Journal of Structural Geology 59 (2014) 19–36

Contents lists available at ScienceDirect

Journal of Structural Geology

journal homepage: www.elsevier.com/locate/jsg

Review article

Overview of continuum and particle dynamics methods for mechanical modeling of contractional geologic structures

Gary G. Gray [a,*], Julia K. Morgan [b], Pablo F. Sanz [a]

[a] *ExxonMobil Upstream Research Company, P.O. Box 2198, Houston, TX 77252-28189, USA*
[b] *Rice University, Dept. Earth Science, Houston, TX 77005, USA*

ARTICLE INFO

Article history:
Received 29 October 2012
Received in revised form
23 November 2013
Accepted 30 November 2013
Available online 12 December 2013

Keywords:
Structural modeling
Finite element
Particle dynamics
Discrete element
Boundary element
Finite difference
Constitutive laws
Contractional structures
Plasticity

ABSTRACT

Mechanically-based numerical modeling is a powerful tool for investigating fundamental processes associated with the formation and evolution of both large and small-scale geologic structures. Such methods are complementary with traditional geometrically-based cross-section analysis tools, as they enable mechanical validation of geometric interpretations. A variety of numerical methods are now widely used, and readily accessible to both expert and novice. We provide an overview of the two main classes of methods used for geologic studies: continuum methods (finite element, finite difference, boundary element), which divide the model into elements to calculate a system of equations to solve for both stress and strain behavior; and particle dynamics methods, which rely on the interactions between discrete particles to define the aggregate behavior of the system. The complex constitutive behaviors, large displacements, and prevalence of discontinuities in geologic systems, pose unique challenges for the modeler. The two classes of methods address these issues differently; e.g., continuum methods allow the user to input prescribed constitutive laws for the modeled materials, whereas the constitutive behavior 'emerges' from particle dynamics methods. Sample rheologies, case studies and comparative models are presented to demonstrate the methodologies and opportunities for future modelers.

1. Introduction

Forward mechanical modeling has become an increasingly popular tool in the study of structural geology, as it can provide fundamental insights into the formation, evolution, and geometries of complex geologic features. In this paper, we present an overview of the current state of mechanical modeling as applied to the structural geology of contractional systems. We focus on methods receiving the majority of usage today, specifically, finite elements and particle dynamics. Finite difference and boundary element techniques are briefly described for comparison. This paper is targeted at the general structural geology community, and assumes only minimal experience with numerical modeling and the concepts behind the different techniques. It is not possible to review the entirety of numerical structural modeling in a short paper, as this topic encompasses scales from the entire crust and lithosphere down to initiation and growth of a single fracture. Therefore, we focus this review on the application of forward mechanical modeling of contractional systems, from the regional cross-section to the individual structure scale, similar to the scale of problems addressed by balanced section analysis.

Many modeling techniques commonly used by the geologic community were developed for solving engineering problems. The goal of most engineering applications is to determine the stress/strain conditions at which a system or structure begins to fail. Such problems range from soil stability for foundation analysis to metal fatigue for bridges, airplane, and automotive parts. It is typically less important for the structural engineer to understand the behavior of the model system once failure is underway (i.e., the behavior of a foundation after it cracks or the airplane wing as it tears and falls off). Most such codes are optimized for these types of low-strain, failure-limit analysis problems. Geologists, of course, are typically more interested in the evolution of systems after the onset of failure. For example, folds and faults begin to form and move, permanently changing the state of the system. These types of geologic behaviors are kinematically discontinuous in nature, and generally involve large displacements and strains, conditions for which few engineering codes are optimized. The accumulation of large strains causes excessive distortion of the mesh used in continuum modeling, preventing such models from converging on a solution. These issues pose unique challenges that must be

---

* Corresponding author. Current address: Rice University, Dept. Earth Science, Houston, TX 77005, USA.
E-mail addresses: graybeau@sbcglobal.net, ggg2@rice.edu (G.G. Gray).

0191-8141/$ – see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.jsg.2013.11.009

