to achieve with a global algorithm; inverting a matrix containing all 22 constraining data and properties. Spatial agents are potentially independent to explore a solution space that is not 23 constrained by regression minimizing criteria, which tend to make smooth solutions at the expense of realism. 24 Importantly, the cohesion of a swarm allows spatial agents to extend beyond the dense data regions, essentially 25 propagating features based on local rules, for example extending a surface along a fold plunge direction. Typically, 26 structural trends are manually traced in 2D, on maps and cross sections, with what are referred to as 'form lines' that 27 match the local planar fabric observations. This can be done also in 3D, automatically (Hillier et al., 2013) but will

not provide feature continuity that the agents could provide. In the code examples, much use is made of what is
termed a 'structural agent'. These are agents that have spatial coordinate location properties for X, Y, Z but also
planar or linear geometric properties of strike, dip, trend, plunge and normal direction cosine components used to
designate a horizon top direction or a fold hinge line. They may also have environmental information that tracks
local or regional eigen-fields. As noted earlier these types of agents may represent data, estimations or interrogators
that can transfer their properties as required. The structural agents enhance the interpretation process by densifying
the form lines and simulating more planar point features to highlight structural changes more clearly (Fig. 2).





**Figure 2.** Structural form traces (orange point streams) estimated from dip data (yellow cuboids) using spatial agents. Red sphere is an interrogator agent. Blue dots are simulated Bézier control points with added random noise. See Appendix A for details.



computed Barycentre with a unit normal vector property. The closest triangle to the model centre will act as a seed
for the meshing and will sense its nearest neighbour triangle and connect to it, maintaining a consistent topology
with each triangle rotating into position, making a proper connection to an adjacent triangle. This proceeds until all
the triangles have been connected into a reasonable continuous surface patch, with no holes or large tears, and all
adjacent triangle normals pointing the same direction. The action is very simple as shown in the pseudo code in
Appendix B.

7



8

- 10 Figure 3. Structural agent demonstrating a quaternion 90° clockwise rotation during linear estimation (SLERP) between two points. Starting
- 11 point A (local), with equivalent orientation to larger observation (yellow and red cuboid) and final rotated point B (distal). Rotation maintains
- smooth topology for top direction. See Appendix B for details.





# Inside Hull:

| Triangles M | lutual Edges | Shared Vertices |
|-------------|--------------|-----------------|
| 12          | 14           | 11              |

| Inside Hull: |              |                 |
|--------------|--------------|-----------------|
| Triangles    | Mutual Edges | Shared Vertices |
| 15           | 17           | 11              |







Figure 4. Spatial agent-based triangular meshing created from the Mesh program. See Appendix B for details.

#### 1

#### 2 2.2 Agent Communication

There are a wide range of functions, behaviours and states that can be encoded into the agent set. These are collectively driving what will be a successful application solution. Facilitating the efficient outcome of an agent model are agent communications. Inter-agent communication is handled through agent property updating (Fig. 5). Each agent is responsible to know what is going on to the extent that it has been programed to, for example a proximity property may be updated that indicates the nearest free agent neighbour, that is an agent not yet belonging to a swarm. Depending on what behavior has been programed into the code, if an agent reaches a certain proximity threshold, an event might get triggered such as to create an association link with that more proximal agent.



10

Figure 5. General summary of structural agent communication using the example from *GeoSwarm*, for details see comments and codes in the open-source programs listed in Appendix B. Thickness of blue lines indicates relative degree of inter-agent communication. Geometry Engine composed of all agent functions for determining eigen directions, proximity, rotation, location and spatial estimation. Grey fold surface in Model Space represents a possible fold realization that emerges from swarming structural agents, given sparse input data (yellow markers). Red arrow indicates principal eigen vector direction, which is also the fold hinge or regional plunge; this can be used as a rotation axis for structural agent geometry updating.

1 An agent can be made to act like an interrogator of space, whereby a continuous sampling may occur, in a given 2 direction rather than through a predefined set of indexed grid cells, such as in a convolution filter. Core to the behavior 3 of agents is the communication of derived weighting parameters for various properties, most importantly, for structural 4 orientation during interpolation. It is in this way that an agent can define a local neighbourhood as a local swarm, not 5 just by proximity, but also with geometric properties such as orientation. An agent might be very close to its neighbour 6 but may not be selected to be in the swarm because it is oriented at too high an angle thus promoting agents that are 7 near co-planar to be working together. Agent interpolation is not actually replacing more classical schemes. SABM's 8 are more of a framework in which interpolation and other spatial operators can be called from as needed. Interpolation 9 schemes from simple to complex could be employed such as, nearest neighbour, inverse distance weighted (IDW) or 10 quaternion based spherical linear interpolation (SLERP) (De Paor, 1995; Shoemake, 1985; Hamilton, 1844). Several 11 schemes could be employed depending on local or global data configurations, property conditions and knowledge 12 constraints. For the demo examples extensive use of SLERP methods ensure that rotations of geologic orientation data 13 are smooth and more realistic with respect to expected structural deformation processes. In the presented examples, 14 there is yet no rheological controls, but these physical parameters could be programed into the agent rule set. Agents 15 can be programed to react to physical laws for example, the barycentre of a 3-tuplet mesh can be dynamically 16 recalculated when neighbour masses, other material and mechanical properties are changed. The location and states of 17 all agents are available and stored at the agent level, passed to a communications centre or just stored as a global 18 variable, if needed. Agent intercommunications is a significant topic of computational science research (Hall and 19 Virrantaus, 2016; Ménager, 2006), which may have implications for geological modelling, for example if moving into 20 the field of geological and geophysical integration and joint modelling, agents may have potential in optimization 21 strategies for inversion of complex geometries, multi-parameter scalar and vector fields (Jessell et al., 2010; Lindsay et 22 al., 2013). It is the way agents can communicate specific local to global information states, and adjust to the combined 23 data and knowledge constraints (Liscano et al., 2000; Friedrich et al., 1999; Gaspari, 1998), that may determine the 24 applicability of their use for geological and no doubt other applications as well. For a comprehensive summary of agent 25 and inter-agent communications and agent system controls see Heppenstall et al. (2012), for spatial agents with GIS see 26 Crooks and Heppenstall (2012), and for a practical introduction Wilensky and Rand (2015) (see also Appendix A).

27

#### 1 2 2.3 Agent Behavior 3 Some interesting qualities of spatial agents: 4 2.3.1 Agents are able to efficiently interrogate irregular and complex model spaces. The model design can result 5 in a wide range of single realizations or solution suites. More traditional approaches are dependent on fixed regular 6 and partitioned structures using standard coordinate systems, with few geological properties. 7 2.3.2 Agents are suitable for modelling natural complex systems. Preserving contributions from multi-scalar and 8 deep multi-property data, such as fold shape parameters, or geophysical rock properties. Global interpolation 9 techniques such as implicit interpolation tend to generalize dense data clusters to a local mean and are optimized for 10 a scale specific purpose, often producing geologically meaningless results (Fig. 1). This could happen when 11 combining point geometry from structure, categorical geology, and continuous geophysics data. Essential details 12 such as fold topology and hinge regions can be ignored or conflict dramatically with geophysical gradients. Agents 13 may be able to more easily incorporate this kind of local information during estimation and feature propagation. 14 2.3.3 Agents can support the domain expert that requires more interpretive skills, with knowledge-based Rules, 15 Missions (Beliefs) and/or Behaviors during data interrogation. Agents could be used in mapping to visualize 16 complex relationships, such as within vector fields; for fabric intersections (bedding – cleavage relationships); 17 vergence relationships on fold trains; disharmonic folds and poly-deformed stratigraphy with early cryptic faulting. 18 Visualization of these relationships within the event history is critical to more accurate geological interpretation. 19 2.3.4 Agents complement rather than replace existing algorithms and approaches. For example, spatial estimation 20 can still be applied (Implicit, IDW- Inverse Distance Weighted, Kriging, DSI - Discrete Smooth Interpolation, SVM 21 Support Vector Machine, etc.) at variable scales as required. Thus, they potentially could provide a framework for 22 calling a variety of interpolators and constructors depending on data density, problem domain and feature 23 complexity. 24 2.3.5 Agent interaction and communication may produce group - swarm behavior. This emergence could

potentially express more complex features or trigger other spatial topological changes, such as new faults or
 unconformities. Agents may also spawn, through their state condition, new geologic events altogether, for example

inserting a new deformation event when a metamorphic fabric is observed in a boulder of apparently undeformed
 conglomerate, or when a high curvature region is detected by inserting a fold hinge or fault control point.

