3.5 Structures and Materials

Group leaders: Keith Hjelmstad and Philippe Geubelle

Faculty: Robert Averback, Armand Beaudoin, Robert Dodds, Philippe Geubelle, Robert Haber, Keith Hjelmstad, Young Huang, Petros Sofronis, Ian Robertson, and Daniel Tortorelli

Research Scientists: Alireza Namazifard and Karel Matous

Research Programmer: M. Scott Breitenfeld

Post-doctoral Associates: Yinon Ashkenazy and Youhong Li

Graduate Research Assistants: Khaled Al-Fadhalah, Kristine Cochran (DOE Krell Fellow), Morgan Hawker, Helen Inglis, Justin Mach, Kalyanbabu Nakshatrala, J. Palaniappan, Arun Prakash, Brad Roe, Cynthia Smith, Michael Tonks, Daniel Turner, Satya Varadhan, Fengbin Xu, Wei Xu, Weixing Zhou

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: (1) system simulation, primarily by finite element methods, and (2) constitutive and failure modeling of components and materials. The technology develop in both of these general areas migrate, when appropriate, to the integrated simulation codes, primarily through the modules *Rocsolid* and *Rocfrac*. The research activities in system simulation primarily concern the groups led by Professors Dodds (CEE), Hjelmstad (CEE), Haber (TAM), and Tortorelli (MIE). The research activities in constitutive and failure modeling primarily concern the groups led by Professors Averback (MatSE), Beaudoin (MIE), Geubelle (AE), Huang (MIE), and Sofronis (TAM). The following sections describe the research accomplishments of the past year.

Integrated Simulation Codes for Solids

Rocfrac (Breitenfeld, Matous, and Geubelle)

Over the past year the explicit structural solver, *Rocfrac*, had numerous enhancements and improvements added. First, new elements were introduced to improve the robustness in bending and in the nearly incompressible finite elasticity behavior. These new elements include: A linear stabilized mixed displacement-pressure tetrahedral, a quadratic tetrahedral satisfying the Babuska-Brezzi condition via a generalization of selective integration, and a mixed-enhanced solid-shell brick element (Figure 3.5.1). Secondly, the ability to solve the thermal transient heat equation with ALE in the solid was added in preparation for the simulation of convective burning of a crack in an energetic

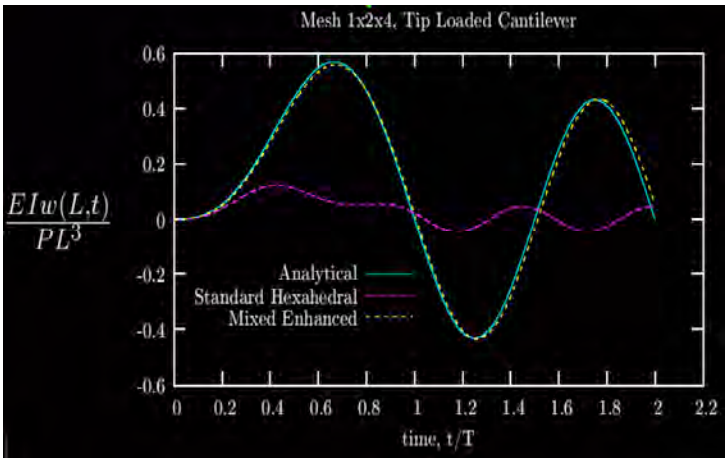

Fig. 3.5.1: Comparison between tip deflection evolution obtained by standard and mixed-enhanced brick elements for cantilever beam subjected to sinusoidal tip loading.

material. The number of verification/validation problems with both analytical and other commercial finite element codes has increased. Other supporting development activities include the investigation of dynamic parallel load balancing using the finite element parallel libraries developed by CSAR's Computer Science team (Figure 3.5.2). New material routines include a porous viscoelastic medium model developed by Sofronis *et al.* Additionally, *Rocfrac* incorporates the new *Rocstar* framework.

