3.5 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: (1) system simulation, primarily by finite element methods, and (2) constitutive and failure modeling of components and materials. The technology developed in both of these general areas migrates, 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). In addition to these two key activities, the S&M Team has been involved, in collaboration with members of other research teams, in integrated simulations of subscale multiphysics problems such as the convective burning of cracks in energetic materials and the mesoscale modeling of burning in a damaged solid propellant. The following sections describe the research accomplishments of the past year.

Integrated Simulation Codes for Structural Response

Substantial progress has been made in the further development and integration of the explicit (*Rocfrac*) and implicit (*Rocsolid*) structural solvers, which are part of the integrated rocket code.

Rocfrac (Breitenfeld, Collins, Matous, and Geubelle)

The development of *Rocfrac* has made rapid progress since its inception at the start of CSAR. The material models have advanced from linearly elastic to hyperelastic and viscoelastic propellant material models, and *Rocfrac* has recently added micro-mechanical models in an effort to improve upon the constitutive behavior of the propellant, including the effects of particle dewetting. The concept of cohe-

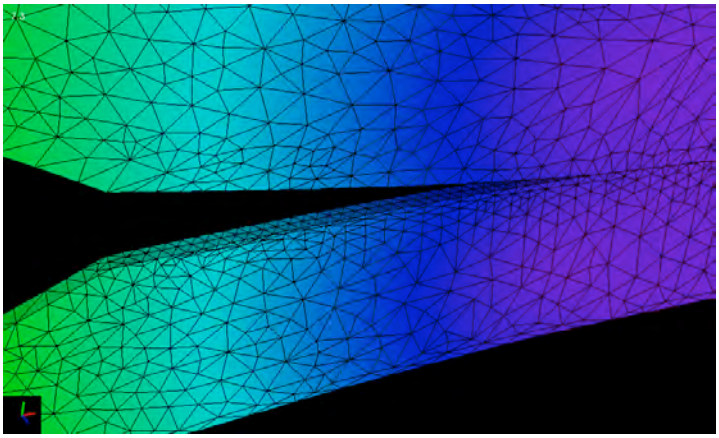

Fig. 3.5.1: Dynamic fracture of Double Cantilever Beam (DCB) specimen modeled with 3D non-matching cohesive finite elements.

sive elements for the study of fracture events is the hallmark of *Rocfrac*, and a recent feature is a cohesive element developed for non-matching meshes (See Figure 3.5.1). This special cohesive element will model the insulation between the case and the propellant and will allow for the use of 8-node mixed-enhanced hexahedral elements for the case and 10-node tetrahedral elements for the propellant. Furthermore, the use of non-matching cohesive elements will allow for burn back of the propellant along the case. Another recently added feature is the solution of the transient heat equation within the ALE framework for coupled thermal-mechanical simulations. This addition allows for the solution of the full 3D temperature field for simulations of convective burning of cracks in solid propellant and other energetic materials. The inclusion of these advanced physics would ordinarily increase the solution time substantially, but due to the remarkable scalability of *Rocfrac* it has had little impact on the overall solution time for the simulations.

Since the pinnacle of *Rocfrac* is the cohesive element concept, future efforts will focus on adaptive activation of cohesive elements and mesh refinement. For the adaptive activation of cohesive elements and adaptive mesh refinement we are using the Parallel Programming Laboratory's (Department of Computer Science, UIUC) FEM framework to handle the following: parallel load balancing, adaptive meshing, and activation of cohesive elements. Additionally, research and implementation of micro-mechanical constitutive models for the propellant will continue. Future features include the ability to adaptively switch to micro-mechanical modeling when the physics warrants it, e.g., a region surrounding a crack tip.

Rocsolid (Namazifard and Hjelmstad)

New Constitutive Material Models in *Rocsolid*: One of the required components in simulating solid rocket motors is computing the structural response of the propellant, case, liner and nozzle. Our parallel structural analysis code *Rocsolid*, 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. The case of the rocket is modeled by using enhanced assumed strain solid elements. The regression of the propellant is implemented by using an arbitrary Lagrangian-Eulerian (ALE) approach in which the mesh moves to allow for the dynamically changing geometry. The code is written in Fortran90, and uses MPI to perform interprocessor communications.

Large deformations are formulated using strains-stresses and their rates defined on an unrotated frame of reference. This model predicts physically acceptable responses for homogeneous deformations of exceedingly large magnitude. The implemented numerical algorithm is suitable for the large strain increments, which may arise in the implicit solution of the global equilibrium equations, employed in *Rocsolid*. The finite rotation effects on strain-stress rates are separated from integration of the rates to update the material response over a time step. This formulation is also adopted in large-scale finite ele-

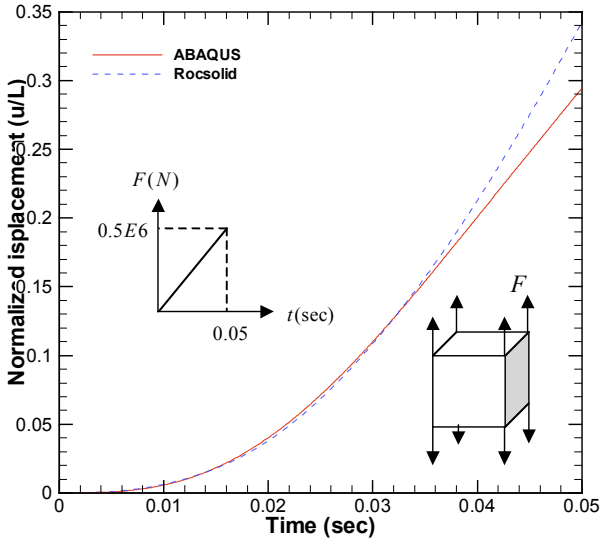

Fig. 3.5.2: Comparison to Abaqus simulation for porous viscoelastic material model.

ment codes, including NIKE, Abaqus-Standard, and Abaqus-Explicit.

