3.2 Structures and Materials

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Overview

The Structures and Materials group is responsible for the analysis of the solid parts of the rocket—the rocket case and the unburned solid fuel. The activities of this group divide into two thrust areas: system simulation, and constitutive and failure modeling of components and materials. The research activities in system simulation primarily concern the groups led by Parsons, Hjelmstad, Haber, and Tortorelli. The research activities in constitutive and failure modeling primarily concern the groups led by Sofronis, Averback, Beaudoin, and Geubelle. The following sections describe the research accomplishments of the past year.

System Simulation

Our principal goal in structural analysis of solid propellant rockets is to develop a scalable parallel finite element code capable of structural modeling of the solid rocket motor. To support the development of this code, we have research efforts in finite element technology to develop more robust elements, contact mechanics, adaptive mesh refinement, implementation of continuum constitutive models, numerical algorithms for time integration, and ALE schemes for moving domains. Parsons and Hjelmstad lead these efforts. Through all of these efforts, the parallel implementation is a key feature. We are also pursuing space-time finite element technology as a possible alternative to ALE. Haber and Tortorelli lead the space-time efforts.

The structural code, *Rocsolid*, is based on a linear multigrid solver, employs a finite element discretization of the problem domain using unstructured meshes, and is capable of solving nonlinear transient problems using an implicit time integrator. The code is written in Fortran 90 and executes in parallel on shared and distributed memory machines using standard MPI libraries. Benchmarking studies demonstrate that the procedure is scalable. Meshes are generated using *TrueGrid*, and partitioned for distributed memory environments using *Metis*.

We have developed an Arbitrary Lagrangian-Eulerian (ALE) formulation capable of modeling the propagation of an interface through a solid. This has produced a working method that is being verified by solving some three-dimensional problems with known analytical solutions. We are currently integrating the ALE methodology into the coupled physics (GEN1) rocket simulation code. Other code development work has considered advanced solid element formulations (e.g., based on assumed strain methods), material model development (linear and nonlinear viscoelastic models), parallel contact enforcement using augmented Lagrangian methods, adaptive mesh refinement, and algorithms designed to couple implicit and explicit solids code together.

To demonstrate the accuracy of our ALE formulation, we have developed several benchmark problems. One of these—the contracting bar—is a 3-D analysis of an essentially 1-D problem. The problem is a bar fixed at one end, contracting due to removal of material, and forced with an end traction. The analytical solution for a non-contracting bar subjected to an end load is well known. This solution can be used to generate the solution for a contracting bar—one in which material is disappearing, not simply contracting under the action of the forces —subjected to an end loading by applying end tractions that are consistent with the fixed length solution. This approach produces a benchmark problem for the moving mesh problem. Figure 3.2.1 shows a comparison between the analytical solution and our numerical solution for this problem; the agreement is excellent, and demonstrates the accuracy of our formulation.

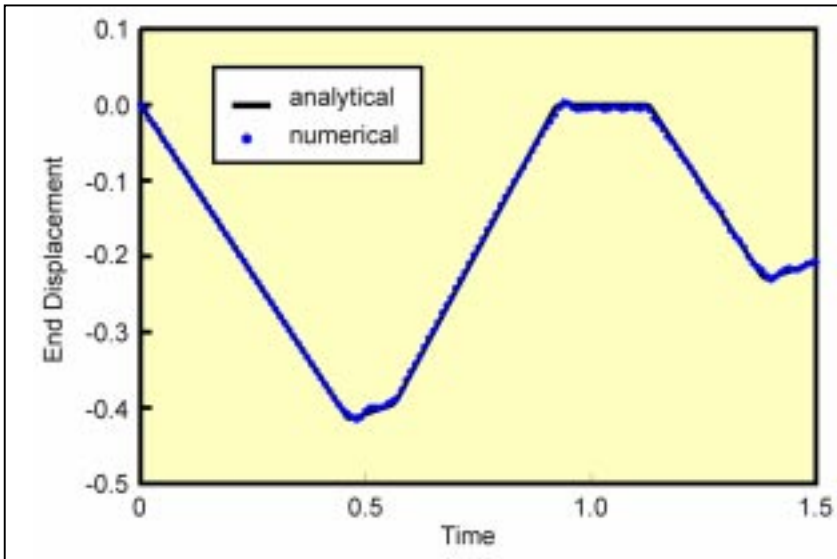

Fig. 3.2.1: ALE formulation for response of contracting bar.