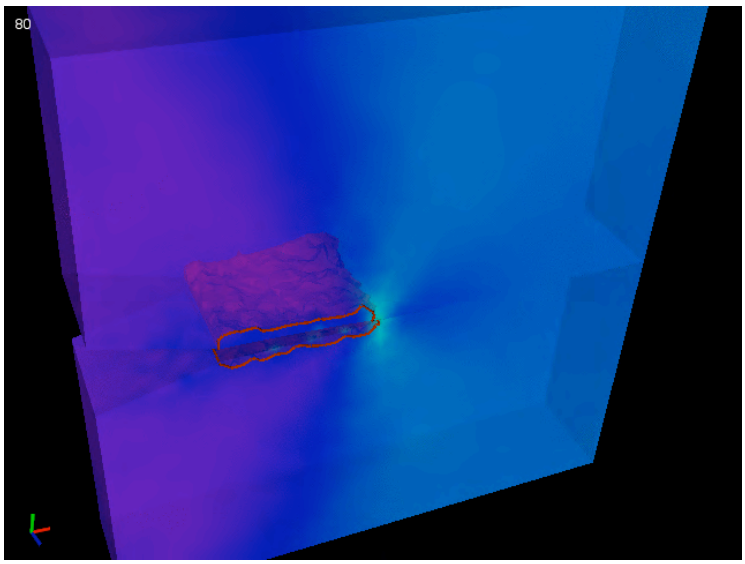

Fig. 3.5.2: Snapshot of elastic-plastic fracture of single edged notched specimen. Isosurface denotes edge of plastic zone and colors correspond to Von Mises stress. Load imbalance is consequence of computation expense of expanding plastic zone.

Future development goals focus on further expanding the rocket simulation capabilities of the code. Additional enhancements include: micro-mechanics based decohesion material models for the propellant response (in collaboration with Matous and Huang), the ability to handle non-matching meshes for propellant walk-back along the case, remeshing/mesh repair (in collaboration with the Meshing Group), and mesh adaptivity (in collaboration with the Computer Science team).

Rocsolid (Namazifard and Hjelmstad)

Rocsolid, the structural analysis code used in the rocket simulations employs a finite 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* can simulate large deformations and Arbitrary Lagrangian-Eulerian method is implemented for moving interfaces. The code is written in Fortran 90, and uses MPI to perform interprocessor communications.

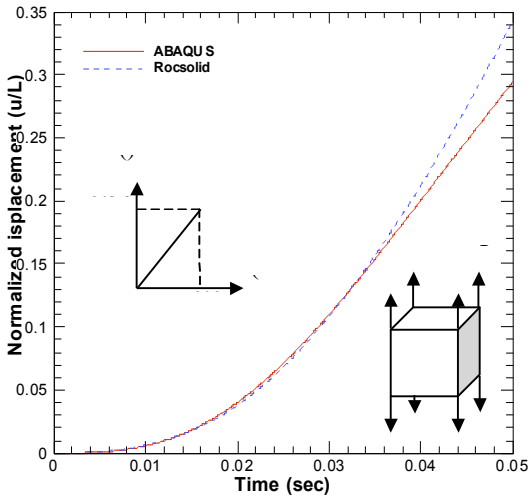

Figure 3.5.3:Benchmark analysis comparing porous viscoelastic model for solid propellant. Comparison is between *Rocsolid* and ABAQUS.

Availability of new material models in *Rocsolid* was the main focus last year to enhance our simulation capabilities. Several modifications were performed to change the material model implementation. In order to make the process of incorporating new constitutive models easier and more efficient, we decided to apply some important structural changes to the code. Material routines are now more modular and new models can

be implemented in the same fashion as ABAQUS UMAT procedures.

Improved constitutive models were added to *Rocsolid* including, incompressible Neo-Hookian and a porous viscoelastic model. A new J2 plasticity model was also implemented in addition to the framework needed for using Shur's compliment in the nonlinear solver. New constitutive modules are usually validated by solving simple problems and comparing the results with available experimental data. The porous viscoelastic model is more appropriate for the solid propellant where evolution of the voids plays a crucial role in the general response of the material. For this model, *Rocsolid* solution for a uniaxial tension problem was verified by comparing with the results obtained from ABAQUS (Figure 3.5.3). *Rocsolid* and ABAQUS give different results for large displacements because they use different strain measures. We also employed this model in a simulation for the Titan IV rocket. Figure 3.5.4 shows the porosity after 200 milliseconds at the stress relief groove where the slumping occurs. A larger initial porosity of 10% was chosen in this simulation. Once the rocket starts to pressurize, the void ratio begins to decrease. The red zones at the lower segments of propellant in this figure will eventually disappear at the later time. A higher ratio of porosity is observed at locations under tension (i.e., the tip of stress relief groove and adjacent to the case), which can be associated to the possibility of cracking at these places.

