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Large-scale application of some modern CSM methodologies by parallel computation

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Abstract

In this paper, the authors demonstrate the significant benefits that High Performance Computing has provided for several large-scale applications of some modern Computational Structural Mechanics (CSM) methodologies. Large complex dynamic analyses, involving large strain/deformation and inelasticity, were reasonably performed by parallel processing with recent constitutive models and modern computational techniques. The predictions were made with finite element and mesh-free method software developed by the authors, using Message Passing Interface on CRAY T3E and IBM SP platforms. Excellent scalability on hundreds of processors was attained, which demonstrated the large-scale viability of the methodologies and greatly improved the authors' research and development productivity.

Keywords: Parallel computing; Finite elements; Meshfree methods; Reproducing kernel particle methods; Large deformation; Inelasticity; Explicit dynamics

1. Introduction

The advent of effective and reliable parallel computing platforms and the creation of extensive communication software standards (e.g. Message Passing Interface, MPI) have increased the use of High Performance Computing (HPC). Several popular Computational Structural Mechanics (CSM) codes (e.g. ParaDyn [1], PRONTO 3D [2], LS-DYNA) have incorporated coarse grain strategies for efficient computation on massively parallel processing systems, making large-scale analysis (e.g. millions of degrees of freedom) by traditional finite element methods feasible. In this paper, the authors demonstrate the significant benefits that HPC has provided for large-scale analyses with some modern CSM methodologies. Large complex analyses with advanced constitutive models and modern computational techniques can be reasonably performed by parallel processing, which can greatly improve the productivity of analysts and researchers. Application of three recent developments for large-scale dynamic problems involving large strain/deformation and inelasticity are presented.

The predictions are made with finite element and meshfree method software [3–5] developed by the authors using coarse grain parallelism and MPI calls. All analyses were conducted on CRAY T3E-1200 and IBM SP platforms at US Army Engineer Research and Development Center (ERDC) and the Army High Performance Computing Research Center (AHPCRC). The basic parallel implementations of each of the methods are similar, but have some important differences. Explicit time integration was used in all analyses. Using METIS [6], separate preprocessing partitioning software was created to distribute computations and minimize communications. Elements and integration points are uniquely defined on processors for finite element analysis and meshfree methods, respectively. Shared nodes/particles are duplicated on processors for data locality. Additional software was written to gather individual processor output files into a single database for postprocessing. To minimize communication costs, transmission of model partition boundary contributions to nodal/particle equations is overlapped with partition of interior computations by nonblocking MPI sends and receives.

2. Explosive detonation in a reinforced concrete wall

The development of a microplane concrete constitutive

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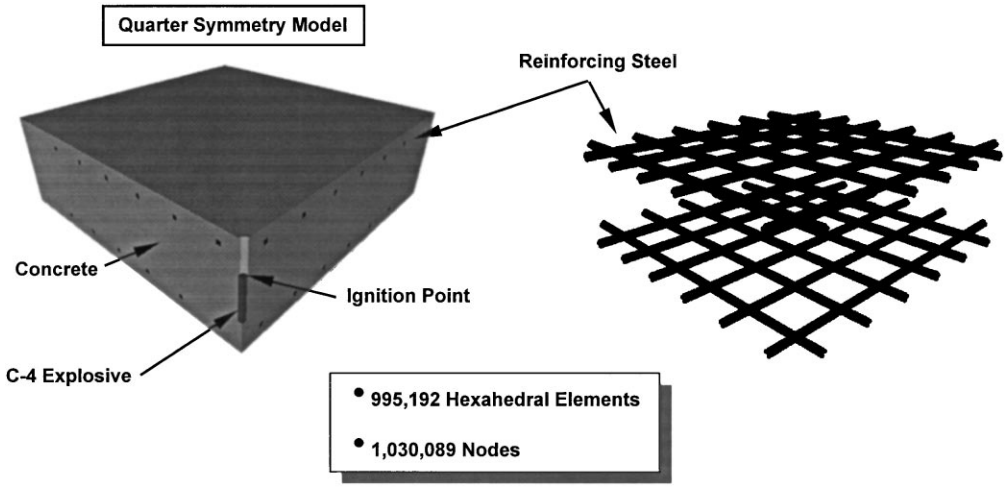

Fig. 1. Finite element model of an explosive detonation in reinforced concrete.

model has been a recent joint Northwestern/ERDC effort [7–10]. The main purpose for its development is to accurately predict concrete behavior under extreme conditions such as large strains and strain rates, large pressures, damage, and strain softening. The fundamental nature of the microplane model yields distinct advantages as data are more accurately fit with simpler experiments, and greater confidence is provided for general loading histories over common three-dimensional constitutive theories. Previous experiences have demonstrated its accuracy for other applications [11,12]. A major disadvantage is that the microplane model is computationally intensive (by more than an order of magnitude greater than typical elasto-plastic models). Leveraging parallel computing, however, its use with the large-scale finite element model was made reasonable.

