SBGf36099

A New Finite Element Strategy for Large-Scale 3-D Tectonic Modeling

Alvaro L.G.A.Coutinho[1], Marcos A.D. Martins[1], José L.D. Alves[1], Luiz Landau[1] and Anderson Moraes[2]

[1]Computational Methods Laboratory ,COPPE / Federal University of Rio de Janeiro
[2]PETROBRAS/CENPES/DIVEX/SETEX

ABSTRACT

A new finite element strategy is presented for solving large-scale three-dimensional and realistic structural geology simulations considering the rheological behavior of the rocks. Special coding techniques and data structures provide the background for computationally feasible 3-d simulations. The main issues of the proposed approach are addressed and application results are shown for a simulation carried out over a full 3D model of a sedimentary basin under extensional conditions, trying to assess strain localization phenomena along heterogeneous strata. All the analyses were carried out on the Cray J-98, a shared memory, parallel vector processor machine, showing remarkable savings in computer time and memory over standard finite element solution techniques.

INTRODUCTION

The finite element method is recognized as the most valuable tool for numerical modeling in structural geology and tectonics. Although the geological literature has some few hundreds of works using finite elements in numerical modeling, a small amount of them are built up in three dimensions. Possibly, the main restriction for the 3D modeling is still the high computational costs involved to reach models with expressive geological significance. In general, numerical models in structural geology and geotectonics aim to show the main structures and their relationships, the stress and deformation distribution and the relative rheological behaviour of rocks. Therefore, realistic simulations should be carried out in 3D models with significant spatial resolution. In addition, 3D finite element models made easy and realistic the understanding of complex structures and geometries found in geological realms. Searching for analysis with more efficient results in terms of quality and cost, tectonic finite-element models should achieve a balance between good geological results and mesh refinement. In many cases, tectonic modeling aims to study the problem of strain localization (that is, faulting) where the need of a fine mesh is almost a rule.

Therefore, we present a novel solution strategy to solve large-scale 3D structural geology problems with special emphasis on computer efficiency and performance. Assuming that the rocks are elastic-plastic materials modeled by Mohr-Coulomb failure criteria, the resulting non-linear equilibrium equations are solved by the Inexact Newton method. At each Inexact Newton iteration, the Jacobian system is approximately solved by preconditioned conjugate gradients. Edge-based data structures are employed to store the coefficients of the Jacobian. The remainder of this paper is organized as follows. In the section that follows, we describe the Inexact Newton method to solve plasticity problems. Next section briefly reviews edge-based data structures for iterative solving of finite element systems of linear equations. In the subsequent section, we present the analysis of the extensional behavior of a sedimentary basin, where we show that our strategy is more computationally efficient than the usual approaches. The paper ends with a summary of the main conclusions of this work.

INEXACT NEWTON METHODS FOR PLASTICITY PROBLEMS

The incremental finite element formulation for plasticity problems with implicit computation of stresses (Simo and Hughes, 1998) requires the solution of a nonlinear system of equations at each load increment. These systems are usually solved by Newton-like methods such as the Initial Stress and Tangent Stiffness methods. In the former the initial Jacobian, that is, the elastic stiffness matrix remains constant, while in the latter the stiffness matrix is usually updated every nonlinear iteration. For solving large-scale problems, particularly in 3D, it is more efficient to solve approximately the Jacobian problems by suitable inner iterative methods, such as preconditioned conjugate gradients. This inner-outer scheme is known as the Inexact Newton method, and the convergence properties of its variants, the Inexact Initial Stress (IIS) and Inexact Tangent Stiffness (ITS) methods have been analyzed for von Mises materials by Blaheta and Axelsson (1997). We introduce here a further enhancement in IIS and ITS methods, by choosing adaptively the tolerance for the inner iterative equation solver according to the algorithm suggested by Kelley (1995). We also include in our nonlinear solution scheme a backtracking strategy to increase the robustness of the overall nonlinear solution algorithm.

EDGE-BASED DATA STRUCTURES FOR ITERATIVE EQUATION SOLVING

At every IIS or ITS nonlinear iterations the inner algebraic systems of linear equations are approximately solved by a nodal-block diagonal preconditioned conjugate gradient (PCG) method. In PCG method, the stiffness matrix is employed only as a linear operator, that is, to compute a sparse matrix-vector product. In this work the stiffness matrix is stored using the edge-based data structures proposed in Martins et al (1997). This data structure is based on the nodal graph of the underlying unstructured grid, storing only the non-zero off-diagonal coefficients of the stiffness matrix. Thus, we have a more compact scheme than the usual element-by-element (EBE) scheme, which stores unassembled stiffness matrix entries.

