Numerical procedures for extreme impulsive loading on high strength concrete structures

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Abstract.   This paper demonstrates numerical techniques for complex large-scale modeling with microplane constitutive theories for reinforced high strength concrete, which for these applications, is defined to be around the 7000 psi (48 MPa) strength as frequently found in protective structural design. Applications involve highly impulsive loads, such as an explosive detonation or impact-penetration event. These capabilities were implemented into the authors' finite element code, *ParaAble* and the PRONTO 3D code from Sandia National Laboratories. All materials are explicitly modeled with eight-noded hexahedral elements. The concrete is modeled with a microplane constitutive theory, the reinforcing steel is modeled with the Johnson-Cook model, and the high explosive material is modeled with a JWL equation of state and a programmed burn model. Damage evolution, which can be used for erosion of elements and/or for post-analysis examination of damage, is extracted from the microplane predictions and computed by a modified Holmquist-Johnson-Cook approach that relates damage to levels of inelastic strain increment and pressure. Computation is performed with MPI on parallel processors. Several practical analyses demonstrate that large-scale analyses of this type can be reasonably run on large parallel computing systems.

Keywords: nonlinear finite element analysis; reinforced concrete; microplane constitutive model; parallel computing.

1. Introduction

A heightened threat to civil infrastructure, government facilities, and military installations has led to an increased use of numerical simulations to evaluate their vulnerabilities to explosive detonations and impacting projectiles. Computer modeling is especially attractive for such applications, since full scale destructive testing on large structures is not economically feasible (e.g., Weerheijm *et al.* 2009). The microplane material model (Bažant *et al.* 1996, 2000) has shown to be an accurate, reliable, and robust constitutive relation for concrete subjected to blast loadings, but it can be nearly an order of magnitude more computationally intensive than other inelastic models. Others have also effectively employed the microplane approach for different applications (e.g., Ožbolt *et al.* 2005, 2008) and parallel computing has been utilized for low rate implicit modeling of nonlinear concrete response (e.g., Paz *et al.* 2005). In this paper, a parallel explicit dynamic finite element code, *ParaAble*, developed by the authors (Danielson and Namburu 1998) is used for three-dimensional

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analysis of blast loading events on concrete structures using the microplane model. The parallel structure of the code is similar to that of other parallel explicit dynamic codes, e.g., Hoover *et al.* (1995) and Plimpton *et al.* (1996). A Single Program Multiple Data (SPMD) paradigm is used with the code written in FORTRAN 95, and all interprocessor communication can be made with explicit Message Passing Interface (MPI) calls. Several numerical developments assist in the efficient calculation of the polar decomposition of the deformation gradient tensor and damage evolution variables. The use of large-scale parallel computing demonstrates the ability to reasonably perform such analyses for production purposes, and the sizes of typical finite element models continue to increase with development of faster computers.

2. Numerical modeling

For the analyses in this paper, eight-noded hexahedral elements (Flanagan and Belytschko 1981) are exclusively used for all geometric modeling and an explicit dynamic formulation is used (e.g., Taylor and Flanagan 1989). Steel reinforcement is modeled with multiple elements through the thickness of each rebar using the Johnson-Cook viscoplastic model (Johnson and Cook 1983). Breakage of rebar elements is performed by erosion of elements to ensure that the restraint of the rebar on the concrete can be dissipated.

2.1. Microplane model

For the microplane (MP) model (Bažant *et al.* 1996, 2000), relations between stress and strain components on planes of multiple orientations (the microplanes) are combined to represent the macroscopic nonlinear material behavior. The strain components acting on individual microplanes are determined by dot products of their respective normal vector and the macroscopic strain tensor. Simple stress-strain relations with bounding curves then determine the stress components on each microplane. Finally, the macroscopic stress tensor is assembled from the microplane stress vectors using a virtual work based averaging transformation. "n" microplanes thus represent an "n^{th}" approximation to reality as an infinite number would exactly model all orientations. To reduce computations, symmetry of plane orientations in three-dimensional space is exploited. The advantage of this approach is its ability to simulate complex three-dimensional nonlinear and path-dependent material responses despite being conceptually and mathematically simple. This approach, however, is also a brute force approach that can be quite computationally intensive. A current implementation with 28 microplanes may require as much as seven times the computational expense as a typical elastic-plastic model. The model, however, is also a total stress-strain (total increment) approach that thus avoids iterative checks that may increase computations or exhibit numerical solution failure. The microplane model has been fit to concrete, where it is able to simulate the triaxial shear behavior in the brittle region as post-peak softening occurs, as well as in the ductile region where continued hardening occurs. Although not explicitly addressed in the model, it inherently exhibits the difference between extension and compression failure typically found in concrete and other geomaterials, which requires special treatments in other models, e.g., a third invariant function in a cap model (Fossum and Brannon 2004). This demonstrates the fundamental motivation for the microplane model: to reasonably predict arbitrary load path behaviors without having to provide specific treatments for each and every case. Predictions can be made with greater confidence that the model will capture any behavior that may occur in an analysis.

