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SPECIAL ISSUE

Towards Stochastic Time-Varying Geological Modeling

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Abstract The modeling of subsurface geometry and properties is a key element to understand Earth processes and manage natural hazards and resources. In this paper, we suggest this field should evolve beyond pure data fitting approaches by integrating geological concepts to constrain interpretations or test their consistency. This process necessarily calls for adding the time dimension to 3D modeling, both at the geological and human time scales. Also, instead of striving for one single best model, it is appropriate to generate several possible subsurface models in order to convey a quantitative sense of uncertainty. Depending on the modeling objective (e.g., quantification of natural resources, production forecast), this population of models can be ranked. Inverse theory then provides a framework to validate (or rather invalidate) models which are not compatible with certain types of observations. We review recent methods to better achieve both stochastic and time-varying geomodeling and advocate that the application of inversion should rely not only on random field models, but also on geological concepts and parameters.

Keywords Geomodeling · Uncertainty · Structural restoration · Inverse methods · Geostatistics

1 Introduction

The geological map has always been a central piece in geology, for it not only synthesizes observations, but also conveys many interpretations made from observations. Whereas a map provides a basis to answer a number of questions, it remains an incomplete representation, especially when it comes to predicting the nature of rocks

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below the earth's surface. During the last decades, geomodeling has been introduced to improve classical maps by providing an unambiguous 3D description of geological volumes. Since then, it has taken a prominent role in quantitative geosciences and management of natural resources. 3D structural modeling is now currently available in various software, such as Dynamic Graphics (2009), Gemcom (2009), Intrepid Geophysics (2009), JOA (2009), Midland (2009), Paradigm Geophysical (2009), Roxar (2009), Schlumberger (2009), Zaparo (2009). However, the nice pictures generated with such software should not obscure the fact that a model is at best an approximation of geological reality and may simply be wrong, especially away from observations. Indeed, geological data used to construct 3D models are generally not evenly distributed over the domain of study, have limited resolution, and provide an incomplete coverage of the physical quantities of interest (Bardossy and Fodor 2001; Mann 1993). Traditionally, geological concepts complement quantitative data in order to obtain a model deemed acceptable. However, modeling methods primarily serve to put a strong focus on spatial data, and only partially account for other geological observations and measurements (e.g., isotopic ages, mineral microstructures, strain analyses, etc.). The need to better integrate the long and often complex geological history into modeling is therefore very acute in order to gain geologic insight and improve the quality of geomodels (Sect. 3).

A second avenue for investigations concerns the representation of uncertainties. It does not matter how good a 3D geological model may be, it will always be underconstrained to some extent. Characterizing this indeterminacy by appropriately varying model parameters is highly desirable, if only to evaluate risks when dealing with natural hazards and underground resources (Sect. 4). Research toward such a stochastic and time-varying modeling would be extremely difficult to address with purely academic modeling systems. The complexity of geological objects and the nature of a computer-based modeling system indeed require significant maintenance efforts. The building of an academic software a nihilo, although desirable, would take significant energy, even to reach the level of existing geomodeling packages. Currently, several commercial software vendors (Paradigm Geophysical 2009; Roxar 2009; Schlumberger 2009) provide development frameworks for universities to capitalize on existing application programming interfaces and test new modeling concepts in an integrated manner, while keeping the maintenance burden for themselves. Because good understanding of prior art is needed to address geomodeling challenges, Sect. 2 will briefly review existing methods to model 3D geological objects.

2 A Short Overview of Geomodeling Methods

2.1 Surface-Based Approaches

Since the early days of geomodeling, surfaces have gained a lot of interest for their use in representing structural geological interfaces such as faults, horizons, and unconformities (Mallet 1988; Turner 1992; Zanchi et al. 2009). One obvious reason for this choice is the ability of surface models to compactly represent complex shapes in 3D. From a mathematical standpoint, two main types of surface representations have been proposed:

Parametric surfaces use polynomial or rational equations describing the surface geometry using two parametric coordinates, u and v. This representation is classically used in computer aided design because it provides convenient user interaction. Moreover, it allows for data conditioning as described by Piegl and Tiller (1997). Parametric surfaces have been used by several authors to represent 3D geological structures (de Kemp 1999; de Kemp and Sprague 2003; Fisher and Wales 1992; Gjøystdal et al. 1985; Hoffman et al. 2003; Sprague and de Kemp 2005; Zhong et al. 2006). In these approaches, discontinuities are addressed using one parametric patch per connected component (fault segment or continuous horizon inside a fault block). These surfaces need then to be truncated along discontinuities for graphical display and structural model queries.