Two different constitutive models for solid propellant materials are available in *Rocsolid*. The first model describes a porous viscoelastic material, i.e., the effect of damage-induced porosity on the constitutive behavior of a solid propellant. The presence of porosity is considered to be a result of complete particle dewetting. The material model is developed by considering a unit cell containing a spherical void under macroscopic axisymmetric stressing. In view of the complexity of the calculations, the pure matrix material is assumed to be described by the standard isotropic linear viscoelastic model. The model is based on small strain formulation. Using the correspondence principle of linear viscoelasticity, a constitutive potential is devised for the response of the porous medium in the transformed domain. By inverting the associated constitutive equation from the Laplace transform domain, the time-dependent response of the porous medium under time-dependent loads is established.

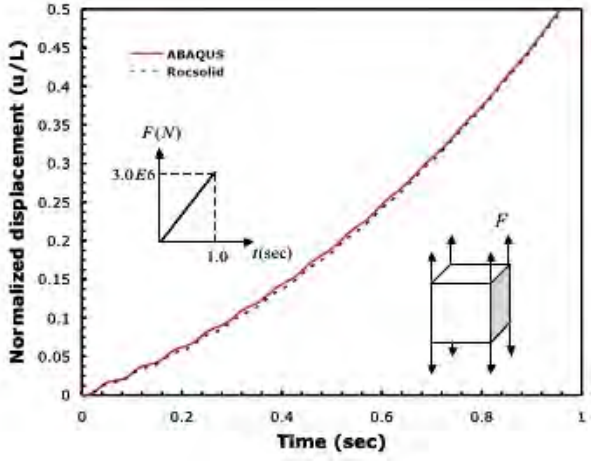

Fig. 3.5.3: Comparison to Abaqus simulation for nonlinear composite material model

The second model (available in the latest version of *Rocsolid*) is a mechanism-based constitutive model using state-of-the-art homogenization procedures for nonlinear composites. The model accounts for the evolution of the microstructure upon straining as is demonstrated by void formation and growth. Since the model addresses the underlying material deformation mechanisms, the model parameters can be determined experimentally. Using this model, the prediction that there are three regimes of deformation for a typical solid propellant material, namely linear, hardening, and softening agrees well with experiment. Also in qualitative agreement with the experiment is the dependence of the response on the strain rate.

Verification of the Material Models Implementation: The solid propellant material models were originally implemented and tested in Abaqus through "User Material" subroutines. In order to verify the numerical procedures in Rocsolid and test the implementation of these constitutive models, results are compared for a uniaxial tension problem. Figure 3.5.2 shows the displacements computed by *Rocsolid* and Abaqus using the porous viscoelastic material model. Since this model is based on small strain formulation, the results do not match as well for very large displacements. The difference for larger strains, when the nonlinear geometric option is active, is caused by different stress rates used in Rocsolid and Abaqus. Figure 3.5.3 shows the comparison between *Rocsolid* and Abaqus for the nonlinear composite material model. The results are in complete agreement through out the solution of a uniaxial tension test problem.

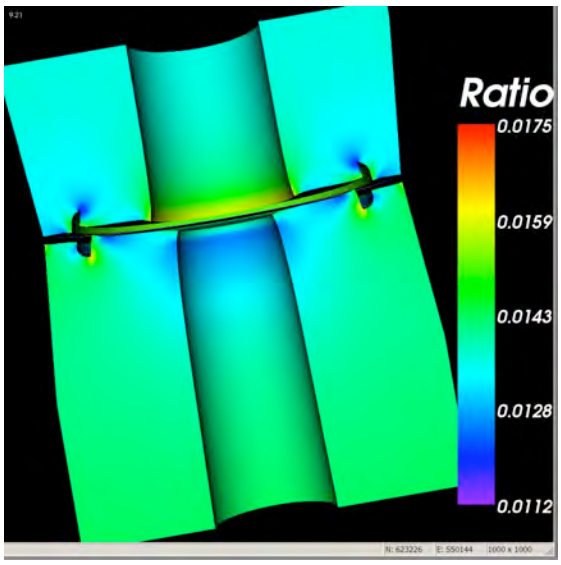

Fig. 3.5.4: Porosity distribution in propellant of Titan IV rocket motor near stress relief groove

Application to Titan IV Slumping Problem: The damage constitutive models available in Rocsolid were used to simulate Titan IV SRMU PQM-1 slumping problem. The generated mesh for this rocket motor consisted of 1,753,600 elements. A coupled fluid-structure-combustion simulation was performed, where the solid propellant was modeled by the porous viscoelastic material model and the predictor-corrector iterations were employed to enhance the stability of the coupling algorithm. The material parameters chosen for this simulation can be found in [Xu et al. AIAA2005] and the time step size was 0.0004 second. Figure 3.5.4 shows the porosity distribution in the deformed grain. The results indicate severe porosity presence at the stress relief groove and the grain/case interface where cracking was observed to initiate during testing.

