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 three broad areas: failure modeling, constitutive behavior of components and materials, and system simulation. The research activities in failure modeling and constitutive properties primarily concern the groups led by Averback, Beaudoin, Geubelle, and Sofronis. The research activities in system simulation primarily concern the groups led by Haber, Hjelmstad, Parsons, and Tortorelli. The following sections describe the research accomplishments of the past year.

Failure Modeling

Crack Propagation in Solid Propellant (Geubelle, Hwang, Breitenfeld, Fiedler, Zaczek)

One of the key goals of CSAR is the simulation of accident scenarios involving the propagation of cracks in the solid propellant rocket. Over the past 12 months, special emphasis has been placed on the development of integrated 2-D and 3-D codes for the simulation of this class of problems. These problems are characterized by inertial effects, by a strong coupling between fluid, structure and combustion, and by substantial geometrical changes.

Hwang, in collaboration with Fiedler, has implemented a 2-D (plane strain and axisymmetric) coupled code that combines an explicit Arbitrary Lagrangian/Eulerian (ALE) formulation of the cohesive/volumetric finite element (CVFE) scheme with an explicit unstructured finite volume Euler solver. The ALE/CVFE code is used to simulate the initiation, propagation and possible arrest of a crack in a discretized domain with a regressing boundary. It includes large deformation effects and a nonlinear constitutive description of the inhibitor and grain (Arruda-Boyce model). The fluid solver includes a robust mesh adaptivity and repair capability, which is essential to handle the complex geometrical changes taking place in the

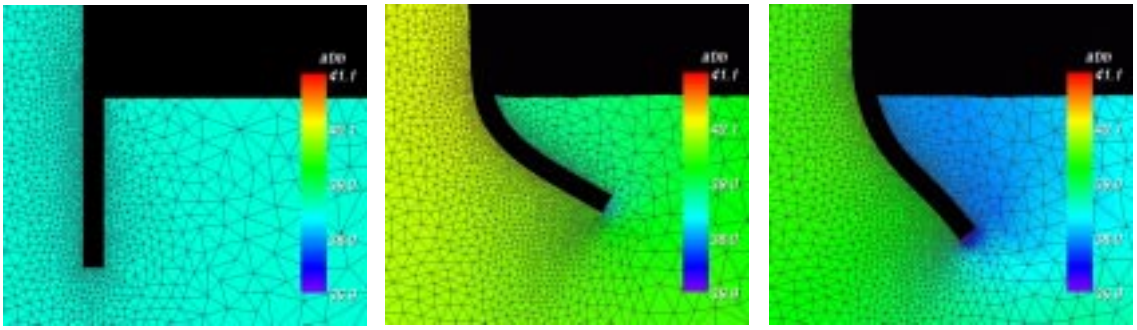

Fig. 3.2.1: Evolution of fluid mesh in vicinity of aeroelastically deforming inhibitor at times $t = 0$ *s.* (left), $t = 0.024$ *s.* (center) and $t = 0.036$ *s.* (right). Sequence demonstrates mesh repair capabilities present in fluid solver and large deformations experienced by flexible inhibitor. Color contours denote pressure.

fluid domain due to the deformation and fracture of the grain. Conservation of mass and linear momentum is enforced explicitly across the interface.

Preliminary axisymmetric simulations using the coupled code have focused on two distinct problems. In the first one, we study the motion of a flexible inhibitor protruding into the core flow (Figure 3.2.1). In the second application, we simulate the Titan IV grain slumping accident (Figure 3.2.2), in which the complex aeroelastic coupling between the grain and the core and slot flows creates excessive deformation of the aft grain segment, eventually leading to the propagation of a crack along the grain/case interface.

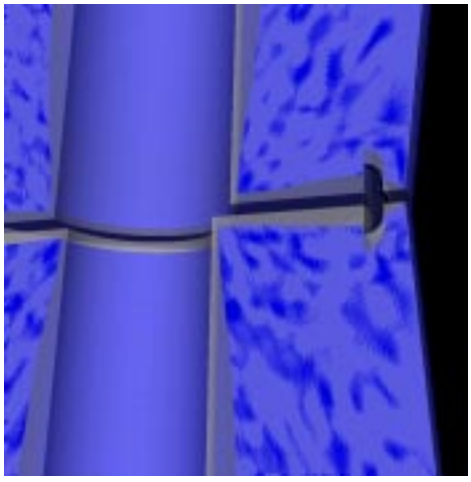

Fig. 3.2.2: *Rocfrac* is used to simulate Titan IV slumping failure. Undeformed (gray) and deformed (blue) solid at $t = 10$ ms, P = 100 MPa.