The explosive detonation in a reinforced concrete wall is depicted by the finite element model in Fig. 1, which consists of 995,192 hexahedral elements and 103,089 nodes. The event was experimentally staged at ERDC. The C-4 explosive was placed in a cylindrical cavity at the center of the wall. Quarter symmetry was assumed for the calculation. The fully coupled explosive-structural analysis uses the microplane constitutive model for the concrete, an elasto-plastic model for the reinforcing steel, and a JWL equation-of-state model for the C-4 explosive. Ignition of the explosive is treated by a programmed-burn algorithm. These procedures were implemented into a parallel finite element code, ParaAble [3], developed by the authors. An example of the METIS partitioning for ParaAble is shown in Fig. 2. Because of the large differences in computational effort among the different constitutive models, the microplane model elements were assigned fourteen times the vertex weighting of the other elements for METIS.

The scalability was excellent, as the analysis required about 8, 4, and 2 CPU hours on 128, 256, and 512 processors (PEs), respectively, of the CRAY T3E-an analysis that

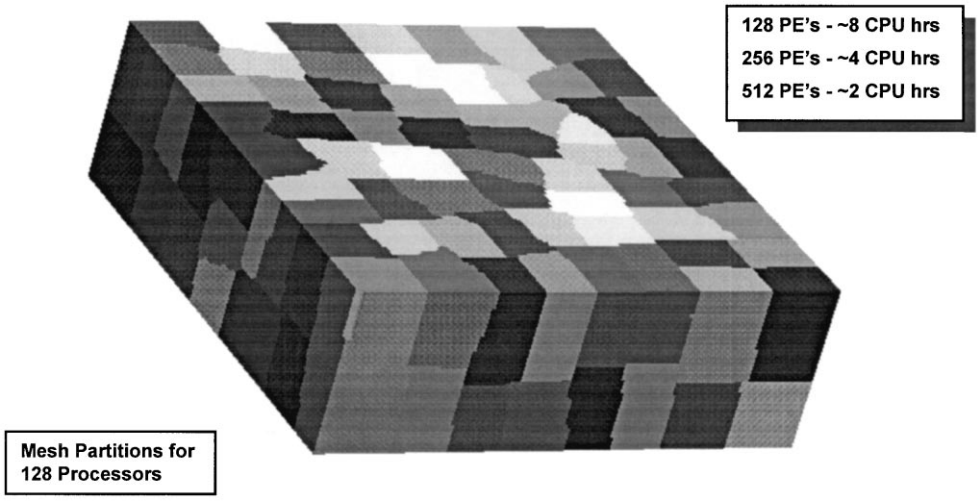

Fig. 2. Finite element mesh partitioning example for explosive detonation analysis.