2.3.6 Agent-based approaches may benefit from denser and faster CPU/GPU architecture and parallelization
schemes. This could be the case, as the simple rules driving agent interaction and communication act more
independently, rather than having to invert large global matrices common in implicit approaches. This has yet to be
tested, since it is perhaps hard to partition on-going spawning processes from independent agents, but could result in
dramatic efficiency gains when combining multi-scalar properties from geophysics and geology within threedimensional structural fields (Burns, 1988; Hillier et al., 2013).

#### 9 3 Agents Examples

10 To demonstrate the general principals of agent behavior for geologic surface development, a number of simple

11 applications were developed, using mostly synthetic data, and one re-scaled data set from an Archean greenstone

12 belt, Caopatina, Québec (de kemp, 2000), in a model space with (X,Y,Z) dimensions = (100,100,100) and model

13 centre at (X,Y,Z) = (0,0,0). The NetLogo codes presented are freely available for download (See

14 https://github.com/Loop3D/GeoSwarm.git or https://doi.org/10.5281/zenodo.4634021).

15 In the following example scenarios, spatial agents may represent control data, interrogators or estimated solutions. 16 They could also morph from one type to another. For example, a data agent could extend itself by expanding 17 incrementally along the dip plane directions into estimation points. They may have properties for tracking local 18 swarm or global states, continuously checking for proximity to neighbours, their status as interrogators or 19 observation sets and their geometric properties, such as strike, dip and polarity (top direction). Agents may have 20 pointers and links to specific topological neighbours as in the case of adjacent triangles but importantly there is no 21 ordered centralized control list, or matrix, which holds all the agents and their relationships. Each type of agent is 22 created and encoded with properties that may change, such as the local anisotropy derived from the eigenanalysis of 23 local supported data. The structural agents are spatial agents, represented herein as tablets or hexagonal glyphs and 24 rotate as quaternions (Fig. 6).



Figure 6. In-put Data constraints. On-contact (white spheres) and dip (blue=upright, red=down, thin hexagonal prisms)
representing simple three-dimensional geological data constraints. Arrows at origin indicate the calculated orthogonal unit
eigenvector directions for the structural data. Depending on the scenario the structural agents will do a SLERP interpolation (De
Paor, 1995; Shoemake, 1985; Hamilton, 1844) using a rotation vector from the major global eigenvector axis to simulate behavior
of bedding rotation due to near coaxial folding (Woodcock, 1977). For specific calculations used in each program see the code
comments or see Davis and Titus (2017) and the Appendix therein and Adamuszek et al. (2011), for a thorough review of structural
data computations. A summary of the quaternion rotation math is in Appendix C.

9

#### 10 3.0.1 Scenarios

Each of the following programs runs inside NetLogo 3D, an agent simulation software which is freely available
from the Northwestern University NetLogo download site: <u>http://ccl.northwestern.edu/NetLogo</u>. The reader should
try the default parameters set when each program is called from NetLogo 3D and then adjust some of the simpler
parameters that control global orientation such as strike and dip. The descriptions below give the name of the
program, its intended behavior, and the main purpose of the demonstration code. Note that not all codes have been

thoroughly tested or gone through performance optimization. It is best to slowly increase the number of agent data
 points for each scenario and experiment with the control parameters for best results.

#### 3 3.1 Trace

4 Demonstrates the modelling of fabric observations (Fig. 2). The search agent (red sphere) travels through the model 5 space randomly until it senses a proximal dip observation. It will then adjust its trajectory towards a down dip vector 6 to this observation and spawn other simulated dip points that are nearest neighbour (NN) or inverse distance 7 weighted (IDW) interpolations from the data. A stream of points is recorded as the search agent moves through the 8 model space. This point stream will form De Casteljau - Bézier (Farin, 1997) curves that are either killed or 9 preserved based on simple user specified shape parameters, such as curve length. Other criteria have not yet been 10 implemented however this could be implemented, such as degree of curvature or mean direction angle from a 11 regional trend. Demonstrates streamline visualization using down dip trajectories. Similar to the three-dimensional 12 Structural Field Interpolation (SFI) from Hillier et al. (2013). The main distinction here is the sampling is random 13 with the potential for multiple search agents acting simultaneously.

14

15 3.2 Poly

Demonstrates simple polyhedral graphics control which is needed for vector-based boundary representations used in many geological modelling environments. Construction agents can perform simple local tasks, such as making a single polyhedron, but also regional tasks, by joining these up until stop-criteria are reached. Modelling of simple closed and connected polyhedra is achieved by joining simple triangles or large loops with many vertices. Each closed polyhedron once formed will connect one link to its adjacent polyhedron, forming a simple object chain. Modelling and visualization of the network are controlled by user-defined edge size, search radius, repulsion, and tension of the edges.

#### 23 3.3 Rotate

24 Demonstrates SLERP rotations, which would be required for estimation in complex geological domains, with

25 folding and sparse data representation (Fig. 3). It is also a testing environment for interpolating planar constraint

26 data with linear rotation axis. The main control dip agent is located at the origin in the centre of the model space and

a user defined target dip agent is set up. A linear quaternion rotation of the control dip is incrementally rotated along
a single or circular radial to the target dip. Users can rotate all dips continuously and dynamically. The agents are
always updating to the new target. Rotation axis is defined by the user which could be in all possible in-plane or out
of plane cross-dip orientations. This is a required method for estimation of local and regional dips and structural
vector fields.

6

# 7 3.4 Mesh

8 Demonstrates the development of topologic surfaces that, at a minimum, are defined by a triangulated mesh that has 9 direction and polarity sensitivity (Fig. 4), also to show that a mesh can be produced from agents without a grid; 10 without having to sample a scalar field value in a partitioned grid (i.e. with marching cube) and that meshes could be 11 grown locally, while conforming to constraint data. Each triangle has a normal that is maintained from the 12 barycentre of the triangle. Triangle vertices have a mass that can be changed by the user to influence the location of 13 the barycentre. A seed triangle senses the nearest neighbour triangle vertex and attracts it, back to itself. The 14 incoming triangle is rotated to be conformable to the evolving surface patch and connected, keeping the normal 15 pointing in the same way, thus maintaining simple surface topology. In this way distributed primitive shapes could 16 act as spatial data interrogators, before being transformed into mesh constructors. Simple topology metrics (edge: 17 vertices: triangles ratios) are reported and plotted on the GUI graph. Once the mesh is complete, and if the on-18 contact constraints are active, the mesh will migrate with its regional barycentre to the nearest on-surface control 19 point, and turn it blue from white, then go on to do the same for the next control point. This functionality is a 20 precursor requirement for adaptive meshes, that could potentially be shaped by various spatial and property data, 21 data quality and data densities. In this instance, a surface mesh is grown through use of simple geological rules. For 22 example, a surface can not intersect itself, and needs to be continuous with consistent surface polarity, and also to 23 avoid large tear faults. These surfaces may move toward on-contact data constraints to extend the local observations. 24 The ratios of triangles to shared edges and shared vertices can be used to check topology and used as a stopping-25 criteria, to reward or penalize during the meshing process.

