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14. ABSTRACT
This project began July 1, 2002 and will expire on November 30, 2004.
During the last two years, the primary focus of this effort has been the creation of a reliable computational capability for the solution of elasto-dynamic moving boundary problems. Specificlly, the PI, along with a student: 1. has formulated a space-time discontinuous Galerkin finite element (DGFEM) formulation that has been shown to be unconditionally stable and capable of adaptive mesh refinement; 2. applied this formulation to the solution of various model problems in isothermal elasto-dynamics as well as isothermal elasto-dynamic phase transition; 3. begun the extension of the DGFEM formultion to fully coupled thermo-elastic problems along withpreliminary numerical results; and 4. begun the creation of a numerical procedure for the solution of double integral equations deriving from the reformulation of fully transient Mode III dynamic fracture problems in thermoelastic media with cohesive zones.

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ANNUAL AND FINAL TECHNICAL REPORT

November 2004

DYNAMIC FRACTURE IN TEMPERATURE SENSITIVE MATERIALS WITH COHESIVE ZONES: A DISCONTINUOUS GALERKIN APPROACH

GRANT NO. F49620-02-1-0318

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1. Objectives

This project intends to expand the understanding of the role of temperature in controlling the dynamic failure behavior of advanced materials subject to combined thermo-mechanical loading. These objectives will be achieved by improving the continuum-based modeling of the fracture properties of materials in conjunction with the formulation and development of a corresponding numerical approach for the solution of the resulting governing equations.

The goal of the proposed modeling effort is the inclusion of temperature dependence in the description of the fracture behavior of the material. In addition to modeling the bulk material as a fully coupled linear thermo-elastic solid, this goal will be achieved by using rate and temperature dependent cohesive zone (CZ) models to account for the highly localized, nonlinear, and softening behavior of the material ahead of the propagating crack. In this project, the cohesive stresses will be assumed to be physically-based constitutive functions of the opening displacement, opening displacement rate and temperature. Finally, the CZ will be assumed to fail in two basic ways: (*i*) by achieving a critical crack opening displacement; and/or (*ii*) by experiencing a critical value of cohesive stress. Both the critical crack opening displacement and the critical cohesive stress will be assumed to be functions of temperature.

The primary objective of the proposed numerical development is the formulation of a high accuracy and unconditionally stable solution scheme for the combined parabolic/hyperbolic problem describing dynamic fracture in a linear thermo-elastic solid. Adaptivity will be a primary feature of the proposed numerical scheme as it will be is crucial for the accurate quantification of the microscopic features that are nucleated during propagation as these features are a means of comparison between theory and experiments. Said numerical approach will be based on the discontinuous Galerkin finite element method (DG FEM). The DG FEM has been shown to be extremely effective in the solution of both parabolic and hyperbolic problems in the presence of moving discontinuities.

To provide an alternative strategy for the assessment of the fracture properties resulting from a given choice of the CZ constitutive law, and to provide a tool to test the efficacy of the proposed DG FEM development, the proposed research also includes the use of a different numerical technique previously developed by the proposer and a collaborator. This technique, based on the notions of Neumann-to-Dirichlet map and product integration, is highly accurate but only applicable to problems with idealized geometry (e.g., dynamic propagation of a semi-infinite crack along a planar bi-material interface). The aforementioned technique will be expanded and refined for the purpose of creating an effective benchmarking tool for the proposed DG FEM.

2. Status of Effort and Accomplishments

This project begub July 1, 2002 and will expire on November 30, 2004.

During the last two years, the primary focus of the this effort has been the creation of a reliable computational capability for the solution of elasto-dynamic moving boundary problems. Specifically, the PI, along with a student,

1. has formulated a space-time discontinuous Galerkin finite element (DGFEM) formulation that has been shown to be unconditionally stable and capable of adaptive mesh refinement;
2. applied this formulation to the solution of various model problems in isothermal elasto-dynamics as well as isothermal elasto-dynamic phase transition;
3. begun the extension of the DGFEM formulation to fully coupled thermo-elastic problems along with preliminary numerical results; and
4. begun the creation of a numerical procedure for the solution of double integral equations deriving from the reformulation of fully transient Mode III dynamic fracture problems in thermoelastic media with cohesive zones.