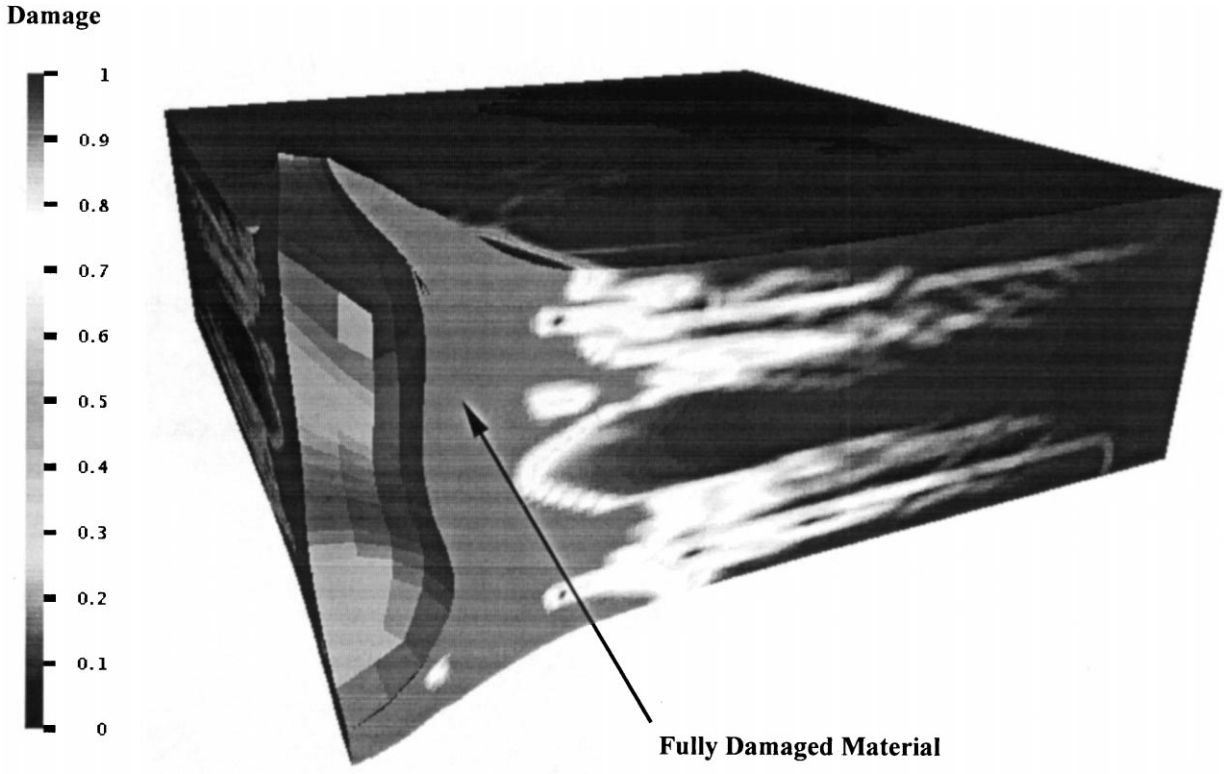

Fig. 3. Predicted shape and damage levels (1.0 = fully damaged) from explosive detonation simulation.

would take over 41 days on a single processor. Because of a communication–computation overlapping algorithm [3], communication time for partition interface data was insignificant, thus achieving the near perfect levels of parallel efficiency. Although the analysis was performed with less analysis time on 512 processors, the turn-around times for the 128- and 256-processor runs were much faster (overnight). The 512-processor run required the entire machine and had to be scheduled appropriately.

Visualization is important for such simulations. Examination of model validity (e.g. material definitions, boundary conditions, partitioning) is crucial. Evaluation of predicted quantities is also improved by visualization (see Figs. 3 and 4). Display of deformed shapes showing scalar quantities (e.g. strains, pressure, damage, etc.) as the explosive event evolves provides the analyst with a better understanding of the structural response in such cases. With the assistance of the scientific visualization staff at the ERDC MSRC, the large-scale visualization package, GMV [13], was linked with the ParaAble output database, ParaGraph. Despite the large model and frequent mirroring of the image for symmetry, typical display procedures (e.g. zoom, rotate, pan) were rendered in a matter of seconds with simple mouse click-and-drag operations.

3. Penetration analysis into three-dimensional targets

The second application type is for modeling the penetration problems like shown in Fig. 5. HPC is beneficial for such applications by making large detailed analyses feasible and improving turn-around times. Projectile component design may require highly refined models. In addition, the design of protective structures requires the assessment of many different attack scenarios (e.g. Fig. 5) and thus, many different analyses.

To achieve these goals, a finite element model of the projectile is coupled with advanced penetration resistance functions to represent the target. Penetration resistance of the target structure is provided by functions derived from principles of dynamic cavity expansion [14–16]. Instead of rigorously modeling the target with elements, the interaction uses a constitutive relation for the penetration resistance of the material and structure, which offers an alternative theory for penetration problems. General geometric descriptive capabilities and intricate searching features are included for the penetrator impacting complex, curvilinear targets composed of geologic and man-made materials such as soil, rock, and concrete [17]. This type of target modeling has recently been coupled with deformable finite element projectile models [18,19] and a parallel implementation placed into ParaAble [4]. The authors also recently collaborated with Lawrence Livermore staff to implement this capability into the DYNA3D/ParaDyn code [1].

During the parallel transient analysis, predicted finite element quantities (e.g. normal surface velocities) are used to compute a resistance pressure, which is then applied