26

#### 2 3.5.1 Swarm Dips: Simple Plane

3 This program demonstrates convergence of a non-meshed swarm toward a common plane. It is useful to 4 demonstrate proximity, vision distance effects, angle of sight and separation. Randomly initialized interrogation 5 agents, represented as smaller hexagons are dynamic, sensing agents and used to estimate or simulate, local 6 structural vector fields, herein referred to as Dip Sims. These Dip Sims slowly behave as a swarm, moving in the 7 plane specified by the controller, respecting vision-proximity and view-angle rules. When the separation and vision 8 distance are low, the sims will converge and produce red balls alerting the user that a proximity threshold has been 9 crossed. The red balls disappear once the sims move apart, and the inter-sim distance is greater than the specified 10 separation. This mode uses a single main dip controlling agent, represented by a large origin (0,0,0) centred, two-11 sided (yellow up/green down) hexagon (see Fig. 7). The displayed data for on-contact and stationary dip data have 12 no influence. Only the main controller, large green-yellow hexagon symbol that is stationary at the model centre 13 with orientation (strike, dip, polarity) defined by the user, is influencing the swarm. The controlling parameters are 14 adjusted dynamically during the simulation run, initiated by pushing first the setup, and then the simulate buttons. 15 Dip Sims sense other Dip Sims within the vision distance and the view angle ( $\phi$ ), they are kept from each other by a 16 user defined separation distance (yellow circle). The user changes the configuration during a simulation with sliders 17 on the NetLogo interface to control strike and dip properties of the Main Dip, which in turn controls the plane upon 18 which agents are moving on. The data in all the swarm examples are generated artificially by randomly positioned 19 sites on the plane of the main controller. The orientation of each dip data point is set by random rotation 20 perpendicular to the E1 (eigen) axis, to achieve a user specified variability (0 = no dip variance and 1 = maximum)21 dip variance). The idea is that each agent can see other agents within a locally controlled environment such as a 22 given vision distance and angle of sight, and these other agents start to coalesce forming a swarm, that could 23 potentially have some task to complete; extending a geologic feature of interest, extending a depositional horizon, 24 for example.

#### 25 3.5.2 Swarm Dips: Moving Plane with Dips

Demonstrates smooth linear interpolation using SLERP (Spherical Linear Rotation Interpolation) with quaternions.
 Parameterizes the rotation with linear segmentation of straight-line distance to controlling dip data. As the Dip Sims

- 1 come close to static dip data control-points they will adjust their local orientation to match the orientation properties
- 2 of the data, but do not move spatially towards these off-contact orientation observations (Fig. 7).



Figure 7. Components of the spatial agent-based model (SABM).

# 4 5

6 The influence of the orientation data on the estimation of orientation properties at the Dip Sim is weighted in an
7 inverse distance manner. There is no migration to on-contact data, only the off-contact dip data points have
8 influence. Outside the vision distance, the main regional controller determines the agent orientation.

## 9 3.5.3 Swarm Dips: Migrate to On-contact Data

Demonstrates that sims can sense and migrate to on-contact feature control points while detecting the structural influence from adjacent data. Dip Sims move toward the nearest on-contact data point while rotating into parallelism with the closest dip observation. At a given tolerance to the on-contact data points, the Dip Sim freezes in an orientation that is close to the neighbourhood dip field. When all on-contact data points have a Dip Sim the rest of the Dip Sims are behaving as a swarm; controlled by the Main controller and moving in the plane specified by the controller and vision-proximity rules.

| 1 |  |
|---|--|
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# 3 3.6 GeoSwarm

4 This example incorporates all of the above swarm methods using 4 separate structural observation files, or a random 5 set. The 4 test sets are taken from actual field data gathered from the Caopatina region, Québec, Canada, from 6 steeply dipping and folded series (Fig. 8) of turbiditic sediments from an Archean Greenstone Belt (de Kemp 2000). 7 Scaling settings can stretch the extents of the data for testing local versus regional influences on swarm cohesion. 8 Several distance sensitive parameters determine how agents are weighted for local surface cohesion versus data 9 migration. A file I/O interface for testing various data configurations representative of common but simple geologic 10 fold scenarios. It could be adapted for custom data configurations and will be used in the future for parameter 11 selection training and testing with a range of real data sets.



Figure 8. Surface model (closed yellow ellipsoid) using implicit calculations with SURFE (Hillier et al., 2015) when using only
 4 on-contact dip data points (a) and then using the GeoSwarm program to extend a fold plunge, with 50 off-contact spatial structural
 agents depicted from the bottom, looking up in (b). Red surface in (c) is a more spatially continuous antiformal structure, when
 using the structural agent approach than with implicit codes alone. Note eigen vector E1 (red stick-ball) is pointing down plunge
 of the fold, the strongest continuity direction.

#### 1 4 Discussion and Conclusions

This study focuses on the rudimentary requirements for geological modelling using spatial agents, primarily their ability to interrogate, communicate and represent solutions to simple sparse geometric or structural constraint data configurations. No doubt future research needs to go much further to see how to build full geological models, optimizing the arsenal of existing geospatial tools within an agent framework. Initial indications are promising for use of agents to develop meshing tools, topologically sensitive surface construction of objects and for respecting simple geological data constraints such as oncontact and dip observations.

8

9 The use of eigenvectors to summarize local anisotropic conditions derived from dip populations was helpful in supporting the 10 propagation of agents, weighting of the spatial continuity direction in a more intuitive manner for structural geological 11 interpretation, and selection of rotation axis for quaternion interpolations. These techniques, more commonly used in the 12 graphics industry, would be beneficial going forward in three-dimensional structural geological modelling in general and 13 potentially for more elaborate spatial agent approaches when solving for multi-property anisotropies such as occur in natural 14 geophysical and geological property distributions (De Paor, 1995). Sparse data configurations with more structural 15 variability, (see Fig. 8) when supported with an agent approach, will better reflect, and extend local structural anisotropy when modelling using other methods such as with implicit estimators. 16

17

With the abundance of machine learning tools currently available it would be potentially useful to investigate how to
optimize structural agents for particular geological use cases, for example using self organizing maps and generalizations for
up-scaling structural data sets based on sampling from Kent distributions (Carmichael and Aillères, 2016) for regional three
dimensional modelling or with application of graph neural networks for more complex geological modelling with sparse data
(Hillier et al., 2020) as well as other emerging deep learning approaches (Guo et al., 2021; Zhang et al., 2019).

23

Natural examples of agent behavior, such as swarm behavior, have emerged over millennia through the embedding of simple rules into organisms that have evolved for optimization of their group survival. This paradigm, although perhaps not obvious for geological applications, could take a similar path and could be an opportunity to leverage geological knowledge through embedding of specific behaviours for given geological processes that are controlled through simple geological rule sets, for example, by programing agents to maintain a range of thickness between stratigraphic layers as they are propagated regionally. Importantly, geological agents would need to operate in a geologically reasonable framework, respecting the
local or regional geological topology network (Thiele et al., 2016). They would need to be able to create solutions from a
suite of possible geological topologies with more complex feature sets, for example from combinations of geologic contacts
and over printings, such as from horizons, faults, ore bodies, intrusions, alteration, and metamorphic fabric relations.