We also employed the nonlinear composite material model available in *Rocsolid* in a structural analysis of the same Titan model. As a prelude to a complete coupled analysis, a uniform pressure was applied over the exposed surfaces of the propellant and increased linearly in time up to 7 MPa. For the parameters used in the material model, see [Aravas et al. AIAA2005]. Figure 3.5.5 shows the voids generated in the propellant around the joint slot as the result of particles dewetting. It also shows the deformation caused by the internal pressure. This result is similar to the response achieved with the previous material model. Since this model considers complete geometric nonlinearities, more accurate response is expected from the simulation.

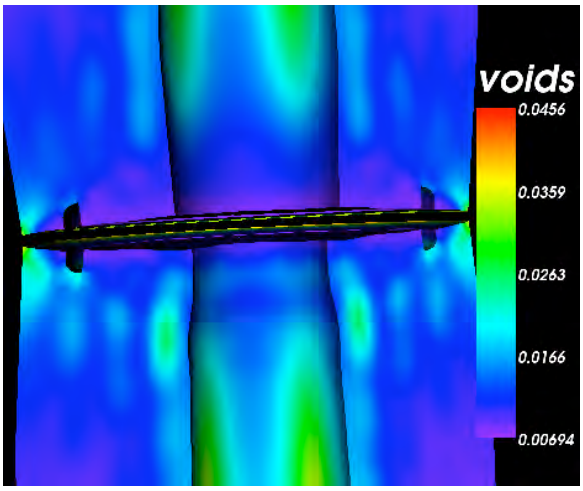

Fig. 3.5.5: Distribution of voids generated by dewetting of particles in Titan IV rocket motor grain

Multiphysics Coupling Algorithms: Our multiphysics code for rocket simulation Rocstar, contains physics modules for solids, fluids and combustion together with software for data transfer and interpolation between non-matching meshes. *Rocsolid* and its nonlinear material models for solid propellant are part of the *Rocstar* framework. Several numerical methods have been constructed and implemented in multiphysics simulation softwares to compute the response of coupled problems. To achieve modularity, partitioned schemes (also known as staggered schemes) are developed where most popular existing modules for the separate resolutions of fluid and structural parts can be coupled. This allows independent treatment of each part and even performing the computation on separate heterogeneous machines. Though the methods used in each module usually have well known decoupled stability limits, the stability of the coupled scheme for a nonlinear problem is unknown.

We investigated the stability characteristics of a few popular coupling algorithms available in *Rocstar*. We considered fluid-structure interaction (FSI) problems for this purpose. A simple coupled problem was analyzed to demonstrate stability of these methods.

Some of the coupling schemes in this investigation were: basic staggered coupling algorithm, basic staggered coupling algorithm with different predictors, staggered coupling algorithm with predictor-corrector and improved second-order staggered scheme. [Namazifard et al. AIAA2005] contains a summary of the results observed in the analysis of these methods. Among the coupling schemes available in *Rocstar*, application of staggered coupling algorithm with predictor-corrector results in a more significant improvement in the stability behavior of coupled system compared to other methods (Figure 3.5.6).

Future Plans: 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. Explicit-implicit coupling of solid solvers is being investigated now and once implemented, we would be able to simulate different regions of the computational domain using different time integrators. 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 repair or remeshing methods developed in the center using four node tetrahedral elements.

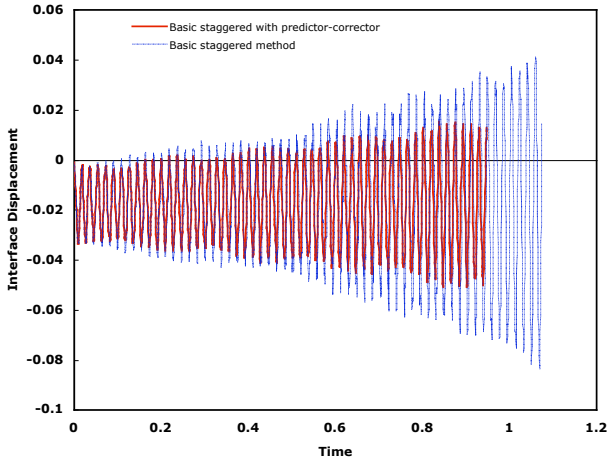

Figure 6. Effect of predictor-corrector iterations on stability of basic staggered coupling algorithm. Time step size is 0.0005

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. Parallel contact formulation is another research topic in our group that would give *Rocsolid* contact simulation capability.

Simulation Methods

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

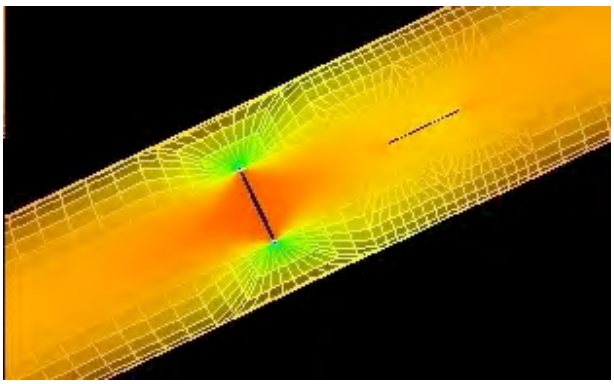

Fig. 3.5.7. Stress response of rocket case with cracks subjected to sudden head pressure. Obtained with multi-time step coupling method with time step ratio 10 between subdomains.