As a second benchmark problem, the analysis of a spherical cavity in an infinite medium with a pressure loading has also been performed. In the analysis, the initially spherical cavity grows into an ellipsoid under a spatially varying velocity field. The method for developing the moving mesh solution is essentially the same as for the contracting bar. The cavity is loaded with a sinusoidal varying load. Good agreement has been observed between the exact (analytical) radial and tangential stress and displacement components and those that are computed with the ALE method.

Nonsymmetric matrix equations are encountered in the ALE formulation, and various solvers, including nonsymmetric multigrid solvers, are being studied to see which gives the best performance. Other future work on this subproject includes implementing improved material models, development of a coupled implicit-explicit time integration scheme, development of parallel contact procedures, and incorporation of adaptive mesh refinement algo-

rithms. Other coupling algorithms will also be studied, and the coupled code will be tested by comparison with available experimental data.

A complete restructuring of *Rocsolid* is underway. This restructuring will allow us to implement constitutive models efficiently to approximate better the material behavior of the solid propellant and the steel casing. The initial implementations of these models will be made for stationary domain problems; the modifications required for the ALE method will follow. We will also work with the computer science integration efforts to help develop the CSAR computational framework

Integrated GEN1 Code

The GEN1 code is the integrated rocket simulation code. *Rocsolid* and *Rocflo,* the fluids solver, form the basis of our rocket motor simulation. A standard predictor-corrector algorithm is employed to treat the fluid-structure interaction. In the current integrated simulation, the combustion rate of the propellant is coupled to the fluid flow via an empirical power law relationship. An interface module, *Rocface*, takes care of the data transfer between the two codes. All of the components of the GEN1 code are fully parallel, and the integrated code has been tested on the NCSA Origin 2000 up to 256 processors and on the PSC Cray T3E on up to 512 processors.

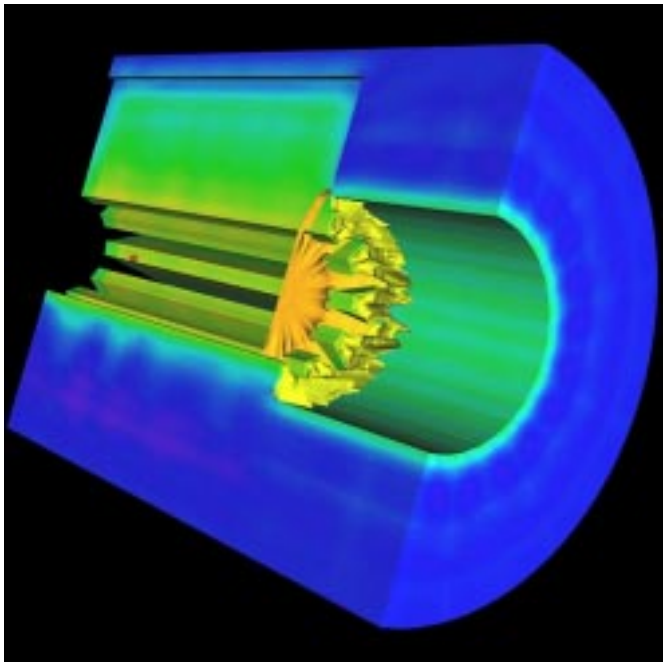

Fig. 3.2.2: Propellant average stress and gas pressure in fully 3-D, integrated GEN1 simulation.

The scalable parallel performance of the primary GEN1 components *Rocsolid* and *Rocflo* has already been shown. The partitioned approach adopted for the coupling algorithms preserves the performance for GEN1. Good scalability is observed up to 512 processors on a CRAY T3E. A short simulation of a shuttle rocket booster was done on 256 processors of an Origin2000, and Figure 3.2.2 shows propellant average stress and gas pressure resulted from this simulation at 0.1 seconds. The ALE capability in *Rocsolid* is currently being tested in the GEN1 coupled code.