Similar capabilities are being developed in 3-D. A parallel 3-D version of the explicit ALE/CVFE code (*Rocfrac*) has been implemented by Breitenfeld, and has been incorporated with *Rocflo* and *Rocface* into the GEN2 version of the integrated code.

Other activities include the development by Zaczek of an adaptive CVFE scheme able to dynamically insert cohesive elements in a finite element domain based on the current stress state in the structure, and the detailed analytical study by Kubair of the effect of rate dependence on the cohesive modeling of dynamic fracture events in rate-dependent materials (such as solid propellant). Finally, a substantial collaborative effort is currently underway with Kale's group on the automatic parallelization of finite element codes using the *Charm++*/FE Framework. The first target code for this parallel implementation effort is Zaczek's adaptive CVFE code.

Constitutive Properties of Materials

As indicated above, the materials involved in the solid propellant rocket problem are quite diverse (steel case, solid propellant, insulation material, etc.) and are characterized by com-

plex constitutive and failure responses. The three projects described hereafter focus on various materials modeling issues at various length scales.

Atomic Scale Modeling of Heterophase Interfaces (Averback, Ashkenazy, and Albe)

At the atomic scale, the fundamental goal of this work is to understand cohesive failures in solid propellants. Building on earlier studies of metal-ceramic interfaces, we have investigated carbon-metal interfaces, which are important for understanding the mechanical behavior of metal/metal-oxide grains embedded in a polymer matrix. For this purpose, we developed a new scheme that integrates the analytical form of Finnis-Sinclair type EAM-potentials for metals with the Brenner bond-order potential for carbon phases. Using experimental and theoretical data from total energy calculations within density functional theory, the parameterization for the Pt/C system was completed and the potential shows good accuracy in describing a wide range of physical properties both for each single phase as well as for a multiphase system.

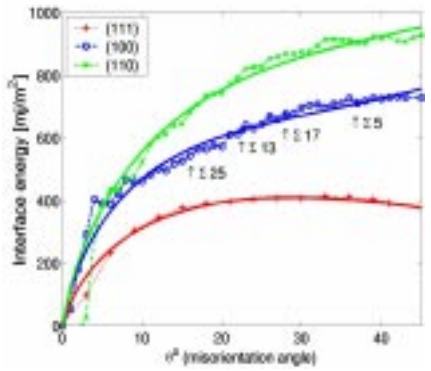

Fig. 3.2.3: Grain boundary energy for pure twist interfaces and different orientations. Points are results of MD calculations while solid lines represent fit to elastic theory-based description.

Large-scale parallel molecular dynamics (MD) simulations have been conducted using this new potential to simulate the stability of grain boundaries. These investigations are directed towards the understanding of dynamics of grain boundary reactions in polycrystalline metals, which for rockets is important owing to the large external loads. We have studied the dynamics within arbitrary interfaces of finite grains on an underlying flat surface. The results on FCC metals reveal that the interface between the particle and the surface can be described using and elastic interactions even for quite small grains (Figure 3.2.3). A new finite size effect was discovered, however, for particles smaller than 5 nm. Below this size, interface dislocations still form, but now they glide to the interface at the free surface of the particle.

The same techniques are currently being employed to simulate a heterogeneous system comprised of a hard particle (amorphous carbon) embedded in a softer matrix (Pt). In this system, a realistic effective traction-separation law is being calculated. The dewetting reaction observed in these simulations is illustrated in Figure 3.2.4.

