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1 **Spatial Agents for Geological Surface Modelling**

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11
12 **Abstract**

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

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

2   (https://doi.org/10.5281/zenodo.4288476).

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

11   is potentially useful for complex geology - sparse data environments where extension, projection and propagation functions

12   are needed to create more realistic geological forms.

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

14   **1   Introduction**

15   The major challenge that this paper is trying to address is the breakdown in achieving geologically realistic model results

16   from sparse data in more complicated geological scenarios when using the existing methods and algorithms. This is no doubt

17   a problem in other modelling domains as well, but is acute in geological applications, where access to data in the subsurface

18   is often extremely expensive, terrain access prohibitive, or the depth of investigation too extreme for direct sampling and

19   must rely on coarser geophysical methods that often do not adequately image the features being modelled. This paper

20   explorers the use of extension, propagation and cohesion methods, which can be considered part of 'swarm' technology,

21   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

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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?

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

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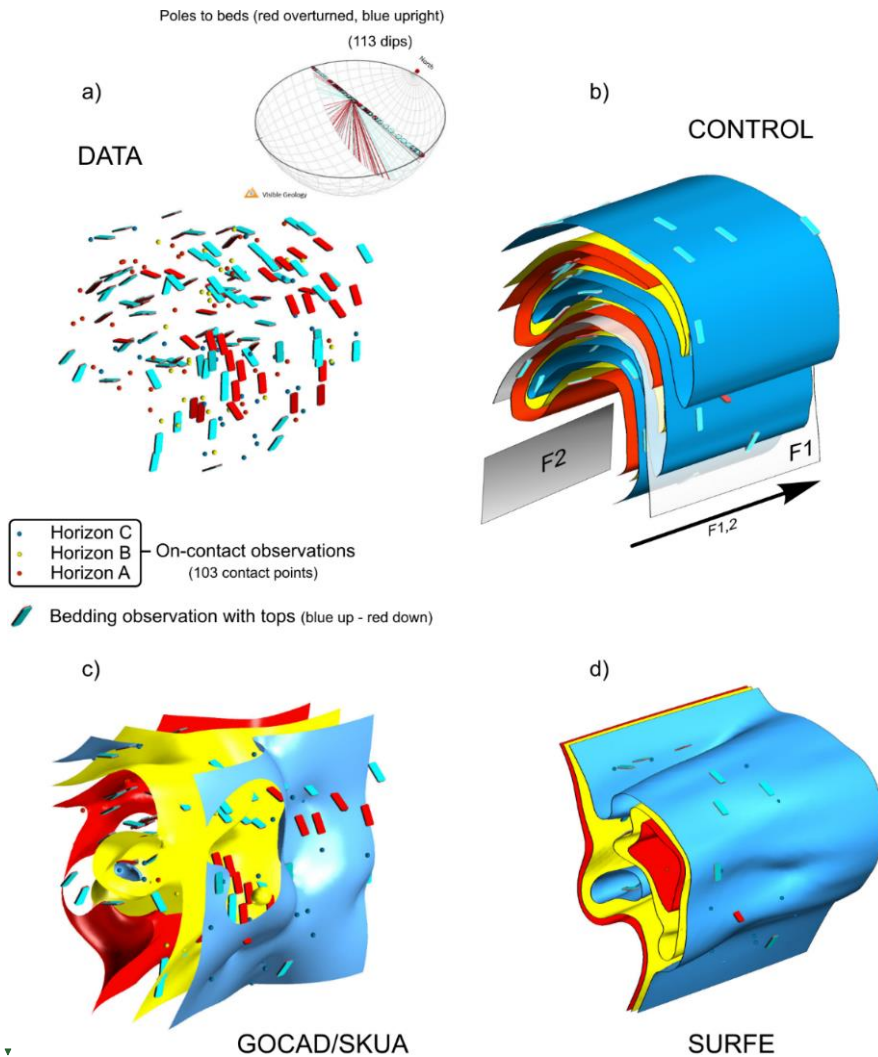
Poles to beds (red overturned, blue upright)