Mesh Adjustment Methods

As the solid propellant of the rocket burns and turns into gas, the finite element mesh of the solid must be adjusted to track the motion of the fluid-solid interface. As the mesh is deformed and the interface is displaced, the mesh must be smoothed to maintain reasonable mesh quality. A smoothing procedure essentially analogous to heat conduction has been implemented in *Rocsolid*. In this paradigm, the motion of the mesh, which is known everywhere

at the solid domain boundary, is treated as a thermal loading. It has been observed that, although with certain deficiencies, this method yields reasonable meshes after minor adjustments.

Eventually the mesh becomes so deformed that mesh smoothing is no longer sufficient. In such cases, a remeshing procedure is necessary. Remeshing may involve element removal, mesh repairing, or other remedial actions. The implementation of a (topological) mesh adjustment algorithm is currently underway. An implementation (independent from *Rocsolid*) has been made and shown to be feasible for domains with a regressing boundary, such as rockets.

The significance of the so-called "mesh motion problem," which is a major component of ALE, requires further examination. The solution of the mesh-motion problem yields the mesh displacements and its gradients. It has been observed that not all strategies for solving this problem yield accurate results in connection with the ALE method. A complete implementation of the topological mesh adjustment strategy will be completed. Also a conservative mapping method that is used to transfer representation of field quantities (displacements, stresses, etc.) between meshes needs to be implemented.

Space-time Finite Element Methods

Our ultimate objective in this research is to demonstrate a coupled solid/fluid rocket simulation based on space-time discontinuous Galerkin (DG) finite element methods. We have leveraged our effort with collaboration and funding with the Center for Process Simulation and Design, a sister center to CSAR in the UIUC Computational Science and Engineering Program.

We have improved the elastodynamic solid mechanics model by developing a novel continuum statement of linear momentum balance. The resulting weak formulation yields a finite element method that outperforms previous DG methods. In addition to balancing linear momentum at the element level, the new procedure virtually eliminates the terminal error in the equation of motion. We tested the new method in 1-D **X** time, proved an *a priori* stability estimate, and extended it to handle material interfaces. We helped to develop a new "tent-pitcher" algorithm for meshing in 2-D and 3-D **X** time—a significant step toward practical applications.

A parallel effort focused on DG methods for nonlinear conservation laws for CFD. We demonstrated a promising new method for Burgers' equation in 1-D **X** time. Conservation is realized at the element level, element-by-element solution procedures are possible, and the method has intrinsic shock-capturing properties.

A further refinement of the elastodynamic formulation is nearly complete. It will balance energy at the element level in addition to momentum—an unprecedented combination. We plan to demonstrate the DG elastodynamic formulation in 2-D **X** time before the end of 2000. Development during Y4 will focus on 2-D applications in dynamic fracture and adaptive analysis. We are working on a DG method for the inviscid Euler equations, and an initial demonstration is planned for Fall 2000. In Y4, we plan to extend this to 2-D **X** time and, ultimately, consider the development of a coupled solid/fluid simulation based entirely on the DG methodology.

Constitutive Behavior and Failure Analysis

An important part of the research effort in the Structures and Materials Team is dedicated to analysis of the constitutive and failure response of various rocket components, and, in particular, the solid propellant and the metallic case. This research activity involves the groups led by Sofronis, Averback, Beaudoin and Geubelle.