Polygonal surfaces consist of a network of nodes connected by polygons. Regular rectangular connection patterns are very easy to represent on a computer and are well suited to the creation of corner-point reservoir grids (Fremming 2002). However, they have shortcomings in representing complex structures. Triangular surfaces provide an interesting alternative. From a mathematical standpoint, they have the beneficial properties of simplicial meshes. From a geological standpoint, they can conform without degeneracy to all types of geometry and topology (densely faulted domains, complex intrusive or erosive contacts, etc.), and can be adaptively refined where needed (Caumon et al. 2009; Jessell 2001; Lemon and Jones 2003; Mallet 1988, 2002).

Whatever the mathematical model retained, surfaces should honor representational validity rules (finite extension, orientability, nonintersection, e.g. Hoffmann (1989)) and geological validity rules like nonintersection of rock boundaries, absence of dangling surface edges except for laterally dying and synsedimentary faults (Caumon et al. 2004c).

2.2 Volume-Based Approaches

Isolated surfaces are the 3D counterpart of the spaghetti format in GIS: they do not necessarily bind well-defined volumes. The simplest volume model is a Cartesian grid whose blocks are flagged depending on the geological unit they belong to (Gjøystdal et al. 1985). As shown in Fig. 1(A), geological interfaces are then stair-stepped; increasing model resolution helps improve model accuracy, but incurs significant memory usage and increases the number of model parameters. Adaptive Cartesian grids such as octrees may be used to more compactly represent structures by using local refinement in areas of high geometric complexity. However, such Cartesian representations do not directly represent fault offset nor locally varying anistrotropy related to rock deformations. Stratigraphic (corner-point) grids, like in Fig. 1(B), address both problems by conforming grid blocks to most structural interfaces. Construction is often achieved by extrusion of a 2D grid vertically (Johnson and Jones 1988; Hoaglund and Pollard 2005; Swanson 1988) or along so-called pillars which define a direction field tangent to the main faults (Bennis et al. 1996; Chambers et al. 1999; Fremming 2002; Mallet 2002). Alternatively, grids may be warped to conform to structural interfaces (Hoffman et al. 2003; Lasseter and Jackson 2004).