NUMERICAL EXAMPLE

We analyse the extensional behavior of a sedimentary basin presenting a sedimentary cover (4 km) over a basement (2 km) with length of 15 km and thickness of 6 km. The model has an ancient fault with 500 m length and 60^o of slope. A two-dimensional elastic analysis of this model was performed earlier by Moraes (1995). The relevant material properties, from Moraes (1995), are compatible with the sediment pre-rift sequence and basement. We have densities of 2450 kg/m^3 and 2800 kg/m^3 respectively for the sediment layer and basement; Young's modulus of 20 GPa for the sedimentary cover and 60 GPa for the basement; Poisson's ratio, 0.3 for both rocks. The ratio between initial horizontal and vertical (gravitational) stresses is 0.429. We assume that both materials are under undrained conditions and modeled by Mohr-Coulomb failure criterion. Thus, we have sedimentary cover cohesion of 30 MPa, basement cohesion of 60 MPa, and internal friction angle of 30^o for both materials. The finite element mesh (see Figure 3) comprises 25,001 tetrahedra, 5,257 nodal points and 32,133 edges. We consider the model simply supported at its left and bottom faces, and we apply tension stresses at the right face and shear stresses at the basement, opposing the basin extension. The loads are applied in 15 increments, ranging from 0.01 to 9.90, and the analysis is performed until the complete failure of the model.

Table 1 presents a comparison of memory requirements to hold the stiffness matrix by a profile solver, by the PCG-EBE storage scheme and by our PCG-Edges scheme. The profile solver is a standard implementation of symmetric Cholesky factorization usually employed in Newton's method. We may see that our solution strategy required 1.5% of the storage area needed by the profile solver and 6 times less memory than the PCG-EBE scheme.

Profile Solver	PCG-EBE	PCG-Edges
19 381 711 (1.000)	1 950 078 (0.100)	289 197 (0.015)

Table 1 - Memory requirements to hold stiffness matrix (64-bit words)

Memory is a very important limiting factor of current large-scale 3d analyses and our scheme presents an inexpensive memory demand compared to the usual procedures. Tables 2 and 3 compare the total number of nonlinear and PCG iterations and the relative CPU times for respectively the Initial Stress (IS) and Tangent Stiffness (TS) as well as their Inexact variants (IIS and ITS). We show in these Tables IIS and ITS solutions where the tolerance for PCG varies adaptively between 10^{-6} to 10^{-2} and 10^{-6} to 10^{-1} according to the convergence of the outer (nonlinear) iterations.

	IS	IIS [10^{-6}, 10^{-2}]	IIS [10^{-6}, 10^{-1}]
Nonlinear Iters	1 587	1 589	1 589
PCG Iters	271 846	146 381	68 626
CPU	1.00	0.55	0.28

Table 2 - Edge-based Initial Stress Solutions – 13 load increments, halted after 950 nonlinear iterations; nonlinear tolerances 10^{-3}.

	TS	ITS [10^{-6}, 10^{-2}]	ITS [10^{-6}, 10^{-1}]
Nonlinear Iters	116	119	156
PCG Iters	27 806	15 726	12 897
Max Stress (MPa)	-122.0	-122.0	-122.0
CPU	0.10	0.07	0.06

Table 3 - Edge-based Tangent Stiffness Solutions – 15 load increments, nonlinear tolerances 10^{-3}.

We may see in these Tables that the Inexact methods are faster than their counterparts, although requiring more nonlinear iterations to achieve the solution. The fastest method is the ITS solution where the PCG tolerance varies between 10^{-6} to 10^{-1}. In Table 3, we may note also that the maximum stress is the same for all solutions. The accuracy of IIS and ITS methods may be observed in Figures 1 and 2, where we show the load-displacement curves for all analyses. In these Figures, the vertical displacements are measured for a node at the model midsection, in the top of the sediment layer, over the fault.