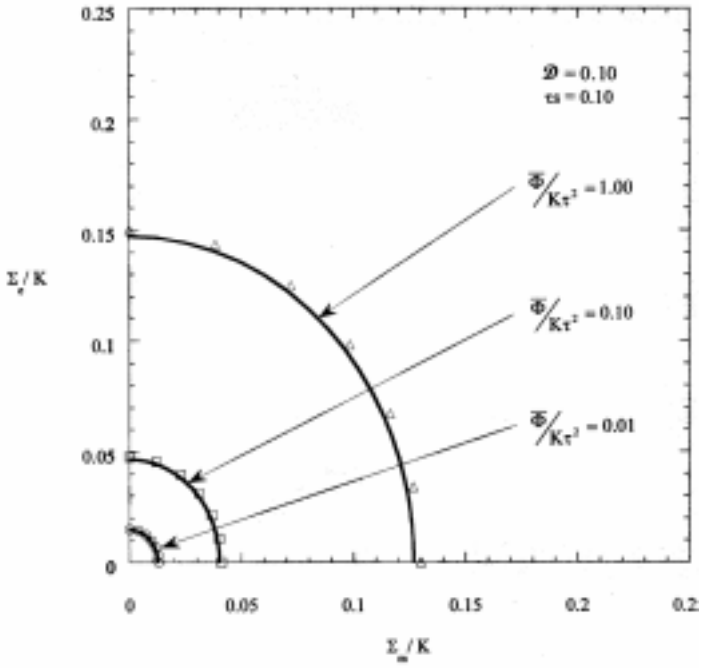

Fig. 3.2.3: Normalized contour plots of $\Phi/K\tau^2$ shown in normalized hydrostatic, Σ_m/K, – deviatoric, Σ_e/K, stress space for analytical approximation (continuous line) and finite element solution (data points) when porosity D is equal to 10%, and time $\tau s = 0.1$. Parameter K denotes bulk modulus of matrix, τ is relaxation parameter for the polymeric binder, and s is Laplace transform parameter.

Sofronis and his graduate student Meyer are working on the development of a micromechanics-based damage model for the grain. Damage in solid propellant manifests itself in various ways: particle cracking, decohesion along particle/polymer interfaces, void opening or even polymer crazing at low temperatures, and inert propellants. The current research activities have focused on the effect of damage due to void formation on the material constitutive response. With the use of the correspondence principle of linear viscoelasticity, a macroscopic constitutive potential has been rigorously devised in terms of the Laplace transform parameter that takes into account the presence of porosity. This potential describes exactly the constitutive response of a porous solid propellant in the case of purely hydrostatic and purely deviatoric loadings. Finite element calculations carried out for arbitrary combination of loads have provided numerical results that point toward an elliptic approximation for the response under general 3-D axisymmetric stress situations, as shown in Figure 3.2.3. This elliptic approximation could be used in a material subroutine to study aspects of solid propellant mechanical behavior such as the deformation fields in the neighborhood of a crack where damage can be severe.

Plans for the coming year start with combining potential Φ with a Gurson-type of work hardening plasticity (non-linear macroscopic response) in which yielding will be identified with the onset of porosity. Once this theory for the overall viscoplastic material response predicated on the form of material degradation (presence of voids) is established, an effort will be made to explain and predict the experimentally observed large macroscopic volume changes that a solid propellant exhibits under load. Subsequently, the analysis will be extended to account for large strain material response and anisotropic evolution of porosity. In this context, the dependence of Φ on the loading rate will be investigated, since it is well

known that strain rate effects on material viscosity are also responsible for the observed non-linearitiy in the behavior of the polymeric binder. The resulting porosity-based damage model will be incorporated into *Rocsolid* for a more accurate description of the grain response in regions where strains and stresses might be large. Longer-term plans include the exploration of other forms of damage such as particle dewetting. For this purpose, the atomistic results of Averback's group on the constitutive characteristics of a solid/soft interface will be used.

Averback, Albe, and Ashkenazy have been modeling heterophase interfaces at the atomic scale. The fundamental goal here is the understanding at the atomic scale level of cohesive failures in solid propellants. Building on their earlier study of metal-ceramic interfaces, they have spent the major part of this past year investigating carbon-metal interfaces, which are important for understanding the mechanical behavior of metal/metal-oxide grains embedded in a polymer matrix. For this purpose, they have developed a new scheme that integrates both the analytical form of Finnis-Sinclair type EAM-potentials for metals and the