Keith Hjelmstad, Dan Tortorelli, Ali Namazifard, Kalyan Nakshatrala, Arun Prakash, Deepak Kularni (CPSD), Dan Turner, and Bono Wasistho, 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 (Arun), integration of elastoplastic material evolution equations (Deepak), implementation of large deformation algorithms (Ali), implementation of the Sofronis constitutive model for SP (Ali), and stability of nearly incompressible elastic materials (Kalyan).

Kalyan has developed a mixed stabilized finite element formulation for the Darcy flow equations based on the Hughes Variational Multiscale (HVM) principle. We refer to this new mixed stabilized finite element formulation as the HVM formulation. We have also developed a systematic procedure to derive the stabilization parameter, and even the stabilization terms are an outcome of this derivation. The procedure employs the notion of multiscale decomposition of the velocity field. A salient feature of the HVM formulation is that there are no mesh-dependent parameters. A major contribution

of this work is the numerical extension of the continuous *v-p* formulation to three-dimensional problems. We have studied the performance of the HVM formulation for various three-dimensional finite elements. Numerical tests were performed for equal-order linear and quadratic brick, tetrahedron and wedge elements, with continuous velocities and pressures. The convergence rates obtained for these elements are in accord with the theory. It has been shown that the HVM formulation passes the three-dimensional constant-flow patch tests even for elements with non-constant Jacobian. To the best of our knowledge, no previous formulation with continuous-field interpolation for the velocity and pressure performs satisfactorily for three-dimensional patch tests using elements with non-constant Jacobian. In particular, the popular Raviart-Thomas element does not pass constant-flow patch tests in three dimensions. Robustness of the HVM formulation was illustrated via numerical simulations of resin injection during GFRP manufacturing process of a complex geometry.

Arun 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 his recursive coupling implementation of the Finite Element Tearing and interconnecting (FETI) method. The method has been extended for non-linear problems and verified for a variety of problems including non-linear elastic and inelastic materials. An efficient parallel implementation of the same using MPI is under way. Future efforts will be directed towards benchmarking the performance of his coupling method in comparison to the uniform time step approach.

Deepak'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.

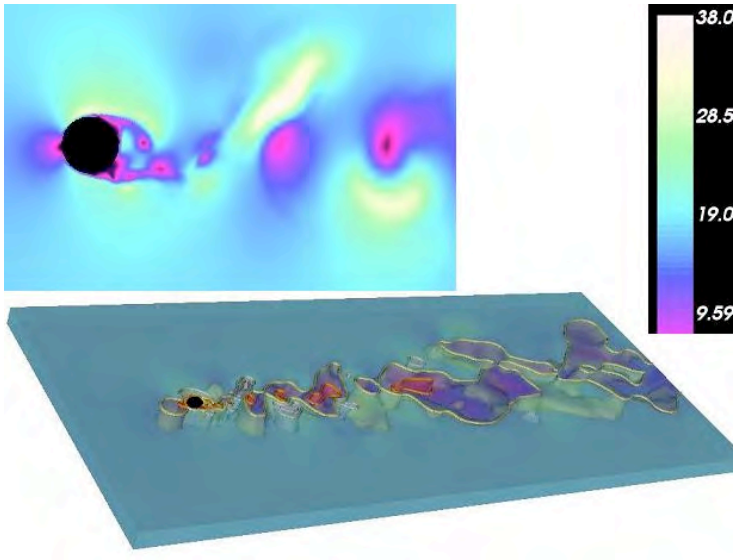

Fig. 3.5.8: Fluid Velocity for flow around cylinder showing vortex shedding.

M. Tonks and D. Tortorelli have been developing an axisymmetric 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 poly crystalline 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 ex-

periments are required to discern its mean and deviation. Mike has spent two summers at LANL as part of this project and will depart UIUC in January to finish his research at LANL.

Dan Turner is studying the flow characteristics around a flexible cylinder. Literature in fluid mechanics contains a wealth of information about flow past a cylinder, but mostly for cases in which the cylinder is rigid. This research investigates changes in flow patterns and the resulting structural forces as the flexibility of the cylinder is incorporated into the analysis. This fluid-solid interaction problem reveals important information that can be used in the design of tall buildings or other structures subject to excessive wind loading. Preliminary results exhibit a Strouhal number for the rigid cylinder of 0.22 , which is slightly higher than the common value of 0.18 in the literature. This difference may be due to the turbulence modeling used in the analysis and may reduce with more numerical fine tuning. Results also show the appearance of alternate modes in the vortex shedding for the flexible cylinder case. This summer, he participated in an internship with Sandia National Labs and worked on coupling a number of independent physics codes to analyze objects heating up in a fire.

In the coming year the group led by Hjelmstad and Tortorelli will continue to focus on algorithm developments associated with the solid code *Rocsolid*, as described above. Additional work will focus on the integration 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 for Multiphysics Rocket Simulation (Haber, Palaniappan and Hawker)

We continued to develop simulation technologies that build on the intrinsic properties of the spacetime discontinuous Galerkin (SDG) finite element method. These include exact balance properties at the element level, O(*N*) computational complexity and greater flexibility for mesh adaptation than conventional methods.

A major revision and expansion of the adaptive spacetime meshing code is mostly complete; it provides a larger vocabulary of adaptive operations, including spacetime edge flips and vertex deletion/insertion. Provisions for inclined tent poles support mesh smoothing and tracking of moving interfaces. Adaptive operations are accomplished in spacetime with zero projection error. Modulo on–going tuning and testing, these capabilities complete our planned research program for meshing in 2D x time, paving the way for meshing in 3D x time.

