https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions
Open Access EGU

Spatial Agents for Geological Surface Modelling

Eric A. de Kemp[1]

Correspondence to: Eric A. de Kemp (edekemp@canada.ca)

[1]Geological Survey of Canada,
Three-dimensional Earth Imaging and Modelling Lab
601 Booth Street, Ottawa, Canada, K0E 1E9
E-mail: eric.dekemp@canada.ca
https://orcid.org/0000-0003-0347-5792
Tel.: 01-613-867-8812

Abstract

Semi-autonomous software entities called spatial agents can be programmed to perform spatial and property interrogation functions, estimations and construction operations for simple graphical objects, that may be usable in building three-dimensional geological surfaces. These surfaces form the building blocks from which full topological models are built and may be useful in sparse data environments, where ancillary or a-priori information is available. Critical in developing natural domain models is the use of gradient information. Increasing the density of spatial gradient information (fabric dips, fold plunges, local or regional anisotropies) from geologic feature orientations (planar and linear) is key to more accurate geologic modelling, and core to the functions of spatial agents presented herein. This study, for the first time, examines the potential use of spatial agents to increase these types of gradient constraints in the context of the Loop 3D project (loop3d.org) in which new complementary methods are being developed for modelling complex geology for regional applications. The Spatial Agent codes presented may act to densify and supplement gradient and on contact control points used in *LoopStructural* (www.github.com/Loop3d/LoopStructural) and *Map2Loop* (https://doi.org/10.5281/zenodo.4288476).

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

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions

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

1 Introduction

This current study highlights the potential use of Spatial Agents in the context of the Loop 3D project (Ailleres et al. 2019), which is developing new methods supporting the modelling of more complex geological terrains. The Loop 3D effort is attempting to address this ongoing challenge, which tends to present itself when geology becomes more complicated, with more elaborate geo-histories. For example, with early cryptic sedimentary and volcanic depositional cycles, and a spectrum of brittle to deeper crustal deformation events, and through masking metamorphic processes. Not to mention overprinting intrusive events, from thin dyke swarms to consuming batholithic intrusions that can completely erase all macroscopic evidence of these 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, conductively 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 to use them to densify input constraints for horizon dips, better model the local anisotropy, and extend features such as regional fold plunges. These derived constraints could be useful as supplemental input to *LoopStructural* (Grose et al. 2020) and *Map2Loop* (Jessell et al. 2021) to increase the accuracy and geological reasonableness of the models. 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 3D, and hopefully other initiatives in the future.

1.1 Agent Characteristics

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). The agent(s) in these systems are software entities that

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

have been programed to work according to specific or general pre-programed beliefs. For example, considering a construction simulation game, a carpenter would be considered as an agent which could be assigned the framing role to construct a house. The house in this case would be an example of a single agent 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). 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. Agents operate as semi-autonomous entities that are not directly controlled by any centralized command structure and may have a great deal of independence from each other as well. For example, 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.

1.2 Agent Applications

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

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

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 anisotropy and gradient type information which the structural agents do in this study. However, these diverse applications do have some common elements which software agents are well suited to. The problem domains have multi-scalar environments with local or global model element interactions, and non-linear, multi-source physical dependencies. 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. The ability to operate in a non-centralized control structure which is environmentally sensitive; being able to adapt to local or globally changing conditions. Their independence allows them to operate as individual elements for example, a single point observation or to work collectively as a team or 'swarm' and change states depending on specific conditions. 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 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. 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 reconciles and respects all the available data.

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions

Spatial agents have the potential to support this interpretive role, if some of their key characteristics can be leveraged towards geological feature estimation and feature to feature relationship extension. For example, through more efficient exploration of the model solution space though extending contacts such as horizons, fault networks and fabrics through the model space.

1.4 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). Section 1 provides an overview, context and review for the current study, surveying various application domains with an eye toward natural and earth sciences systems agent solutions. A summary of current geological surface modelling approaches is given in section 2 with some argumentation that highlights the need for new approaches particularly when data is sparse and geology is more complex. Section 3 outlines the use of spatial agents for structural geology. 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 4 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.

The code implementation was done 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 implementation version that can run the code (see Appendix B). Section 5 discusses some of the possible future research directions such as developing agent sensitivity to thickness and other property constraints as well as some challenging issues that need to be considered such as geological relationship or geological topology modelling with agents. The conclusion summarizes the results of the study which is essentially affirming that spatial agents can be used for geological surface modelling and encourages further development to more complete applications for a wider range of geological scenarios and data configurations. 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.

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

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, these 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 missing representation of horizon C in 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.