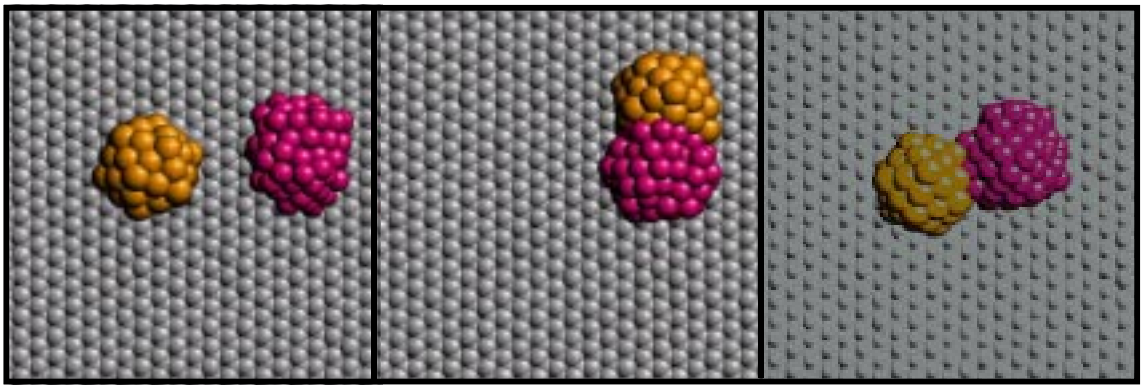

Fig. 3.2.4: Thermally activated diffusion and sintering of Pt nanoclusters on (111) diamond. Shown are snapshots after 15ps, 45ps and 250 ps.

Brenner bond-order potential for carbon phases. Using experimental and theoretical data from total energy calculations within density functional theory, a parameterization was first performed for the Pt/C system, which is an ideal model system that also has great scientific and technological interest (e.g., catalysts). Several large-scale molecular dynamics (MD) simulations using their massively parallel MD-code were run using this model. One example is the thermally activated diffusion and sintering of Pt nanoclusters on a diamond surface (Figure 3.2.4). Other applications of this model include the investigation of the initial stages of ion-induced nanostructuring of a thin metal film on carbon and the modeling the compound semiconductor GaAs. This latter result is especially significant as it represents the first potential for this technologically important system that includes both the chemistry and complicated structure of the gallium and arsenic constituents.

Future plans for Averback's group involve extending the new potential scheme on metal-hydrocarbons, which makes necessary a detailed analysis of the metal-hydrogen interaction. The objective here is to model decohesion at polymer-metal interfaces in a chemically more accurate manner. Fundamental mechanisms and materials parameters will be exported to programs that are based on continuum mechanics approaches, such as the damage models

described above. Other efforts include extending the group's initial investigations of grain boundary dynamics in polycrystalline metals to multi-grain configurations including triple-junctions. The emphasis here is to gain valuable insights in order to understand plasticity of poly- and nanocrystalline materials on an atomic level scale. These results will then be used to further refine the microscale continuum analysis conducted by Beaudoin and his group.

Beaudoin and his coworkers (Kok, Acharya, and Tortorelli) have developed a material model to describe plastic deformation of the D6AC steel case. There are two distinct components to the model: a finite element discretization of the polycrystalline microstructure for the steel that renders detailed microscale response; and a material point model that provides characterization of polycrystal response and is suitable for introduction into the finite element code to be used to simulate deformation of the rocket motor case.

From the detailed finite element studies of the polycrystalline microstructure, fundamental understanding of the large strain behavior and grain-size dependence on work hardening has been gained. In particular, a study of grain-size effect, being carried out at Los Alamos National Laboratory, was accurately characterized by the model. The results led to a publication with co-authors Chen, Korzekwa and Stout from LANL.

At the macroscale level, Kok is developing polycrystalline plasticity models with incorporation of strain rate and temperature effects. To date a novel integration algorithm has been formulated for the plastic spin evolution equation and identification studies have been performed in which the material parameters of a tantalum plate and an HY100 steel are identified in accordance with the MTS (mechanical threshold stress) material model. The US Naval Surface Warfare Center and LANL provided experimental data for these studies. Dr. Carlos Tome (LANL) has introduced the formulation developed by Mr. Kok into the LANL code VPSC (viscoplastic self-consistent model).

Future efforts will address the evolution of damage in the finite element model of a metal polycrystal. Using the same approach as was done for work hardening, results will be distilled for introduction into a material point description suitable for use in *Rocsolid*.

Grain Failure

The final component of the constitutive and failure response modeling effort of Structures and Materials Group is dedicated to the development of the numerical tools needed to perform macroscale analysis of grain failure. In this research effort led by Geubelle, special emphasis is placed on the capture of the possible spontaneous debonding of the solid propellant from the case or the insulation layer. A major part of the past year has been dedicated to the incorporation of ALE capability into the existing 2-D and 3-D cohesive-based finite element code used by Geubelle's group to simulate complex dynamic fracture events. An example of such 2-D simulation is shown in Figure 3.2.5, illustrating the spontaneous propagation of an interface crack and the accompanying erosion of the grain. An explicit coupling algorithm including both ALE and fracture capabilities has also been developed with Hwang, Acharya and Fiedler that addresses the complex fluid/structure/combustion interaction characterizing this fracture problem as new burning surfaces are dynamically created as the crack propagates. This coupling algorithm has been first implemented in a 2-D setting, taking advantage of the explicit 2-D unstructured finite volume code developed by Fiedler. The objective of

this study is to model ultimately a 1991 Titan IV SRMU accident in which an excessive deformation of the grain initiated an interfacial failure resulting in failure of the rocket.