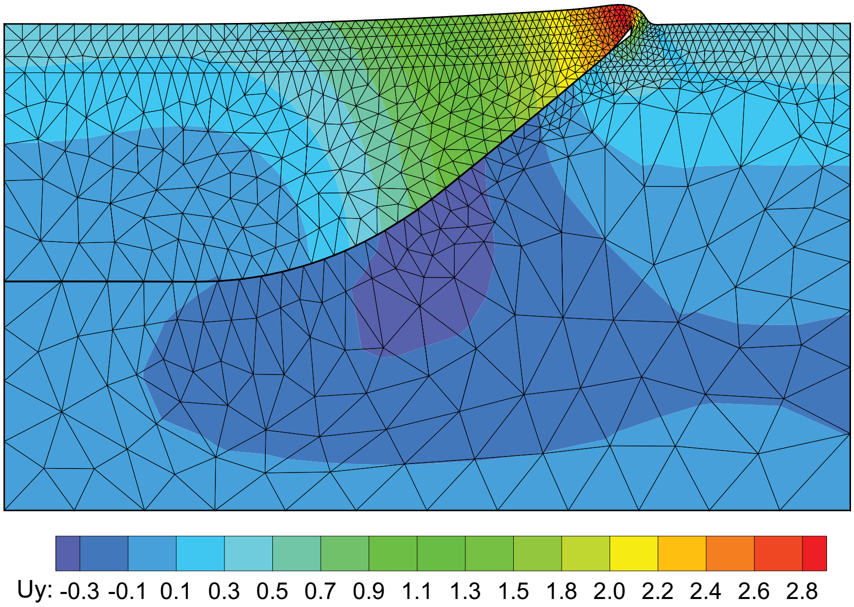

Fig. 1. Diagram showing a typical finite element model with the mesh and a pre-defined slip surface. This view shows the model after significant lateral contraction. Colors are contours of displacement in the vertical direction. Modified from Sanz (2008).

overcome when modeling discontinuous processes, such as faulting, with many of these methods (Munjiza, 2004).

Despite these cautionary comments regarding the abilities of forward mechanical modeling in structural geology, numerical models offer powerful ways to identify and assess feasible solutions to structural interpretations, and provide important insights into the mechanical conditions under which they must form. For these reasons, forward modeling is becoming increasingly popular, rapidly advancing the state of knowledge in structural studies with a wide range of applications.

2. Continuum and particle-based numerical methods

Numerical methods are required to study geologic problems that are too complex for simple analytical solutions. The linear momentum balance law is the governing equation for the deformation of solids and these methods are capable of solving this equation in problems with irregular geometries and boundaries, and non-linear material behavior. The mechanical behavior of geologic materials can be modeled as a continuous mass or as discrete particles. A spectrum of different modeling approaches have been developed for wide variety of applications. The following section examines the most common continuum and discrete numerical methods utilized in forward modeling of contractional geologic structures.

2.1. Continuum methods

The basic strategy of the continuum methods (finite element, finite difference, and boundary element) is to discretize the model geometry into smaller subdomains (e. g., Laursen and Simo, 1993, and many others). The subdomains share nodes and edges, and any surfaces that are defined within the model. The nodes, edges and surfaces comprise a mesh that provides the framework within which the calculations are made (Fig. 1). The models runs are divided into a series of time-steps. At each time-step, the mesh is moved by pre-defined loads and/or displacements at the model boundaries, and the effect of these changes on adjacent nodes and elements propagates via a system of mathematical equations throughout the rest of the mesh as needed to maintain equilibrium.

Continuum methods assume that the processes and properties being modeled can be represented as smoothly varying fields. The three methods discussed herein deal with this continuum in different ways. Finite element and finite difference models use a similar meshing strategy for the entire domain. The primary distinction between these two techniques is that the finite element method solves an equivalent weighted-integral, or weak form of the problem (e.g., Zienkiewicz, et al., 2005). The finite difference method directly approximates the partial differential equation, or strong form of the problem, using finite difference equations (e.g., Detournay and Hart, 1999). The finite element approach is generally better suited for non-linear problems with irregular geometries and complex boundary conditions. In addition, there are many well-developed and verified academic and commercial finite element codes with large capacities in terms of computing power and material complexities. For these reasons, it is the most widely applied numerical method for modeling in structural geology (Melosh and Williams, 1989; Mäkel and Walters, 1993; Braun and Sambridge, 1994; Erickson and Jamison, 1995; Mohapatra and Johnson, 1998; Smart et al., 1999; Cardozo et al., 2003; Ellis et al., 2004; Kwon and Mitra, 2004; Panian and Wiltschko, 2004; Crook et al., 2006b; Sanz et al., 2007; Simpson, 2009; Albertz and Lingrey, 2012; Albertz and Sanz, 2012; see also Table 1).

The finite difference method is the oldest member in this family of numerical methods. This method transforms the original partial differential equations into systems of algebraic equations with unknowns at the grid points. As with the finite element method, the solution of the system of equations is obtained after imposing the necessary initial and boundary conditions. Finite difference methods are excellent for static problems such as heat flow and temperature modeling, and have some strong adherents for lithospheric-scale viscous models (e.g., Gerya, 2010).

A commonly used finite difference code for geologic structures is FLAC (Fast Lagrangian Analysis of Continua) (http://www.itascacg.com/flac/overview.html), first released in 1986. FLAC utilizes an explicit integration scheme and considers large strains (geometric nonlinearities) in the solution. An important advantage