The study of stability problems in high pressure response was continued and a new stabilized mixed finite element method for finite elasticity is being incorporated into *Rocsolid*. Integration into *Rocstar* is also well under way and all the new modifications including the improved constitutive modules will be integrated into *Rocstar*.

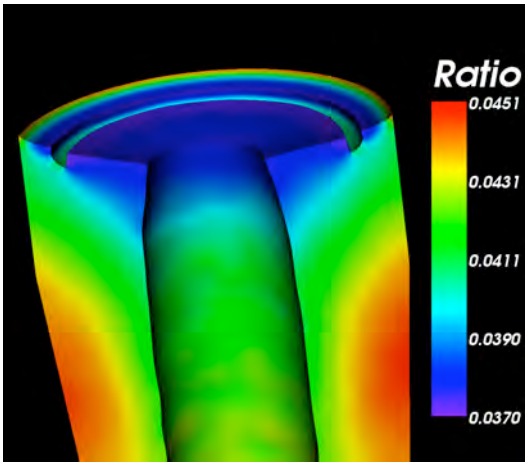

Figure 3.5.4: Titan slumping simulation showing evolution of porosity in tensile regions of solid propellant.

Future enhancements for *Rocsolid* will include new features that would not only help us to simulate solid propellant rockets more accurately, they would also make this module more suitable for other possible applications. Availability of the new stabilized mixed finite element method for finite elasticity (four node tetrahedral and eight node hexahedral elements) will also facilitate the modification of the ALE procedure to include large deformations and *Rocsolid* will benefit from any mesh modification or remeshing methods developed in the center using four node tetrahedral elements.

New material models including micromechanics will be helpful in getting more accurate response from the solid propellant. This will also construct a suitable framework for other physical applications involving similar materials. Explicit-implicit coupling of solid solvers are being investigated now and, once implemented, we would be able to simulate different regions of the computational domain using different time integrators.

Simulation Methods

Numerical Algorithms for Coupled Problems (Hjelmstad, Tortorelli, Namazifard, Nakshatrala, Prakash, Kulkarni, Turner, and Wasistho)

We have been focused on problems associated with the coupling algorithms for fluid/structure interaction. These discussions have included characterizations of multiple time stepping algorithms for coupled problems (Prakash), integration of elastoplastic material evolution equations (Kulkarni), im-

plementation of large deformation algorithms (Namazifard), implementation of the Sofronis constitutive model for SP (Namazifard), and stability of nearly incompressible elastic materials (Nakshatrala).

Kulkarni's Schur's complement scheme for the solving coupled nonlinear equations that arise in domain decomposition has been applied to resolve the coupled equations that arise in the mechanical analyses of complex materials (e.g., the viscoelastic propellant). In this latter application the need for time consuming local material point constitutive iterations has been eliminated. Simulations of the uniaxial tension of a bar modeled with an elastoplastic isotropic hardening material have demonstrated the effectiveness of his method.

Nakshatrala has used multiscale methods to stabilize the analyses of nearly incompressible materials that arise in propellant model. These developments also consider Arbitrary Eulerian Lagrangian (ALE) formulations and the mesh motion problem. Several improved mesh motion methods have been developed. To eliminate local element iterations, Kulkarni's Schur's complement scheme is combined with Nakshatrala's multiscale formulation. Finally, Nakshatrala has written both compressible and incompressible Neo-Hookean material models in an effort to more accurately model the propellant material behavior under large deformation. The improved accuracy will also eliminate instabilities that appear in some of our verification/validation analyses but do not appear to be associated with a physical instability.

Prakash has developed algorithms for utilizing different Newmark time-stepping schemes in various subdomains of the solid mesh (solid-solid coupling). The algorithm could be used to efficiently analyze dynamically growing microcracks (using small time steps in an explicit scheme) in the bulk propellant (using large time steps in an implicit scheme). Multiple subdomains and multiple time steps are accommodated by using the "tree" implementation of the Finite Element Tearing and Interconnecting (FETI) method. Nonlinearities are also treated. Initial verification has been completed using simple spring-mass models; verifications using three-dimensional finite element models are forthcoming.