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions
Open Access
EGU

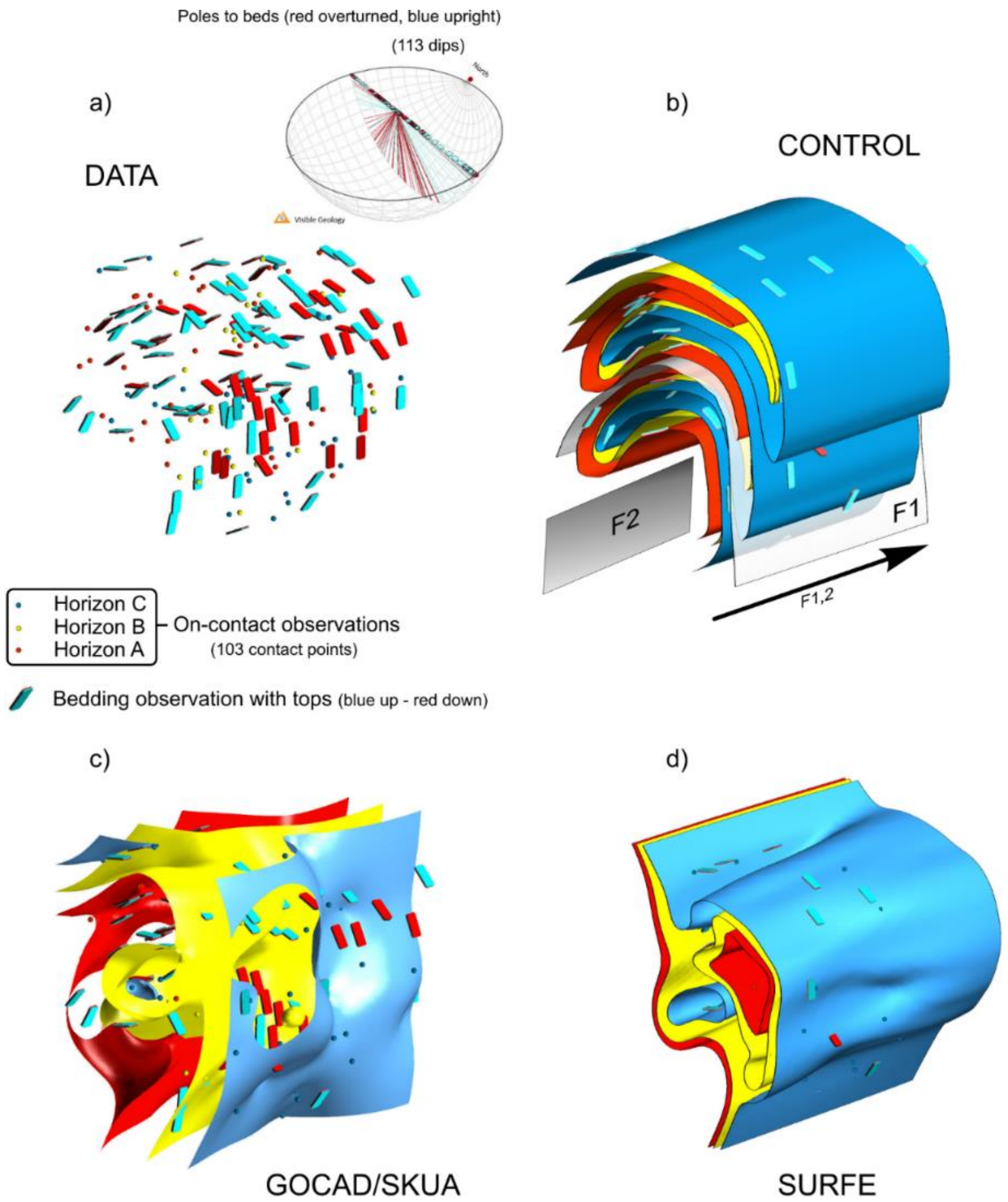

Figure 1. Comparison of synthetic geological three-dimensional models of classic Ramsay type 3 interference folds, with identical data. (a) Uniaxial dip data, with local opposing tops, represented on equal-angle Wulf plot (https://app.visiblegeology.com/stereonet.html). (b) Control model developed with 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).

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions
Open Access
EGU

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

2.1 Spatial Agents

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. Geoscience applications employing spatial agent-based modelling (SABM) have largely been focused on solving time series problems, like land use change due to climate, urbanization and hazards (Torrens 2010). Herein however, the focus is on spatial variability, and distribution, rather than temporally changing environments. The study demonstrates how simple fold solutions can be achieved using sparse data, such as would be acquired from ground traversing, through form line and fabric densification, as well as on contact estimation using structural agents (Figure 2). Spatial agents are employed to visualize and interpolate planar and linear structures, respecting the polarity of the observations and resulting estimations (Figure 3), essential for interpreting folded geology. Spatial agent triangulated meshes are produced from point observations, that use proximity and topologic rules for accepting or reject the meshing criteria in order to maintain local and overall continuity (Figure 4).