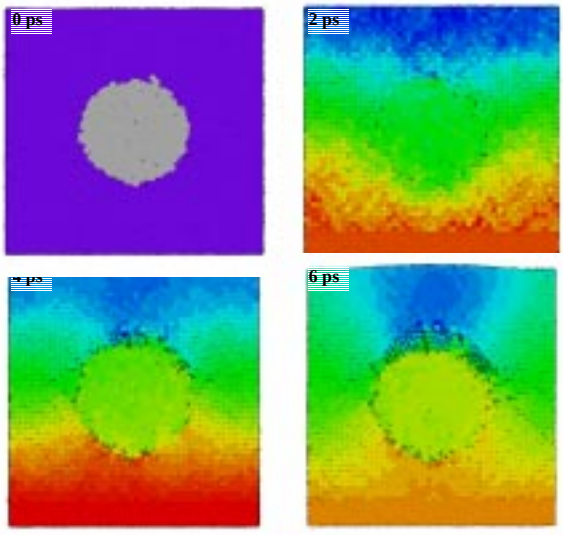

Fig. 3.2.4: Dewetting process of amorphous carbon inclusion in Pt matrix. Images show system at initial conditions and 2, 6 and 8 ps after activating stress on top layer while holding bottom layer fixed. Colors represent displacement of each atom.

Work Hardening at Large Strains (Beaudoin, Tortorelli, Kok, Acharya)

We have developed a mesoscale model for study of grain size effects in the hardening behavior of metals. Slip plane lattice incompatibility—a gradient measure that follows from spatial variations in crystallographic slip in metal grains—is naturally developed through grain-to-grain interactions (Figure 3.2.5). Over the course of metal deformation, lattice incompatibility is associated with an increased contribution to work hardening, ultimately rendering a transition in the fundamental character of the hardening response. The transition indicated by mesoscale simulations has been used to formulate a material model appropriate for (macroscale) analysis of engineering components. The material model includes grain size, temperature and strain rate effects and physically-based transition in hardening response at large strains. This approach has been applied in the *EPIC* finite element code by researchers at Los Alamos and in the *Rocsolid* finite element code described below. Future efforts will be directed at the study of fracture in metals, with ultimate application to the D6AC case of the solid rocket motor. Stress gradients follow naturally from grain interaction in the mesoscale simulations. These gradients provide a natural driving force for the progression of intergranular fracture. Cohesive elements (developed by R. Dodds) will be introduced into the model, and the progression of fracture detailed at the scale of individual grains. Following an approach similar to the work hardening model, results will be condensed for application in macroscale continuum models appropriate for analysis of engineering structures.

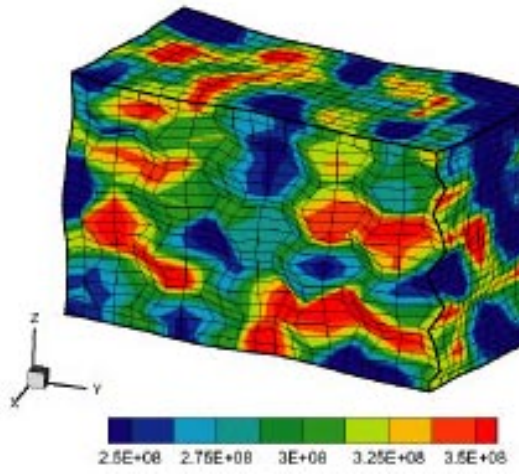

Fig. 3.2.5: Simulation of work hardening in Ag polycrystals shows effective compressive stress.

Constitutive Modeling of Voids (Sofronis, Meyer, F. Xu)

The effect of voids on the material constitutive response of solid propellant has been investigated by Sofronis, Meyer and F. Xu from a solid mechanics perspective. With the use of the correspondence principle of linear viscoelasticity, a macroscopic constitutive potential Φ has been rigorously devised such that $\bar{E}_{ij} = \partial\bar{\Phi}/\partial\bar{\Sigma}_{ij}$, where the overbar denotes the Laplace transform of a function in the time domain and $\bar{E}_{ij}$ is the macroscopic strain in response to a macroscopic stress Σ_{ij} on the "homogenized" material. This potential describes exactly the constitutive response of a porous propellant in the case of purely hydrostatic and purely deviatoric loadings. Finite element calculation results for arbitrary combination of loads suggest an elliptic approximation for the material response under general 3-D axisymmetric stress situations. The usefulness of this constitutive law is that it can be used in a user material subroutine in a general purpose finite element code to study the mechanical behavior of a solid propellant in the presence of internally evolving porosity.