2.1. DGFEM: early developments

The choice of a discontinuous Galerkin method for the solution of dynamic fracture problems was motivated by several reasons:

(a) The fragmentation processes occurring ahead of a running crack tip are intrinsically discontinuous in both space and time. However, second order accurate numerical methods with no artificial viscosity are likely to predict severe high frequency spurious oscillations when the boundary data are non-smooth. Clearly, one could resort to methods which introduce *artificial viscosities* (see, for example, the discussion on the β-Newmark's method by Hughes, 1987 or Johnson, 1987). However, this practice is questionable in the present context due to the fact that the CZ constitutive equations are rate dependent and it would be extremely complicated to distinguish the rate effects due to the physical behavior of the near crack tip environment from the behavior induced by the choice of the numerical solution scheme. In addition, one must remember that high frequency crack tip velocity oscillations are one of the *physical* phenomena that one wishes to be able to predict. The PI intended to formulate a solution scheme free from the suspicion that high frequency oscillations are induced by the solution strategy itself. Furthermore, it should be remembered that no rigorous studies have been done which discuss error estimation in dynamic fracture problems and therefore it is very difficult to assess the stability/accuracy properties of current solution schemes. By contrast, as shown by Hughes and Hulbert (1988), Hulbert and Hughes (1990), and Johnson (1993) (see also French, 1993; Hulbert, 1992a,c) second order hyperbolic problems can be given a DG formulation which leads to unconditionally stable and high accuracy algorithms *without* the addition of artificial viscosities. In addition, the space-time formulation of the problem makes it possible for one to conduct a very transparent error analysis.

(b) A DGFEM in dynamic fracture requires that the meshing of the space-time domain be *dynamic*, that is, that the FEM grid be generated along with the rest of the computation. This is crucial if one wants to avoid the *pre-meshing* (that is, the *a priori* assigning) of the crack path as it is done in any gradual node release algorithm, the latter being by far the most used computational strategy in dynamic fracture to date.

(c) The third important reason for proposing the use of a DGFEM approach is that the present proposal intends to explore the fully-coupled thermo-mechanical dynamic fracture problem. This problem is notoriously difficult to confront numerically due to the fact that semi-discrete FEM formulations (i.e., FEM schemes which discretize the space domain only) of the heat equation lead to *stiff* initial value problems for the time component of the problem. In the context of parabolic problems (such as the heat equation) the advantage of the use of DGFEM has long been demonstrated.* Therefore the use of a DGFEM approach to the problem of interest herein seems rather "natural" since one will be able to construct solutions schemes for which error estimates can be assessed in a rational and unified way for both the mechanical and thermal parts of the problem, thus leading to the possibility of adaptive and parallelizable solution schemes.

As part of the work done in the last 2 years (although some of the work was begun before August 1, 2002, as part of the Ph.D. thesis of Hao Huang, one of the PI's students), the PI revisited the DGFEM formulation proposed Hughes and Hulbert (1988); Hulbert and Hughes (1990) and adapted it to the study of moving boundary problems in isothermal elasto-dynamics. This extension has been reported in Huang and Costanzo (2002), in which basic properties of the extended formulation were discussed and along with a number of results concerning a 1D model problem with dynamic solid/solid phase transition as depicted in Fig. 1,. The motion considered is that of a linear elastic

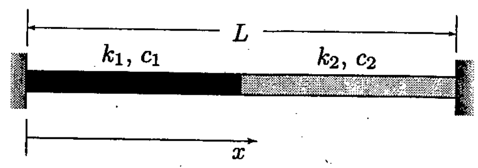

Figure 1: Bi-material bar in tension fixed at both ends.

1D bi-material bar subjected to an initial stretch. The two halves of the bar are given the same density ρ_0 but different stiffness, k_1 and k_2, respectively, with $k_1 < k_2$, and correspondingly different wave speeds, c_1 and c_2, with $c_1 < c_2$. At time $t = 0$ the interface separating the two halves of the bar is made to move in a prescribed manner such that the less stiff part of the bar grows at the expense of the stiffer part. Said motion is therefore analogical to a damage or fracture process since it causes a weakening of the overall structure. The results reported below are presented in non-dimensional form. In particular, the quantities reported in the graphs have been non-dimensionalized as follows:

$$x^* = \frac{x}{L}, \quad t^* = \frac{c_2}{L}t, \quad n^* = \frac{1}{k_2}n, \tag{1}$$

*There is vast literature on the use of discontinuous Galerkin FEM in the solution of linear and nonlinear parabolic problems and its review is outside the scope of this proposal. Here are a few references which focus on the heat equation: Cockburn and Shu (1998); Eriksson and Johnson (1991, 1995); Eriksson et al. (1985); French (1998, 1999); Hulbert (1992b); Johnson (1987); Makridakis and Babuska (1997); Schotzau and Schwab (2000); Shaw and Whiteman (1996, 2000).