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions
Open Access

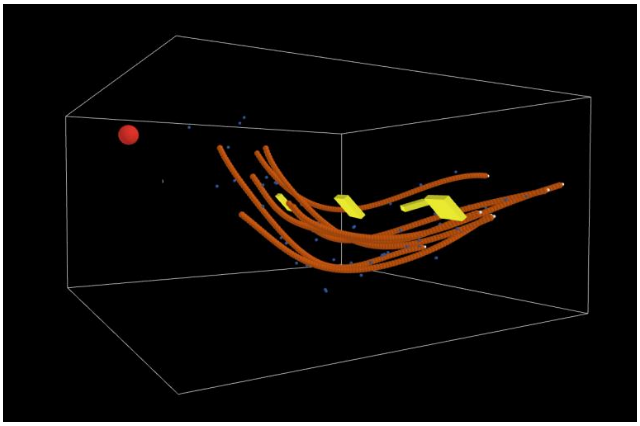

Figure 2. Structural form traces (orange point streams) estimated from dip data (yellow cuboids) using spatial agents. Red sphere is an interrogator agent. Blue dots are simulated Bézier control points with added random noise. See Appendix A for details.

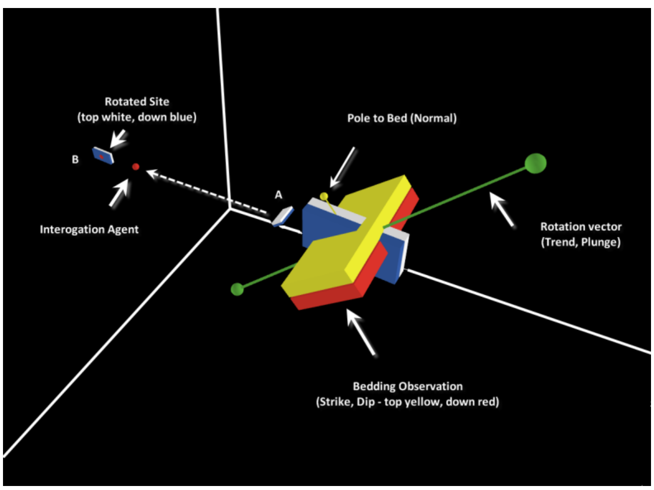

Figure 3. Structural agent demonstrating a quaternion 90° clockwise rotation during linear estimation (SLERP) between two points. Starting point A (local), with equivalent orientation to larger observation (yellow and red cuboid) and final rotated point B (distal). Rotation maintains smooth topology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