(113 dips)

a)

DATA

b)

CONTROL

F2

F1

F1,2

- Horizon C
- Horizon B ⎤ On-contact observations
- Horizon A ⎦ (103 contact points)

Bedding observation with tops (blue up - red down)

c)

d)

GOCAD/SKUA

SURFE

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2

3 **Figure 1.** Comparison of synthetic geological three-dimensional models of classic Ramsay type 3 interference folds (Ramsay, 1967;1962), with identical

4 data. (a) Uniaxial dip data, with local opposing tops, represented on equal-angle Wulf plot (https://app.visiblegeology.com/stereonet.html). (b) Control

5 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

6 al., 2008) and (d) SURFE (Hillier et al., 2104).

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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.

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

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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.

1.2 Agent Applications

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

http://www.gravitysim.net/index.html. 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. This allows them to behave in a flexible and efficient manner, without the need for global partitioned data structures or tightly coupled deterministic algorithms. Many agent examples are biologically based such as the classic flock of birds examples; 'murmurings' and geese in V-formation, beehive and anthill construction examples (Mnasri et al., 2019; Carrillo et al., 2014; Johnson and Hoe, 2013). These examples highlight the potential to capture multi-scaler and complex interaction that has enhanced the uptake of this technology for medical and biology fields (An et al., 2017; Rigotti and Wallace, 2015).

1.3   Agent Characteristics

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

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

1.4 Role of Interpretation

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

1.5 Demonstration Codes

The properties and general behavior of spatial agents is demonstrated for the simplest of geological data, through several agent demonstration programs. These codes and data can be freely downloaded (See https://github.com/Loop3D/GeoSwarm.git or https://doi.org/10.5281/zenodo.4634021). The code implementation was done in NetLogo 3D agent-based modelling software (Wilensky, 1999), taking inspiration from some earlier model examples such

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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.

2   Current Geological Surface Modelling

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

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

14 extension methods (Torrens, 2010; de kemp and Jessell, 2013) using sparse data, for regional geological domains.

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

1   not provide feature continuity that the agents could provide. In the code examples, much use is made of what is

2   termed a 'structural agent'. These are agents that have spatial coordinate location properties for X, Y, Z but also

3   planar or linear geometric properties of strike, dip, trend, plunge and normal direction cosine components used to

4   designate a horizon top direction or a fold hinge line.   They may also have environmental information that tracks

5   local or regional eigen-fields. As noted earlier these types of agents may represent data, estimations or interrogators

6   that can transfer their properties as required. The structural agents enhance the interpretation process by densifying

7   the form lines and simulating more planar point features to highlight structural changes more clearly (Fig. 2).
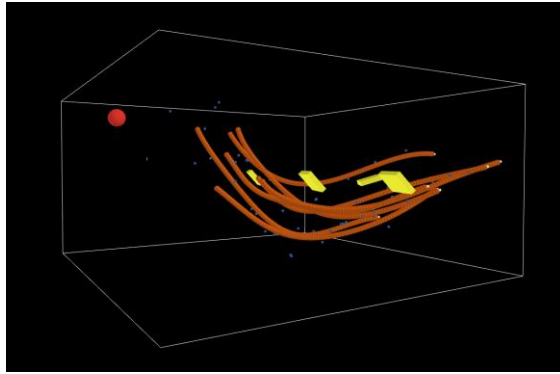
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11   **Figure 2.** Structural form traces (orange point streams) estimated from dip data (yellow cuboids) using spatial agents. Red sphere

12   is an interrogator agent. Blue dots are simulated Bézier control points with added random noise. See Appendix A for details.