Since the microplane model uses only stress-strain relations, it does not directly contain a damage metric to predict zones of failure for inspection or for use with erosion/deposition algorithms. Therefore, a damage evolution model that uses a linear relation between pressure and effective inelastic strain increments was appended to the microplane model. This relationship allows the model to predict reduced damage accumulation that generally occurs in concrete at high pressures, e.g., near explosive detonations, and typical increased damage at low pressures, e.g., surface spall. The approach is a modified Holmquist-Johnson-Cook (1993) damage model that also includes both the volumetric and deviatoric strain in the effective inelastic strain computation. Specifically, the model uses increments of inelastic Green-Lagrange strain (total minus the elastic strains) that is input into the Holmquist-Johnson-Cook (1993) damage relationship. A cohesive relationship can also be used with a fully damaged material. That is, when the damage variable reaches the value of full damage, another variable can be used to indicate those elements that are both fully damaged and in tension. In addition, another variable reports a displacement magnitude when both these criteria (full damage and tension) are met. These different variables provide a variety of options to visualize damage, erode Lagrangian elements, and/or deposit them into Eulerian codes. Therefore, fully damaged concrete can be treated as slightly cohesive sand so that it can still transmit compressive waves, but cannot sustain either much tension or displacement magnitude.

2.2. Polar decomposition of the deformation gradient tensor

A critical step in using the microplane model is the polar decomposition of deformation gradient tensor, $\mathbf{F}$, which is defined by (Malvern 1969).

$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \mathbf{I} + \frac{\partial \mathbf{u}}{\partial \mathbf{X}}; \quad |\mathbf{F}| > 0 \tag{1}$$

where $\mathbf{x}$ is the current position, $\mathbf{X}$ is the undeformed position, and $\mathbf{u}$ is the displacement vector of any point. $\mathbf{I}$ is the identity tensor. For the highly nonlinear applications described herein, a multiplicative decomposition is necessary such that the product of a pure rigid body rotation tensor and a symmetric positive definite tensor representing a stretching defines $\mathbf{F}$. This is frequently referred to as application of the polar decomposition theorem (Malvern 1969), whereby

$$\mathbf{F} = \mathbf{V} \cdot \mathbf{R} = \mathbf{R} \cdot \mathbf{U} \tag{2}$$

$\mathbf{V}$ and $\mathbf{U}$ are symmetric positive-definite and are the left and right stretch tensors, respectively. $\mathbf{R}$ is the rotation tensor that defines the rigid body rotation of the material point.

Since the microplane model already requires Green-Lagrange strains, they are conveniently used to develop an efficient and robust modified Newton-Raphson procedure for polar decomposition of the deformation gradient. First, the six unique components of the Green-Lagrange strain tensor, $\mathbf{E}$, are readily computed by the same displacement gradients used to compute $\mathbf{F}$, via (Malvern 1969).

$$\mathbf{E} = \frac{1}{2}\left[\frac{\partial \mathbf{u}}{\partial \mathbf{X}} + \left(\frac{\partial \mathbf{u}}{\partial \mathbf{X}}\right)^{T} + \left(\frac{\partial \mathbf{u}}{\partial \mathbf{X}}\right)^{T} \cdot \frac{\partial \mathbf{u}}{\partial \mathbf{X}} \right] \tag{3}$$

An alternate definition of $\mathbf{E}$ and Eq. (2) provides the following quadratic relationship between these components and the components of the right stretch tensor (Malvern 1969).

$$\mathbf{E} = \frac{1}{2}(\mathbf{F}^{T} \cdot \mathbf{F} - \mathbf{I}) = \frac{1}{2}(\mathbf{U} \cdot \mathbf{U} - \mathbf{I}) \tag{4}$$