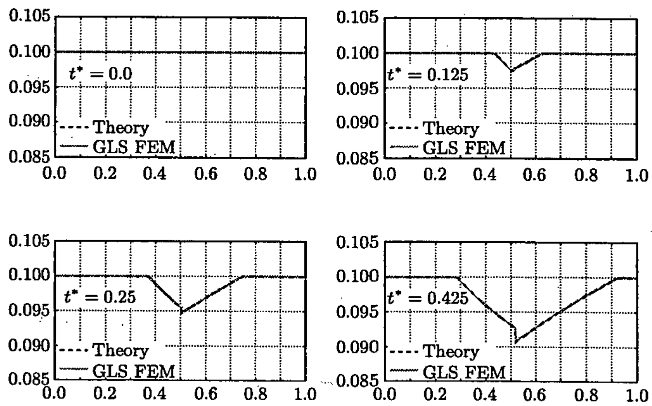

Figure 3: Distribution of the axial internal force at various time instants for the case of the interface traveling at a constant acceleration α. Here $(\alpha L)/c_2^2 = 0.2$, $c_1/c_2 = 0.5$, $k_1/k_2 = 0.25$, and $n^*(t = 0) = 0.1$. Every plot has the same horizontal and vertical axes. The horizontal axis represents the non-dimensional position x^* along the bar, while the vertical axis represents the non-dimensional axial force n^*. The space time domain was discretized using 400 bi-quadratic isoparametric space-time elements.

where x and x^* denote the position and the non-dimensional position along the bar, respectively, t and t^* denote time and non-dimensional time, respectively, n and n^* denote the bar's internal axial force and its non-dimensional counterpart, respectively. The first set of results concerns the case of an interface traveling along a prescribed trajectory. Two cases are reported here: at a constant speed case and a constant acceleration case reported in Fig. 2 and Fig. 3, respectively. For the constant velocity case, it should be noted that the growth process modeled is *discontinuous* in two distinct ways. Firstly, the process is discontinuous because the motion of the interface is such that the interface simply *jumps* from rest a steady state regime. Secondly, the process is discontinuous in that the internal axial force in the bar suffers jumps across the propagating acoustic wave fronts. Despite these discontinuity sources the calculated results are remarkably close to those given by the exact solution, especially in view of the fact that the quantity n^* is obtained from the derivative of the primary unknown, the latter being the axial displacement of the bar.

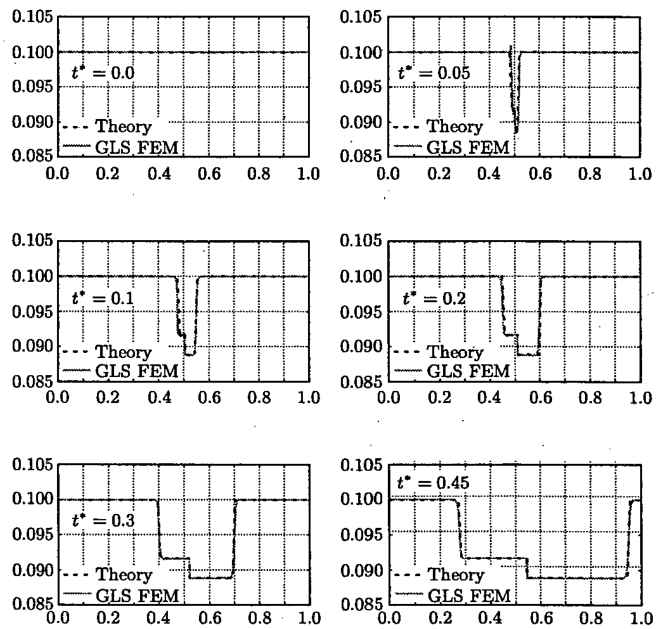

Figure 2: Distribution of the axial internal force (stress) at various time instants for the case of the interface traveling at a constant speed v, with $v/c_2 = 0.1$. $c_1/c_2 = 0.5$, $k_1/k_2 = 0.25$, and $n^*(t = 0) = 0.1$. Every plot has the same horizontal and vertical axes. The horizontal axis represents the non-dimensional position x^* along the bar, while the vertical axis represents the non-dimensional axial force n^*. Each space-time slab was discretized using 400 bi-quadratic isoparametric space-time elements.

To quantify the accuracy of the method, convergence rates for the two cases reported herein have been explicitly computed along with the convergence rate for a problem yielding a smooth solution. In particular, as suggested in Hulbert and Hughes (1990), the solution for the case of a homogeneous bar fixed at both ends with a quiescent past is subjected to a given initial displacement field coinciding with the displacement distribution given by the first harmonic of the system. For this test case the convergence rate is 3, as theoretically predicted by Hulbert and Hughes (1990). Clearly, the convergence rate is negatively affected by the loss of smoothness in the solution of the moving interface problem. However, as Fig. 4 indicates, the convergence rates for the moving interface problems discussed herein are still quite satisfactory.