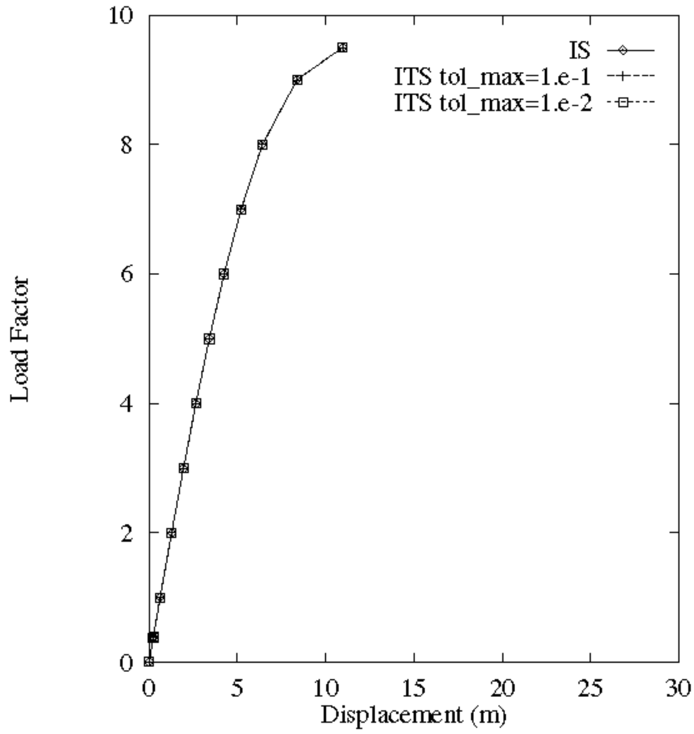

Figure 1. Initial Stress Load-displacement curves

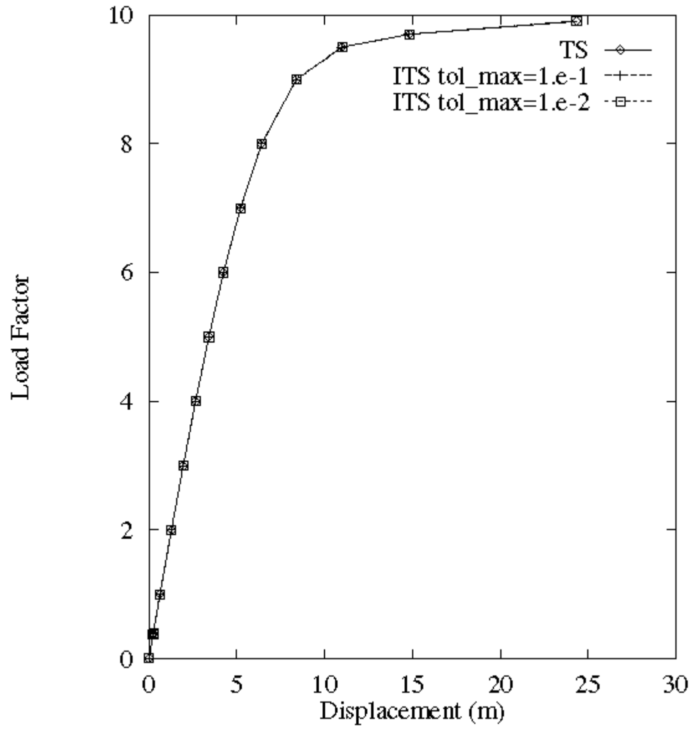

Figure 2. Tangent Stiffness Load-displacement curves

We may note the complete rupture of the model, particularly in the ITS analysis. The IIS analyses were halted in the 13^{th} load increment, after 950 nonlinear iterations. Figure 2 shows the deformed mesh obtained by ITS methods at the last load increment. We may also see in this Figure the fringes of the ratio between the current equivalent stresses to the unidimensional yield stress for the Mohr-Coulomb criterion at basin midsection. It can be observed the development of failure zones at the sedimentary cover and embankment, mostly in the righ portion of the model, with an incision to the left underneath the fault. Thus, the fault is acting as a barrier for the spread of the failure zones. Similar behavior has been noted earlier by Moraes (1995) for two-dimensional models.