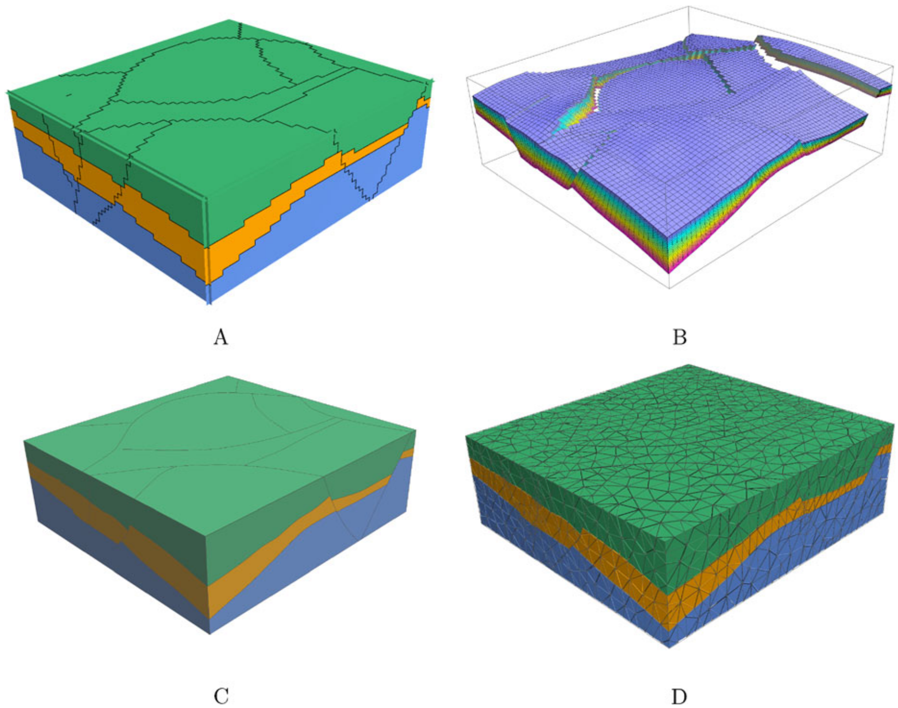

Fig. 1 For a given structural model, several volumetric representations may be built, for instance a Cartesian grid (**A**), a corner-point stratigraphic grid (**B**), a boundary representation (**C**) or a tetrahedral mesh (**D**). (Structural model courtesy of Total)

These grids have become standard in the modeling of underground reservoirs. Indeed, they approximate the coordinate transformation needed to apply geostatistical methods in depositional space, thereby accounting for depositional heterogeneities (Mallet 2004). Also, they offer a support to finite-volume based flow simulation. However, conforming to geological structures generally yields nonorthogonal grids, which may introduce distortions in geostatistical models (Gringarten et al. 2008; Jayr et al. 2009) and discretization errors in flow simulation (Wu and Parashkevov 2009). Moreover, from a practical standpoint, these grids are very difficult to create in the presence of low-angle faults and subhorizontal fault contacts. This explains why Fig. 1(B) only covers a subset of the volume of study. These shortcomings make corner-point grids difficult to apply at basin scale as well as to igneous and metamorphic formations.

Boundary representations, or sealed geological models, stitch surfaces together to define rock volumes, as can be seen in Fig. 1(C). The full structural complexity can therefore be captured by these models, which have been widely used in geomodeling (Apel 2006; Caumon et al. 2004c; Euler et al. 1998; Frøyland et al. 1993; Gjøystdal et al. 1985; Lemon and Jones 2003; Mello and Henderson 1997; Zhong et al. 2006). Analytical properties may be defined within each region to support seismic velocity modeling (Gjøystdal et al. 1985; Guiziou et al. 1996; Sword 1991) or numerical integration with the boundary element method (Thomas 1993;

Maerten et al. 2000). When a higher level of detail is needed, conformable meshes are generated within each region. Among these, tetrahedral meshes are simple and can in principle adapt to complex boundary geometries; as for triangulated surfaces, tetrahedral level of detail can be variable in space in order to honor data or geological features (Frank et al. 2007; Zhang and Thurber 2005). In spite of recent advances in mesh generation (Tournois et al. 2009), accounting for complex constraints such as sharp geological contacts, thin layers, or fracture networks is still a challenge (Mustapha and Mustapha 2007; Owen 1998).

One way to address these mesh generation problems is to use implicit surfaces or level sets to represent geological structures. In this representation, some structural interfaces are equipotential surfaces of some 3D scalar field $f(x,y,z)$. Although this idea is quite old (Houlding 1994), it has democratized for the last few years thanks to widely available computer memory. Several approaches have been described to build the 3D scalar field $f(x,y,z)$ from a set of data points, using radial basis functions (Cowan et al. 2003), dual kriging with polynomial drift (Calcagno et al. 2008; Chilès et al. 2004), or discrete interpolation on Cartesian grids (Ledez 2002) or tetrahedral meshes (Frank et al. 2007; Moyen et al. 2004). As compared to surface-based structural modeling, implicit methods are very attractive because they provide some built-in model consistency rules, and do not rely on data-to-surface projections which raise a number of problems in classical approaches.

2.3 Heterogeneity Modeling

Notwithstanding the intrinsic value of 3D structural mapping, it is often only a step to generate petrophysical models which can be later used in numerical simulation of physical processes. This petrophysical modeling is the realm of geostatistics (Chilès and Delfiner 1999; Deutsch 2002; Goovaerts 1997; Journel and Huijbregts 1978; Matheron 1970; Rémy et al. 2008). These methods provide either an estimate of expected values at all locations, or a set of simulated possible values that honor some random function model. A significant challenge in geostatistics is to define stationary domains where the intrinsic stationarity hypothesis is deemed acceptable, and to estimate spatial trends when sharp domain boundaries cannot be defined. Such trends may come from ancillary information provided by geophysical data, or from geological knowledge (Kedzierski et al. 2008; Massonnat 1999).