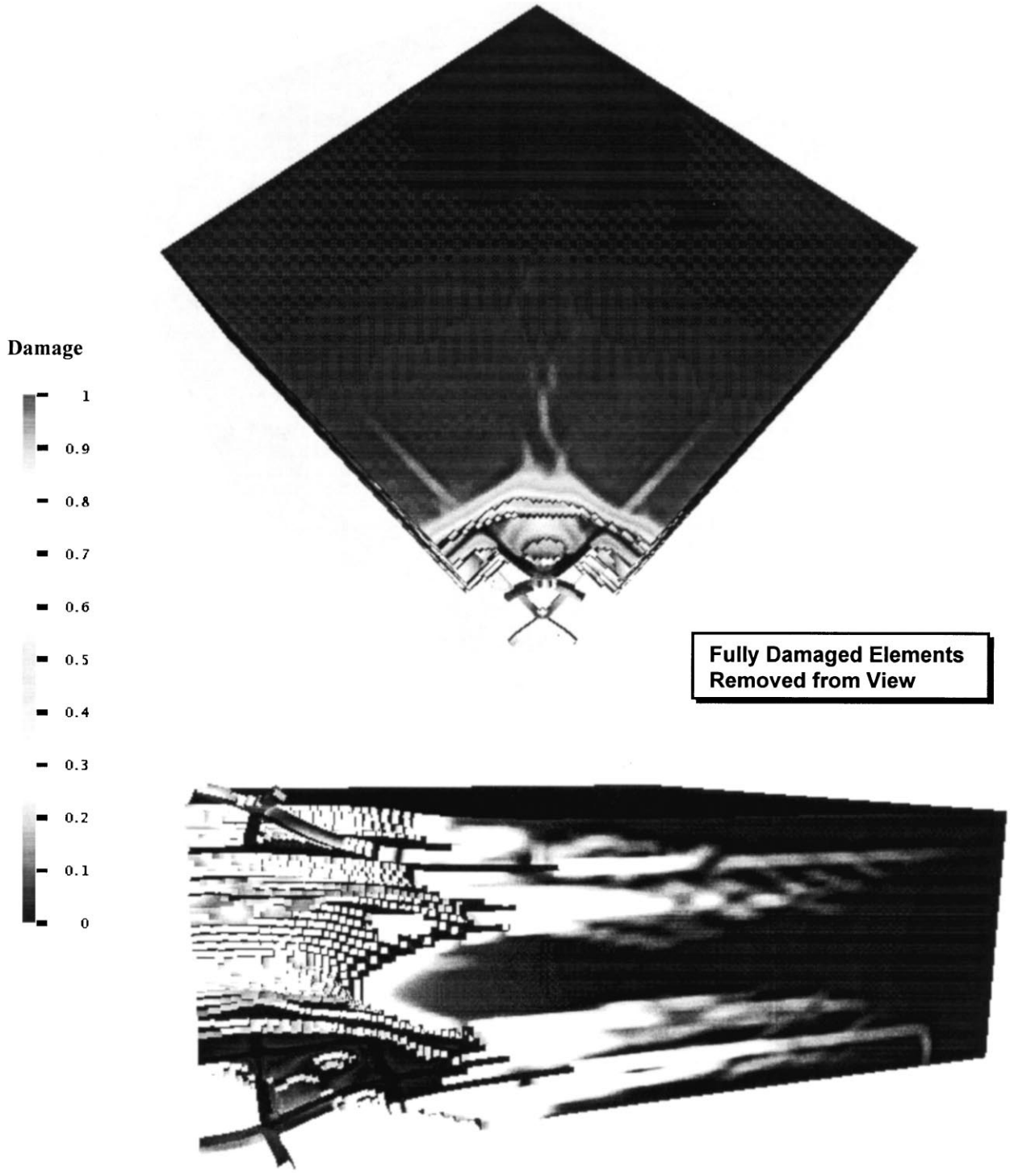

Fig. 4. Predicted shape and damage levels with fully damaged elements removed from explosive detonation simulation.

to the projectile finite element mesh. Therefore, the target is efficiently modeled without a mesh. In addition, the traction calculation is local to the processors with unique definitions of the projectile's outer elemental faces. The latest ParaAble and ParaDyn implementations require several scalar quantities to be communicated among processors with outer faces at each time increment. The quantities are used to properly terminate the execution (e.g. the projectile has stopped in the target) and to determine the need to apply an impact induced turning algorithm. Therefore, the penetration calculations are primarily local as the communications consist of only a few MPI reduction calls.

A model of about 95,000 eight-noded hexahedral elements was partitioned with METIS (see Fig. 6) and

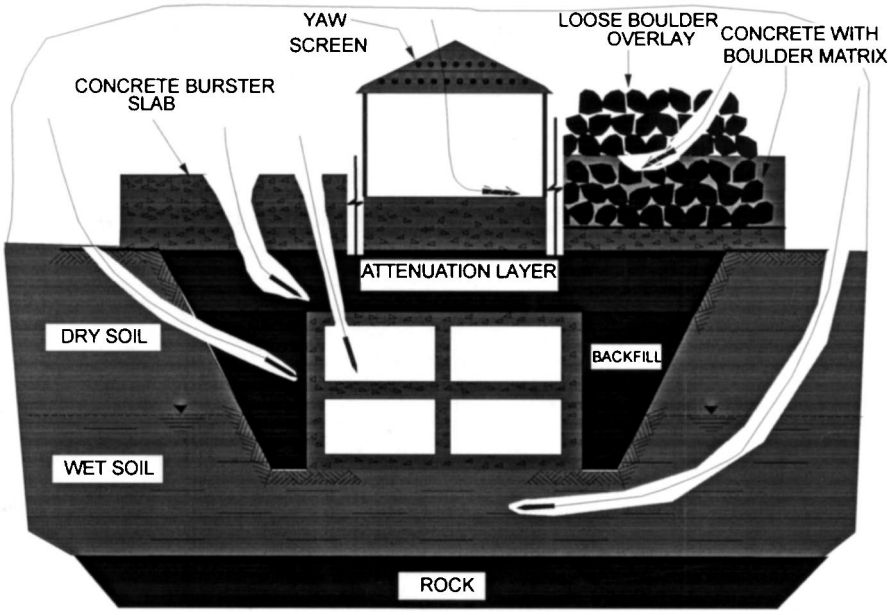

Fig. 5. Typical penetration events for protective structures.

analyzed for different numbers of processors on the two computing platforms. As depicted in Fig. 7, the parallel efficiency at 128 processors was 93 and 80% (with a 16 processor baseline) on the Cray T3E and IBM SP, respectively. An analysis that would require over four days on a single processor of the Cray T3E was performed on 512 processors in about 15 min. Analysis of the more complex and longer duration event shown in Fig. 8 was performed in less than five hours with 256 processors—an analysis that would take over 44 days on a single processor.