- 5 From this study it is clear that spatial agents can be used to develop simple meshed surfaces, fabric traces, visualize
- 6 anisotropies and structurally sensitive swarm surfaces. Structural agent interrogators exploring a model space can update
- 7 local or group behavior to conform to on-contact or within volume topological dip constraints.
- 8 Agent-based tools as applied to geological applications are yet in their infancy but can be used to interpolate or extrapolate
- 9 from data to produce fabric trajectories, gradients, vector fields and continuous or discontinuous polyhedral meshed surfaces.
- 10 The amplification of local anisotropies is particularly useful with sparse data and increased structural complexity scenarios.
- 11 These characteristics can provide support for simulated input using existing methods for spatial estimation, such as implicit
- 12 approaches.
- 13 Finally, more in-depth investigation into the use of and optimization of spatial agents needs to be undertaken to demonstrate
- 14 the range of benefits for complex geological modelling in a variety of data configurations that could represent typical
- 15 geological scenarios.
- 16 Code and Data Availability
- 17 These codes and data can be freely downloaded. (Please see: https://github.com/Loop3D/GeoSwarm.git or
- 18 <u>https://doi.org/10.5281/zenodo.4634021</u>)

#### 19 Video Supplement

- 20 The video files (mp4) related to this article are available online. (Please see
- 21 https://github.com/Loop3D/GeoSwarm/tree/master/Docs or within https://doi.org/10.5281/zenodo.4634021).
- 22 Author contributions
- 23 EdK developed the GeoSwarm system, performed the literature review of spatial agents and wrote the paper.
- 24 Competing interests
- 25 The author declares that there is no conflict of interest.

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2

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#### 19 References

- Adamuszek, M., Schmid, D. W. and Dabrowski, M.: Fold geometry toolbox Automated determination of fold shape,
   shortening, and material properties, Jour. Struct. Geol., 33(9), 1406-1416, 2011.
- Ailleres, L., Jessell, M., de Kemp, E. A., Caumon, G., Wellmann, F. J. and Grose, L.: Loop Enabling 3D stochastic
   geological modelling, ASEG Extended Abstracts, 1-3, <u>https://doi.org/10.1080/22020586.2019.12072955</u>, 2019.
- Amadou, M. L., Villamor, G. B. and Kyei-Baffour, N.: Simulating agricultural land-use adaptation decisions to climate
   change: An empirical agent-based modelling in northern Ghana, Agric. Syst., 166, 196-209, 2018.
- An, G., Fitzpatrick, B. G., Christley, S., Federico, P., Kanarek, A., Miller, N. R., Oremland, M., Salinas, R., Laubenbacher,
   R. and Lenhart, S.: Optimization and Control of Agent-Based Models in Biology: A Perspective, Bull. Math. Biology,
   79(1), 63–87, 2017.
- Azam, F., Sharif, M. and Mohsin, S.: Multi agent-based model for earthquake intensity prediction, Jour. Comp. Theor. Nano., 12(12), 5765-5777, 2015.
- Barrett, B.J., Hodgson, D.M., Collier, R.E. Ll, Dorrell, R.M.: Novel 3D sequence stratigraphic numerical model for syn-rift
   basins: Analysing architectural responses to eustasy, sedimentation and tectonics, Marine and Petroleum Geology, 92,
   270-284, ISSN 0264-8172, https://doi.org/10.1016/j.marpetgeo.2017.10.026., 2018.
- Bürkle, A.: Collaborating miniature drones for surveillance and reconnaissance, Proceedings of SPIE The Intern. Soc. Opt.
   Eng., 7480:74800H, 2009.
- Brodaric, B.: Characterizing and representing inference histories in geologic mapping, Int. Jour. Geog. Info. Sci., 26 (2), pp. 265-281,https://doi.org/10.1080/13658816.2011.585992, 2012.
- Brodaric, B., Gahegan, M., Harrap, R.: The art and science of mapping: Computing geological categories from field data,
   Comp. Geos., 30 (7),719-740,https://doi.org/10.1016/j.cageo.2004.05.001, 2004.
- Carmichael, T., and Ailleres A.: Method and analysis for the upscaling of structural data, Jour. Struct. Geol., 83, 121-133, 2016.

- Carrillo, J. A., Huang, Y. and Martin, S.: Nonlinear stability of flock solutions in second-order swarming models, Nonlinear
   Analysis: Real World Applications, 17(1), 332-343, 2014.
- Caumon, G., Jessell M. W., de Kemp, E. A., Nemeth, B., Peron, G. and Schetselaar, E. M.: Introduction to special section:
   Building complex and realistic geological models from sparse data, Interpretation 4(3):Smi, 2016.
- Caumon, G. and Collon-Drouaillet, P.: Editorial, Special Issue on Three-Dimensional Structural Modelling, Math. Geos., 46, 905-908, <u>https://doi.org/10.1007/s11004-014-9571-9</u>, 2014.
- Caumon, G., Collon-Drouaillet, P., Carlier L., de Veslud, C., Viseur, S. and Sausse, J.: Surface-based 3D modelling of
   geological structures. Math. Geos., 41(8), 927-945, <u>https://doi.org/10.1007/s11004-009-9244-2</u>, 2009.
- 9 Cervelle J., Formenti E.: Algorithmic Complexity and Cellular Automata, in: Meyers R. (eds) Encyclopedia of
   10 Complexity and Systems Science, Springer, New York, NY. <u>https://doi.org/10.1007/978-0-387-30440-3\_17</u>,
   11 2009.
- Cloetingh, S., Burov, E., Matenco, L., Beekman, F., Roure, F., Ziegler, P.A.: The Moho in extensional tectonic settings: Insights from thermo-mechanical models, Tectonophysics, 609, 558-604, ISSN 0040-1951, <u>https://doi.org/10.1016/j.tecto.2013.06.010</u>., 2013.
- Courrioux, G., Nullans, S., Guillen, A., Boissonnat, J.D., Repusseau, P., Renaud, X., Thibaut, M.: 3D volumetric modelling
   of Cadomian terranes (Northern Brittany, France): An automatic method using Voronoï diagrams,
   Tectonophysics,331(1-2),181-196, https://doi.org/10.1016/S0040-1951(00)00242-0, 2001.
- Crooks, A. T. and Heppenstall, A. J.: Introduction to Agent-Based Modelling, in: Agent-Based Models of Geographical
   Systems, edited by: Heppenstall, A. J., Crooks, A. T., See, L. M., Batty, M. Springer, Chapter 5:85-105, 2012.
- Damiano, R., Lombardo, V. and Nunnari, F.: Virtual agents for the production of linear animations, Entert. Comp. 4(3):187 194, 2013.
- Davis, J. R., and Titus, S. J.: Modern methods of analysis for three-dimensional orientational data, Jour. Struct. Geol., 96, 65 89, 2017.
- de Kemp, E. A., Jessell, M. W., Aillères, L., Schetselaar, E. M., Hillier, M., Lindsay, M. D. and Brodaric, B.: Earth model
   construction in challenging geologic terrain: Designing workflows and algorithms that makes sense, in: Proceedings of
   Exploration'17: Sixth DMEC Decennial International Conference on Mineral Exploration, edited by: Tschirhart, V.
   and Thomas, M.D., Integrating the Geosciences: The Challenge of Discovery (October 21-25, 2017), 419-439, 2017.
- de Kemp, E. A. and Jessell, M. W.: Challenges in 3D modelling of complex geologic objects, in: Proceedings 33'rd gOcad
   meeting (Nancy, September 2013):12, 2013.
- de Kemp, E.A., Sprague, K., and Wong, W.: Interpretive Geology with Structural Constraints: An introduction to the
   SPARSE © plug-in, Americas GOCAD User Meeting, Houston Texas: 1-16, 2004.
- de Kemp, E. A.: 3-D visualization of structural field data: Examples from the Archean Caopatina Formation, Abitibi
   greenstone belt, Québec, Canada, Comp. Geos., 26 (5): 509-530, 2000.
- de la Varga, M., Schaaf, A., and Wellmann, F.: GemPy 1.0: open-source stochastic geological modeling and inversion,
   Geosci. Model Dev., 12, 1–32, <u>https://doi.org/10.5194/gmd-12-1-2019</u>, 2019.
- 36 De Paor, D. G.: Quaternions, raster shears, and the modelling of rotations in structural and tectonic studies. in: Proceedings
   37 and abstracts: Geol. Soc. Amer., New Orleans, LA, USA, November 6-9, 27(6), 72, 1995.
- de Swarte, T., Boufous, O., and Escalle, P.: Artificial intelligence, ethics and human values: the cases of military drones and companion robots, Artificial Life and Robotics, 24:291–296, <u>https://doi.org/10.1007/s10015-019-00525-1</u>, 2019.