The potential Φ will be used next to construct a Gurson-type of work hardening plasticity (non-linear macroscopic response) in which yielding will be identified with the onset of po-

rosity. Such a theory will be used to explain and predict the experimentally observed large macroscopic volume changes a solid propellant exhibits under load. The dependence of Φ on the loading rate will be investigated since strain rate effects on material viscosity strongly affect the response of the polymeric binder. The analysis will be extended to account for large-strain material response and anisotropic evolution of porosity. Also, other forms of damage will be explored such as partial particle dewetting. For this purpose, the atomistic results of Averback on the cohesive characteristics of a hard particle/soft matrix interface will be used.

System Simulation

Rocsolid Code Development (Parsons, Namazifard)

As a scaleable parallel finite element code, *Rocsolid* is capable of forming the backbone for structural model development of the solid rocket motor. *Rocsolid* is based on a linear multigrid solver and solves nonlinear transient problems using an implicit time integrator. The code executes in parallel on shared and distributed memory machines using standard MPI libraries. Benchmarking studies demonstrate that the procedure is scaleable. Meshes are generated using *Truegrid*, and partitioned for distributed memory environments using *Metis* (Figure 3.2.6).

This year's activities have focused on extending the functionality of *Rocsolid*, working with the CSAR integration team to produce demonstrations of CSAR's multiphysics simulation capability; and developing research that will enhance CSAR's program in future years. Recent additions to *Rocsolid* include scalable implicit contact, large deformations, transient heat conduction and multiscale material models. Initial steps towards a rigorous validation and verification program have also been undertaken. Contributions to the multiphysics simulation demonstrations include improved models of the lab scale rocket, specification and discretization of the Titan IV slumping problem, and scalability problems employing a moving interface. Research activities have continued in the areas of parallel adaptive mesh refinement, coupling of implicit and explicit time integrators in a solid mechanics code, and fundamental algorithmic studies of fluid-structure coupling with a moving interface.

Future work will be concentrated on developing the research activities outlined above so that new capabilities can be added to *Rocsolid*. This will help to expand CSAR's simulation capabilities and add crucial understanding to the basic algorithms used in the coupled simulations. *Rocsolid*, the structural analysis code used in the rocket simulations, employs a finite

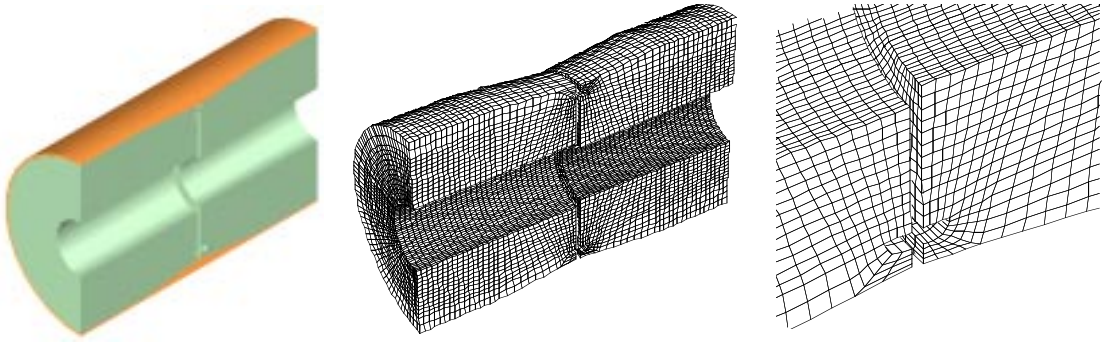

Fig. 3.2.6: Mesh generation for Titan IV slumping simulation.

element discretization of the problem domain using unstructured meshes. Dynamic problems are solved using the implicit Newmark time integrator. The linear matrix equations encountered within the Newton iterations at each time step are solved using a scalable parallel multigrid solver. *Rocsolid* is written in Fortran 90 and uses MPI to perform interprocessor communications.

Nonsymmetric matrix equations are encountered in the ALE formulation and different solvers, including nonsymmetric multigrid solvers, are being studied to see which gives the best performance. Other future work on this project includes implementing improved material models, development of a coupled implicit-explicit time integration scheme, integration of parallel contact procedures, incorporation of adaptive mesh refinement algorithms. Also, other coupling algorithms will be studied and the coupled code will be tested by comparison with the available experimental data.