4. Meshfree prediction of three-dimensional shear bands

The last application type is a highly detailed analysis of failure events, like the three-dimensional tensile shear band development depicted in Figs. 9 and 10. The predictions were made with a meshfree Reproducing Kernel Particle Method (RKPM) code [5] using a viscoplastic material law. RKPM has distinct advantages to capture such detailed failure mechanisms over other methods, but is also typically more computationally intensive.

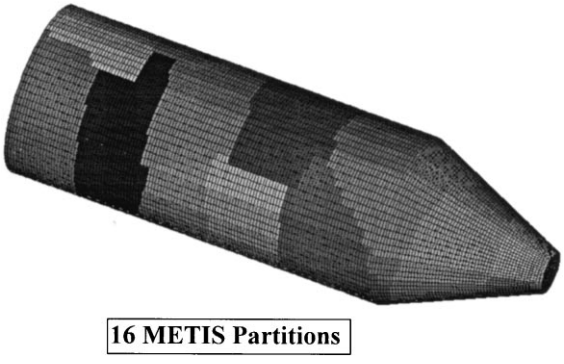

Fig. 6. METIS mesh partitioning of a projectile finite element mesh (~95,000 hexahedral elements).

RKPM formulations use a kernel approximation to the displacements, whereby the kernel function is typically taken as the Smoothed Particle Hydrodynamic (SPH) [20] interpolation function that is modified by a correction function to accommodate the presence of boundaries of finite domains in order to satisfy consistency (reproducing) conditions. This produces a nonlocal interpolation in terms of an arbitrary number of particle values within the subregion of influence. The size and shape of the influence region can be general and can vary within the domain and between different analyses. The support nodes are determined by searching within each individual support zone for any desired point (e.g. node, integration point, etc.). A Lagrangian formulation is used, so that the search for neighboring support nodes and the calculation of interpolation function are only done once at the beginning of the analysis. Detailed descriptions of RKPM procedures can be found, for example, in Refs. [21–25].

Separate pre-analysis software was created to partition any general unstructured RKPM model. Similar to explicit finite element codes [1–3], the partitioning is made with regard to the numerical integration of the internal virtual work terms, since it involves more computational effort than the lumped mass equation solving. Therefore, integration points are distributed to processors and nodes (particles) are shared by integration points on different processors. In contrast to finite elements, the amount of computations will vary among integration points, since each may contribute to a different number of particles/nodes. Despite the lumped mass matrix associated with the explicit temporal integration, systems of simultaneous

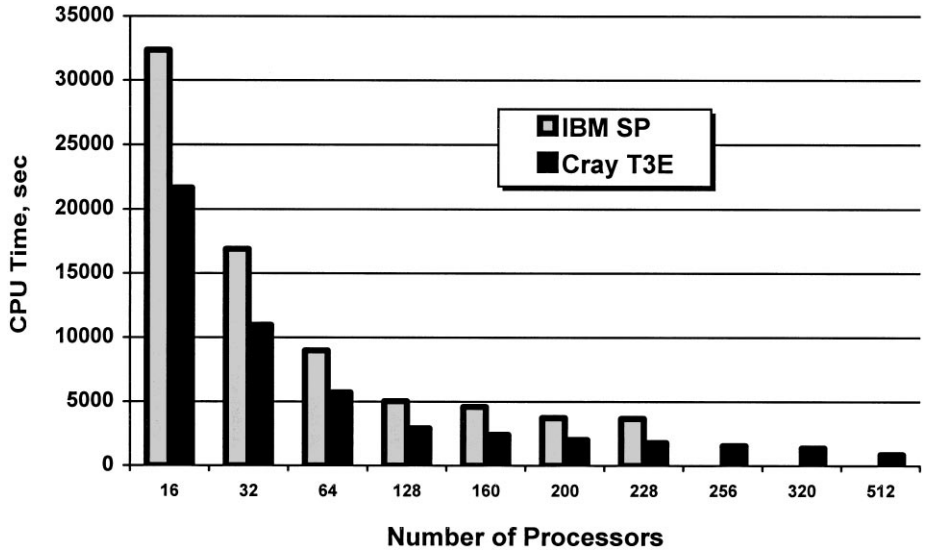

Fig. 7. Parallel performance of penetration analysis into semi-infinite concrete medium; (~95,000 hexahedral elements, ~128,000 time increments).

equations must usually be solved during each time increment to enforce essential boundary conditions. The nonlocal nature of the RKPM interpolant produces a coupling between nodes, which requires additional parallel computational considerations for essential boundary condition enforcement over finite element applications [5].