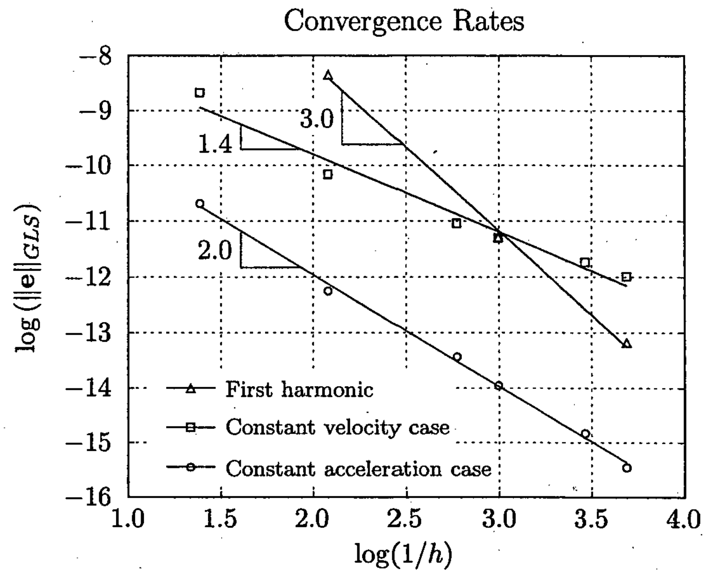

Figure 4: Convergence rates for a problem with smooth solution along with those of the solid-solid phase transition problems preciously discussed.

The proposed DGFEM has also been tested by the PI in the solution of a few fracture model problems with excellent results, which have been reported in Huang and Costanzo (2004). Problems with sharp cracks as well as with a Dugdale zones have been considered. For the purpose of comparison, we report the energy release rate computation for this problem provided by Nakamura et al. (1985) using a nodal relaxation scheme. The loading and geometry for this example are displayed in Fig. 5. The loading is applied "suddenly" at the top and bottom edge of the plate. The crack is allowed to propagate with a prescribed motion. In particular, the crack is kept stationary for a prescribed amount of time after which the crack is made to advance in with a constant speed. Because of this, the problem solution is expected to reflect the discontinuous nature of the crack propagation process. Clearly, the problem is somewhat artificial in that the crack tip motion is a *given* of the problem. However, the problem is mathematically well posed and it is interesting to demonstrate the effectiveness of the proposed DGFEM in dealing with discontinuous loading. For the time interval considered, in which the crack tip is not hit by reflected waves, the problem affords a closed-form solution provided by Freund (1990). The nondimensional energy release rates calculated by the formulation developed by the PI, by the semidiscrete method used by Nakamura et al. (1985), as well as by the exact solution are shown in Fig. 6 for $v_c = 0.4c_s$ and Fig. 7 for $v_c = 0.6c_s$, v_c being elastic shear wave speed. It can be observed that the numerical results calculated by the DGFEM formulation is not only closer to the closed-form solution, but, most importantly, it captures the energy release rate jump discontinuity caused by the onset of the crack motion.

2.2. DGFEM: most recent developments

The result discussed above were obtained with a FORTRAN code developed from scratch. The code in question was rather crude and not easily expandable to include a good automatic mesh

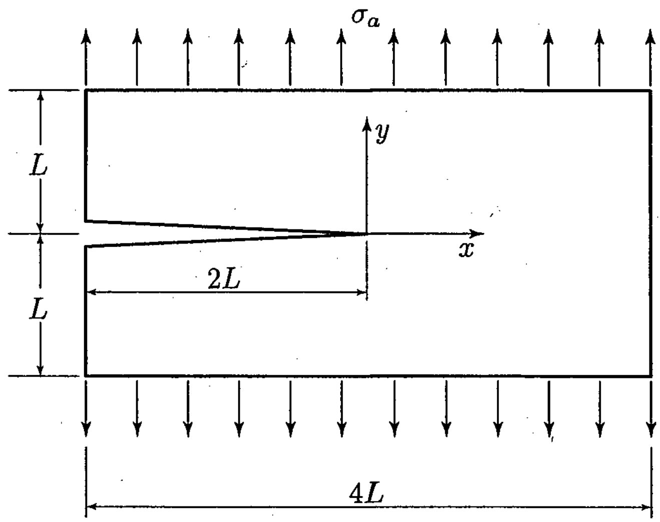

Figure 5: The geometry, crack position and boundary conditions of for the results in Figs.6 and 7.

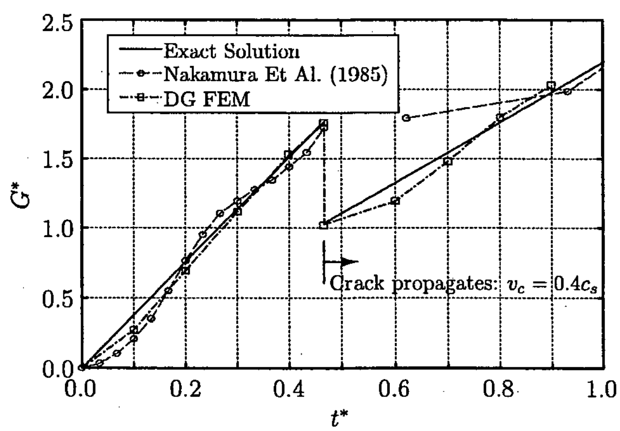

Figure 6: Energy release rate estimates for $v_c = 0.4\, c_s$ and step size $\Delta t = 1.0\, L/c_1$.