Newton-Raphson iteration is used to solve the nonlinear set of simultaneous equations for the six components. Although this solution must be done for every element, on average, the mild quadratic nonlinearity typically only requires a few iterations. Several additional numerical procedures also facilitate these computations. Using engineering instead of tensorial components, along with a rearrangement of the equations, results in a symmetric coefficient matrix with a minimum bandwidth. For additional efficiency, the small matrix is easily factored with a special closed-form solver. Convergence is rapid, if the initial iteration starts with $\mathbf{U} = \mathbf{I}$. This also permits a cheap first iteration, since the matrix is a trivial diagonal. Time increments are typically quite small in explicit simulations, however, so convergence was found to be typically much faster if the initial guess for $\mathbf{U}$ was the stretches from the previous time. Furthermore, a modified Newton-Raphson was found to only require about as many iterations as full Newton-Raphson in conjunction with this initial guess. The modified method is thus much more efficient, as it only updates and factors the coefficient matrix at the beginning of the time increment, and then back substitutes into the old factored matrix for further iterations. Finally, once $\mathbf{U}$ is found, it is inverted and $\mathbf{R}$ is then obtained by

$$\mathbf{R} = \mathbf{F}\mathbf{U}^{-1} \tag{5}$$

2.3. Parallel code development

The parallel procedure primarily consists of a mesh partitioning pre-analysis phase, a parallel analysis phase that includes explicit message passing among each partition on separate processors, and a post-analysis phase to gather separate parallel output files into a single coherent database. Each partition can be optionally placed on individual cores of multi-core processors to further exploit this new parallelism of modern chip architectures. In *ParaAble*, a material-weighting scheme using METIS (Karypis and Kumar 1995a, 1995b) was developed for parallel analysis involving multiple material types. For METIS, elements are weighted according to their relative computational cost. Numerical investigations were made to determine individual material model costs, which indicate that the microplane model is approximately seven times more expensive than typical elastic-plastic models. In the upcoming 4.1 version of METIS/ParMETIS, a new general interface permits direct specification of elemental weights along with the connectivities to more easily accomplish this task while also permitting the mixing of multiple element types. METIS outputs a list of processor numbers for the elements, so that each is uniquely defined on a single processor. Additional software was written to use this information and create separate input files for each processor. The diagonal nature of the mass matrix permits the nodal equation of each degree of freedom to be solved independent of other degrees of freedom. To retain data locality, nodes are redundantly defined on all processors with elements possessing these nodes. All elements, nodes, loads, boundary conditions, material properties, constraints, etc., are only defined on the processors for which they apply. The entire preprocessing software can be reasonably executed for large models on a workstation in only a matter of minutes.

The basic parallel approach is for each processor to perform an analysis on its own partition. These are performed as if they were separate analyses, except that contributions to the force vectors are sent to and from other processors for the shared nodes. At each time increment the basic parallel scheme first consists of creating a force vector (global for the partition) for the partitions on each processor from elemental contributions to the force vectors. Next, the forces belonging to redundant nodes are gathered into vectors and sent to the processors possessing duplicate definitions. The

partial force vectors are then received from the other processors and added to the global force vector on the current processor. Finally, the critical time increment and energies on each processor are sent to all processors in order to determine the global values. At this point, other boundary conditions are accommodated in the force vector, and the new accelerations, velocities, and displacements are determined. Using the new configuration, the process is then started all over again for a new time increment.

Interprocessor communication can be made entirely with MPI calls. Using the Catamount Virtual Node (CVN) capability on the Cray XT3 platform, each partition can be optionally placed on individual cores of their dual-core processors for further parallelism. Although each partition/core will have less than half the memory and cache of the full processor, this approach has the potential to reduce CPU times by half. Scalable I/O is performed by using separate files (input, output, restart, etc.) for each partition. In addition to the pre-analysis mesh partitioning tools, accompanying software was also developed for post-analysis assemblage of separate partition output files when necessary.