- Dickinson, P., Gerling, K., Hicks, K., Murray, J., Shearer, J., and Greenwood, J.: Virtual reality crowd simulation: effects of agent density on user experience and behaviour, Virt. Real., 23(1), 19–32, 2019.
- Fagnant, D. J., and Kockelman, K. M.: The travel and environmental implications of shared autonomous vehicles using
   agent-based model scenarios, Transportation Research Part C: Emerging Technologies, 40:1-13, 2014.
- Farin, G.: Curves and Surfaces for Computer Aided Geometric Design. (4<sup>th</sup> edition), Academic Press, San Diego, California.
   ISBN-13: 9780444511041, 1997.
- Frank, T., Tertois, A.-L. L., and Mallet, J.-L. L.: 3D-reconstruction of complex geological interfaces from irregularly
   distributed and noisy point data, Comput. Geosci., 33, 932–943, <u>https://doi.org/10.1016/j.cageo.2006.11.014</u>, 2007.
- 9 Friedrich, H., Rogalla, O. and Dillmann, R., Communication and propagation of action knowledge in multi-agent systems.
   10 Robot. and Auto. Syst., 29(1):41-50, 1999.
- 11 Gaspari, M.: Concurrency and knowledge-level communication in agent languages, Artif. Intel., 105(1-2):1-45, 1998.
- Grose, L., Ailleres, L., Laurent, G. and Jessell, M.W.: LoopStructural 1.0: Time aware geological modelling, GEOSCI.
   MODEL DEV., 14(6), 3915-393, <u>https://doi.org/10.5194/gmd-14-3915-2021</u>, 2021.
- Grose, L., Laurent, G., Aillères, L., Armit, R.,Jessell, M.W., Guillaume Caumon,G.: Structural data constraints for implicit modeling of folds, Jour. Struct. Geol., 104, 80-92, ISSN 0191-8141,
   https://doi.org/10.1016/j.jsg.2017.09.013, 2017.
- Groshong, R. H. Jr.: 3-D Structural Geology a Practical Guide to Quantitative Surface and Subsurface Map Interpretation,
   (2<sup>nd</sup> Edition), Springer-Verlag Berlin Heidelberg., ISBN-13, 978-3540310549, 2006.
- Guo, J., Li, Y., Jessell, M.W., Giraud, J., Li, C., Wu, L., Li, F., Liu, S.: 3D geological structure inversion from Noddy generated magnetic data using deep learning methods, Comp. Geos., 149, art. no. 104701, https://doi.org/10.1016/j.cageo.2021.104701, 2021.
- Guo, R. G., and Sprague K.S.: Replication of human operators' situation assessment and decision making for simulated area
   reconnaissance in wargames, The Journal of Defense Modelling and Simulation, 13(2), 213-225,
   <u>https://doi.org/10.1177/1548512915619499</u>, 2016.
- Guo, Z. and Li, B.: Evolutionary approach for spatial architecture layout design enhanced by an agent-based topology finding
   system, Frontiers of Architectural Research, 6(1), 53-62, 2017.
- Hall, A., and Virrantaus, K.: Visualizing the workings of agent-based models: Diagrams as a tool for communication and knowledge acquisition, Computers, Environment and Urban Systems, 58, 1-11, 2016.
- Hamilton, W. R.: On a new species of imaginary quantities connected with a theory of quaternions, Proceedings of the Royal
   Irish Academy, 2, 424-434, 1844.
- Heppenstall, A. J., Crooks, A. T., See, L. M., and Batty, M. (editors), Agent-Based Models of Geographical Systems,
   Springer, ISBN-10: 9048189268, 2012.
- Hillier, M., Wellmann, F., Brodaric, B., de Kemp, E., Schetselaar, E.: Three-Dimensional Structural Geological Modeling
   Using Graph Neural Networks, Math. Geos., <u>doi: 10.1007/s11004-021-09945-x</u>, 2021.
- Hillier, M., Wellmann, F. J., de Kemp, E. A., Brodaric, B. and Schetselaar, E. M.: Towards Topologically Constrained 3D
   Geological Modelling, Presentation, Loop3D Sponsor Review Meeting, (March 10-13, 2020), Busselton, Western
   Australia, 2020.

- Hillier, M., Schetselaar, E. M., de Kemp, E. A. and Perron, G.: 3D modelling of geological surfaces using generalized interpolation with radial basis functions, Special Issue, Math. Geos., 46, 931-953, 2014.
- Hillier, M., de Kemp, E. A. and Schetselaar, E. M.: 3D Formline construction by structural field interpolation (SFI) of
   geologic strike and dip observations, Jour. Struct. Geol., 51,167-179, 2013.
- Hoy, G. E. and Shalaby, A.: Use of agent-based crowd simulation to investigate the performance of large-scale intermodal
   facilities: case study of union station in Toronto, Ontario, Canada. Transportation Research Record: Journal of the
   Transportation Research Board, 2540(1), <u>https://doi.org/10.3141/2540-03</u>, 2016.
- 8 Hu, H., Ye, G., Dong, J., Wei, W., Jin, S.: 3-D lithospheric conductivity structures in the Cathaysia Block and the Jiangnan suture zone: implications for origins of metallogenic belts, Journal of Applied Geophysics, 177, 104045, ISSN 0926-9851, <u>https://doi.org/10.1016/j.jappgeo.2020.104045</u>, 2020.
- Jaxa-Rozen, M., Kwakkel, J. H. and Bloemendal, M.: A coupled simulation architecture for agent-based/geohydrological modelling with NetLogo and MODFLOW. Environmental Modelling and Software, 115, 19-37, <u>https://doi.org/10.1016/j.envsoft.2019.01.020</u>, 2019.
- Jayr, S., Gringarten, E., Tertois, A.-L., Mallet, J.-L. and Dulac, J.-C.: The need for a correct geological modelling support: The advent of the UVT-transform, First Break, 26, 73-79, <u>https://doi.org/10.3997/1365-2397.26.10.28558</u>, 2008.
- Jessell, M.W., Ogarko, V., Lindsay, M., Joshi1, R., Piechocka, A., Grose, L., de la Varga, M., Ailleres, L. and Pirot, G.:
   Automated geological map deconstruction for 3D model construction, GEOSCI. MODEL DEV., Preprint gmd-2020-400, <u>https://doi.org/10.5194/gmd-2020-400</u>, 2021.
- Jessell, M. W., Aillères, L., de Kemp, E. A., Lindsay, M., Wellman, F., Hillier, M., Laurent, G., Carmichael, T. and Martin,
   R.: Next Generation Three-Dimensional Geologic Modelling and Inversion. Soc. Econ. Geol., Spec. Pub., 18, 261-272,
   2014.
- Jessell, M. W., Aillères, L. and de Kemp, E. A.: Towards an Integrated Inversion of Geoscientific data: what price of
   Geology? Tectonophysics, 490(3-4), 294-306, 2010.
- Johnson, J. F. and Hoe, D. H. K.: Designing an agent-based model for the efficient removal of red imported fire ant colonies.
   Sim. Ser. 45(11), 361-367, 2013.
- Lajaunie, C., Courrioux, G., Manuel, L.: Foliation fields and 3D cartography in geology: principles of a method based on
   potential interpolation, Mathematical Geology, 29, 571–584, 1997.
- Laurent, G., Ailleres, L., Grose, L., Caumon, G., Jessell, M. and Armit, R.: 2016, <u>Implicit Modeling of Folds and</u>
   <u>Overprinting Deformation</u>, Earth and Planetary Science Letters, 456, 26-38, 2016.
- Levy, S., Martens, K. and Van Der Heijden, R.: Agent-based models and self-organisation: Addressing common criticisms
   and the role of agent-based modelling in urban planning, Town Plan. Rev. 87(3), 321-338, 2016.
- Lindsay, M. D., Jessell, M. W., Aillères, L., Perrouty, S., de Kemp, E. A. and Betts, P. G.: Geodiversity: Exploration of 3D geological model space, Tectonophysics, 594:27-37, 2013.
- Liscano, R., Baker, K. and Meech, J.: The use of ontologies and meta-knowledge to facilitate the sharing of knowledge in a
   multi-agent personal communication system, Lecture Notes, in: Computer Science, Springer, Berlin, Heidelberg,
   (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics), 1822, 187-200,
   <u>https://doi.org/10.1007/3-540-45486-1\_16</u>, 2000.
- Liu, W., Lu, L., Lévy, B., Yang, C. and Meng, X., Centroidal voronoi tessellation of streamlines for flow visualization, ISVD
   2013 10th International Symposium on Voronoi Diagrams in Science and Engineering, 75-81, https://doi.org/10.1109/ISVD.2013.8, 2013.