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions

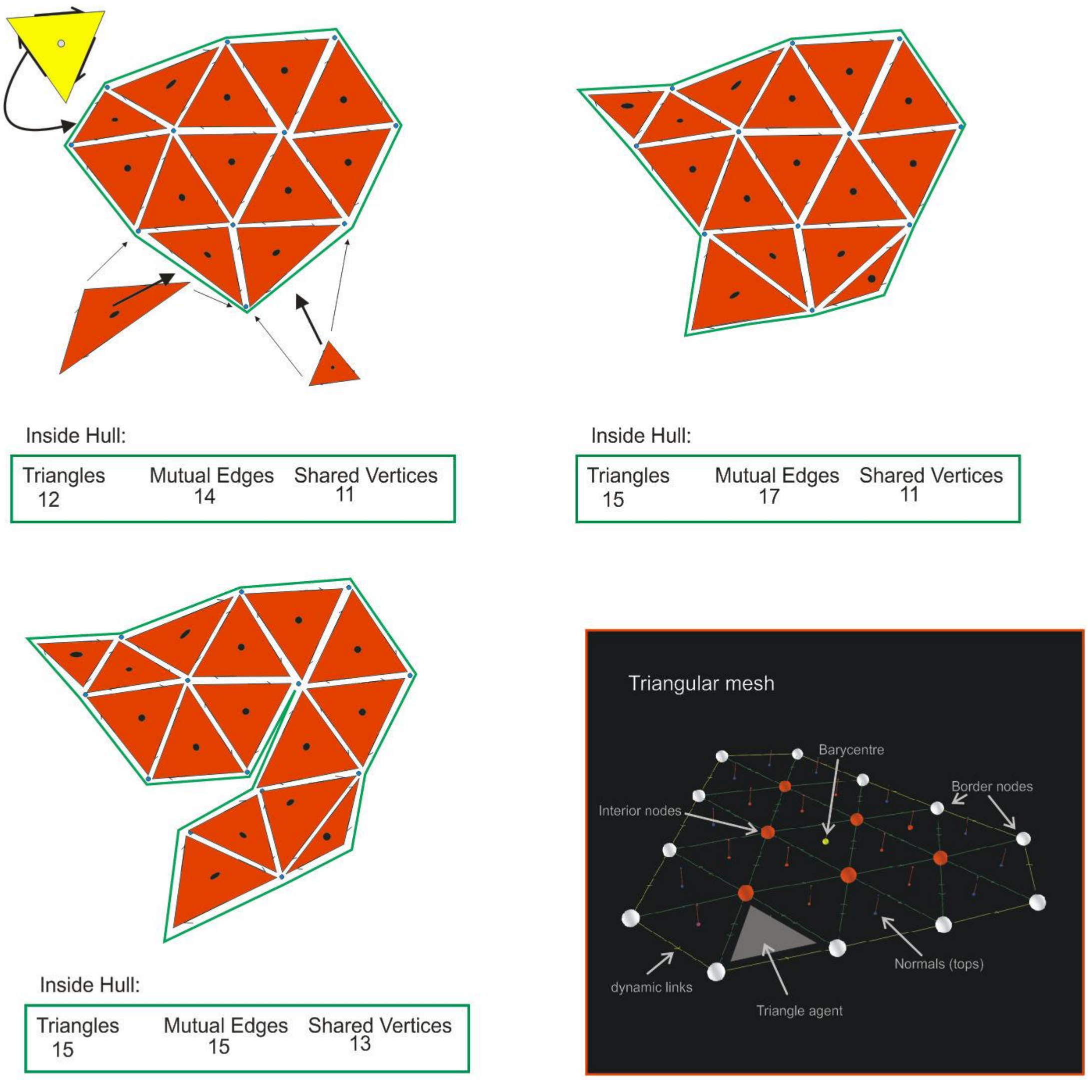

Figure 4. Spatial agent-based triangular meshing created from the Mesh program. See Appendix A for details.

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

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. 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. 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. An agent can be made to act like an interrogator of space whereby a continuous sampling may occur, in a given direction rather than through a predefined set of indexed grid cells, such as in a convolution filter. Core to the behavior of agents is the communication of derived weighting parameters for various properties, most importantly, for structural orientation during interpolation. Interpolation schemes from simple to complex could be employed such as, nearest neighbour, inverse distance weighted (IDW) or quaternion based spherical linear interpolation (SLERP) (De Paor 1995, Shoemake 1985, Hamilton 1844). Several schemes could be employed depending on local or global data configurations, property conditions and knowledge constraints. For the demo examples extensive use of SLERP methods ensure that rotations of geologic orientation data are smooth and more realistic with respect to expected structural deformation processes. In the presented examples, there is yet no rheological controls, but these physical parameters could be programed into the agent rule set. Agents can be programed to react to physical laws for example, the barycentre of a 3-tuplet mesh can be dynamically recalculated when neighbour masses, other material and mechanical properties are changed. The location and states of all agents are available and stored at the agent level, passed to a communications centre or just stored as a global variable, if needed. Agent intercommunications is a significant topic of computational science research (Hall and Virrantaus 2016, Ménager 2006), which may have implications for geological modelling. For example, if moving into the field of geological and geophysical integration and joint modelling, agents may have potential in optimization strategies for inversion of complex geometries, multi-parameter scalar and vector fields (Jessell et al. 2010, Lindsay et al. 2013). It is the way agents can communicate specific local to global information states, and adjust to the combined data and knowledge constraints (Liscano et al. 2000, Friedrich et al. 1999, Gaspari 1998), that may determine the applicability of their use for geological and no doubt other applications as well. For a comprehensive summary of agent and inter-agent

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions

communications and agent system controls see Heppenstall et al. (2012), for spatial agents with GIS see Crooks and Heppenstall (2012), and for a practical introduction Wilensky and Rand (2015) (see also Appendix A).

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. 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. For example, 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.

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.

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

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 will likely benefit from denser and faster CPU/GPU architecture and parallelization schemes. Since 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 but could result in dramatic efficiency gains when combining multi-scalar properties from geophysics and geology within three-dimensional structural fields (Burns 1988, Hillier et al. 2013).

3 Agents Examples

To demonstrate the general principals of agent behavior for geologic surface development, a number of simple applications were developed, using mostly synthetic data, and one re-scaled data set from an Archean greenstone belt (Caopatina Québec, from dekemp 2000), in a model space with (X,Y,Z) dimensions = (100,100,100) and model centre at (X,Y,Z) = (0,0,0). The Netlogo codes presented are freely available for download (See https://github.com/Loop3D/GeoSwarm.git or https://doi.org/10.5281/zenodo.4634021).

In the following example scenarios, spatial agents have properties for tracking local or global states, continuously checking for proximity to neighbours, their status as interrogators or observation sets and their geometric properties, such as strike, dip and polarity (top direction). Agents may have pointers and links to specific topological neighbours as in the case of adjacent triangles but there is no ordered centralized control list or matrix which holds all the agents and their relationships. Each type of agent is created and encoded with properties that may change, such as the local anisotropy derived from the eigenanalysis of local supported data. The structural agents are spatial agents, represented herein as tablets or hexagonal glyphs and rotate as quaternions (Figure 5).