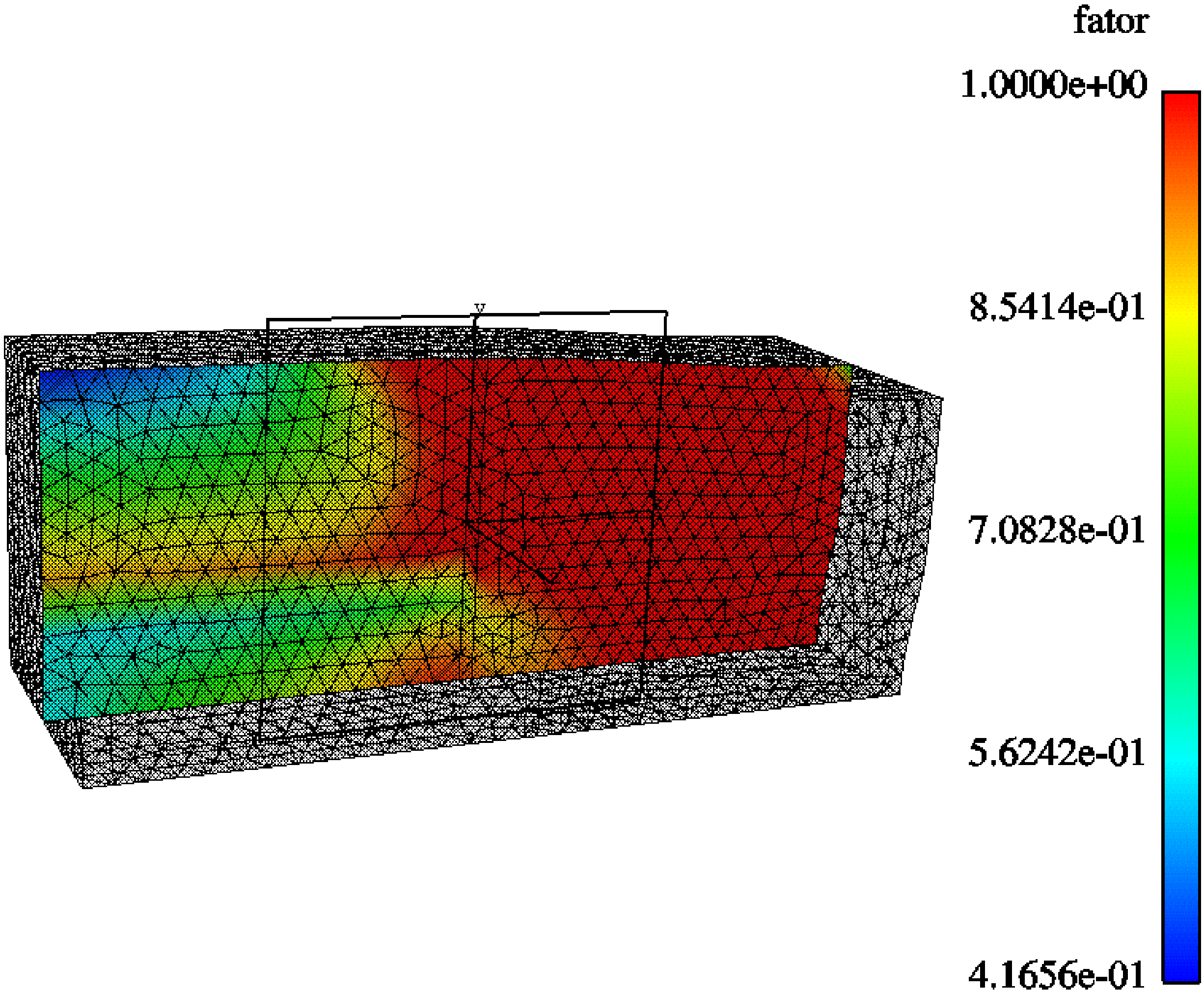

Figure 2. Fringes of Mohr-Coulomb failure index ("fator") at basin midsection. Unit failure index stands for full failure.

CONCLUSIONS

We presented a fast, memory inexpensive and accurate finite element solution scheme for analysing large-scale 3d tectonic models. Our scheme employ novel nonlinear solution strategies and suitable data-structures, allowing us to tackle challenging problems in their full complexity.

REFERENCES

Simo J.C and Hughes, T.J.R. , 1998, Computational Inelasticity, Springer-Verlag, New York.

Blaheta, R. and Axelsson, O. , 1997, Convergence of Inexact Newton-like Iterations in Incremental Finite-element Analysis of Elasto-plastic Problems, Comp. Meth. Appl. Mech. Engng., 141, pp. 281-295.

Kelley, C.T. , 1995, Iterative Methods for Linear and Nonlinear Equations, SIAM, Philadelphia.

Martins, M.A.D., Coutinho, A.L.G.A. and Alves, J.L.D. , 1997, Parallel Iterative Solution of Finite Element Systems of Equations Employing Edge-based Data Structures, 8th SIAM Conf. on Parallel Processing for Scientific Computing, CD-ROM, SIAM, Philadelphia.

Moraes A., 1995, A Study of Local Stress Fields and Fault Generation in Extensional Regimes by the Finite Element Method: MSc Thesis, Federal University of Ouro Preto, Ouro Preto, Brazil (in Portuguese).

ACKNOWLEDGMENTS

This work is partially supported by grants CNPq 142318/1996-5 and CNPq 522692/95-3. The authors gratefuly acknowledge the Center for Parallel Computing of COPPE/UFRJ (NACAD/COPPE) for the computer time provided in the Cray J-98.