3 The Time Dimension

Geological interpretation highly relies on one's understanding of a succession of geological events through time. However, most current geomodeling techniques only provide limited or indirect integration of this temporal dimension. Indeed, a model honoring basic topological validity rules is not necessarily compatible with a plausible geological history. The concepts of time-stratigraphy (Wheeler 1958; Vail 1987; Mallet 2004) introduce geological time more directly into interpretation and geomodeling methods. From identified chronostratigraphic surfaces, it is possible to define a mapping between present-day physical space to chronostratigraphic space, where depositional heterogeneities can be modeled using geostatistical methods (Mallet 2004;

Caumon et al. 2004a; Gringarten et al. 2008; Jayr et al. 2009). In this view, chronostratigraphic horizons are seen as the equipotentials of the depositional time.

3D model quality controls reviewed by Caumon et al. (2009), such as layer thickness variations and fault juxtaposition diagrams, are also connected to depositional and kinematic concepts. Such principles may be included directly in the modeling method, for instance by constraining sedimentation and compaction rates with thickness constraints (Kaven et al. 2009; Mallet 2002, p. 269). Structural kinematic constraints may also be used during model construction to generate developable horizons (Thibert et al. 2005) or compatible geometry of fault surfaces (Thibault et al. 1996). A more direct integration of time as an explicit model parameter is readily available in process-based geological simulations of sedimentary processes (Harbaugh et al. 1999) or tectonic processes (e.g., Braun 1993; Jessell and Valenta 1996). In principle, inverse theory may be used to constrain these models to spatial data (Cross and Lessenger 1999). However, in practice, only sparse observations may be accounted for. Moreover, present observations result from a complex succession of depositional or setup processes, diagenetic and tectonic transformations; process-based models are generally concerned with only one of these aspects.

An alternative is to start from 3D models built with current geomodeling methods, and perform balanced restoration to move back in time. Structural geologists have been performing such restorations for decades, mostly on cross-sections using geometric criteria (Dahlstrom 1969; Elliott 1983). Because cross-section restoration assumes planar strain, a significant effort has been made to adapt structural restoration techniques to 3D structural models during the last 15 years. This first concerned geological horizons (Gratier et al. 1991; Rouby et al. 2000; Dunbar and Cook 2003), then volumes, using either geometric methods (Mello and Henderson 1997) or geomechanical principles (Muron 2005; Maerten and Maerten 2006; Moretti 2008; Guzofski et al. 2009). As compared to other approaches, geomechanical restoration is able to reproduce heterogeneous mechanical behavior depending on rock type. Geomechanical restoration is applied on conformable meshes by specifying boundary conditions to sequentially flatten layer hanging walls. However, mesh generation itself is often time-consuming, and honoring fine-scale structural features tends to generate a very large number of elements. This limitation has been addressed by Durand-Riard et al. (2010): using an implicit scalar field $f(x, y, z)$ to represent chronostratigraphic horizons, geomechanical restoration can be performed on a coarser mesh, conforming only to faults. In the presence of unconformities, several scalar fields may be used, which also allows for easily making hypotheses about the amount of eroded material.

Restoration can be used for three major purposes. First, it helps produce geometries which are kinematically acceptable from limited data. Second, it provides ways to assess the interplay between sedimentary and tectonic processes and to analyze basin evolution by providing a view at paleostructures. Lastly, it generates a 3D map of rock strain which can be used to predict fracture location, under the assumption that the deformation mechanism is correct (Fig. 2). As compared to cross-section balancing, the quantitative usage of restoration for correcting 3D structural interpretations is still an active topic, which calls for fast model updating methods (Sect. 4).

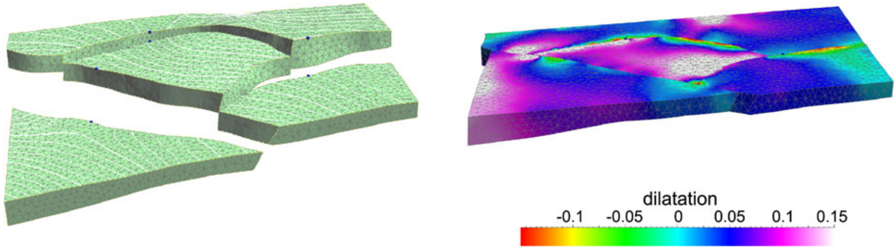

Fig. 2 Present state (*left*) and restored state (*right*) of a faulted structural model. Dilation between restored and present states is color coded (model courtesy of Pierre Muron)

Other challenges lie in the definition of appropriate boundary conditions (Guzofski et al. 2009) and the choice of good rheological behavior to obtain realistic deformations. Coupling 3D restoration with quantitative sedimentological models is another area for future research.