ALE Methods (Parsons, Hjelmstad, Geubelle, Namazifard, Breitenfeld)

The matrix-free implementation and the verification of the ALE method that is used in tracking the fluid-solid interface is completed and documented. In the particular implementation of the ALE method in *Rocsolid*, a novel mesh smoothing procedure has been employed.

Further research is needed, especially in extending the ability of the current implementation of the ALE method to track the interface as the solid propellant completely burns out. A novel technique to achieve this via topological mesh modifications and smoothing had been studied and shown to be feasible. This method can now be implemented as a module to the simulation code to perform the following tasks: 1) track the quality of mesh and drive other applications to perform mesh adaptation and maintain mesh quality; 2) apply topological modifications to repair the mesh; 3) apply smoothing based on quality measures to the mesh; and 4) transfer field variables once a mesh modification is made (material history variables, stress, strains and displacement) from the old mesh to the new one.

Another topic of interest is the study of the accuracy and the stability of the fluid-solid coupling algorithm that is currently employed in the simulation code. New algorithms may be needed to employ larger time-steps in the simulations to reduce the computational effort. The performance of these algorithms in the ALE context are not currently well understood.

Also, the coupling of explicit (*Rocfrac*) and implicit (*Rocsolid*) codes may be required as the first one is essential in tracking the propagation of cracks through the solid-propellant and the latter is essential in doing very large-scale computations due to its scalability. Algorithms exist to perform the aforementioned task but they are currently not suitable to be employed in large-scale computations as they require the solution of secondary systems of equations to resolve the continuity of fields across the explicit-implicit interfaces. Implementation and analysis of this coupled algorithm is made more complicated in the ALE context.

Modeling Strategies for Rocket Motor Case (Tortorelli, Duesterhaus)

The analysis of “thin” and incompressible components of solid rocket motors, such as the steel casing, the propellant, and the inhibitors with the finite element method requires special element formulations. The so-called mixed enhanced elements provide a means to tackle the problems associated with such problems, i.e., volumetric locking and locking in bending. The group directed by Hjelmstad and Parsons have implemented a state of the art mixed-

enhanced element in the simulation code *Rocsolid* and verified the implementation via standard benchmark problems. A matrix-free implementation of the aforementioned element is completed. This particular implementation is well suited for use with the multigrid method that is employed in *Rocsolid* and provides a computational efficiency that is essential in carrying out large-scale computations.

Tortorelli and Duesterhaus (now employed at Sandia-Albuquerque) have been developing continuum finite elements that can be used to model plates. The advantages of these elements are the ability to consistently model the junctions between plates and continuum structures and the ability to incorporate complex constitutive models, e.g., plasticity.

The theory behind the plate model is simple. We use the basic governing equations that describe the continuum system and to that add constraints to mimic plate behavior, i.e., that plane sections perpendicular to the mid plane remain plane throughout the deformation. For small deformation elasticity this is accomplished by equating to zero those shear strain components in the mid-plane normal direction. As expected, the Lagrange multipliers that are used to enforce the constraints are related to the section forces of traditional plate models.

To date we have incorporated the theory with various element interpolation schemes for the deformation and the Lagrange multipliers. What we have found is that the presence of the constraints restricts the element deformation more than that of an unconstrained element and that is problematic. In an attempt to create a more flexible element we will augment our deformation interpolation with an enhanced strain method (Kasper and Taylor).

Space-time Discontinuous Galerkin Finite Elements (Haber, Tortorelli, Sheffer, Sobh, Guoy, Pattilo, Bammann [SNL-Livermore])

We are developing a new class of space-time discontinuous Galerkin (STDG) finite element methods for applications in computational solid and fluid mechanics. These methods offer element-wise conservation properties, scalable computational complexity, and a rich structure for parallel execution. They can track moving boundaries, including topology change, without discrete remeshing and data projection. They support simultaneous spatial and temporal mesh adaptation, and are very promising for large-scale simulations of solid fuel rocket engines. Funding from the NSF Center for Process Simulation and Design substantially leverages DOE funds.