Morgan Hawker implemented an adaptive cohesive failure model that is the first to guarantee satisfaction of the cohesive traction–separation relation to within specified error tolerances. This approach yields unprecedented resolution and led to the discovery of a crack-tip velocity singularity for dynamic cohesive crack growth (Figure 3.5.9) — an unexpected result with significant physical implications.

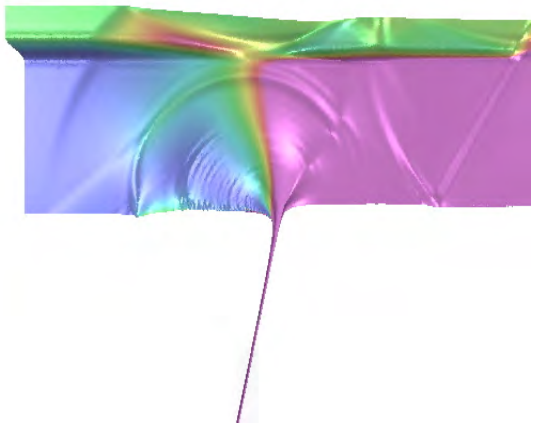

Fig. 3.5.9: Elastodynamic cohesive crack propagation due to shock loading. Newly–discovered velocity singularity is visible as crack tip propagates to right. Color indicates strain energy density and the height field (positive out of page) indicates velocity magnitude. Symmetry conditions model cohesive zone along bottom edge to right of crack tip.

We implemented a unified software architecture to facilitate adaptive multi-physics simulations. Jayandran Palaniappan used this framework to combine our elastodynamics and gas dynamics codes in a fluid-structure interaction model with exact element–level balance between the phases. The method is free of spurious oscillations around shocks, as occur in some other methods. We are currently integrating this code with the new adaptive front–tracking capabilities to simulate burnback in solid fuel engines.

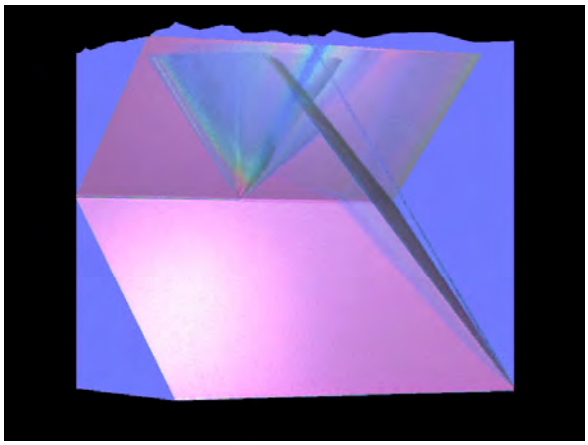

Fig. 3.5.10: Spacetime visualization of shock trajectories in crack–tip wave scattering. Vertical axis is time. (Visualization by Y. Zhou and M. Garland)

Our results demonstrate that the SDG approach addresses a number of drawbacks in conventional methods to deliver superior accuracy. Our new findings in cohesive fracture demonstrate the importance of computational technique in making valid scientific predictions. However, the restriction that continuing work must focus on the *Rocstar* software precludes a continuation proposal for this work within CSAR. We will make further results available to CSAR as we complete our current studies.

Constitutive Modeling

This section summarizes recent advances in the wide range of modeling efforts in the constitutive and failure response of the solid propellant and the metallic case. These constitutive modeling efforts take place at a wide range of length and time scales, and special effort has been placed over the past year in developing computational methods and framework to link these various scales.

Multiscale Modeling of Damage in Solid Propellant (Matous, Inglis and Geubelle)

Substantial progress has been made in the area of the multi-scale numerical modeling of the damage evolution in solid propellants. The framework of hierarchical numerical modeling has been formulated and work has begun on the calibration of the micromechanics-based models used in the Rocstar suite. The 3D numerical apparatus, including the implicit cohesive model, has been created for nearly incompressible solids subjected to finite deformations. This model allows in detail studies of damage evolution in solid propellants. Furthermore, we have developed the high-performance parallel multiscale solver, which will be used to investigate more complex and representative 3D unit cells. In addition, a 2D semi-explicit scheme consists of cohesive and volumetric response has been derived and implemented. The mathematical theory of homogenization has been employed and implemented in both 2D and 3D theories (Figure 3.5.11). This theory with natural scale bridging mechanism is used in predicting both meso and macroscale behavior of the solid propellant under progressive debonding. Thus using the 3D and 2D theories, low-resolution models such as micromechanics will be enhanced by the multiscale analysis corrections in order to capture the complex mechanical behavior of heterogeneous solid propellants. Moreover, we have created the module to compute the probability functions of first and second order to characterize the propellant. Such characterization will be used for the periodic unit cell construction, which has the same and/or similar statistics as the original pack generated by *Rocpack* code.