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14   Spatial agents are also employed to better visualize and interpolate planar and linear structures, respecting the

15   polarity of the observations and resulting estimations (Fig. 3), essential for interpreting folded geology. Spatial agent

16   triangulated meshes are produced from point observations, that use proximity and topologic rules for accepting or

17   reject the meshing criteria to maintain local and overall continuity, meaning the surface has no holes or branches

18   (Fig. 4). In this triangular meshing application, a random field of moving unconnected and randomly oriented

19   triangles is initialized. Each triangle is an agent set comprised of 3 node agents and 3D directed edges, as well as a

1   computed Barycentre with a unit normal vector property. The closest triangle to the model centre will act as a seed

2   for the meshing and will sense its nearest neighbour triangle and connect to it, maintaining a consistent topology

3   with each triangle rotating into position, making a proper connection to an adjacent triangle. This proceeds until all

4   the triangles have been connected into a reasonable continuous surface patch, with no holes or large tears, and all

5   adjacent triangle normals pointing the same direction. The action is very simple as shown in the pseudo code in
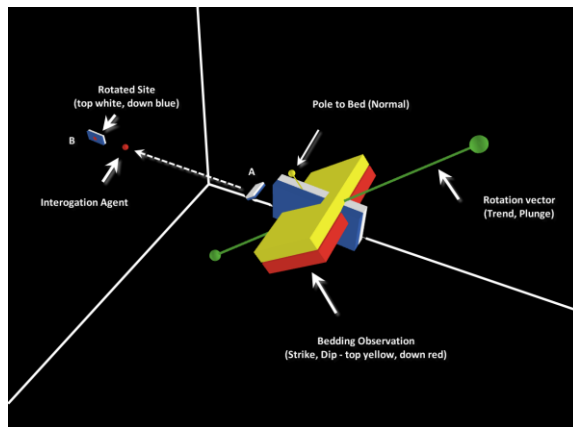
6   Appendix B.

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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

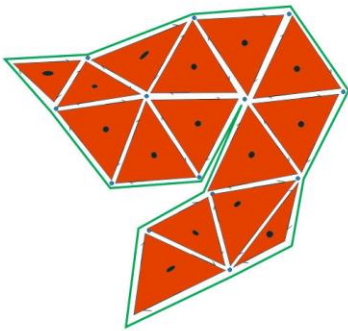12   smooth topology for top direction. See Appendix B for details.

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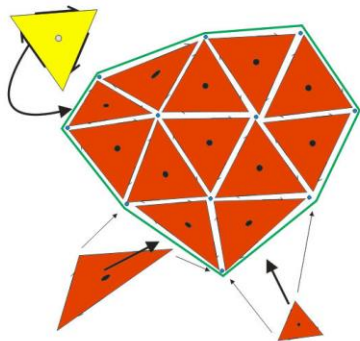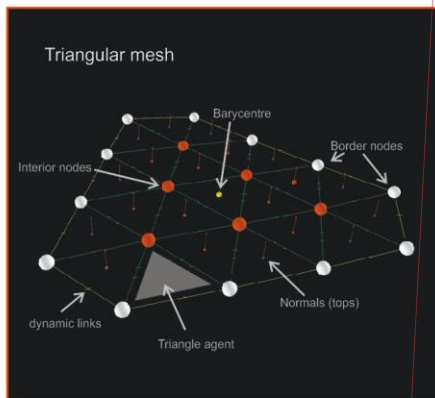

Inside Hull:

Triangles	Mutual Edges	Shared Vertices
12	14	11
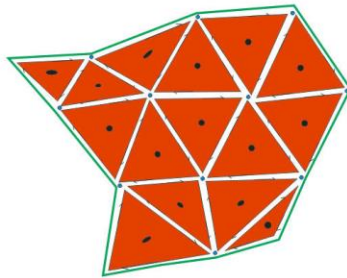
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Triangles	Mutual Edges	Shared Vertices
15	17	11

Inside Hull:

Triangles	Mutual Edges	Shared Vertices
15	15	13

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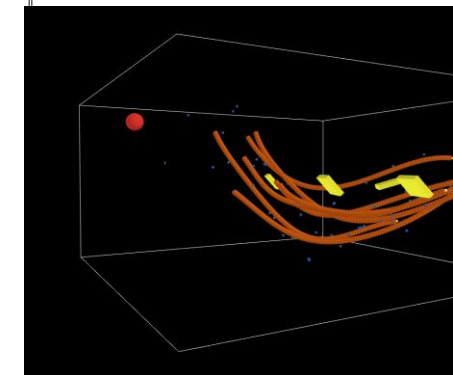**Figure 2.** Structural form traces (orange point streams) estimated from dip data (yellow cuboids) using spatial agents. Red sphere is an interrogator agent. Blue dots are simulated Bézier control points with added random noise. See Appendix A for details.¶