A hybrid geometric graph-based scheme is used to partition the integration points. The support node list for each RKPM integration point is used to create the graph edges by identifying integration points with common support nodes. For the graph, vertex weighting is applied according to the number of nodes to which an integration point contributes. All graph edge weights are defined to be the same. RKPM integration points typically contribute to many more nodes than those of similar finite element models do. Thus, RKPM graphs can be very large with many edges. To reduce the number of edges, a reduced support size is used solely for graph creation. Therefore, only the nearest neighbors (edge members) of each integration point (vertex) were included in the graph. The graph is then input into METIS as usual. Experience has shown that this produces effective partitions and it greatly reduces the computational effort involved in the partitioning.

For these problems, detailed post-bifurcation formations of three-dimensional shear bands are seen in the numerical simulation, which can provide better insight into this failure phenomenon. The first specimen is $2 \times 0.2\ \text{mm}^2$ with a length of 4 mm. The RKPM model uses 16,605 nodes and the undeformed and deformed configurations are shown in Fig. 9. The analysis was performed in about 45 min on 128 processors of the Cray T3E-1200, instead of over 100 h on a single processor.

The second specimen has cross-section dimensions of $2 \times 2\ \text{mm}^2$ and a length of 4 mm. The RKPM model uses 18,081 nodes and 128,000 integration points, shown in Fig. 10. The original graph of the model averaged approximately

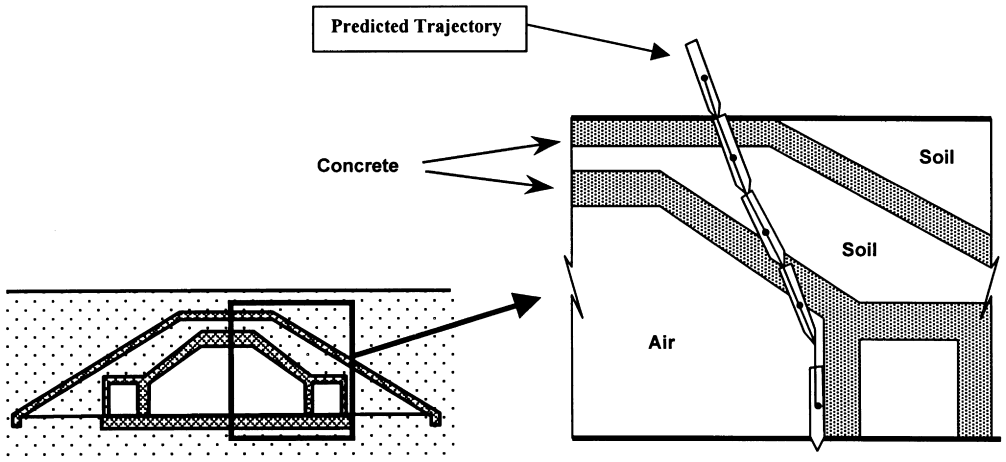

Fig. 8. Projectile penetration into a buried protective structure.

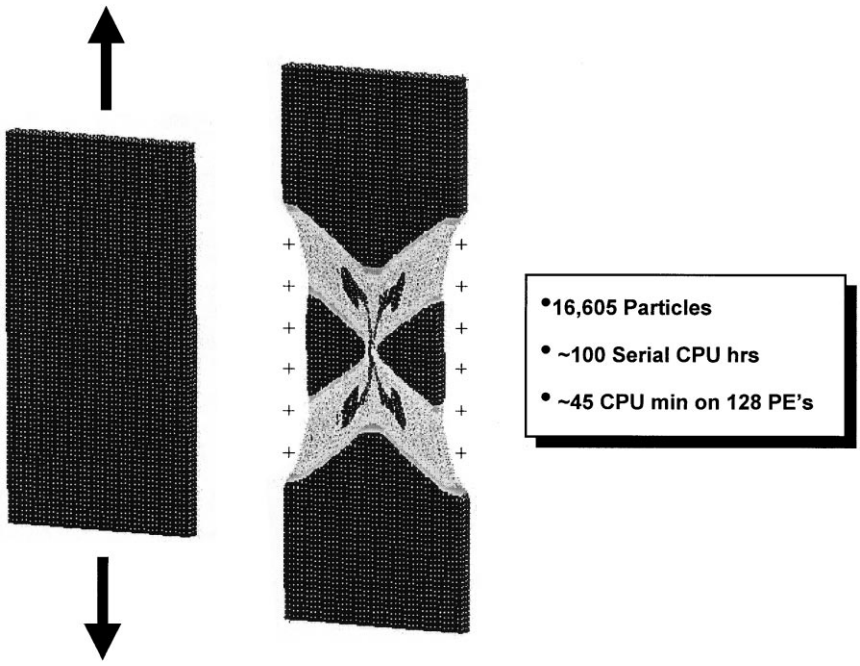

Fig. 9. Predicted three-dimensional tensile shear band development by meshfree RKPM analysis (shown by plotted effective plastic strain).