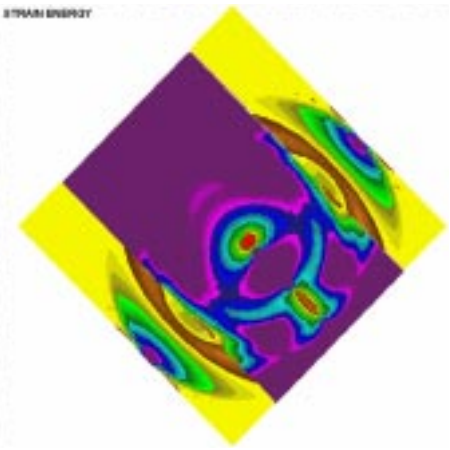

Fig. 3.2.7: Strain energy isosurfaces for wave scattering off elastic crack tip.

The STDG formulation for elastodynamics has been improved and extended from 1-D to 2-D x time. A recent simulation involves wave scattering off an elastic crack tip (Figure 3.2.7). A second part of the effort involves new methods for nonlinear conservation laws. A new shock-limiting technique has been introduced and the previous work on Burgers equation has been extended to address the Euler equations of compressible gas dynamics. Tent-pitcher, a new space-time meshing algorithm, has been extended to 2-D x time and integrated with the elastodynamic analysis (Figure 3.2.8).

In the coming year the elastodynamic problem will be extended by adding a cohesive interface model to simulate crack propagation and by formulating a new STDG method to simultaneously enforce local energy and momentum balance. A parallel implementation will be done using the *Charm++* system and adaptive analysis capabilities will be added. In the realm of nonlinear conservation laws, the code will be extended to handle systems of equations in 2-D x time (for the Euler equations) with special treatment of transmitting boundary conditions. We will incorporate parallel execution and adaptive analysis and extend the meshing procedures to track moving interfaces and to adaptively grade space-time meshes.

Tortorelli, Sheffer, Guoy, Pattillo (a PhD student who works summers at Sandia-Livermore but is not funded by CSAR) and Doug Bammann (Sandia-Livermore) are developing a space-time finite element program that can track interfaces. The immediate application of this program will be to model the rigid contact phenomena in nanoindentation tests. These tests are part of a material identification study for the Sandia BCJ material model.

The advantages of this method are that we will be able to eliminate the inequality contact constraints from our analyses which plague the convergence of traditional approaches and refine locally in time as well as space.

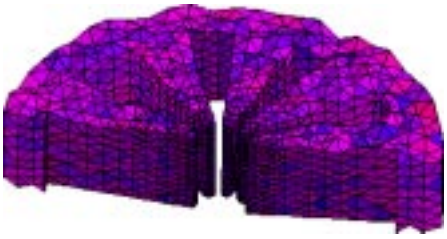

Fig. 3.2.8: "Tent-pitcher" algorithm applied to RSRM head end geometry.

The algorithm uses Sheffer's meshing library to refine and unrefine elements, Guoy's element flipping algorithm to retain good quality meshes, and Pattillo's space-time finite element program. Surface elements are introduced over the potential contact surface. Those elements for which the nodal gap function values range from positive to negative are subdivided to form element edges that are defined by zero nodal gap function values. These edges serve as the boundary of the contact region. Given the mesh topology, iterations commence to satisfy equilibrium and the contact conditions. Nodes interior to and on the boundary of the contact surface are given prescribed displacements in accordance to the motion of the rigid indenter. These same nodes are also given traction conditions in accordance with the given friction model. Finally, the node locations (in space and time) on the boundary of the contact surface are perturbed to ensure that their normal reaction forces are identically zero.

GEN1 Simulations

The GEN1 integrated rocket simulation code is the main product of this effort. *Rocsolid* and *Rocflo* form the basis of our rocket motor simulation. A standard predictor-corrector algorithm is employed to treat the fluid-structure interaction. The combustion module *Rocburn* was added to the coupled code. An interface module, *Rocface*, takes care of the data transfer across the three codes. All of the components of the GEN1 code are fully parallel.

GEN1 version 2.0 was released this year. It features a parallel ALE formulation for the moving interface. Parallel performance of this formulation has been tested and the results are available in AIAA-2001-3954. We are now using GEN1 version 2.0 to run several simulations including the Space shuttle solid rocket booster (with more detailed meshes), lab-scale rockets to test the ALE capability and the Titan IV slumping problem.