In a shorter time scale, time-varying geological models mostly aim to represent fluid transport, reactive or not, and geomechanical transformations such as subsidence during hydrocarbon reservoir depletion, stability of rocks in underground cavities, etc. Many of these problems are currently addressed by simulating numerical processes on a static geomodel, and possibly assimilating observations to update the model (Sect. 4.2).

4 The Uncertainty Dimension(s)

Progresses in geomodel representation, construction and restoration can never remove ambiguity present in subsurface data (Bond et al. 2007). In many cases, creating several possible models reflecting the uncertainty is therefore preferable to building one single best model, which tends to smooth features in areas of high local uncertainty. Indeed, this smoothing effect is often unrealistic, and may lead to significant biases in the modeling output (e.g. simulated behavior of an aquifer or hydrocarbon field). Multirealization approaches better reproduce realistic geological features and assess the impact of subsurface uncertainty on modeling response, as demonstrated by many authors (Charles et al. 2001; Manzocchi et al. 2008).

Many geostatistical methods exist to sample petrophysical uncertainties using either classical two-point covariance, multipoint statistics carried by a training image or object models. However, the application of geostatistical simulation calls for defining stationary domains and providing global target statistics, whereas both are questionable. Therefore, realistic uncertainty assessment methods must go beyond standard geostatistical simulation. For example, uncertainty about a global parameter (e.g. global rock type proportion) can be assessed by spatial resampling from geostatistical realizations (Journel 1993; Norris et al. 1993). This method is a good way to assess uncertainty about a global parameter while honoring spatial variability models. However, to be representative, it should be performed on several realizations sampling the prior uncertainty distribution of this parameter (Caumon et al. 2004b; Maharaja et al. 2008).

4.1 Structural Model Uncertainties

We will now review methods to look into uncertainty about geological structures. Indeed, structural uncertainty is often first-order as compared to other types of subsurface uncertainty, especially when observations are sparse. Even in the presence of 3D seismic data, poorly known velocity models and interpretation errors may induce significant uncertainties about position and relative layout of structural objects (Thore et al. 2002; Bond et al. 2007). Perturbation or randomization of the structural model parameters are therefore needed to sample these uncertainties, then assess their impact on volumetrics, heterogeneities, and response of hydrodynamic or other physical forward models.

With most structural parameterizations reviewed in Sect. 2, stochastic structural modeling is very difficult, or only samples a subset of the possibilities. For instance, Abrahamsen (1992), Charles et al. (2001), Goff (2000), Lecour et al. (2001) have proposed to perturb a reference structural model by moving surfaces along some predefined direction field, generally vertically or aligned along faults. The amount of surface displacement is evaluated by simulating 2D realizations of a 2D Gaussian random field or p-field simulation to sample from an existing uncertainty map. Another approach may use free-form deformation methods to interpolate a displacement field and distort discrete meshes (Caumon et al. 2007). However, this approach warps the whole model and does not easily allow for different displacement fields across faults. In hard rocks, Guillen et al. (2008) propose perturbing the geometry of a reference model, using random sampling of region boundaries and mathematical morphology operators. Because all these methods can only generate models with the same topology, Hollund et al. (2002) and Holden et al. (2003) introduce a fault operator which can be introduced to alter fault block definitions and connectivity. Fault/horizon consistency is maintained by applying this operator on pillar-based corner-point grids. This practical decision is convenient to directly assess the effect of structural uncertainty on flow predictions in reservoirs, but can only simulate faults aligned on grid pillars. The range of structural uncertainty which can be represented with this approach is therefore smaller than desirable.