3. Numerical applications

The first application consists of a simulation of a reinforced concrete bridge deck atop a prestressed concrete girder assembly subjected to a truck bomb detonation. These types of simulations were used for vulnerability assessments and improved design and retrofit concepts and are typical of those performed with *ParaAble*. The deformed damaged finite element model, shown in Fig. 1, consists of approximately 3 million elements and nodes. For a spectrum of charge sizes, the BLASTX code (Britt *et al.* 2001) was used to predict pressure histories that were applied to the deck as radial varying concentric surface tractions. A three by three element mesh density was used
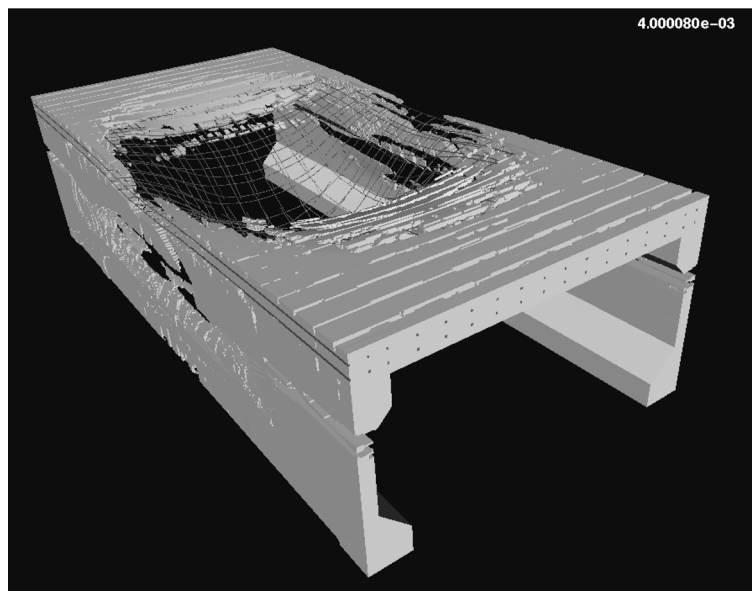

Fig. 1 Finite element simulation of a bridge deck and girder assembly subjected to a truck bomb detonation; placement of the bomb in between beams

for the cross-section of the reinforcing steel. The top boundary nodes were fixed in the lateral directions to represent the restraint of the rest of bridge deck. The analyses were executed on both single-core and dual-core Cray XT3 and on a quad-core Cray XT4 systems. The simulation used only about 1.5 CPU hours on 256 processors. The newer Cray XT4 is slightly slower per core than the XT3, but both platforms can reasonably perform these analyses on a moderate to medium number of processors. The fully damaged concrete elements, which are determined from solely post-processing the damage evolution data, are removed from the views depicted in Fig. 1. The performance of the analyses is depicted in Fig. 2, where both systems are seen to scale well for this application. Furthermore, the dual-core XT3 and quad-core XT4 processors performed the analyses in the same time as the single-core processors, but with only half and a fourth as many processors, respectively.
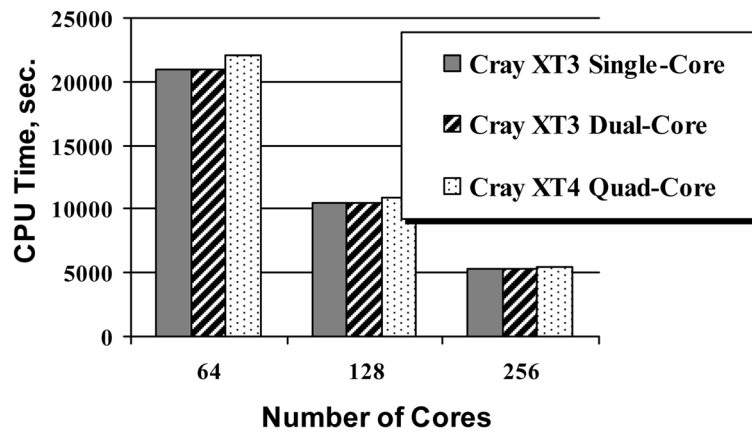

Fig. 2 Parallel performances of bridge deck blast analysis on Cray XT3 and XT4 platforms

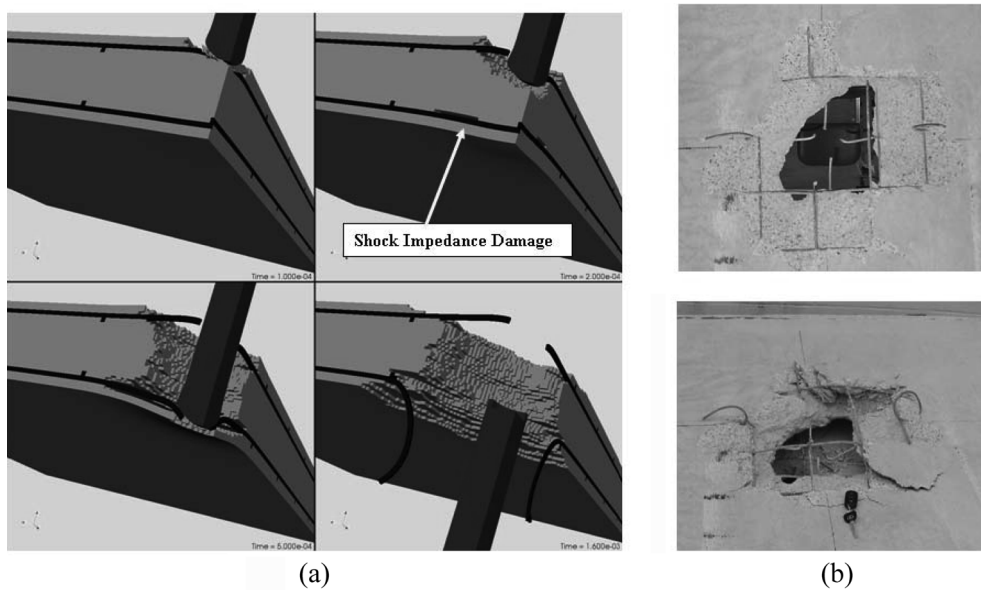(a)   (b)