- MacCormack, K.E., Eyles, C.H.: Assessing the impact of program selection on the accuracy of 3D geologic models,
   Geosphere, 8(2), 534-543, https://doi.org/10.1130/GES00732.1, 2012.
- Ménager, L.: Consensus, communication and knowledge: An extension with Bayesian agents, Mathematical Social Sciences
   51(3), 274-279, 2006.
- Mnasri, S., Nasri, N., van den Bossche, A. and Val, T.: A new multi-agent particle swarm algorithm based on birds accents
   for the 3D indoor deployment problem, ISA Transact. 91, 262-280, 2019.
- Motieyan, H. and Mesgari, M. S.: An Agent-Based Modelling approach for sustainable urban planning from land use and
   public transit perspectives, Cities, 81, 91-100, 2018.
- 9 Nelson, J., Hugh, O., Angel, N., García, E., Chahine, J. and Socci, N.D.: The energy landscape theory of protein folding:
   10 Insights into folding mechanisms and scenarios, Advances in Protein Chemistry, 53, 87-130,
   11 <u>https://doi.org/10.1016/S0065-3233(00)53003-4</u>, 2000.
- Parquer, M., Yan, N., Colombera, L., Mountney, N.P., Collon, P., Caumon, G.: Combined inverse and forward numerical
   modelling for reconstruction of channel evolution and facies distributions in fluvial meander-belt deposits, Marine and
   Petroleum Geology, 117, 104409, ISSN 0264-8172, <u>https://doi.org/10.1016/j.marpetgeo.2020.104409</u>, 2020.
- Parunak, H.V., Baker, A. D., and Clark, S. J.: AARIA agent architecture: from manufacturing requirements to agent-based
   system design, Integrated Computer-Aided Engineering 8(1), 45-58, 2001.
- Pellerin, J., Botella, A., Bonneau, F., Mazuyer, A., Chauvin, B., Lévy, B., Caumon, G.: RINGMesh: A programming library
   for developing mesh-based geomodeling applications, Comp. Geos., 104, 93-100, ISSN 0098-3004,
   <u>https://doi.org/10.1016/j.cageo.2017.03.005</u>, 2017.
- 20 Ramsay, J.G.: Folding and Fracturing of Rocks, McGraw-Hill, New York, 568 pp, ISBN 13: 9780070511705, 1967.
- Ramsay, J.G.: The Geometry of Conjugate Fold Systems, Geol. Mag., 99(6), 516 526,
   <u>https://doi.org/10.1017/S0016756800059823</u>, 1962.
- Reynolds, C. W.,: Flocks, herds and schools: A distributed behavioral model, SIGGRAPH '87 Proceedings of the 14th annual conference on Computer graphics and interactive techniques, 25-34, https://doi.org/10.1145/37401.37406
   <u>http://www.red3d.com/cwr/boids/</u>, 1987.
- Rigotti, N. A. and Wallace, R. B.: Using agent-based models to address "wicked problems" like tobacco use: A report from the institute of medicine, Annals of Internal Medicine, 163(6), 469-470, 2015.
- 28 Schatten, K.: Large-scale solar magnetic field mapping: I. SpringerPlus, Virtual Journal, 2013, 2-21, 2013.
- Schlögl, M., Richter, G., Avian, M., Thaler, T., Heiss, G., Lenz, G. and Fuchs, S.: On the nexus between landslide
   susceptibility and transport infrastructure- an agent-based approach, Natural Hazards and Earth Systems Sciences 19, 201–219, 2019.
- Semenchenko, A., Oliveira, G. and Atman, A. P. F.: Hybrid agent-based model for quantitative in-silico cell-free protein
   synthesis. BioSystems, 150, 22-34, https://doi.org/10.1016/j.biosystems.2016.07.008, 2016.
- 34 Shoemake, K.: Animating Rotation with Quaternion Curves, Comp. Graph. (ACM), 19(3), 245-254, 1985.
- Siegfried, R.: Modeling and Simulation of Complex Systems: A Framework for Efficient Agent-based Modeling and
   Simulation, Springer Fachmedien, Wiesbaden , 227 pp, <u>https://doi.org/10.1007/978-3-658-07529-3</u>, 2014.
- Skirrow, R.G., Murr, J., Schofield, A., Huston, D. L., van der Wielen, S., Czarnota, K., Coghlan, R., Highet, L.M.,
   Connolly, D., Doublier, M., Duan, J.: Mapping iron oxide Cu-Au (IOCG) mineral potential in Australia using a

- knowledge-driven mineral systems-based approach, Ore Geology Reviews, 113, 103011, ISSN 0169-1368, https://doi.org/10.1016/j.oregeorev.2019.103011, 2019.
- Sprague, K., de Kemp, E.A., Wong, W., McGaughey, J., Perron, G., Barrie, T.: Spatial targeting using queries in a 3-D GIS
   environment with application to mineral exploration, Comp. Geos., 32, (3), 396-418, ISSN 0098-3004,
   <u>https://doi.org/10.1016/j.cageo.2005.07.008</u>, 2006.
- Thiele, S. T., Jessell, M. W., Lindsay, M., Ogarko, V., Wellmann, J. F. and Pakyuz-Charrier E.: The topology of geology 1:
   Topological analysis, Journ. Struct. Geol. 91, 27–38, 2016.
- 8 Tieskens, K. F., Shaw, B. J., Haer, T., Schulp, C. J. E. and Verburg, P. H.: Cultural landscapes of the future: using agent-based modelling to discuss and develop the use and management of the cultural landscape of South West Devon.
   10 Landscape Ecology, 32(11), 2113-2132, <u>https://doi.org/10.1007/s10980-017-0502-2</u>, 2017.
- 11 Torrens, P. M.: Agent based models and the spatial sciences. Geography Compass, 4(5), 428-448, 2010.
- Valbuena, D., Verburg, P. H., Veldkamp, A., Bregt, A. K., and Ligtenberg, A.: Effects of farmers' decisions on the landscape
   structure of a Dutch rural region: An agent-based approach, Landscape and Urban Planning, 97(2), 98-110,
   https://doi.org/10.1016/j.landurbplan.2010.05.001, 2010.
- Von Neumann, J.: Theory of self-reproducing automata. Edited by A. W. Burks, Urbana, University of Illinois Press, 408 pp, 1966.
- Wellmann, F., Schaaf, A., de la Varga, M., von Hagke, C. : Chapter 15 From Google Earth to 3D Geology Problem 2:
   Seeing Below the Surface of the Digital Earth, Editor(s): Andrea Billi, Åke Fagereng, Developments in Structural
   Geology and Tectonics, Elsevier, 5, 189-204, ISSN 2542-9000, ISBN 9780128140482, <u>https://doi.org/10.1016/B978-0-12-814048-2.00015-6</u>, 2019.
- Wellmann, F., Caumon, G.: Chapter One 3-D Structural geological models: Concepts, methods, and uncertainties, Editor(s):
   Cedric Schmelzbach, Advances in Geophysics, Elsevier, 59, 1-121, ISSN 0065-2687, ISBN 9780128152089,
   <a href="https://doi.org/10.1016/bs.agph.2018.09.001">https://doi.org/10.1016/bs.agph.2018.09.001</a>, 2018.
- White, D.: Seismic characterization and time-lapse imaging during seven years of CO2 flood in the Weyburn field,
   Saskatchewan, Canada, International Journal of Greenhouse Gas Control,16, S1, S78-S94, ISSN 1750-5836,
   <a href="https://doi.org/10.1016/j.ijggc.2013.02.006">https://doi.org/10.1016/j.ijggc.2013.02.006</a>, 2013.
- Wilensky, U., and Rand, W.: An Introduction to Agent Based Modelling Modelling Natural, Social and Engineered
   Complex Systems with NetLogo, Massachusetts Institute of Technology, ISBN: 9780262731898, 2015.
- Wilensky, U.: NetLogo, Center for Connected Learning and Computer-Based Modelling, Northwestern University, Evanston,
   IL. <u>http://ccl.northwestern.edu/NetLogo/</u>, 1999.
- Wilensky, U.: NetLogo Flocking model, Center for Connected Learning and Computer-Based Modelling, Northwestern
   University, Evanston, IL. <u>http://ccl.northwestern.edu/NetLogo/models/Flocking</u>, 1998.
- Wilensky, U.: NetLogo Wave Machine 3D model., Center for Connected Learning and Computer-Based Modelling,
   Northwestern University, Evanston, IL., <u>http://ccl.northwestern.edu/NetLogo/models/WaveMachine3D</u>, 1996.
- Wolfram, S.: Cellular Automata and Complexity; Collected Papers, 1<sup>st</sup> Edition, Westview Press, USA, 1994, 596 pp, https://doi.org/10.1201/9780429494093, 1994.
- 37 Woodcock, N. H.: Specification of Fabric Shapes using an eigenvalue method, Geol. Soc. Amer. Bull., 88, 1231-1236, 1977.