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

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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.
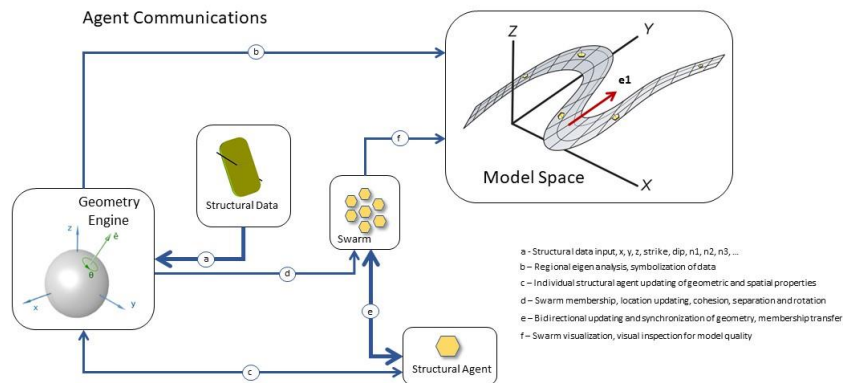

Figure 5. General summary of structural agent communication using the example from *GeoSwarm*, for details see comments and codes in the open-source programs listed in Appendix B. Thickness of blue lines indicates relative degree of inter-agent communication. Geometry Engine composed of all agent functions 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.

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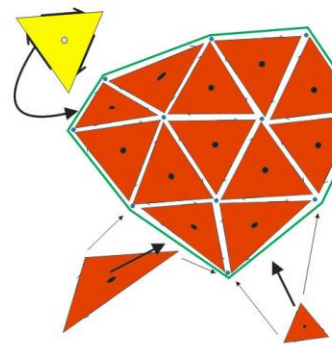
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Triangles	Mutual Edges	Shared
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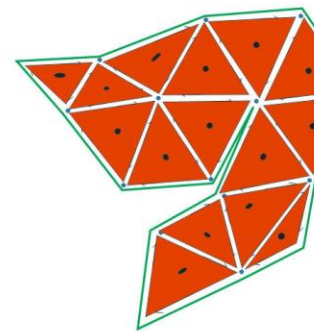
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Triangles	Mutual Edges	Share
15	15	13

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

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2.3 Agent Behavior

Some interesting qualities of spatial agents:

2.3.1   Agents are able to efficiently interrogate irregular and complex model spaces. The model design can result in a wide range of single realizations or solution suites. More traditional approaches are dependent on fixed regular and partitioned structures using standard coordinate systems, with few geological properties.

 2.3.2   Agents are suitable for modelling natural complex systems. Preserving contributions from multi-scalar and deep multi-property data, such as fold shape parameters, or geophysical rock properties. Global interpolation techniques such as implicit interpolation tend to generalize dense data clusters to a local mean and are optimized for a scale specific purpose, often producing geologically meaningless results (Fig. 1). This could happen when combining point geometry from structure, categorical geology, and continuous geophysics data. Essential details such as fold topology and hinge regions can be ignored or conflict dramatically with geophysical gradients. Agents may be able to more easily incorporate this kind of local information during estimation and feature propagation.

2.3.3   Agents can support the domain expert that requires more interpretive skills, with knowledge-based Rules, Missions (Beliefs) and/or Behaviors during data interrogation. Agents could be used in mapping to visualize complex relationships, such as within vector fields, for fabric intersections (bedding – cleavage relationships); vergence relationships on fold trains; disharmonic folds and poly-deformed stratigraphy with early cryptic faulting. Visualization of these relationships within the event history is critical to more accurate geological interpretation.