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions Open Access EGU

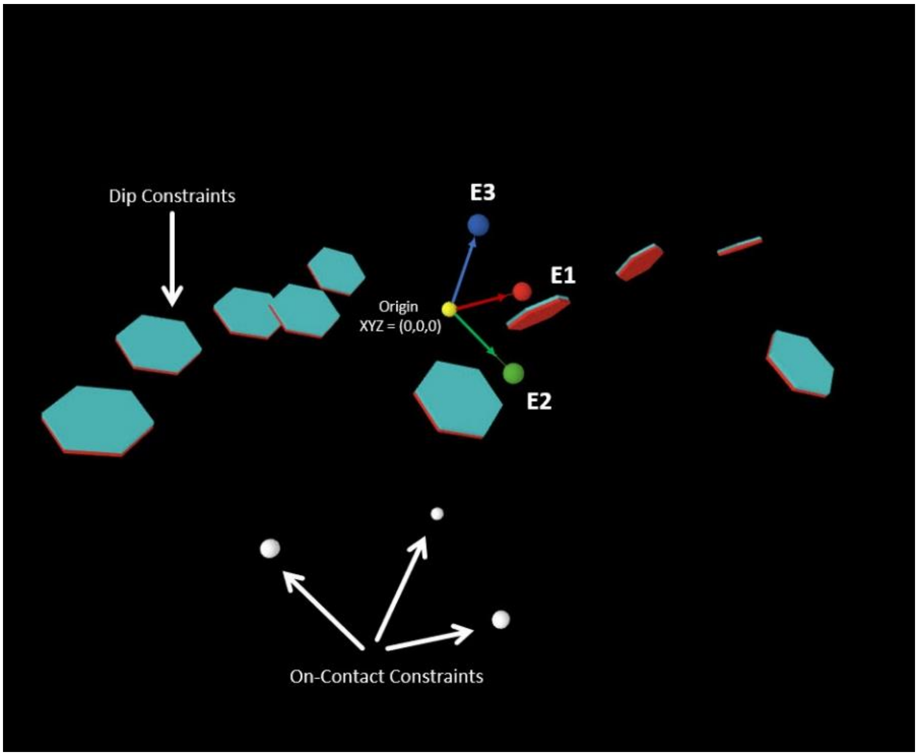

Figure 5. On contact (white spheres) and dip (blue=upright, red=down, thin hexagonal prisms) representing simple three-dimensional geological data constraints. Arrows at origin indicate the calculated orthogonal unit eigenvector directions for the structural data Depending on the scenario the structural 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 located 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 thoroughly tested or gone through performance optimization. It is best to slowly increase the number of data points for each scenario and experiment with the control parameters for best results.

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions

3.1 Trace

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.

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 a stop criteria is 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.

3.3 Mesh

Demonstrates the development of topologic surfaces that, at a minimum, are defined by a triangulated mesh that has direction and polarity sensitivity. Also, to show that a mesh can be produced from agents without a grid. For example, without having to sample a scalar field value in a partitioned grid (i.e. with marching cube) and that meshes could be grown locally, while conforming to constraint data. Each triangle has a normal that is maintained from the barycentre of the triangle. Triangle vertices have a mass that can be changed by the user to influence the location of the barycentre. A seed triangle senses the nearest neighbour triangle vertex and attracts it, back to itself. The incoming triangle is rotated to be conformable to the evolving surface patch and connected, keeping the normal pointing in the same way, thus maintaining simple surface topology. In this way distributed primitive shapes could

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

act as spatial data interrogators, before being transformed into mesh constructors. Simple topology metrics (edge: vertices: triangles ratios) are reported and plotted on the GUI graph. Once the mesh is complete, and if the on contact constraints are active, the mesh will migrate with its regional barycentre to the nearest on-surface control point, and turn it blue from white, then go on to do the same for the next control point. This functionality is a precursor requirement for adaptive meshes, that could potentially be shaped by various spatial and property data, data quality and data densities. In this instance, a surface mesh is grown through use of simple geological rules. For example, a surface can not intersect itself, and needs to be continuous with consistent surface polarity, and also to avoid large tear faults. These surfaces may move toward on contact data constraints to extend the local observations. The ratios of triangles to shared edges and shared vertices can be used to check topology, and used as a stopping criteria or to reward or penalize during the meshing process.

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.

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-

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions

sided (yellow up/green down) hexagon (see Figure 6). 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 such as 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 come close to static dip data control points they will adjust their local orientation to match the orientation properties of the data, but do not move spatially towards these off-contact orientation observations (Figure 6).

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions
Open Access
EGU

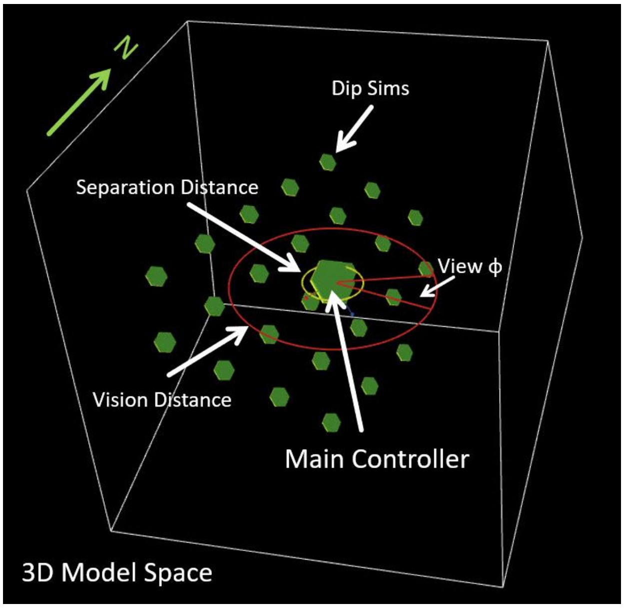

Figure 6. Components of the spatial agent-based model (SABM).