Namazifard has continued his work to modularize and verify *Rocsolid*. Modular material subroutines routines are now available similar to the UMAT subroutines in ABAQUS. Using this modularity he implemented Nakshatrala's incompressible Neo-Hookean model and Sofronis' porous viscoelastic model to more accurately model the propellant. Kulkarni's elastoplastic isotropic hardening material model was also implemented with the intent of extending the Schur's complement algorithm to viscoplastic propellant material models. Verifications of the finite deformation features and Nakshatrala's stabilized finite elements for nearly incompressible material behavior were also performed. Namazifard has prepared the required input files (including mesh generation) for the RSRM inhibitor and full scale Titan IV rocket for use in the coupled simulations. He also completed the migration to *Rocstar*.

Tonks and Tortorelli have been developing an axi-symmetric FEM element that can be used to model the usual axisymmetric geometries, but with the ability to accommodate nonaxisymmetric loadings and material properties for both linear and nonlinear analyses. This work can be used to model the development of orientation distribution functions in polycrystalline metals, such as the casing. Additional efforts in this work have/will address the identification problem (i.e., the problem of using experimental data to garner the material parameter values for use in subsequent analyses). This latter effort will utilize sensitivity analyses and probability theory to assign the means and deviations of material parameters, based on the means and deviations of the experimental data. In this way we can assess whether or not a material parameter is needed, if it is influential, and if further experiments are required to discern its mean and deviation. Tonks has spent two summers at LANL as part of this project and will depart UIUC in January to finish his research at LANL.

In the coming year the group led by Hjelmstad and Tortorelli will continue to focus on algorithm developments associated with *Rocsolid*, as described above. Additional work will focus on the inte-

gration between the fluids, combustion, and solids codes, and specifically the development and verification of efficient, stable time integration of the coupled equations. A variety of implicit-explicit and explicit-explicit schemes will be developed, analyzed, and tested on a simple one-dimensional benchmark problem (the piston problem) to examine the advantages and disadvantages of the formulations. Specifically we will investigate accuracy, stability, convergence, and computational efficiency. Our findings will be integrated into the Rocstar codes.

Space-Time DG Simulation Methods (Haber, Hawker, and Palaniappan)

In conjunction with Jeff Erickson, Michael Garland, Laxmikant Kale and Robert Jerrard we continued to develop simulation technologies that build on the intrinsic properties of the space-time discontinuous Galerkin (SDG) finite element method. These include exact balance (or conservation) properties at the element level, O(*N*) computational complexity, greater flexibility for mesh adaptation than conventional methods and a rich parallel structure.

The completion of a new "Tent Pitcher" meshing software that supports *h*-adaptive analysis on unstructured space-time grids (2-D x time) represents a significant step forward. This software is implemented within an application–independent object-oriented framework, so its capabilities are immediately available to all of our solids and CFD applications. Compared with other finite element software, it delivers unprecedented solution resolution, even in serial, desktop implementations.

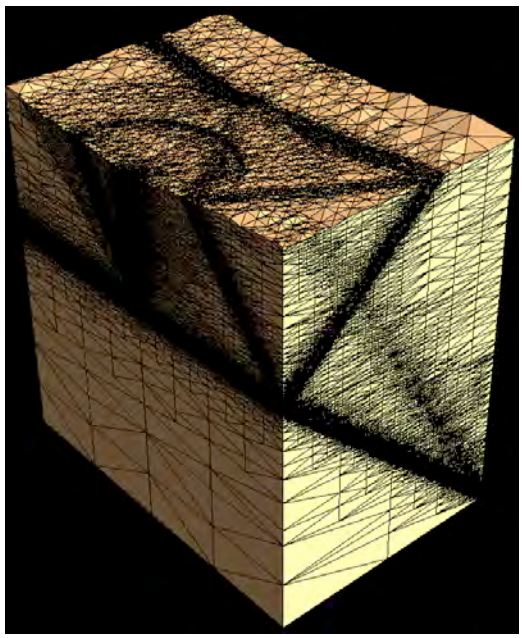

Fig. 3.5.5: Adapted space-time mesh for crack-tip wave scattering. Vertical axis represents time. Detailed shock trajectories are clearly evident in refinement pattern, including separation of dilatation, shear and Rayleigh surface waves. Maximum refinement ratio is 1024:1.