700 edges per vertex. Using the reduction scheme, the graph was reduced to about 50 edges per vertex. A plot of the deformed shape for the RKPM model is also shown in Fig. 10. For this specimen, a detailed transition process from localization necking to diffuse necking is seen in the numerical simulation. For an 8×10^{-5} s simulation, the analysis required about 400 CPU seconds on 256 processors of the Cray T3E-1200. The parallel performance is given in Fig. 11 for the 10,000 time increment analysis. For economical reasons, this scalability study was performed with no less than four processors. The speedup is significant for this model. The analysis on 256 processors was about 47 times faster than the one on four processors.

5. Conluding remarks

Parallel computational capability was shown to be invaluable for large-scale application of several modern developments in computational structural mechanics. Analyses that would require over 1000 serial computing hours were performed in only a few hours on large CRAY T3E and

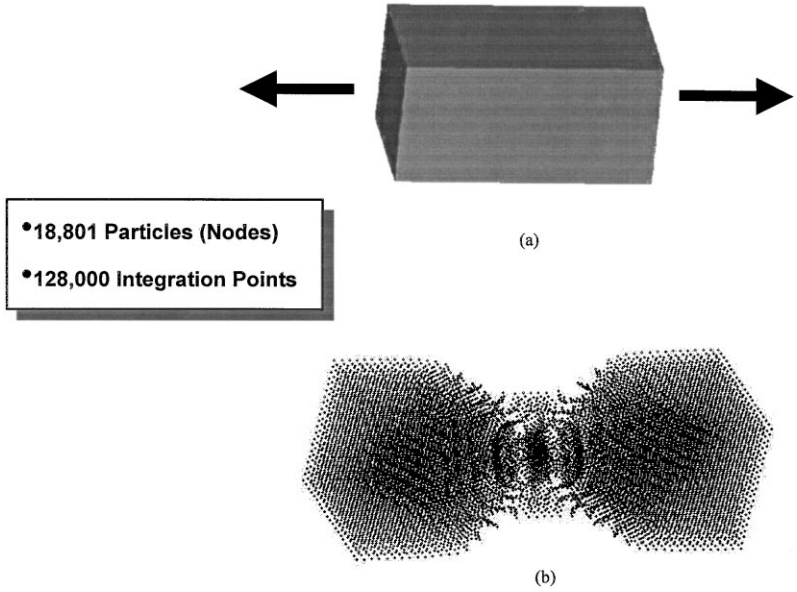

Fig. 10. RKPM model for the three-dimensional tensile shear band development: (a) undeformed shape; (b) deformed particle configuration.

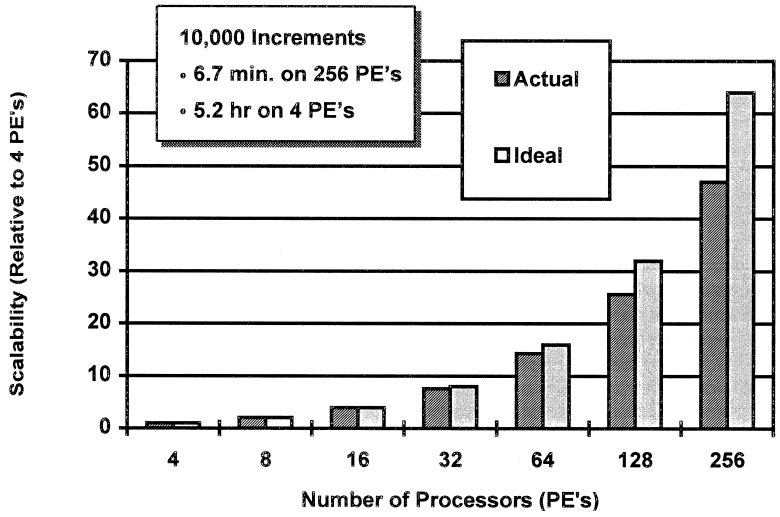

Fig. 11. Parallel performance on a Cray T3E-1200 of RKPM for the three-dimensional tensile shear band development.

IBM SP platforms. Although the methodologies possess some distinct benefits for complex modeling of nonlinear structural behavior, the computational expense of these methods may preclude their frequent use for large applications on serial computers. Leveraging high performance computing, however, the viability of these methods has been greatly extended.