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

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 only controlled by the Main controller and moving in the plane specified by the controller and vision-proximity rules.

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development
Discussions

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 (Figure 7) 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.

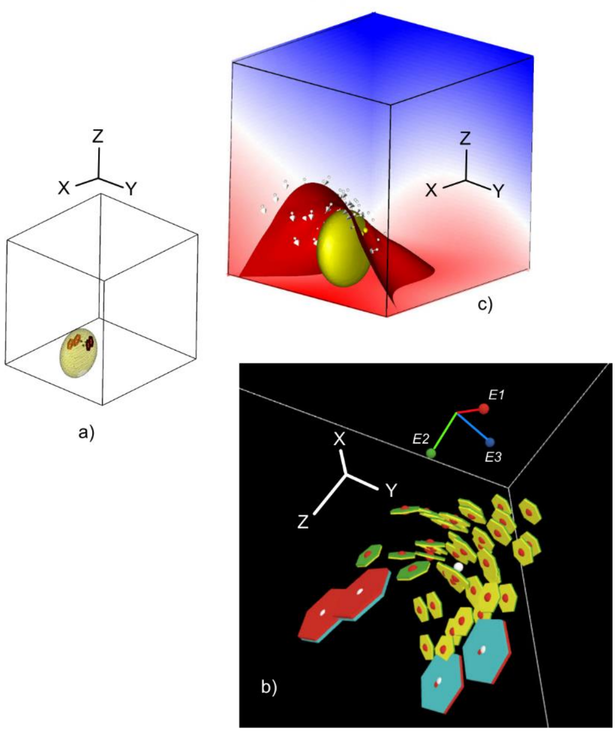

Figure 7. Surface model (closed yellow ellipsoid) using implicit calculations with SURFE (Hillier et al. 2015) when using only 4 on contact dip data points (a) and then using the GeoSwarm program to extend a fold plunge, with 50 off-contact spatial structural agents depicted from the bottom, looking up in (b). Red surface in (c) is a more spatially continuous antiformal structure, when using the structural agent approach then with implicit codes alone. Note eigen vector E1 (red stick-ball) is pointing down plunge of the fold, the strongest continuity direction.

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

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 on contact and dip observations.

The use of eigenvectors to summarize local anisotropic conditions derived from dip populations were helpful in supporting the propagation of agents, weighting of the spatial continuity direction in a more intuitive manner for structural geological interpretation, and selection of rotation axis for quaternion interpolations. These techniques, more commonly used in the graphics industry, would be beneficial going forward in three-dimensional structural geological modelling in general and potentially for more elaborate spatial agent approaches when solving for multi-property anisotropies such as occur in natural geophysical and geological property distributions (De Paor 1995). Sparse data configurations with more structural variability, (see Figure 7) when supported with an agent approach, will better reflect and extend local structural anisotropy when modelling using other methods such as with implicit estimators.

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).

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

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions Open Access EGU

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.

From this study it is clear that spatial agents can be used to develop simple meshed surfaces, fabric traces, visualize anisotropies and structurally sensitive swarm surfaces. Structural agent interrogators exploring a model space can update local or group behavior to conform to on contact or within volume topological dip constraints.

Agent based tools as applied to geological applications are yet in their infancy but can be used to interpolate or extrapolate from data to produce fabric trajectories, gradients, vector fields and continuous or discontinuous polyhedral meshed surfaces. The amplification of local anisotropies is particularly useful with sparse data and increased structural complexity scenarios. These characteristics can provide support for simulated input using existing methods for spatial estimation, such as implicit approaches.

Finally, more in depth investigation into the use of and optimization of spatial agents needs to be undertaken to demonstrate the range of benefits for complex geological modelling in a variety of data configurations that could represent typical geological scenarios.

Code and Data Availability

These codes and data can be freely downloaded. (Please see: https://github.com/Loop3D/GeoSwarm.git or https://doi.org/10.5281/zenodo.4634021)

Video Supplement

The video files (mp4) related to this article are available online. (Please see https://github.com/Loop3D/GeoSwarm/tree/master/Docs or within https://doi.org/10.5281/zenodo.4634021).

Author contributions

EdK developed the GeoSwarm system, performed the literature review of spatial agents and wrote the paper.

Competing interests

The author declares that there is no conflict of interest.

Special Issue Statement: This contribution is part of The Loop 3D stochastic geological modelling platform – development and applications, edited by Laurent Ailleres.

