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Comput. Methods Appl. Mech. Engrg. 195 (2006) 1499–1516

Computer methods in applied mechanics and engineering

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Solution verification for explicit transient dynamics problems in the presence of hourglass and contact forces

James R. Stewart *, Arne S. Gullerud, Martin W. Heinstein

Sandia National Laboratories, P.O. Box 5800, MS 0382, Albuquerque, NM 87185-0382, USA

Received 22 October 2004; received in revised form 18 March 2005; accepted 10 May 2005

Abstract

This paper presents solution verification studies applicable to a class of problems involving wave propagation, frictional contact, geometrical complexity, and localized incompressibility. The studies are in support of a validation exercise of a phenomenological screw failure model. The numerical simulations are performed using a fully explicit transient dynamics finite element code, employing both standard four-node tetrahedral and eight-node mean quadrature hexahedral elements. It is demonstrated that verifying the accuracy of the simulation involves not only consideration of the mesh discretization error, but also the effect of the hourglass control and the contact enforcement. In particular, the proper amount of hourglass control and the behavior of the contact search and enforcement algorithms depend greatly on the mesh resolution. We carry out the solution verification exercise using mesh refinement studies and describe our systematic approach to handling the complicating issues. It is shown that hourglassing and contact must both be carefully monitored as the mesh is refined, and it is often necessary to make adjustments to the hourglass and contact user input parameters to accommodate finer meshes. We introduce in this paper the hourglass energy, which is used as an "error indicator" for the hourglass control. If the hourglass energy does not tend to zero with mesh refinement, then an hourglass control parameter is changed and the calculation is repeated.

Keywords: Solution verification; Verification and validation; Transient dynamics; Contact; Hourglass control; Error estimation; Mesh refinement

* Corresponding author.
E-mail addresses: jrstewa@sandia.gov (J.R. Stewart), asgulle@sandia.gov (A.S. Gullerud), mwheins@sandia.gov (M.W. Heinstein).

0045-7825/$ - see front matter
doi:10.1016/j.cma.2005.05.043

1. Introduction

Verification and validation are increasingly important components of numerical simulations that are used to make critical design and policy decisions. Verification is the assurance that the underlying mathematical equations are being solved correctly, while validation ensures that the equations adequately represent the physics (i.e., reality). The process of validation usually involves comparisons of numerical results to experimental data. Often, the validation activity is focused on a specific mathematical model developed to approximate the governing physics in some simplified way.

Verification, in turn, has two main components: *code* verification and *solution* verification. Code verification involves finding and fixing algorithmic and coding bugs. This usually requires performing simulations of problems with an analytical or some other very accurate known solution (see, for example, [1]). One popular technique is to generate problems with analytical solutions through the method of manufactured solutions [2]. It is important to note that code verification activities precede the solution verification and model validation phases.

Solution verification involves the assurance that parameters of the numerical discretization do not prevent the goals of the numerical simulation from being achieved. In other words, it addresses the question "is this particular solution accurate enough?". Typically, solution verification is adequately addressed through *a posteriori* error estimation, which attempts to assess the adequacy of the mesh resolution. If the discretization error is too large, then one refines the mesh and repeats the calculation.

This paper addresses solution verification for a generally hard class of problems—explicit, transient dynamics problems with contact, solved using finite elements that give rise to spurious energy modes called *hourglass* modes. In the engineering community, code performance and robustness are typically viewed as being more important than solution accuracy or solution verification for this problem class. There has been very little attention paid to rigorous verification of solutions. Despite this lack of attention, solution verification is becoming more important and, in fact, is supplanting other issues in importance in emerging applications such as model validation. This paper is a novel study that highlights some critical issues that arise in the solution verification process. The theory and application presented herein are not new. However, the systematic approach to solution verification in the presence of complex issues including geometry, friction, contact, wave propagation, localized incompressibility, and hourglassing, is new. Furthermore, this study is carried out on a scale not generally realizable in the academic community, involving in one case millions of elements run on thousands of parallel processors. Thus, these methods are being pushed in ways not commonly seen before.

The calculations are performed using PRESTO [3], which is a rewrite of PRONTO3D [4] using the SIERRA [5] computational mechanics framework developed at Sandia National Laboratories. PRESTO implements commonly used methods for explicit transient dynamics applications. The standard Galerkin finite element method is used in space, while the time derivative is handled by the explicit central-difference method. To render the time integrator fully explicit, the mass matrix is lumped (i.e., diagonalized). We use four-node fully-integrated tetrahedral elements, as well as eight-node mean quadrature hexahedral elements. The mean quadrature hexahedra require the addition of terms to control the spurious energy modes (the "hourglass" modes) that are introduced (Section 3.2 reviews the description of the hourglass modes and how they arise—a complete description is given in [6]). Improper treatment of the hourglass control terms can cause a calculation to fail. *We will show that hourglass control parameters that are appropriate for a nominal coarse mesh may not be sufficient for a refined mesh*. In this paper, we introduce a new indicator for monitoring the adequacy of the hourglass control. The indicator is essentially an energy term, which we refer to as the *hourglass energy*. We use the hourglass energy the same way that an error indicator for adaptive mesh refinement would be used. If the hourglass energy grows too large, then we refine the hourglass viscosity parameter and repeat the calculation.