refinement capability. Furthermore, the PI intended to avoid the non-trivial tack of creating an efficient program with error estimation and adaptivity. Therefore, the PI, along with Scott T. Miller, a Master's student of his, decided to undergo a complete restructuring of the numerical capability discussed earlier, so as to rely on a very well established FEM library. After some searching, it was decided that any new FEM development was to be based on the "deal.II" FEM library developed and maintained by W. Bangerth, G. Kanschat, and R. Hartmann Bangerth, 2002; Hartmann and Houston, 2002a,b.* deal.II is a C++ program library specifically designed to support adaptive finite elements and error estimation. It uses state-of-the-art programming techniques of the C++ programming language so as to allow one to use complex data structures and algorithms required for adaptivity from 1D through 4D. As it can be learned from the supporting literature on deal.ii,

deal.II emerged from work at the Numerical Methods Group of the University of Heidel-

*For detailed information concerning the deal.II library see <www.dealii.org>.

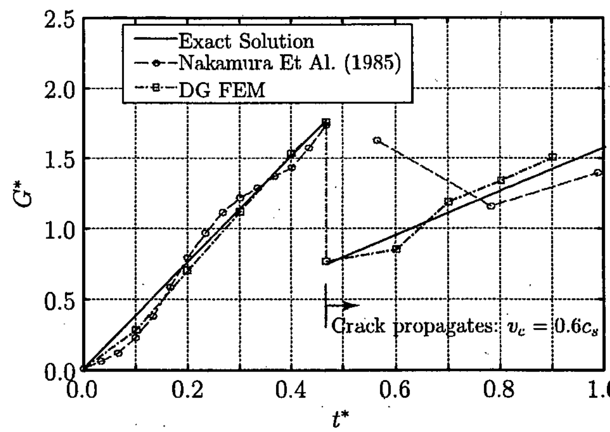

Figure 7: Energy release rate estimates for $v_c = 0.6\, c_s$ and step size $\Delta t = 1.0\, L/c_1$.

> berg, Germany, which is at the forefront of adaptive finite element methods and error estimators. It is presently developed in Heidelberg, at the Institute of Aerodynamics and Flow Technology of the German Aerospace Center (DLR) in Braunschweig, and at the Institute for Computational Engineering and Sciences (ICES, formerly TICAM) in Austin, Texas. It is used in several large research projects around the world. deal.II presently has about 220,000 lines of code and has several hundred users around the world.

Among other features, the deal.ii library is extremely thoroughly documented and it provides fast algorithms that enable you to solve problems with up to several millions of degrees of freedom, a complete stand-alone linear algebra library (including sparse matrices, vectors, Krylov subspace solvers, support for blocked systems, and interface to other packages such as PETSc and METIS. Finally, deal.ii is freely available under the Q Public Licence.

The most recent developments of the PI activities consist of the recasting of the DGFEM discussed earlier using deal.II. The reformulation in question has been successful and automatic self refinement is now part of the numerical capability created by the PI. In the process of recasting the proposed DGFEM to include adaptivity, it was discovered that the formulation used until then suffered from loss of unconditional stability when using completely unstructured space-time grids. Hence, the recent efforts included a correction of the formulation and the derivation of a proof of unconditional stability of the new formulation. The proof in question has been presented in a Costanzo and Huang (2004). This paper includes the discussion of a variant of the proposed DGFEM formulation which, in the absence of physically-based dissipation, is energy conserving (although the computer implementation of this variant has not been pursued yet). The unconditional stability of the new formulation has been also numerically verified. Figure 8 presents the solution in terms of a simple 1D problem in which a homogeneous stretched bar initially at rest is suddenly released. The solution was obtained a completely unstructured space-time grid. The total energy of the true solution to the problem is conserved. The plot of the total energy vs. time of the approximate solution is displayed in Fig. 9, which shows a (very slight) monotonic decreasing behavior for the energy, thus providing a numerical verification for the unconditional stability claim.