We extended our inviscid gas dynamics model (Euler equations) into 2-D x time; Figure 3.5.5 shows a solution for a Mach reflection that uses the space-time adaptive meshing capability. We added a cohesive damage model to our elastodynamics code and carried out simulations of fracture and particle dewetting in rocket grains subjected to shock loads.

Special visualization methods are required to display information computed on unstructured space-time meshes. We developed a per-pixel-accurate visualization system that exploits the programmable capabilities of the latest generation of graphics hardware to deliver high–fidelity renderings of our SDG solutions.

We completed and tested a parallel implementation of our SDG system that delivers linear scaling (tested on clusters of up to 64 processors) with better than 95% processor utilization. This initial implementation is limited to nonadaptive models; work is underway to remove this restriction.

Plans for CSAR–related work during the next year include:

- Generalization of the parallel code to provide load balancing in adaptive runs using *Charm++*
- Coupled simulations of fluid-solid interaction based on the elastodynamics and Euler codes
- Extension of Tent-Pitcher to track moving boundaries (e.g., for burn-back, phase change, etc.)

- Extension of the software for nonlinear conservation laws to handle Hamilton–Jacobi equations that describe the motion of moving interfaces
- Implementation of adaptive procedures to enforce cohesive models accurately
- Various production runs

We hope to begin work on extensions of this technology to 3-D x time in the spring. We're also starting to look at methods for solving elliptic and parabolic problems with this technology.

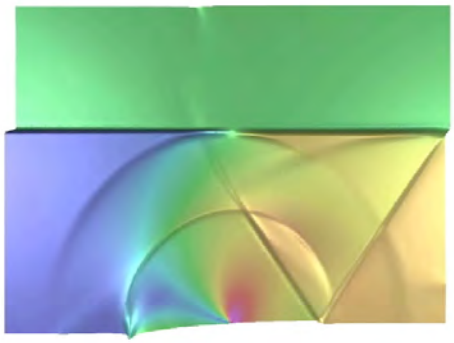

Fig. 3.5.6: Visualization of crack-tip wave scattering modeled by adaptive space-time discontinuous Galerkin finite element method. Light-source shaded height field indicates velocity magnitude; color field indicates strain energy density on logarithmic scale. One quarter of center–cracked plate subjected to shock loading is shown; crack tip is at bottom center.

Constitutive Modeling

A key component of the activities of the Structures and Materials Group involve the constitutive modeling of the materials present in the rocket, with special emphasis on the modeling of the solid propellant. This modeling effort takes place at a wide range of length scales, from the microscale with the discrete molecular dynamics simulations of the dynamic response of heterogeneous materials, to the mesoscale with continuum description of damage evolution in SP that accounts for its particle reinforcements, and to the macroscale, with fully homogenized description of the material response incorporated in the two structural solvers, *Rocfrac* and *Rocsolid*.

Micromechanics Modeling (Huang, Sofronis, Xu, and Zhou)

Two complementary micromechanics-based constitutive modeling effort are currently underway: the first one, led by Huang, aims at modeling the particle debonding process (often referred to as *dewetting* in the SP community), while the second, led by Sofronis, focuses on the evolution of voids present in the viscoelastic binder.

Since many of the damage mechanisms present in SP are similar to those observed in other heterogeneous energetic materials, such as explosives, Huang and his coworkers have been collaborating extensively with scientists at LANL Laboratory to develop the constitutive models of solid propellants and high explosives accounting for the effect of particle dewetting from the binder matrix in these materials. They have used the homogenization technique such as the Mori-Tanaka method to study the effect of nonlinear interface debonding on the constitutive behavior of solid propellants. The interface debonding is characterized by a nonlinear cohesive law determined from the fracture test conducted at LANL (Figure 3.5.7). Over the past year, they have established a general theoretical framework to