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Acknowledgements

Many thanks to Uri Wilensky, NetLogo team of developers and contributors who continue to enhance applications and extend the functionality of NetLogo with extensions to 3D, GIS, numerical functionality and other shared codes. Several examples such as wave and flocking codes have been the starting codes for this work presented here. Many thanks to Sarah D'Ettorre (2013) who initiated the first agent meshing codes now incorporated into Mesh.nlogo3d. Thanks to Doron Nussbaum, Carleton University, School of Computer Science who provided supervision of D'Ettorre while working on her MSc. Thanks to Mike Hiller and Boyan Brodaric (GSC), for valuable feedback. Early consultation on AI methods from Éric Beaudry, (Université du Québec a Montréal), Khalid Djado and Mathieu Bouyrie (Kinna Technologies) is appreciated. Thanks to all the LOOP 3D team https://loop3d.org/ especially Mark Jessell and Laurent Ailleres for their patience and support of the project. Thanks to RING https://www.ring-team.org/ for academic support for use of Gocad/SKUA software and to Guilaume Caumon of who provided critical feedback for the research. Many thanks to Kevin Sprague who was inspired with the original notion of using agents for 3D geological modelling at the Geological Survey of Canada.

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, https://doi.org/10.1080/22020586.2019.12072955, 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.

Bürkle, A.: Collaborating miniature drones for surveillance and reconnaissance, Proceedings of SPIE - The Intern. Soc. Opt. Eng., 7480:74800H, 2009.

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.

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions

Caumon, G. and Collon-Drouaillet, P.: Editorial, Special Issue on Three-Dimensional Structural Modelling, Math. Geos., 46, 905-908, https://doi.org/10.1007/s11004-014-9571-9 , 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., 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, 2009.

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 Paor, D. G.: Quaternions, raster shears, and the modelling of rotations in structural and tectonic studies. in: Proceedings 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, https://doi.org/10.1007/s10015-019-00525-1 , 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^{th} edition), Academic Press, San Diego, California. ISBN-13: 9780444511041, 1997.

Friedrich, H., Rogalla, O., and Dillmann, R., Communication and propagation of action knowledge in multi-agent systems. Robot. and Auto. Syst., 29(1):41-50, 1999.

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, GMD, Preprint gmd-2020-336, https://doi.org/10.5194/gmd-2020-336 , 2020.

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions

Groshong, R. H. Jr.: 3-D Structural Geology A Practical Guide to Quantitative Surface and Subsurface Map Interpretation, (2nd Edition), Springer-Verlag Berlin Heidelberg., ISBN-13, 978-3540310549, 2006.

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, https://doi.org/10.1177/1548512915619499 , 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. 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), https://doi.org/10.3141/2540-03 , 2016.

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, https://doi.org/10.1016/j.envsoft.2019.01.020 , 2019.

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.

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., 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, GMD, Preprint gmd-2020-400, https://doi.org/10.5194/gmd-2020-400, 2021.

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.

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, https://doi.org/10.3997/1365-2397.26.10.28558, 2008.

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.

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.

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, https://doi.org/10.1007/3-540-45486-1_16, 2000.

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.

Nelson, J., Hugh, O., Angel, N.,.García, E., Chahine, J. and Socci, N.D.: The energy landscape theory of protein folding: Insights into folding mechanisms and scenarios, Advances in Protein Chemistry, 53, 87-130, https://doi.org/10.1016/S0065-3233(00)53003-4, 2000.

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 http://www.red3d.com/cwr/boids/, 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.

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.

Shoemake, K.: Animating Rotation with Quaternion Curves, Comp. Graph. (ACM), 19(3), 245-254, 1985.

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. Landscape Ecology, 32(11), 2113-2132, https://doi.org/10.1007/s10980-017-0502-2, 2017.

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.

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.

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.

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 Flocking model, Center for Connected Learning and Computer-Based Modelling, Northwestern University, Evanston, IL. http://ccl.northwestern.edu/netlogo/models/Flocking, 1998.

Wilensky, U.: NetLogo Wave Machine 3D model., Center for Connected Learning and Computer-Based Modelling, Northwestern University, Evanston, IL., http://ccl.northwestern.edu/netlogo/models/WaveMachine3D, 1996.

Wilensky, U.: NetLogo, Center for Connected Learning and Computer-Based Modelling, Northwestern University, Evanston, IL. http://ccl.northwestern.edu/netlogo/, 1999.

Woodcock, N. H.: Specification of Fabric Shapes using an eigenvalue method, Geol. Soc. Amer. Bull., 88, 1231-1236, 1977.

Zuparic, M., Jauregui, V., Prokopenko, M. and Yue, Y.: Quantifying the impact of communication on performance in multi-agent teams, Artificial Life and Robotics, 22(3), 357-373, 2017.

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions Open Access EGU

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.