2.3.4   Agents complement rather than replace existing algorithms and approaches. For example, spatial estimation can still be applied (Implicit, IDW- Inverse Distance Weighted, Kriging, DSI - Discrete Smooth Interpolation, SVM Support Vector Machine, etc.) at variable scales as required. Thus, they potentially could provide a framework for calling a variety of interpolators and constructors depending on data density, problem domain and feature complexity.

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

1 inserting a new deformation event when a metamorphic fabric is observed in a boulder of apparently undeformed

2 conglomerate, or when a high curvature region is detected by inserting a fold hinge or fault control point.

3 **2.3.6**   Agent-based approaches may benefit from denser and faster CPU/GPU architecture and parallelization

4 schemes. This could be the case, as the simple rules driving agent interaction and communication act more

5 independently, rather than having to invert large global matrices common in implicit approaches. This has yet to be

6 tested, since it is perhaps hard to partition on-going spawning processes from independent agents, but could result in

7 dramatic efficiency gains when combining multi-scalar properties from geophysics and geology within three-

8 dimensional 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).

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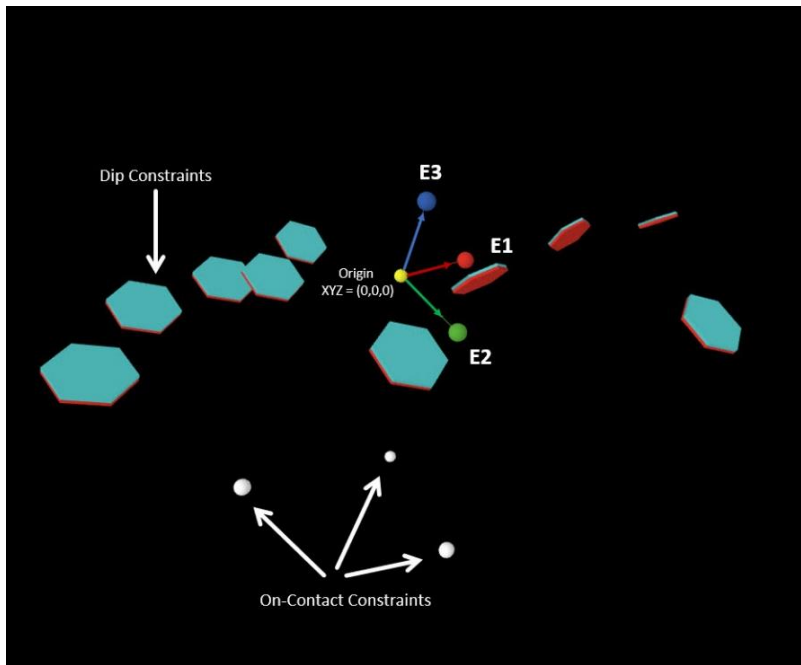Deleted: Netlogo

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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.

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: http://ccl.northwestern.edu/NetLogo. 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

18

1   thoroughly tested or gone through performance optimization. It is best to slowly increase the number of agent data

2   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*

16   Demonstrates simple polyhedral graphics control which is needed for vector-based boundary representations used in

17   many geological modelling environments. Construction agents can perform simple local tasks, such as making a

18   single polyhedron, but also regional tasks, by joining these up until stop criteria are reached. Modelling of simple

19   closed and connected polyhedra is achieved by joining simple triangles or large loops with many vertices. Each

20   closed polyhedron once formed will connect one link to its adjacent polyhedron, forming a simple object chain.

21   Modelling and visualization of the network are controlled by user-defined edge size, search radius, repulsion, and

22   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

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Demonstrates the modelling of fabric observations. The search agent (red sphere) travels through the model space randomly until it senses a proximal dip observation. It will then adjust its trajectory towards a down dip vector to this observation and spawn other simulated dip points that are nearest neighbour (NN) or inverse distance weighted (IDW) interpolations from the data. A stream of points is recorded as the search agent moves through the model space. This point stream will form De Casteljau – Bézier (Farin 1997) curves that are either killed or preserved based on simple user specified shape parameters. Demonstrates streamline visualization using down dip trajectories. Similar to the three-dimensional Structural Field Interpolation (SFI) from Hillier et al. (2013). The main distinction here is the sampling is random with the potential for multiple search agents acting simultaneously.