The proposed work for the final two years is focused on the multi-scale modeling of the complex material behavior. The hierarchical approach will be continuously integrated into *Rocstar* and should substantially improve the existing framework. The complicated material systems, particularly the class of reinforced elastomers, can be studied with great accuracy and efficiency. First, the microme-

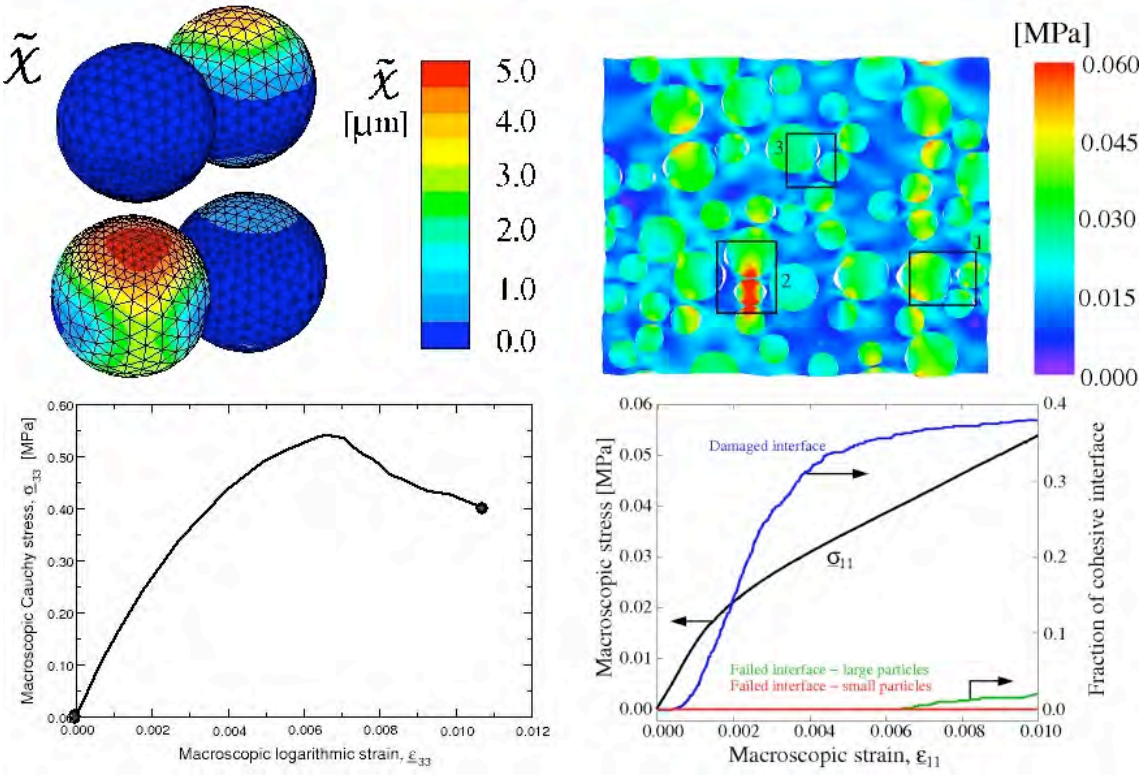

Figure 3.5.11: Multiscale analysis of constitutive response of reinforced elastomers in 3D (left) and 2D (right). Upper figures provide some details on microstrctural solution (effective displacement jump along reinforcing particles on left and heterogeneous effective stress on right), while lower ones present macroscopic stress-strain responses.

chanics based theories integrated in the *Rocstar* will be calibrated and enhanced by the multiscale solutions. Next, the mathematical theory of homogenization will be employed to study particular loading histories. The 3D multiscale solver will be completed to allow for particle debonding also. The unit cell construction procedures will be completed both in 2D and 3D in order to reduce the number of particles, but preserve the correct statistics of the investigated packs. The correct description of the underling physics will improve upon existing theories and will be applicable in many *Rocstar* applications.

Multiscale Cohesive Modeling Framework (Matous and Geubelle)

Over the past year we have derived a novel multi-scale cohesive modeling framework, incorporating the important physical processes in the adhesive/interfacial layer and allowing for the natural scale bridging. Such theory is advantageous in cohesive failure mechanisms and can capture physical phenomena missed by the most conventional approaches. The proposed method for coupling the macro- and micro- domains relies on a hierarchical decomposition of the approximation space. At the macroscale, we define the cohesive layer kinematics in order to obtain the strain of the adhesive layer in terms of the displacement jump, across the cohesive faces (Figure 3.5.12). The material periodicity is assumed in the discontinuity plane and an asymptotic expansion is employed, whereas the intrinsic cohesive length scale, defined by the layer thickness, is introduced and the space dimension reduction is performed perpendicular to the interface. The macroscopic displacement jump across the adhesive layer is then used as a forcing term in order to derive the homogenized cohesive traction-separation law used at the macro-scale by the common-refinement cohesive elements. This framework will be

very advantageous in modeling the heterogeneous insulation layer and allow for accurate mode mixity.

In the remaining two years, we will focus on completing multiscale cohesive model development. Efficient and accurate damage mechanisms will be incorporated into the multiscale cohesive finite element code. We will also employ the mesh localization limiters to eliminate mesh bias. The multiscale cohesive module will be then employed in the *Rocstar* framework in order to model the insulation between the grain and the case. This will likely be done through the look-up table pre-computed for several loading histories and insulation layer configurations. The correct description of the underling physics will improve substantially upon existing theories and will be applicable in many *Rocstar* applications, while providing great flexibility when used in conjunction with the aforementioned non-matching cohesive element method.