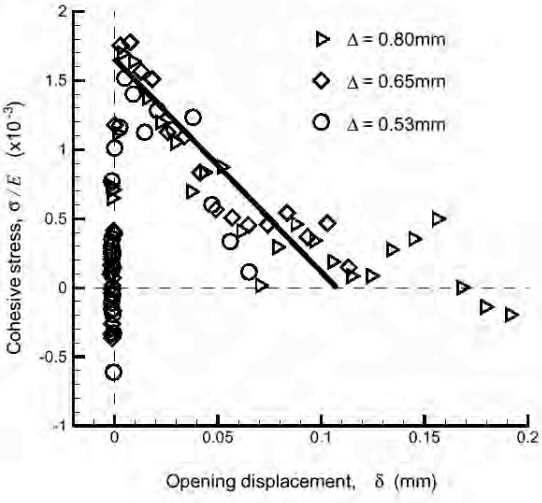

Fig. 3.5.7: Cohesive law for high explosive PBX 9501 under quasi-static loading condition

incorporate the nonlinear cohesive law of the particle/matrix interface. The nonlinear behavior of the solid propellants is predicted in terms of the properties of the energetic particles, binder matrix, and interfaces. It is established that the size of energetic particles has an important effect on the constitutive behavior of the solid propellants, namely hardening for fine particles and softening for coarse particles. The critical particle size that separates the hardening and softening behavior of the solid propellants is obtained analytically. For the solid propellants with large particles, the particle/matrix interface may under catastrophic debonding, i.e., sudden, dynamic debonding even under static load. The energy release during catastrophic debonding can be very large, thus may trigger the detonation of solid propellants and the high explosives. For the high explosive PBX 9501, the energy release due to catastrophic debonding of coarse (large) particles is equivalent to the free drop of the high explosive from a height of 110 meters.

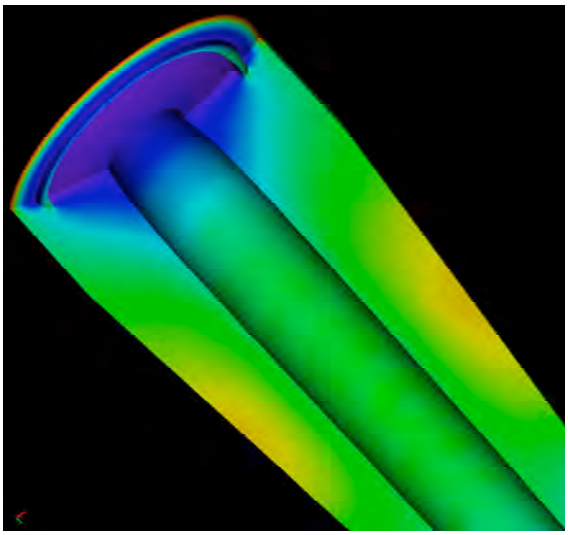

Fig. 3.5.8: Numerical simulation of Titan IV grain slumping accident, showing enhanced porosity at bottom of groove and propellant/case interface.

To address the continuously evolving microstructure upon dewetting, Sofronis and co-workers have developed over the past year a more sophisticated damage model that is based on non-linear homogenization theory and accounts for nonlinearity in the viscoelastic response of the binder. This "finite-strain" model takes into account the possible growth of voids and the resulting changes in the volume fractions of the different phases as the material deforms. The predictions of the model in uniaxial tension response at constant strain rate provide very good agreement with the experiment over a wide range of applied strains and strain rates. Another key accomplishment is the incorporation of the damage model into the implicit structural solver *Rocsolid* and its application to the Titan IV grain slumping problem. As shown in Figure 3.5.8, integrated simulations of this accident scenario have revealed enhanced porosity at the bottom of grooves and the propellant/case interface, the sites where cracking of the grain has been observed to initiate.