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1 a user defined target dip agent is set up. A linear quaternion rotation of the control dip is incrementally rotated along

2 a single or circular radial to the target dip. Users can rotate all dips continuously and dynamically. The agents are

3 always updating to the new target. Rotation axis is defined by the user which could be in all possible in-plane or out

4 of plane cross-dip orientations.   This is a required method for estimation of local and regional dips and structural

5 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.

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3.4 Rotate¶
Demonstrates SLERP rotations which would be required for estimation in complex geological domains with folding and sparse data representation. It is also a testing environment for interpolating planar constraint data with linear rotation axis. 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 useful for modelling of local and regional dips for structural vector fields.

1

3.5.1 *Swarm Dips: Simple Plane*

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

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

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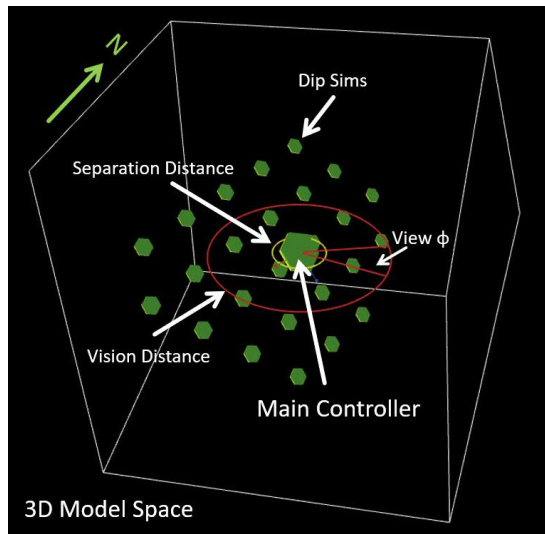
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4 **Figure 7.** Components of the spatial agent-based model (SABM).

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*

10 Demonstrates that sims can sense and migrate to on-contact feature control points while detecting the structural

11 influence from adjacent data. Dip Sims move toward the nearest on-contact data point while rotating into parallelism

12 with the closest dip observation. At a given tolerance to the on-contact data points, the Dip Sim freezes in an

13 orientation that is close to the neighbourhood dip field. When all on-contact data points have a Dip Sim the rest of

14 the Dip Sims are behaving as a swarm; controlled by the Main controller and moving in the plane specified by the

15 controller and vision-proximity rules.

16

22

3.6   GeoSwarm

This example incorporates all of the above swarm methods using 4 separate structural observation files, or a random set. The 4 test sets are taken from actual field data gathered from the Caopatina region, Québec, Canada, from steeply dipping and folded series (Fig. 8) of turbiditic sediments from an Archean Greenstone Belt (de Kemp 2000). Scaling settings can stretch the extents of the data for testing local versus regional influences on swarm cohesion. Several distance sensitive parameters determine how agents are weighted for local surface cohesion versus data migration. A file I/O interface for testing various data configurations representative of common but simple geologic fold scenarios. It could be adapted for custom data configurations and will be used in the future for parameter selection training and testing with a range of real data sets.
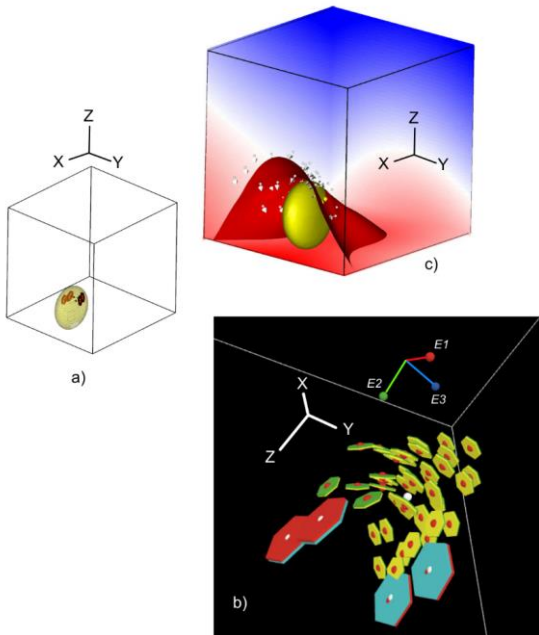
1   **Figure 8.**   Surface model (closed yellow ellipsoid) using implicit calculations with SURFE (Hillier et al., 2015) when using only