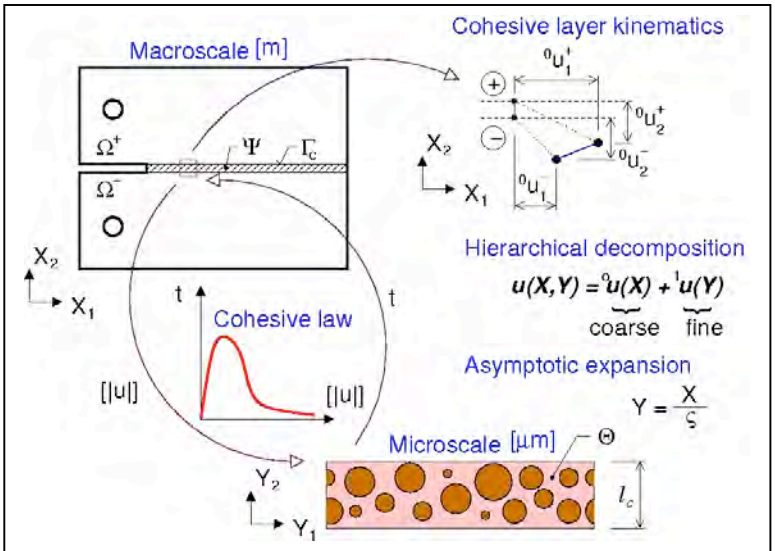

Fig. 3.5.12: Multiscale cohesive modeling heterogeneous adhesive. Macroscopic and microscopic domains and cohesive layer kinematics.

Micromechanics Modeling of Particle Dewetting in Energetic Materials (Huang)

In collaboration with scientists at Los Alamos National Laboratory, we have developed a constitutive model for solid propellants and have extended it high explosives accounting for the effect of particle dewetting from the binder matrix. We have implemented the constitutive model in Rocfrac, and it has been used in the simulation of advanced rockets. The debonding of particle/matrix interfaces has an important effect on the macroscopic behavior of solid propellants and high explosives. There are extensive analytical and numerical studies on interface debonding in composite materials based on cohesive zone models which assume a phenomenological relation between the normal (and shear) traction(s) and opening (and sliding) displacement(s) across the particle/matrix interface. However, there are little or no experiments to determine the cohesive law for particle/matrix interfaces in composite materials. In collaboration with Los Alamos National Laboratory, we have developed a method to determine the cohesive law for particle/matrix interfaces in the high explosive PBX 9501 and in solid propellants. We use the digital image correlation technique to obtain the stress and displacement around a macroscopic crack tip in the modified compact tension experiment of PBX 9501. The extended Mori-Tanaka method (which accounts for the effect of interface debonding) and the equivalence of cohesive energy on the macroscale and microscale are used to link the macroscale compact tension experiment to the microscale cohesive law for particle/matrix interfaces. Such an approach enables us to quantitatively determine key parameters in the microscale cohesive law, namely the linear modulus, cohesive strength, and softening modulus of particle/matrix interfaces in the high explosive PBX 9501 and solid propellant. The present study shows that Ferrante *et al.*'s (1982) cohesive law, which is established primarily for bimetallic interfaces, is not suitable to the high explosive PBX 9501 nor to solid propellants.

Micromechanics of Damage in Solid Propellant (Xu, Aravas and Sofronis)

A nonlinear, "finite-strain," 3-D, constitutive model for solid propellant materials in the presence of continuously evolving microstructure due to particle dewetting has been developed and implemented in *Rocsolid* through an Abaqus type "User Material" subroutine. The model is based on rigorous homogenization theory for nonlinear viscous-matrix composites and accounts for particle dewetting and void growth. The predictions of the model in uniaxial tension at a given strain rate are in excellent agreement with the experiment (Figure 3.5.13) even for high elongation solid propellants over a wide range of applied strains and strain rates. The model is currently used to investigate the small scale yielding behavior ("boundary layer" formulation) of a solid propellant at a crack tip. Possible scaling of the solution is currently being explored in an effort to establish a fracture criterion based on crack advance resulting from severe damage accumulation at a notch root. Since an essential component of the model is a physically sound dewetting criterion, research was carried out on the micromechanics of particle dewetting. It is for the first time that a rigorous criterion for particle dewetting has been established by accounting for the viscous response of the binder. The criterion that is based on the energy changes upon dewetting predicts a critical dewetting stress which is very sensitive to the particle/binder interfacial energy. The important implication of this result on the manufacturing of solid propellants is obvious.

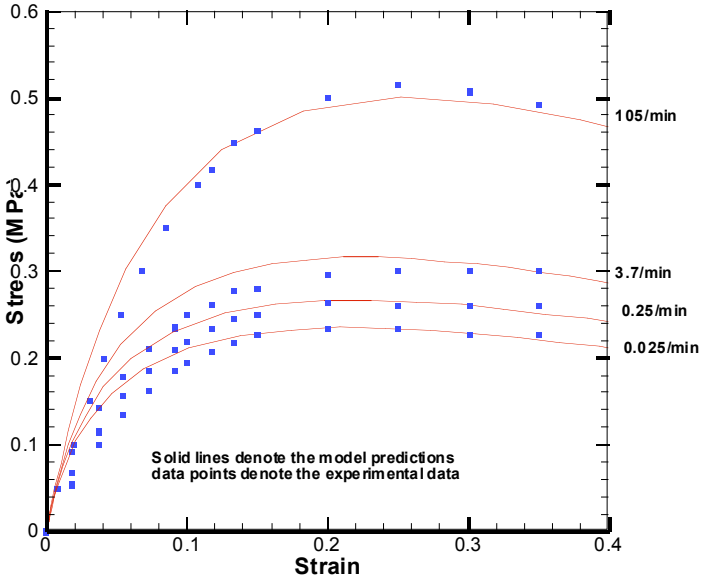

Fig. 3.5.13: Model predictions in uniaxial tension compared with experimental data for high elongation solid propellant under various applied strain rates. Model accounts for nonlinear viscous response of binder and allows for void opening and growth due to particle dewetting.