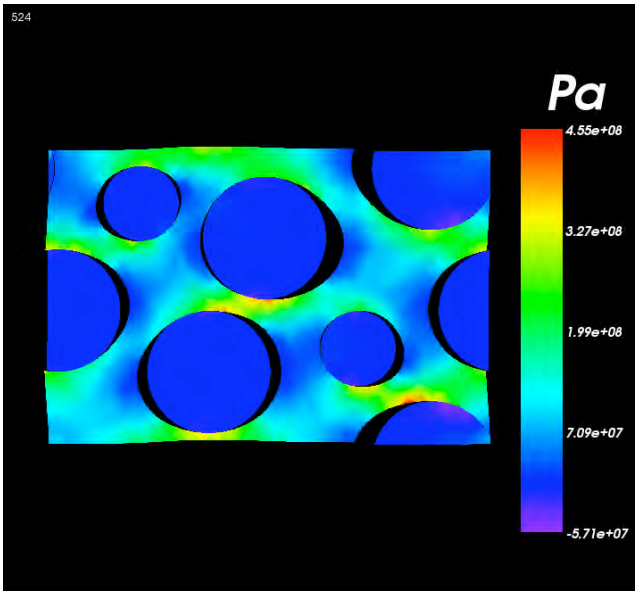

Fig. 3.5.9: 2-D analysis of debonding of particles in periodic RVE showing heterogeneous stress distribution.

Mesoscale Modeling (Mateous, Geubelle, and Inglis)

Complementing these two micromechanical modeling efforts, Matous, Geubelle and co-workers have been developing a hierarchical multiscale framework to simulate damage in SP, starting at the mesoscale with detailed 2-D and 3-D cohesive-volumetric finite element (FE) descriptions of the damage process that captures the heterogeneous stress and strain fields in a representative volume element (RVE) including a set of AP particles and a binder

blend (Figure 3.5.9). A new class of stable finite elements has been developed to improve the accuracy and efficiency of the FE solution of the near-incompressible matrix material (binder). The mathematical theory of homogenization has been employed and implemented in both 2-D and 3-D. This theory with natural scale bridging mechanism is used to predict both the meso- and macro-scale behavior of SP under progressive debonding. The other key component of the hierarchical constitutive model is a state-of-the-art micromechanics model, based on the Hashin-Shtrikman variational principle, that has also been derived for the damage evolution in particulate reinforced elastomers. The next step consists in developing and implementing accurate error measures allowing for an adaptive transition between the various components of the model hierarchy.

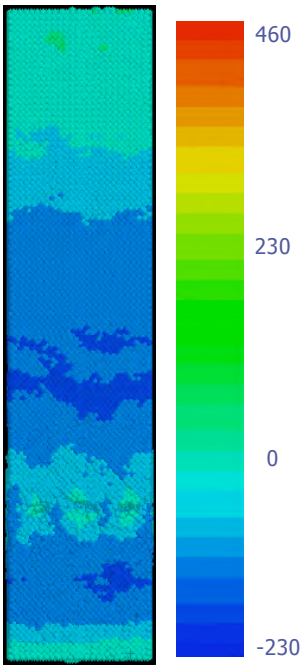

Fig. 3.5.10: Cross section of 3-D pressure analysis for 10% vacancies at interface at 15ps. The unit is in kbar. Pressure release at interface is accompanied by void formations.

Atomic Scale Modeling (Averback, Li, and Ashkenazy)

At a much lower physical scale, Li, Ashkenazy and Averback have conducted large-scale Molecular Dynamics (MD) studies on both homogeneous and heterogeneous metal systems. The goal is to understand shock wave propagation in such a system, its interaction with interfacial defects, and shock wave induced temperature, pressure, and microstructure change in the materials system (Figure 3.5.10). Such work is closely related to hot spot generation in energetic materials for rocket applications. For this work, empirical potentials in the Embedded Atom Method (EAM) framework were adopted for Cu and CuTi, and another potential having the same lattice constant and cohesive energy as Cu but with the mass of Au. This computational trick was employed to create a heterogeneous interface, but one that eliminates any possible effects at the interface arising from strain due to a lattice mismatch or weaknesses due to bonding. In addition to the potential construction, interfacial defects in the form of vacancies and at different fractions are deliberately introduced into the computational models for the purpose of evaluating their effects on shock propagation and dynamic failure process. Visualization of atomic structure change is extremely important in understanding shock physics. Atomic positions, velocities, and virials are output at relevant time intervals from the parallel MD code, and a series of subsequent data analyses for atomic microstructure, temperature, pressure, and defect structures are performed for each set of output data. Several codes have therefore been developed for the data analyses. The state-of-art spatial decomposition algorithm was implemented in these codes, which tremendously improved the efficiency in data analysis. An accurate method was also developed for calculating atomic volumes, which is needed for the calculation of pressure.