- Zhang, T.-F., Tilke, P., Dupont, E., Zhu, L.-C., Liang, L., Bailey, W.: Generating geologically realistic 3D reservoir facies
   models using deep learning of sedimentary architecture with generative adversarial networks, Petroleum
   Science, 16 (3), 541-549, https://doi.org/10.1007/s12182-019-0328-4, 2019.
- Zuparic, M., Jauregui, V., Prokopenko, M. and Yue, Y.: Quantifying the impact of communication on performance in multiagent teams, Artificial Life and Robotics, 22(3), 357-373, 2017.
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- 7
- 8

#### C

9

#### 10 Appendix A: Agent resources

An excellent starting point to become familiar with agent-based applications and approaches is Paul Torrens' web site at <a href="http://geosimulation.org/">http://geosimulation.org/</a> from the Computer Science and Engineering, Tandon School and Center for Urban Science and

13 Progress, at New York University.

14 The agent-based codes used in this paper are written in Net Logo-3D, a spatial agent-based modelling language and

15 development environment that is supported from the Center for Connected Learning and Computer-based modelling in

16 Evanston, Illinois, USA. The NetLogo project is affiliated with Northwestern University Centre on Complex Systems

17 (NICO) <u>https://www.nico.northwestern.edu/</u>. To download and run the NetLogo codes, for tutorials and documentation on

18 the NetLogo language see http://ccl.northwestern.edu/NetLogo. The code must be minimally compatible with the NetLogo

19 3D version as listed in the programs below. Current and early 3D versions of the program are all available on the main

20 NetLogo homepage.

21 Codes presented in this paper are freely downloadable from the Git Hub Open Source web site at

22 <u>https://github.com/Loop3D/GeoSwarm.git</u> (<u>https://doi.org/10.5281/zenodo.4634021</u>) with accompanying power point, pdf

and animations presented at the annual meeting of the International Association of Mathematical Geoscientists at Penn State

24 University, USA, August 2019.

| 1  | Appendix B:             | List of NetLog                        | List of NetLogo 3D Programs                            |  |
|----|-------------------------|---------------------------------------|--|--|
| 2  | Program Name            | Version                               | Purpose  |  |
| 3  | Trace.nlogo3d           | 6.0.4                                 | Propagation and interpolation (NN and IDW)             |  |
| 4  | Poly.nlogo3d            | 6.0.4                                 | Closed and connected polyhedral growth                 |  |
| 5  | Mesh.nlogo3d            | 6.0.4                                 | Simple surface meshing by triangulation growth         |  |
| 6  | Rotate.nlogo3d          | 6.0.4                                 | Dips with polarity rotation (SLERP - eigenvectors)     |  |
| 7  | Swarm_Dips.nlog         | go3d 6.0.4                            | Structural dip cohesion mimicking deformed surfaces    |  |
| 8  | GeoSwarm.nlogo          | 3d 6.0.4                              | Simple geometry solving from steep fold limb pairs     |  |
| 9  | Wave.nlogo3d            | 6.0.4                                 | Simple non-meshed elastic surface motion               |  |
| 10 |                         |                                       |  |  |
| 11 | <u>Shape Libraries:</u> |                                       |  |  |
| 12 | 3d_HexShape.txt         | > 5.3                                 | Required to generate hexagon dip glyphs with polarity  |  |
| 13 | 3d_Shape.txt            | 4.1,5.1,6.0.4                         | Required to generate tabular dip glyphs with polarity  |  |
| 14 |                         |                                       |  |  |
| 15 | Example Psuedo Code:    |                                       |  |  |
| 16 |                         | Mesh.nlogo3d                          |  |  |
| 17 |                         |                                       |  |  |
| 18 |                         | Start                                 |  |  |
| 19 |                         | Create Nodes agent set                |  |  |
| 20 |                         | Create Triangles agent set with rande | om directed normals                                    |  |
| 21 |                         | Define a seed Triangle                |  |  |
| 22 |                         | Do while [ mesh growing ] [           |  |  |
| 23 |                         | if [nearest neighbour to see          | ed <i>Triangle</i> exists] [                           |  |
| 24 |                         | connect an edge                       | e of the seed Triangle to its nearest neighbour's edge |  |
| 25 |                         | repeat along the                      | seed until all its edges are fused                     |  |
| 26 |                         | repeat along the                      | outer edge of the mesh                                 |  |
| 27 |                         |                                       |  |  |
| 28 |                         | ]                                     |  |  |
| 29 |                         | if [all Triangles meshed] [           |  |  |
| 30 |                         | quality check the                     | emesh  |  |
| 31 |                         | if [mesh is not re                    | easonable] [   |  |
| 32 |                         | set me                                | esh to growing   |  |
| 33 |                         | discon                                | nnect the mesh by killing shared edges                 |  |
| 34 |                         | Scatte                                | er all <i>Triangles</i>                                |  |
| 35 |                         | Re-de                                 | fine the seed Triangle                                 |  |

| 1 |     |      | ]                         |
|---|-----|------|---------------------------|
| 2 |     | Else |                           |
| 3 |     |      | [set mesh to not growing] |
| 4 |     |      | ]                         |
| 5 |     | ]    |                           |
| 6 | End |      |                           |
| 7 |     |      |                           |

- 8 Once all the meshing is complete, there is a quality control check to determine if the result is a 'reasonable' surface.
- 9 This could be a simple rule that looks for holes, and surfaces with low connectivity, for example by calculating a
  10 low node count to edge count ratio; with 1 = no triangles connected, ~ .72 = single node connected chain, ~ .62 =
- 11 single edge connected chain,  $\sim .58 =$  hexagonal mesh).
- 12
- 13