Fig. 3 Finite element simulation of a wall penetration analysis

The second application consists of a simulation of a wall penetration by a projectile with circular shaped nose at approximately 800 m/s. The deformed damaged finite element model, shown in Fig. 3, consists of approximately 4.5 million elements and nodes. A three by three element mesh density was used for the cross-section of the reinforcing steel. An erosion value of 0.3 (a reasonable fracture value in steel) was used for the effective plastic strain in the rebar and the very large value of 80 was used for the erosion criterion of the concrete. Since the concrete model has strain softening, it will not produce artificial forces in a damaged material (they go to zero). Highly damaged materials, however, can significantly distort so as to terminate the analysis. Therefore, as a numerical trick, concrete elements are eroded with a very large damage value so as to minimize the inherent erosion error, which is also reduced by the very fine mesh. The analyses were made using PRONTO 3D and executed again on both single-core and dual-core Cray XT3 and on a quad-core Cray XT4 system. The simulation used less than 1.5 CPU hours on 1200 processors. The fully damaged (Damage = 4) concrete elements, which are determined from solely post-processing the damage evolution data, are removed from the views depicted in Fig. 3(a). This value of damage predicted by the modified Holmquist-Johnson-Cook damage model has been determined by experience whereby the concrete is essentially rubble or sand. Note that due to the impedance differences between steel and concrete, a significant level of damage occurs at the top of the rebar concrete interface as a result of the impact stress wave reaching that depth prior to the projectile. Note that the predicted rebar deformation is similar to the test shown in Fig. 3(b). The top layer is sheared through, but the bottom layer of rebar has more of a bending mode failure from the stress wave. The simulation was stopped shortly after the projectile exited the wall, but the bottom layer of rebar still have high velocities and should thus continue to bend significantly. The performance of the analyses are depicted in Fig. 4, where both systems are seen again to scale well for this application.

4. Conclusions

The microplane constitutive model, which is effective for predicting complex nonlinear behavior of reinforced concrete subjected to explosive detonations and high speed impact, was implemented
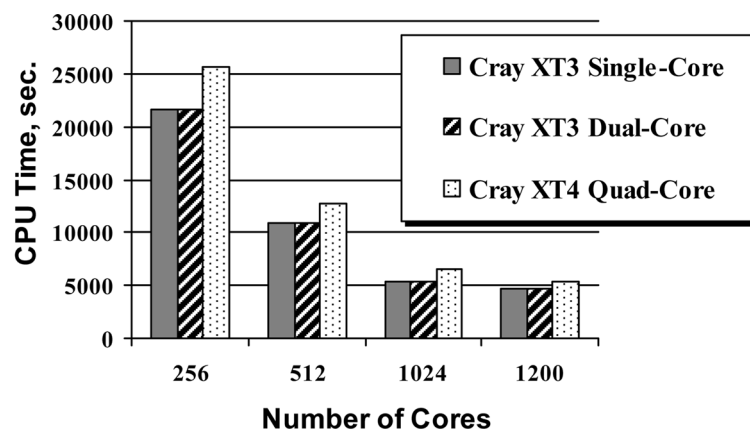

Fig. 4 Parallel performances of wall penetration analysis on Cray XT3 and XT4 platforms

into MPI based massively parallel finite element codes. A material weighting scheme was used to reduce parallel load imbalances for multiple material analyses. A modified Newton-Raphson method was developed to efficiently perform the polar decomposition of the deformation gradient tensor. Parallel computational capability was shown to be invaluable for large-scale applications of this type and that the expensive microplane constitutive model is computationally viable using parallel processing. Finally, it was shown that separate processes spawned on individual cores of dual and quad core processors provided nearly perfect speedup (double and quadruple) over use of a single core alone.

Acknowledgments

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