11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

A modified Hager-Zhang nonlinear conjugate gradient algorithm for efficient solution of finite element models

Sam L. Evans[1]

[1] School of Engineering, Cardiff University, Cardiff CF24 3AA, UK; email EvansSL6@cardiff.ac.uk

Key Words: conjugate gradient; surgical simulation.

INTRODUCTION

This paper presents a novel nonlinear conjugate gradient solution algorithm with modified line search and compares its performance to an explicit solver and a conventional implicit solver. All three solvers were implemented in the FEBio finite element package [1] which provides a convenient test bed to compare their performance; in the future they could be implemented in a more efficient form for surgical simulation.

METHODS

The default solver used in FEBio and other nonlinear FE codes such as Abaqus is an implicit modified Newton – Raphson algorithm in which the tangent stiffness matrix is calculated on the first iteration and then updated approximately using a BFGS algorithm. The tangent stiffness matrix is recalculated at intervals or if an iteration fails. This algorithm is much faster than a standard Newton – Raphson solver and is very efficient for many problems, especially with the use of the highly optimised Pardiso linear solver.

We have implemented two other algorithms in FEBio, a Hager – Zhang nonlinear conjugate gradient solver and a simple explicit solver, and these can perform much better for some problems.

The Hager – Zhang solver uses a conjugate gradient method to find the solution directly rather than as a linear equation solver. The residual is calculated at each iteration and used to find a line search direction in combination with previous directions; the Hager – Zhang method [2] has guaranteed convergence even with an inexact line search for certain nonlinear problems, although unfortunately this is typically not the case for finite element models.

An efficient line search algorithm is critical to the success of this algorithm, since it determines how many times the residual must be calculated on each iteration, which is the main computational effort required. An improvement on Hager and Zhang's line search is to use the step length from the penultimate iteration as an initial estimate of the step length for the current iteration. Since the steps are typically alternately long and short this is much more efficient than using the step length from the previous iteration.

Another way in which the efficiency of the conjugate gradient method can be greatly improved for finite element problems is to continue to increment the load while iteration continues. A combined incremental – iterative scheme can be used in which the load is increased in many small increments and this can be much faster than a conventional incremental scheme where full convergence is achieved on each increment. This has great potential for surgical simulation because external inputs could continue to vary in parallel as iterations continue without necessarily needing full convergence. A measure of the resulting

error is provided by the residual. Such a scheme is similar to an explicit solver but potentially more efficient and has many of the same advantages such as the possibility of efficient parallelisation.
The various algorithms were tested using standard models. The mesh density was varied to determine how the performance of the different algorithms scales with the size of the model. A single processor was used in all cases to ensure a proper comparison between the algorithms, since some parts of the code have been parallelised more efficiently than others.

RESULTS

The Hager – Zhang solver does not require the tangent stiffness matrix and hence uses much less memory than the BFGS solver. It could therefore be used to solve problems an order of magnitude larger on a given computer. Although slower for small problems, the Hager – Zhang algorithm scales better with problem size and is competitive with BFGS for very large models. The modified line search algorithm improves performance by at least a factor of two. The performance of an explicit solver is difficult to compare to that of implicit methods. The relative performance varies widely depending on the stiffness, mass and time scale but in general explicit solvers are slower than implicit solvers. For large problems, high speed dynamic events such as impacts or with careful modification of the mass and damping parameters they may be faster. Their structure and operation is similar to the Hager – Zhang solver and they also scale well for large problems and can be parallelised very efficiently.

CONCLUSIONS

The Hager – Zhang conjugate gradient solver with modified line search is much faster than conventional conjugate gradient methods and competitive with the best conventional solvers for large models while using much less memory. The load can be continually varied during the solution and this has interesting possibilities for surgical simulation applications.

ACKNOWLEDGEMENTS

The assistance of the FEBio team and in particular Steve Maas in implementing the algorithms in FEBio is gratefully acknowledged.

REFERENCES

[1] S. A. Maas, B. J. Ellis, G. A. Ateshian and J. A. Weiss, FEBio: Finite elements for biomechanics. *J. Biomech. Engng.*, Vol. **134**, pp. 011005-1 – 011005-10, 2012.
[2] W. W. Hager and H. Zhang, A new conjugate gradient method with guaranteed convergence and an efficient line search. *SIAM J. Optimization*, Vol. **16**(1), pp. 170-192, 2005.