Figure 10 presents the solution for the same phase transition problem discussed in relation to Fig. 2, this time achieved with the new formulation and automatic mesh refinement. Despite the fact that half as many elements were used in each space-time slab (with respect to the calculation

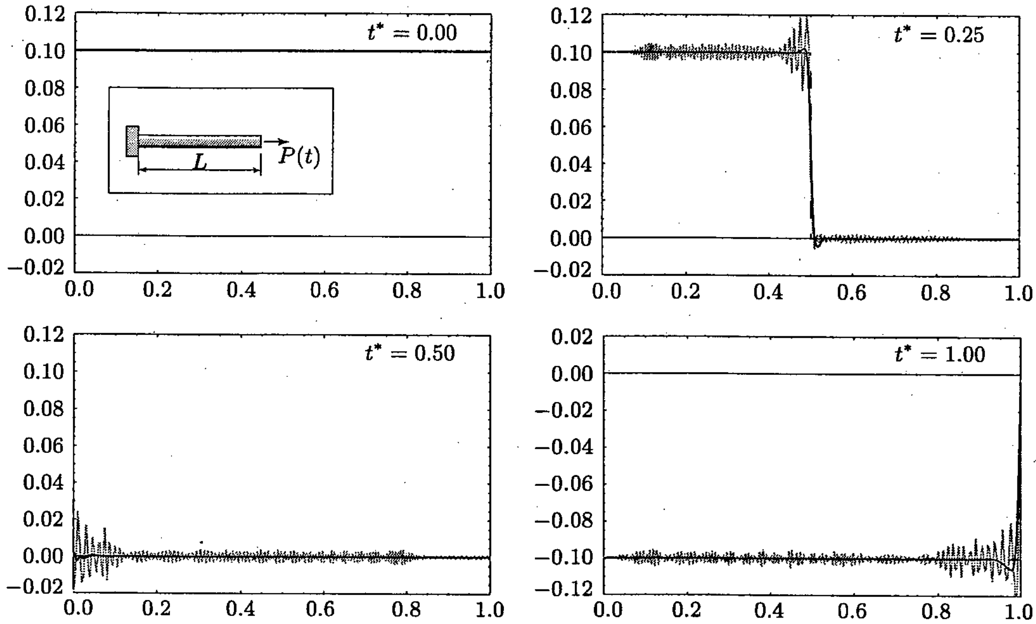

Figure 8: Plots of the (nondimensional) axial internal force (stress) in a homogeneous bar (shown in the inset in the upper left) which was initially at rest and stretched. At time $t = 0$, the bar is released thus causing a stress pulse to propagate to the left. The **solid black** line denotes the DGFEM solution. The **dashed black** line denotes exact solution, whereas the **gray line** denotes the solution obtained using FEMLAB.

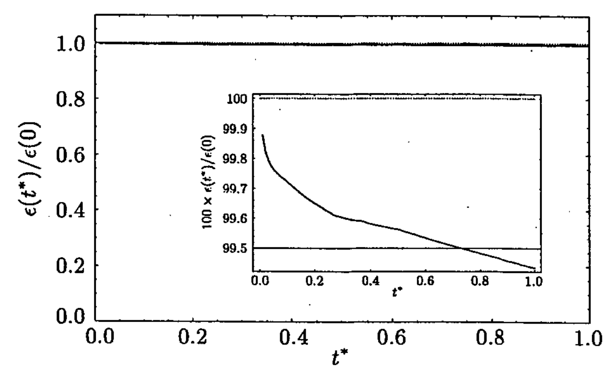

Figure 9: Plot of the total energy normalized with respect to the initial total energy for the case described in Fig. 8. The **solid black** line denotes the DGFEM solution. The **dashed black** line denotes exact solution. The inset plot is simply is a magnification of the main plot by a factor of 100 to show the monotonic decay of the energy.