Constrained editing of sealed geological models is more flexible, but its implementation is very complicated, and difficult to automate without infringing model validity (Euler et al. 1998; Caumon et al. 2004c). Recently, promising works have been presented to automatically update or perturb implicit models on tetrahedral meshes (Caumon et al. 2007; Tertois and Mallet 2007; Cherpeau et al. 2009). In this case, perturbation of a given implicit model simply amounts to adding realizations of a random field $r(x, y, z)$ to the 3D scalar field $f(x, y, z)$. In the frame of estimation, Aug et al. (2004) has established a relationship between the local uncertainty of the 3D scalar field and the probability for the implicit surface to go through a point, under Gaussian assumption. In the frame of stochastic simulation, the approach to sample uncertainties of Caumon et al. (2007) is still heuristic, and only imposes values of the random field to be 0 at exact data location (in first approximation, the isosurface at location (x, y, z) is displaced by a distance equal to $r(x, y, z)/\|\nabla f(x, y, z)\|$). In practice, the random field $r(x, y, z)$ is controlled by a locally varying anisotropy aligned on the gradient ∇f of the scalar field f. Variogram range along this gradient controls layer thickness variations in the case of chronostratigraphic models; ranges orthogonal to ∇f control the sinuosity of the perturbation. Although additional work is needed to account for more complex types of uncertainties about geological surfaces (Thore et al. 2002), this method benefits from the built-in topological integrity of implicit models and does not make simplifying assumptions on structural features. When coupled with constructive solid geometry principles and random tree generation rules, it also allows for significant topological changes (Cherpeau et al. 2009).

4.2 Updating Prior Geological Uncertainties

The methods we have reviewed so far are based on spatial data and geological concepts to build geomodels. One of the target applications of geomodels is to simulate physical processes (flow, heat transfer, wave propagation, etc.). The result of these numerical simulations may differ from the actual observations (flow rates/pressures at wells, heat flux, seismic waveform, etc.). Inverse theory is concerned with the search for model parameters compatible with this type of observation (Tarantola 1987). Essentially, inverse methods look for the probability distribution $f_{\text{post}}(\mathbf{m}|\mathbf{d})$ of model parameters $\mathbf{m}$ given a set of observations $\mathbf{d}$. Following Bayes' rule, this probability is proportional to the product of the probability of model parameters $f_{\text{prior}}(\mathbf{m})$ before making the observations $\mathbf{d}$ times the likelihood probability $f(\mathbf{d}|\mathbf{m})$ of the data for a given model. This data likelihood probability is derived from the difference between the true and simulated data, generally under the Gaussian assumption of both measurement and forward simulation errors.

This theoretical framework is very general, but raises a number of challenges when applied to complex geomodels. Structural parameters are very diverse, and may include the absence or presence of a fault, the connection (or not) of two faults, the geometry of a layer, etc. It is not currently possible to cast such a heterogeneous set of features into a random vector of parameters characterized by covariances. Finding a model parameterization which honors geological consistency is very difficult, and often relies on simplifications (Lelièvre et al. 2008). In the case of random fields describing petrophysical heterogeneity, gradual deformation (Hu et al. 2001) and probability perturbation method (Caers and Hoffman 2006) provide effective ways of blending models while preserving their consistency. Ensemble Kalman Filter offers another avenue for updating stochastic models through data assimilation, generally under Gaussian assumption (Evensen 2007; Aanonsen et al. 2009). Notably, this approach benefits from the time-varying nature of most inverse problems by successively updating the ensemble of models at successive time steps. However, the application of these methods to structures can account for continuous uncertain parameters, but not categorical parameters or different structure scenarios. Such simplifications may prevent many possible configurations to ever occur in a realization; this is not appropriate for sound uncertainty assessment.

To avoid simplifying assumptions, it is convenient to consider that an ensemble of possible models define the prior uncertainty. Solving the inverse problem then amounts to eliminating those of the prior models which are not consistent with observations. This may be achieved naively by simulating the forward physical model for every single model in the prior space. This is not practically feasible due to the