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development
Discussions
Open Access

Appendix B: List of Netlogo-3D Programs

Program Name	*Version*	*Purpose*
Trace.nlogo3d	6.0.4	Propagation and interpolation (NN and IDW)
Poly.nlogo3d	6.0.4	Closed and connected polyhedral growth
Mesh.nlogo3d	6.0.4	Simple surface meshing by triangulation growth
Rotate.nlogo3d	6.0.4	Dips with polarity rotation (SLERP - eigenvectors)
Swarm_Dips.nlogo3d	6.0.4	Structural dip cohesion mimicking deformed surfaces
GeoSwarm.nlogo3d	6.0.4	Simple geometry solving from steep fold limb pairs
Wave.nlogo3d	6.0.4	Simple non-meshed elastic surface motion

Shape Libraries:

3d_HexShape.txt	> 5.3	Required to generate hexagon dip glyphs with polarity
3d_Shape.txt	4.1,5.1,6.0.4	Required to generate tabular dip glyphs with polarity

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions

Appendix C: Quaternion Calculations

Quaternion codes are used in Dip_Swarm and Rotate programs and implemented in NetLogo within the **Spin()** procedure. Used for smooth rotation along specified axis such as an eigenvector of a structural observation set and for inverse distance weighted (IDW) and Spherical Linear Interpolation (SLERP). For details see De Paor (1995), Shoemake (1985), Hamilton (1853).

C.1 Provide a normalized unit vector to the Spin procedure from common structural observation data

Convert strike and dip (RHR) to a Unit Normal vector. Input is in degrees. Normal is perpendicular to plane

strike = a scalar angle of in degrees azimuth in the horizontal plane measured clockwise from north (0^o) representing 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 structural geological measuring standard for planar field observation data. It assumes that the strike direction vector is pointing such that the geological surface dips to the right of the observer as they face the strike direction.

(Note east = 90^o , south = 180^o, west = 270^o)

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

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^o to the strike direction. The dip angle (dip) is the maximum vertical angle from the horizontal to the geological surface.

$dip \in \{0{,}90\}$

$polarity \in \{-1{,}1\}$

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, 1 = upright. This value is used to give topological information in modelling.

strdip2norm (*strike, dip, polarity*)

Returns a 3 element unit normal vector.

Calculate down dip vector

$ddx = \cos(-1 * strike) * \cos(-1 * dip)$

$ddy = \sin(-1 * strike) * \cos(-1 * dip)$

$ddz = \sin(-1 * dip)$

Calculate the strike vector

$sx = -1 * ddy$

$sy = ddx$

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

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

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

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

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

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions

Normalize the normal for unit length *L*.

$$L = \sqrt{NNx^2 + NNy^2 + NNz^2}$$

Adjust for polarity

Nx = (polarity * NNx) / L

Ny = (polarity * NNy) / L

Nz = (polarity * NNz) / L

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.

TrendPlunge2Vec (*trend*, *plunge*)

Returns a 3 element unit normal vector.

VVx = sin (trend) * cos (plunge)

VVy = cos (trend) * cos (plunge)

VVz = sin (plunge)

Unit Normalize

$$M = \sqrt{VVx^2 + VVy^2 + VVz^2}$$

Vx = *VVx* / *M*

Vy = *VVy* / *M*

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.

Spin ***(A V P)***

A = spherical angle of rotation in degrees (not Euler angles) $A \in \{-\infty, \infty\}$

V = Unit vector 3D axis of rotation (Vx, Vy, Vz,). Can be any of the eigenvectors, a down dip vector, strike vector etc.

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

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

Geoscientific Model Development Discussions
Open Access
EGU

Returns ***S*** a matrix with full orientation description including the normal to bedding or new rotated linear element, the *strike* and *dip* components, *overturned* (polarity) and 4 quaternion elements (*qw*, *qx*, *qy*, *qz*).

Transform from single vector to quaternion with rotation *A* about an axis **Q**

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* as a single matrix from the normal

Returns RHR_Orientation array using Right Hand Rule planar orientation for STRIKE, DIP, N1, N2 ,N3, OVERTURNED

$\boldsymbol{Q} = (s, V)$ scalar , vector

$qx = (\sin(A/2)) * \mathrm{Vx}$

$qy = (\sin(A/2)) * \mathrm{Vy}$

$qz = (\sin(A/2)) * \mathrm{Vz}$

$qw = (\cos(A/2))$

$\mathbf{Q} = (qw, qx, qy, qz)$

C.3 Create the Rotation Matrix

Use quaternion identities to derive the rotation matrix

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

$q2x = qx^2$

$q2y = qy^2$

$q2z = qz^2$

Compose ***R*** the rotation matrix

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

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

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

$\boldsymbol{S} = \boldsymbol{P}\ X\ \boldsymbol{R}$

https://doi.org/10.5194/gmd-2021-66
Preprint. Discussion started: 19 April 2021

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*). Note with the inverse distance weighted (IDW) form of SLERP a set of structures can all influence the agent depending on the agents 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 $\boldsymbol{G}$ the estimated orientation at x by adjusting the contributing quaternion components of the data with the distance weights,

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

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

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