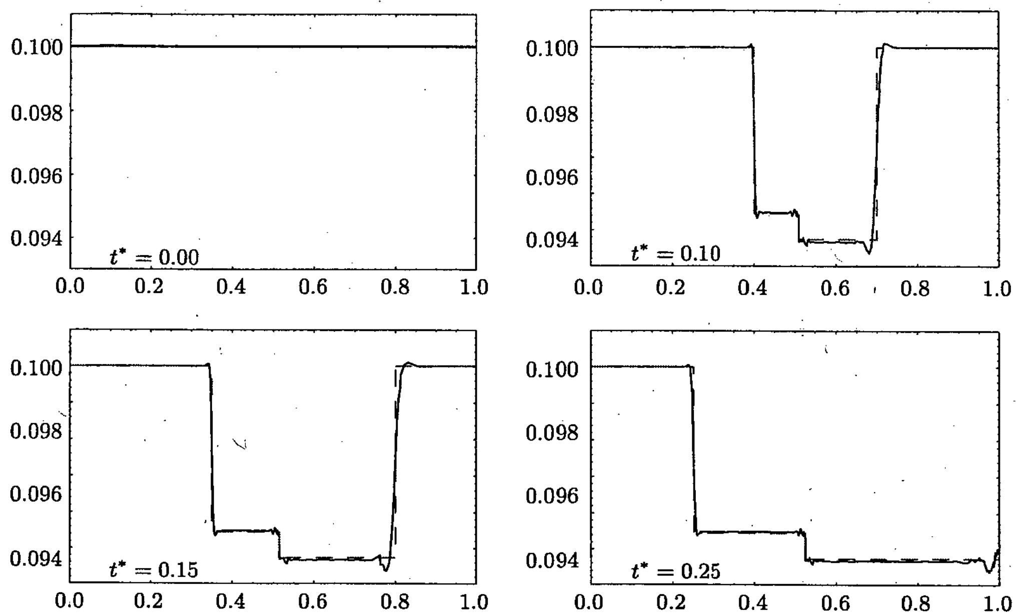

Figure 10: The **dashed line** represents the exact solution. The **solid back line** represents the distribution of the axial internal force (stress) at various time instants for the case of the interface traveling at a constant speed v, with $v/c_2 = 0.1$. $c_1/c_2 = 0.5$, $k_1/k_2 = 0.25$, and $n^*(t=0) = 0.1$. Every plot has the same horizontal and vertical axes. The horizontal axis represents the non-dimensional position x^* along the bar, while the vertical axis represents the non-dimensional axial force n^*. Each space-time slab was discretized using 100 bi-quadratic isoparametric space-time elements and then automatically refined. The final number of elements per slab is approximately 200.

in Fig. 2), the solution accuracy remains very satisfactory. Figure 11 displays the FEM grid that was automatically generated over the space-time solution domain using automatic refinement. In this figure, the automatic refinement captures the propagation of shock wave fronts as well as the propagation of the interface. Figure 12 shows the total energy vs. time plot for the propagating interface problem. Note that the dissipation due to the formulation is essentially negligible when compared to the physical dissipation due to the advancement of a moving boundary. Finally, the computational capability created thus far was used to *predict* the motion of an interface in a 1D dynamic solid-solid phase transition process using as evolution law of the type

$$V_{\text{int}} = \begin{cases} \eta(f - f_{CR}), & \text{for } f > f_{CR} \\ 0, & \text{for } f \leq f_{CR}, \end{cases} \tag{2}$$

where V_{int} is the velocity of the interface, η is a material parameter, f is the energy release rate and f_{CR} is a threshold value of the energy release rate below which interface propagation does not occur. Formally, the structure of this 1D problem is vary similar to that of the dynamic propagation of Griffith crack in a linear elastic material. Figure 13 depicts the interface trajectories for several values of the η parameter and under the same loading conditions of the problem discussed in Fig. 10.

The results reported here are being compiled into a paper, which is currently in preparation.

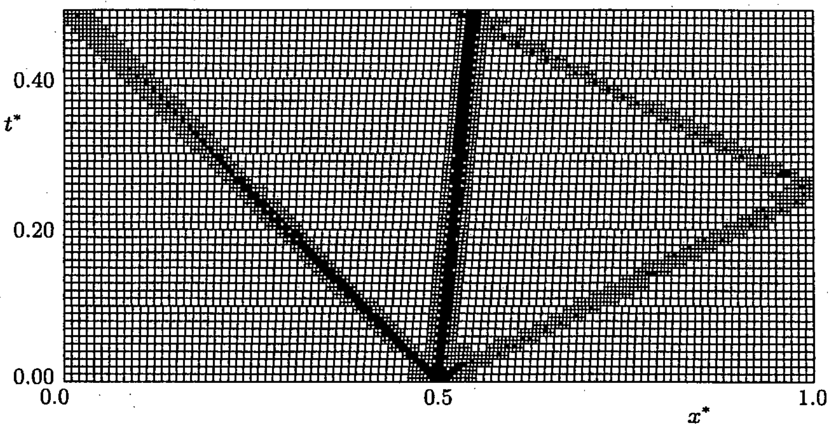

Figure 11: Space-time grid automatically generated by the adaptive refinement for the solution in Fig. 10.

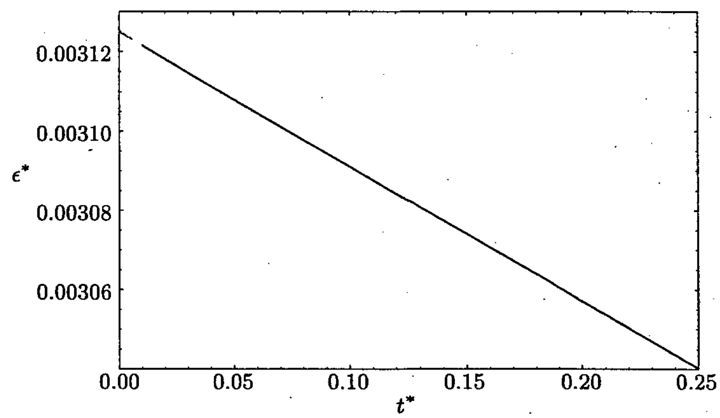

Figure 12: Plot of the nondimensional total energy vs. nondimensional time for the solution in Fig. 10. Both exact and approximate solutions are presented in the plot.