2   4 on-contact dip data points (a) and then using the GeoSwarm program to extend a fold plunge, with 50 off-contact spatial structural

3   agents depicted from the bottom, looking up in (b). Red surface in (c) is a more spatially continuous antiformal structure, when

4   using the structural agent approach than with implicit codes alone. Note eigen vector E1 (red stick-ball) is pointing down plunge

5   of the fold, the strongest continuity direction.

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1   **4   Discussion and Conclusions**

2   This study focuses on the rudimentary requirements for geological modelling using spatial agents, primarily their ability to

3   interrogate, communicate and represent solutions to simple sparse geometric or structural constraint data configurations. No

4   doubt future research needs to go much further to see how to build full geological models, optimizing the arsenal of existing

5   geospatial tools within an agent framework. Initial indications are promising for use of agents to develop meshing tools,

6   topologically sensitive surface construction of objects and for respecting simple geological data constraints such as on-

7   contact 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

16   when modelling using other methods such as with implicit estimators.

17

18   With the abundance of machine learning tools currently available it would be potentially useful to investigate how to

19   optimize structural agents for particular geological use cases, for example using self organizing maps and generalizations for

20   up-scaling structural data sets based on sampling from Kent distributions (Carmichael and Aillères, 2016) for regional three

21   dimensional modelling or with application of graph neural networks for more complex geological modelling with sparse data

22   (Hillier et al., 2020) as well as other emerging deep learning approaches (Guo et al., 2021; Zhang et al., 2019).

23

24   Natural examples of agent behavior, such as swarm behavior, have emerged over millennia through the embedding of simple

25   rules into organisms that have evolved for optimization of their group survival. This paradigm, although perhaps not obvious

26   for geological applications, could take a similar path and could be an opportunity to leverage geological knowledge through

27   embedding of specific behaviours for given geological processes that are controlled through simple geological rule sets, for

28   example, by programing agents to maintain a range of thickness between stratigraphic layers as they are propagated

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1 regionally. Importantly, geological agents would need to operate in a geologically reasonable framework, respecting the

2 local or regional geological topology network (Thiele, et al., 2016). They would need to be able to create solutions from a

3 suite of possible geological topologies with more complex feature sets, for example, from combinations of geologic contacts

4 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 https://doi.org/10.5281/zenodo.4634021)

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.

26 **Special Issue Statement:** This contribution is part of the Loop stochastic geological modelling platform – development and
27 applications, edited by Laurent Ailleres.

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Appendix A: **Agent resources**

An excellent starting point to become familiar with agent-based applications and approaches is Paul Torrens' web site at http://geosimulation.org/ from the Computer Science and Engineering, Tandon School and Center for Urban Science and Progress, at New York University.

The agent-based codes used in this paper are written in Net Logo-3D, a spatial agent-based modelling language and development environment that is supported from the Center for Connected Learning and Computer-based modelling in Evanston, Illinois, USA. The NetLogo project is affiliated with Northwestern University Centre on Complex Systems (NICO) https://www.nico.northwestern.edu/ . To download and run the NetLogo codes, for tutorials and documentation on the NetLogo language see http://ccl.northwestern.edu/NetLogo. The code must be minimally compatible with the NetLogo 3D version as listed in the programs below. Current and early 3D versions of the program are all available on the main NetLogo homepage.

Codes presented in this paper are freely downloadable from the Git Hub Open Source web site at https://github.com/Loop3D/GeoSwarm.git (https://doi.org/10.5281/zenodo.4634021) with accompanying power point, pdf and animations presented at the annual meeting of the International Association of Mathematical Geoscientists at Penn State University, USA, August 2019.