#### 1 Appendix C: Quaternion Calculations

- 2 Quaternion codes are used in Dip\_Swarm and Rotate programs and implemented in NetLogo within the **Spin**()
- 3 procedure. Used for smooth rotation along specified axis such as an eigenvector of a structural observation set and
- 4 for inverse distance weighted (IDW) and Spherical Linear Interpolation (SLERP). For details see De Paor (1995),
- 5 Shoemake (1985), Hamilton (1853).
- 6 C.1 Provide a normalized unit vector to the Spin procedure from common structural observation data
- 7 Convert strike and dip (RHR) to a Unit Normal vector. Input is in degrees. Normal is perpendicular to plane
- 8 strike = a scalar angle of in degrees azimuth in the horizontal plane measured clockwise from north (0°) representing
- 9 the angle between a topographic surface trace of a geological feature, such as a horizon intersecting with
- topography, and the north direction. Strike in this study uses the Right Hand Rule (RHR) which is a common
- 11 structural geological measuring standard for planar field observation data. It assumes that the strike direction vector
- 12 is pointing such that the geological surface dips to the right of the observer as they face the strike direction.
- 13 (Note east =  $90^{\circ}$ , south =  $180^{\circ}$ , west =  $270^{\circ}$ )

14 *strike* 
$$\in$$
 {0,360}

- 15 *dip* = a scalar angle in degrees indicating maximum slope from the horizontal taken in the direction of the dipping
- surface. The dip direction is always 90° to the strike direction. The dip angle (dip) is the maximum vertical angle
   from the horizontal to the geological surface.
- 18  $dip \in \{0,90\}$
- 19 *polarity*  $\in \{-1,0,1\}$
- 20 polarity = a signed unit integer indicating if a geological surface is upside down, that is overturned with respect to its
- original depositional configuration. -1 = overturned, 0 = unknown, 1 = upright. This value is used to give topological information in modelling.
- 23 strdip2norm ( *strike*, *dip*, *polarity* )
- 24 Returns a 3 element unit normal vector.
- 25 Calculate down dip vector
- 26  $ddx = \cos(-1 * strike) * \cos(-1 * dip)$
- 27  $ddy = \sin(-1 * strike) * \cos(-1 * dip)$
- $ddz = \sin\left(-1 * dip\right)$
- 29 Calculate the strike vector
- $30 \qquad sx = -1 * ddy$
- $31 \qquad sy = ddx$
- 32  $s_z = 0$  (note the strike vector is always in the horizontal plane)
- Cross down dip vector with strike vector ( $V_{dd} \times V_s$  to get the normal (N) or pole to bedding.
- $34 \qquad NNx = (ddy * sz) (ddz * sy)$
- $35 \qquad NNy = (ddz * sx) (ddx * sz)$
- $36 \qquad NNz = (ddx * sy) (ddy * sx)$

| 1              | Normalize the normal for unit length <i>L</i> .   |
|----------------|---|
| 2              |   |
| 3              | $L = \sqrt{NNx^2 + NNy^2 + NNz^2}$  |
| 4              |   |
| 5              | Adjust for polarity   |
| 6              | Nx = (polarity * NNx) / L   |
| 7              | Ny = (polarity  * NNy) / L  |
| 8              | Nz = (polarity  * NNz) / L  |
| 9              |   |
| 10<br>11<br>12 | Convert a Trend and Plunge to a normalized unit Vector. A common fabric element for various linear structural features such as fold hinge lines joining maximum curvatures along the plunge of a fold, or stretching features located along E3. Used to get a vector from an agent heading and pitch state. |
| 13             | TrendPlunge2Vec (trend, plunge)   |
| 14             | Returns a 3 element unit normal vector.   |
| 15             |   |
| 16             | $VVx = \sin(\text{trend}) * \cos(\text{plunge})$  |
| 17             | $VVy = \cos(\text{trend}) * \cos(\text{plunge})$  |
| 18             | $VVz = \sin(\text{plunge})$   |
| 19             |   |
| 20             | Unit Normalize  |
| 21             | $M = \sqrt{VVx^2 + VVy^2 + VVz^2}$  |
| 22             | Vx = VVx / M  |
| 23             | Vy = VVy / M  |
| 24             | Vz = VVz / M  |

C.2 Input the rotation increments (A) the rotation vector (Q) and the normal of the structural observation (P)
 into the Spin procedure to rotate the structural elements with quaternion calculations.

- 28 Spin (A VP)
- 29 A = spherical angle of rotation in degrees (not Euler angles)  $A \in \{-\infty, \infty\}$
- 30 V = Unit vector 3D axis of rotation (Vx, Vy, Vz,). Can be any of the eigenvectors, a down dip vector, strike vector 31 etc.
- 32  $P = \text{Normal unit vector } (n_x, n_y, n_z)$  (such as Poles to beds, a fold hinge etc.)

- 1 Returns *S* a matrix with full orientation description including the normal to bedding or new rotated linear element,
- 2 the *strike* and *dip* components, *overturned* (polarity) and 4 quaternion elements (*qw*, *qx*, *qy*, *qz*).
- 3 Transform from single vector to quaternion with rotation A about an axis **Q**
- 4 This procedure can be used to convert normal to strike and dip RHR by input A = 0 rotation and V = P just cast the *P* 5 as a single matrix from the normal
- 6 Returns RHR\_Orientation array using Right Hand Rule planar orientation for STRIKE, DIP, N1, N2, N3,
- 7 OVERTURNED
- 8
- 9 Q = (s, V) scalar, vector
- 10  $qx = (\sin(A/2) * Vx)$
- 11  $qy = (\sin(A/2) * Vy)$
- 12  $qz = (\sin(A/2) * Vz)$
- 13  $qw = (\cos(A/2))$
- 14  $\mathbf{Q} = (qw, qx, qy, qz)$
- 15
- 16 C.3 Create the Rotation Matrix
- 17 Use quaternion identities to derive the rotation matrix

$$18 \qquad q^2w = 1 - qx^2 - qy^2 - qz^2$$

- **19**  $q2x = qx^2$
- 20  $q2y = qy^2$
- **21**  $q2z = qz^2$
- 22 Compose *R* the rotation matrix
- 23

24 
$$\mathbf{R} = \begin{array}{ccc} q2w+q2x-q2y-q2z & 2qxqy-2qzqw & 2qzqx+2qyqw \\ 2qxqy+2qzqw & q2wq2x+q2y-q2z & 2qyqz-2qwqx \\ 2qzqx-2qyqw & 2qyqz+2qwqx & q2wq2x-q2y+q2z \end{array}$$

$$\mathbf{26} \qquad \mathbf{R} = \begin{array}{c} R_{xx} & R_{xy} & R_{xz} \\ R_{yx} & R_{yy} & R_{yz} \\ R_{zx} & R_{zy} & R_{zz} \end{array}$$

- 27
- 28 C.4 Matrix multiply the Rotation matrix with the input observation normal P
- S = P X R
- 30

- 1 C.5 Interpolate, by calling the spherical linear interpolator (SLERP) for any interpolation on parameter *t*, a
- 2 normalized distance between data and the spatial starting point of an agent (A) as it is rotated towards the structural
- 3 constraint (*B*). Details of SLERP can be located in De Paor (1995). Note with the inverse distance weighted (IDW)
- 4 form of SLERP a set of structures can all influence the agent depending on the agent's ability to sense the data, for
- 5 example the structural search agent needs to be within the vision distance.
- For the IDW SLERP calculate the data weights based on inverse distance, adjust exponent <sup>*p*</sup> if needed for stronger
   local influence,

8 
$$W_i = \frac{1}{D_i^p \sum_{j=1}^n (\frac{1}{D_i^p})}$$

10 Calculate G the estimated orientation at x by adjusting the contributing quaternion components of the data with the 11 distance weights,

12 
$$G(x) = \sum_{i=1}^{n} (W_i * Q_i)$$

13 To use the simpler linear form with A and B orientations,

14 
$$SLERP(x) = (1 - t)Q_A + tQ_B \quad (t = |dist|)$$