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References

[1] Hoover CG, DeGroot AJ, Maltby JD, Procassini RJ. ParaDyn—DYNA3D for massively parallel computers. Engineering, Research, Development and Technology FY94, Lawrence Livermore National Laboratory, UCRL 53868-94, 1995.

[2] Plimpton S, Attaway S, Hendrickson B, Swegle J, Vaughan C, Gardner D. Transient dynamics simulations: parallel algorithms for contact detection and smoothed particle hydrodynamics. In: Proceedings of SuperComputing 96, Pittsburgh, PA, 1996.

[3] Danielson KT, Namburu RR. Nonlinear dynamic finite element analysis on parallel computers using FORTRAN 90 and MPI. Adv Engng Software 1998;29(3-6):179–86.

[4] Danielson KT, Adley MD. A meshless treatment of three-dimensional penetrator targets for parallel computation. Comput Mech 1999 (in press).

[5] Danielson KT, Hao S, Liu WK, Uras RA, Li S. Parallel computation of meshless methods for explicit dynamic analysis. Int J Numer Meth Engng 1999 (in press).

[6] Karypis G, Kumar V. A fast and high quality multilevel scheme for partitioning irregular graphs. Technical Report TR 95-035, Department of Computer Science, University of Minnesota, 1995.

[7] Bazant ZP, Xiang Y, Prat PC. Microplane model for concrete. I: stress–strain boundaries and finite strain. J Engng Mech 1996;122(3):245–54.

[8] Bazant ZP, Xiang Y, Adley MD, Prat PC, Akers SA. Microplane model for concrete II: data delocation and verification. J Engng Mech 1996;122(3):255–62.

[9] Bazant ZP, Caner FC, Adley MD, Akers SA. Incorporation of rate effects of fracturing and creep into microplane model for concrete dynamics. Submitted for publication.

[10] Bazant ZP, Adley MD, Carol I, Jirasek M, Akers SA, Cargile JD, Rohani B, Caner FC. Large-strain generalization of microplane model for concrete. Submitted for publication.

[11] Adley MD, Cargile JD, Akers SA, Rohani B. Numerical simulation of projectile penetration into concrete. In: Proceedings of the 14th US Army Symposium on Solid Mechanics, Myrtle Beach, SC, October 16–18, 1996. p. 189–96.

[12] Akers SA, Windham JE. Structure medium interaction calculations of DIPOLE FAÇADE 8. In: Proceedings of the 14th US Army Symposium on Solid Mechanics, Myrtle Beach, SC, October 16–18, 1996. p. 481–8.

[13] Ortega FA. GMV: General Mesh Viewer users Manual, Version 1.8. Los Alamos National Laboratory, LAUR 95-2986, 1995.

[14] Bernard RS, Creighton DC. Projectile penetration in soil and rock: analysis for non-normal impact. Technical Report SL-79-15, US Army Engineer Waterways Experiment Station, Vicksburg, MS, 1979.

[15] Forrestal MJ, Norwood FR, Longcope DB. Penetration into targets described by locked hydrostats and shear strength. J Appl Mech 1981;55(4):275–9.

[16] Forrestal MJ, Altman BS, Cargile JD, Hanchak SJ. An empirical equation for penetration depth of ogive-nose projectiles into concrete targets. Int J Impact Engng 1994;15(4):395–405.

[17] Adley MD, Danielson KT, Rohani B, Moxley RE. Coupling penetration resistance functions and finite elements for deformable projectile impact analysis. Submitted for publication.

[18] Adley MD. PENCO2D/ABAQUS: a simply coupled penetration

trajectory/structural dynamics model for deformable projectiles. Technical Report SL-92-26, US Army Engineer Waterways Experiment Station, Vicksburg, MS, 1991.

[19] Warren TL, Tabbara MR. Spherical cavity-expansion forcing function in PRONTO 3D for applications to penetration problems. SAND97-1174, Sandia National Laboratories, Albuquerque, NM, 1997.

[20] Lucy LB. A numerical approach to the testing of the fission hypothesis. The Astronomical Journal 1977;82(12):1013–24.

[21] Liu WK, Jun S, Li S, Adee J, Belytschko T. Reproducing kernel particle methods for structural dynamics. Int J Numer Meth Engng 1995;38:1655–79.

[22] Liu WK, Chen Y, Uras RA, Chang CT. Generalized multiple scale reproducing kernel particle methods. Comput Meth Appl Mech Engng 1996;139:91–158.

[23] Jun S, Liu WK, Belytschko T. Explicit reproducing kernel particle methods for large deformation problems. Int J Numer Meth Engng 1998;41:137–66.

[24] Chen JS, Pan C, Wu CT, Liu WK. Reproducing kernel particle methods for large deformation analysis of nonlinear structures. Comput Meth Appl Mech Engng 1996;139:195–228.

[25] Günther FC, Liu WK. Implementation of boundary conditions for meshless methods. Comput Meth Appl Mech Engng 1998;163(1-4):205–30.