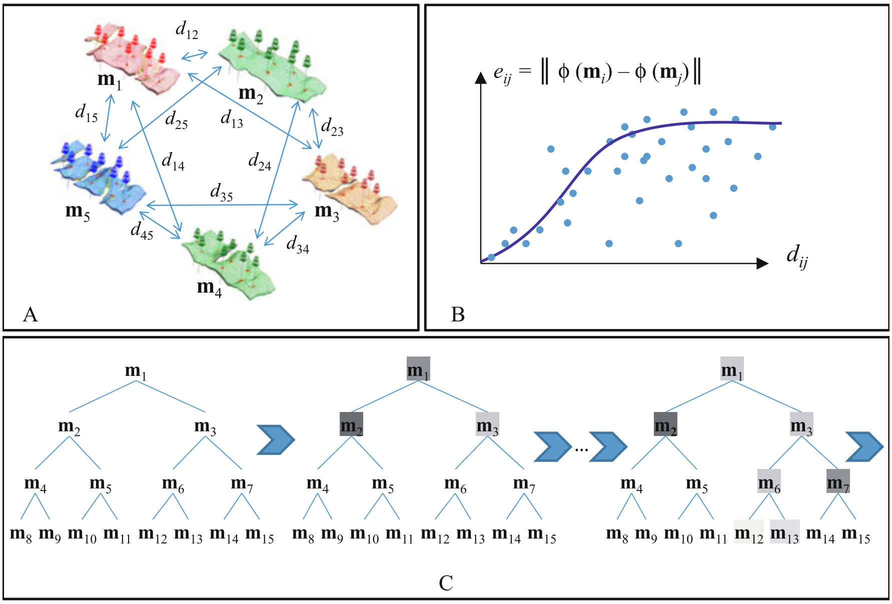

Fig. 3 Sampling from a population of models to solve a history matching problem (Suzuki et al. 2008). Hausdorff distances between models are computed (**A**), and are correlated differences in flow response (**B**). Efficient search of model space (**C**) can then be achieved with a proximity tree (Brin 1995). The error magnitude between simulated and actual production is shown as grey intensity

high computational cost of forward computations. To address this problem, Suzuki and Caers (2008), Suzuki et al. (2008) propose computing a distance between prior models, as seen in Fig. 3(A), and then use this distance to search more efficiently for acceptable models, as seen in Fig. 3(C). In the case of history matching, the Hausdorff distance between structural models was shown to be correlated to flow response, like in Fig. 3(C). Discrete optimization techniques (Sambridge 1999a, 1999b; Brin 1995) can then exploit this to rapidly find models which are compatible with observed production history. Scheidt and Caers (2009) also propose to use distances to project models into a feature space in order to speed up selection of representative models. A practical problem with these approaches is that the prior set of models must be very large in order to cover the space of uncertainty. Therefore, further research is still needed to generate new and consistent models in a given area of the search space, as with gradual deformation or probability perturbation methods.

Another avenue for further research is to look into ways of computing the likelihood of a structural model using concepts related to geological time (Sect. 3). For instance, characterization of rock microstructures provides clues about the successive phases of deformation of a rock. Comparing such micro-scale observations to retrodeformations obtained by 3D restoration could provide indices about 3D structural model consistency.

5 Conclusions

Ideally, geological models should result from numerical simulations of the physical processes which led to the present state (Tarantola 2006). The parameters of these processes should be inferred from qualitative observations, and matched with all quantitative data using stochastic inverse methods. The ensemble of models obtained that way would describe our level of knowledge about a geological domain; every new observation would then reduce the number of possible models. Currently, this vision cannot be put into practice (and this will probably remain so for a while). Physical processes are coupled and still being described and improved by the geosciences community, forward model parameters are unlikely to be multivariate Gaussian, time-varying boundary conditions are poorly constrained, and problem dimensionality is huge, even with parsimonious models.

I advocate a more pragmatic approach toward the integration of time and uncertainties in 3D geological modeling. Advances in the specifications and formulations of 3D model representations opens new perspectives to more easily generate possible structural models honoring prior geological concepts. For each of these models, a vast range of methods can assess petrophysical uncertainty. In the future, we believe that further progresses in parameterization of geological models will help address inverse problems in order to reconcile numerical simulation of physical processes and observations. Geological time may be incorporated in this parameterization through indirect rules or backward process-based simulation. Additional reasons to be optimistic are to be found in sensitivity analysis (to find the most significant parameters to a given problem), progresses in optimization methods, and hardware evolution. All these will hopefully converge toward making truly integrated, stochastic, and time-varying models a reality.

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