2.3. Additional developments

Thorough a cooperation with Prof. Jay R. Walton, the PI is working on a formulation of dynamic fracture in unbounded media based on the use of complex variables and integral transforms. The PI work in this field has been discussed in a number of papers preceding the beginning the present research project Costanzo and Walton, 1998a,b, 2002. With the present research project, the PI has begun to extend the solution methods already developed to the solution of a Mode III transient dynamic propagation of a CZ in a fully coupled thermo-elastic solid. The progress achieved on this component of the project consists of extending the computational capability already created by the PI to solve transient (i.e., not steady state) dynamic fracture mode III problems with a CZ undergoing fragmentation. The new components of the computational capability in question regard the addition of adaptivity as well as being able to deal with a a fragmented CZ, that is, a multiply connected domain. The complication introduced by the presence of fragmentation is rather substantial from a computational geometry viewpoint. The progress to date on this part of

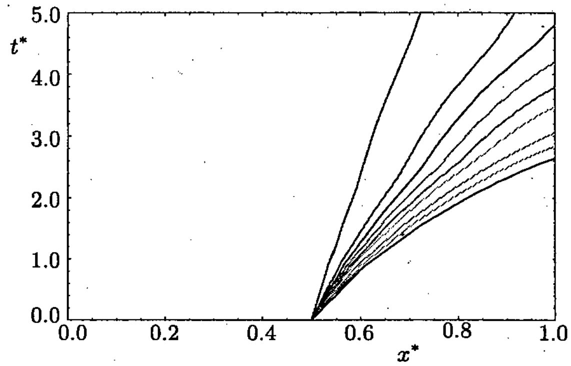

Figure 13: Interface trajectory as a function of the non-dimensional time t^*. From left to right, The various curves correspond to the following value of the nondimensionalized parameter η in Eq. (2): 20, 25, 30, 35, 40, 45, 50, 60, 75.

the project, consists in the creation of a triangulation capability which can in indeed cope with an evolving and fragmenting CZ. In addition, an algorithm for the use of product integration scheme to deal with the double-singular-integral Neumann-to-Dirichlet map which is at the core of the numerical scheme in question has also been formulated. This integration scheme guarantees that all of the numerical integrations to be carried out are exact for the interpolation functions selected to represent the solution.

Finally, an additional development is the extension of the DGFEM formulation discussed earlier to the solution of a fully coupled thermo-elasto-dynamic moving boundary problems. This component of the project has begun in the last month and, while a few results have been already obtained, a more careful validation of the numerics is needed.

2.4. Publications

The work done since the beginning of the project has resulted in the following publications, which acknowledge AFOSR funding:

1. F. Costanzo and H. Huang, "Proof of Unconditional Stability for a Single-field Discontinuous Galerkin Finite Element Formulation for Linear Elasto-dynamics," *Computer Methods in Applied Mechanics and Engineering*, to appear, 2004.

2. H. Huang and F. Costanzo, "On the Use of Space-time Finite Elements in the Solution of Elasto-dynamic Fracture Problems," *International Journal of Fracture*, to appear, 2004.

3. Scott T. Miller, "A Space-Time Finite Element Method for Second Order Hyperbolic Problems," Master of Science thesis, The Pennsylvania State University, August 2004.

Mr. Scott T. Miller has defended his thesis work, carried out under the supervision of the PI, in June 2004. Mr. Miller is going to continue his graduate studies in the Department of Theoretical and Applied Mechanics at the University of Illinois—Urbana.

3. Interactions

2002 Along with his collaborator Jay R. Walton (Department of Mathematics, Texas A&M University), the PI has had the opportunity to give a seminar to the GERC in April 2002, illustrating a number of preliminary results obtained on the use of the DG FEM in dynamic fracture of linear elastic isothermal materials. The PI intends to expand his collaboration with Dr. Walton aimed at the derivation of the Neumann-to-Dirichlet maps for coupled linear thermo-elastic dynamic fracture problems. Furthermore, while at GERC in April, the PI had the opportunity to meet Dr. Molly Hughes (Damage Mechanisms Branch of the Ordinance Division within the Munition Directorate at AFRL/Eglin AFB). From the brief discussion with her, it appears that Dr. Hughes is interested in the PI's project and possible future collaborations.

2003 The PI has been contacted by Prof. Barna Szabo (Professor of Mechanics, Washington University) for exploring the full-scale development of the DG FEM scheme proposed herein. Furthermore, the PI will be spending two weeks visiting with Prof. Walton (October 16–November 1, 2003) to further their development on the derivation of Neumann-to-Dirichlet maps for transient thermo-elastic fracture problems.

2004 The PI continues to interact with prof, Jay R. Walton on matters that very closely related to this project. Furthermore, the PI is still in coontact with Prof. Szabo for exploring the full-scale development of the DG FEM scheme proposed herein. Finally, the PI has recently hired as a post-doctoral researcher on this project Dr. Dinara Khalmanova who received her Ph.D. in mathematics at Texas A&M University under Prof. Walton's supervision.

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