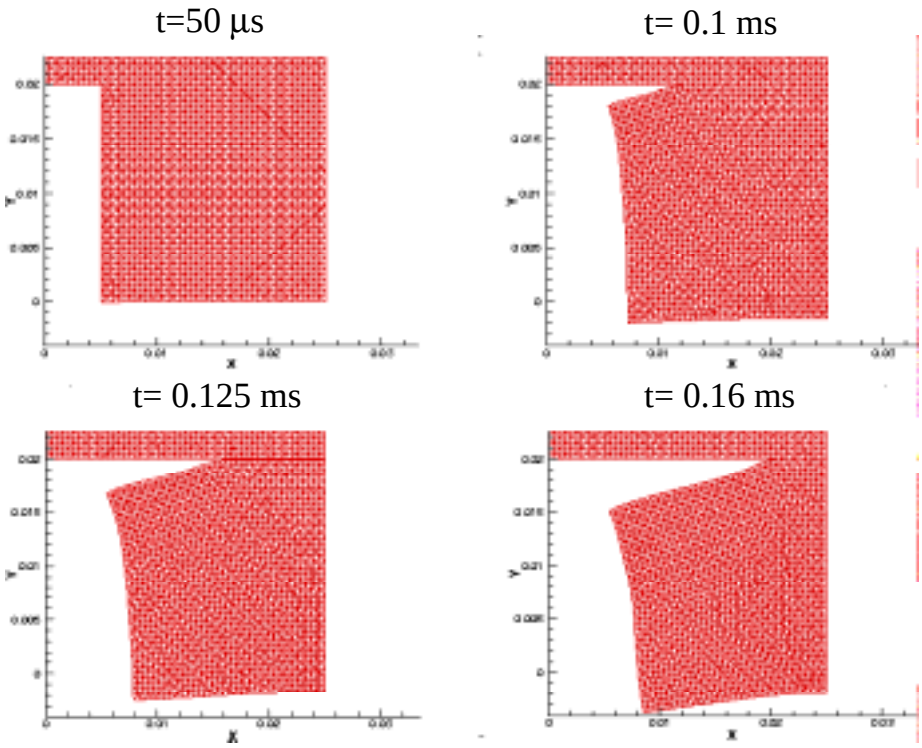

Fig. 3.2.5: Model problem illustrating ALE CVFE analysis of grain/case dynamic debonding event showing spontaneous propagation of interfacial crack and progressive erosion of grain.

In concert with that effort, Breitenfeld and Hwang are developing a parallel version of the explicit dynamic fracture code. Scalability of the resulting F90/MPI CVFE code has been studied on very large models (with almost 500M degrees of freedom) up to 2048 processors. Current investigations include collaboration with Kale and his group in CS to incorporate their recently completed *Charm*++ FE "chunk-based" framework. At a more fundamental mechanics level, Kubair is investigating various basic dynamic fracture issues associated with the introduction of rate dependence in cohesive failure models with the aid of a spectral scheme and other analytical tools. Finally, in preparation of more adaptive simulations of dynamic failure in which cohesive elements would be introduced "on the fly" in the discretized domain, Zaczek is investigating issues such as mesh refinement, cohesive element insertion and subcycling. This initial study is first conducted in a simpler 1-D setting and will be expended to 2-D and eventually to 3-D over the next two years. Other plans include the development of the fully 3-D ALE-based fluid/structure code and its incorporation into the *Rocface* interface code that will enable the treatment of more general fluid/structure interfaces. Mesh generation issues are also critical in this part of the program, especially with regard to the possible remeshing required after substantial mesh motion, the dynamic incorporation of cohesive elements, and the adaptive refinement of the mesh in the region where failure is occurring or is bound to occur. Collaboration with Tim Baker of Princeton University is currently underway to address these issues.