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1	**Appendix B:**		**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.nlogo3d	6.0.4	Structural dip cohesion mimicking deformed surfaces
8	GeoSwarm.nlogo3d	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	*Shape Libraries:*		
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

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15 **Example Pseudo Code:**

16 **Mesh.nlogo3d**

```
17            Start
18            Create Nodes agent set
19            Create Triangles agent set with random directed normals
20            Define a seed Triangle
21            Do while [ mesh growing ] [
22                    if [nearest neighbour to seed Triangle exists] [
23                            connect an edge of the seed Triangle to its nearest neighbour's edge
24                            repeat along the seed until all its edges are fused
25                            repeat along the outer edge of the mesh
26                    ]
27                    if [all Triangles meshed] [
28                            quality check the mesh
29                            if [mesh is not reasonable] [
30                                    set mesh to growing
31                                    disconnect the mesh by killing shared edges
32                                    Scatter all Triangles
33                                    Re-define the seed Triangle
34                            ]
35                    Else
```

1   [set mesh to not growing]

2   ]

3   ]

4   End

5

6 Once all the meshing is complete, there is a quality control check to determine if the result is a 'reasonable' surface.

7 This could be a simple rule that looks for holes, and surfaces with low connectivity, for example by calculating a

8 low node count to edge count ratio; with 1 = no triangles connected, ~ .72 = single node connected chain, ~ .62 =

9 single edge connected chain, ~ .58 = hexagonal mesh).

10

11

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 (0º) representing
9   the angle between a topographic surface trace of a geological feature, such as a horizon intersecting with
10   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 = 90º, south = 180º, west = 270º)

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
16   surface. The dip direction is always 90º to the strike direction. The dip angle (dip) is the maximum vertical angle
17   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
21   original depositional configuration. -1 = overturned, 0 = unknown, 1 = upright. This value is used to give topological
22   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*)

28   *ddz* = sin (-1 * *dip*)

29   Calculate the strike vector

30   *sx* = -1 * *ddy*

31   *sy* = *ddx*

32   *sz* = 0 (note the strike vector is always in the horizontal plane)

33   Cross down dip vector with strike vector (V_{dd} X V_s to get the normal (*N*) or pole to bedding.

34   *NNx* = (*ddy* * *sz*) - (*ddz* * *sy*)

35   *NNy* = (*ddz* * *sx*) - (*ddx* * *sz*)

36   *NNz* = (*ddx* * *sy*) - (*ddy* * *sx*)

1   Normalize the normal for unit length *L*.

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   Convert a Trend and Plunge to a normalized unit Vector. A common fabric element for various linear structural
11   features such as fold hinge lines joining maximum curvatures along the plunge of a fold, or stretching features
12   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 (trend) * cos (plunge)

17    $VVy =$ cos (trend) * cos (plunge)

18    $VVz =$ sin (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

25

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

28   **Spin (A V P)**

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    $P =$ Normal unit vector (n_x, n_y, n_z)   (such as Poles to beds, a fold hinge etc.)

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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 $Q = (qw, qx, qy, qz)$

15

16 **C.3** Create the Rotation Matrix

17 Use quaternion identities to derive the rotation matrix

18 $q2w = 1 - qx^2 - qy^2 - qz^2$

19 $q2x = qx^2$

20 $q2y = qy^2$

21 $q2z = qz^2$

22 Compose **R** the rotation matrix

23

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

25

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

27

28 **C.4** Matrix multiply the Rotation matrix with the input observation normal P

29 $S = P \, X \, R$

30

C.5 Interpolate, by calling the spherical linear interpolator (SLERP) for any interpolation on parameter t, a normalized distance between data and the spatial starting point of an agent (A) as it is rotated towards the structural constraint (B). Details of SLERP can be located in De Paor (1995). Note with the inverse distance weighted (IDW) form of SLERP a set of structures can all influence the agent depending on the agent's ability to sense the data, for 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 p if needed for stronger local influence,

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

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

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

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

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