To promote our research collaboration with the Lawrence Livermore National Laboratory (Roger Minich, contact scientist), research will be carried out on the study of void collapse under projectile impact (Figure 3.5.14). Such studies are of interest to LLNL as they pertain to the void size and shape evolution behavior under shock loading. The mechanical response of a solid propellant will be coupled to chemical reaction theory in order to understand hot spot generation in solid propellants resulting from the coupling and interaction between severe shear localization around microstructural defects and internal heat conduction mechanisms. Detailed numerical studies of "edge-cracked" specimens with different crack-to-ligament ratios are also currently being carried out to determine the region of dominance of the asymptotic stress and deformation fields that develop in real-world fracture toughness specimens. These studies will address the role of damage on interpreting fracture toughness results for solid propellants obtained through standard linear elastic fracture mechanics procedures.

Atomic Scale Modeling (Li and Averback)

We performed constant strain rate cyclic deformation simulations using the Parallel Molecular Dynamics code *PARCAS* to examine deformation mechanisms in various materials. With coworkers (Bellon, Odunuga, and Krasnochtchekov), we developed a new scheme based on the relative mean square displacement of atoms to determine relative diffusion coefficients between atoms that are separated by a distance, R, apart. This scheme has the wonderful property that it yields directly the length scale of the deformation mechanism, without the need to visualize the atomic displacements. As illustrated in Figure 3.5.15, we find that in single crystalline materials the length scale of the deformation at ultra high strain rates is proportional the size of the system (dislocation glide), while it is limited to the grain size in nanocrystalline materials. For metallic glasses, the deformation occurs by atomic motion in units of about 1 nm. Initial results were published in Physical Review Letters [Odunuga et al. 2005].

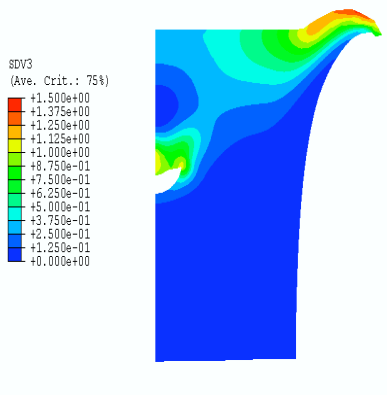

Fig. 3.5.14: Contour plot of effective viscous strain from finite-strain finite element simulation of collapsing void in specimen subjected to dynamic impact at 50m/s. Constitutive response of solid propellant material surrounding void accounts for nonlinear viscous response of binder and allows for void opening and growth due to particle dewetting.

We also continued our research on shock wave interactions with heterogeneous metal systems. Structure analysis coupled with stress and temperature analysis for those systems were completed. The results are given in a paper presented at fall 2004 MRS meeting. The shock induced stress and shock propagation speed as calculated from these atomic level simulations are compared well with results from experiments.

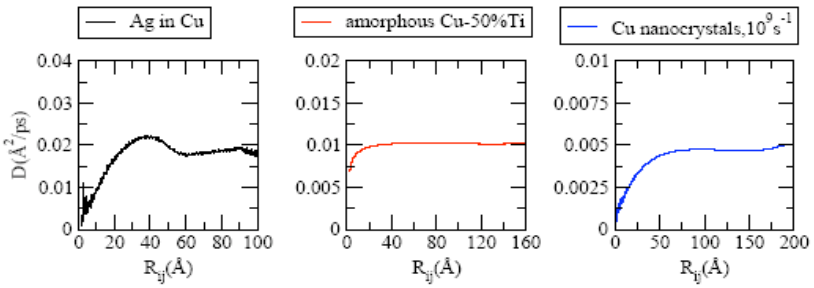

Fig. 3.5.15. Relative diffusion coefficient between atoms as function of distance apart.

We will continue our work on high strain rate deformation, focusing on the behavior on nanocrystalline materials. We will determine whether the deformation results primarily from grain boundary sliding or dislocation motion within the grains. We will also use our new method of analysis to look for shear bands in metallic glasses.

Constitutive Modeling of Metallic Components (Beaudoin)

The modeling effort for metals has focused on the study of rate-dependent and anisotropic properties. Models are derived with a physical basis and address the strain rate and temperature dependence of metal plasticity, effect of microstructural length scale, and impact of grain boundaries on deformation. The detailed mesoscale models have been condensed into relations appropriate for "engi-

neering scale" analysis of components. The temperature and strain rate dependent properties of the barrel-rolled D6AC steel case material have been characterized, and the hardening response of steels – as well as other metals -- at large strains has been derived through consideration of an intrinsic length scale. The mesoscale model is now applied to the study of fracture in the presence of rate effects, such as dynamic strain aging (DSA). In DSA, routinely observed in metal alloys, plasticity occurs in sharp bursts. The Aluminum-Lithium (Al-Li) alloys used in the "super lightweight" external fuel tank used on the space shuttle to increase payload capacity provide an example. The parallel finite element code for mesoscale fracture, developed under the CSAR program, is presently utilized in a NASA funded program to study a delamination fracture mode in the Al-Li alloy C458. This alloy is under consideration for structural application in the next generation launch vehicle (NGLV). Modeling efforts are presently carried out in coordination with an extensive experimental program for Al-Li alloy C458, sponsored by NASA Marshall and presently underway at UIUC.

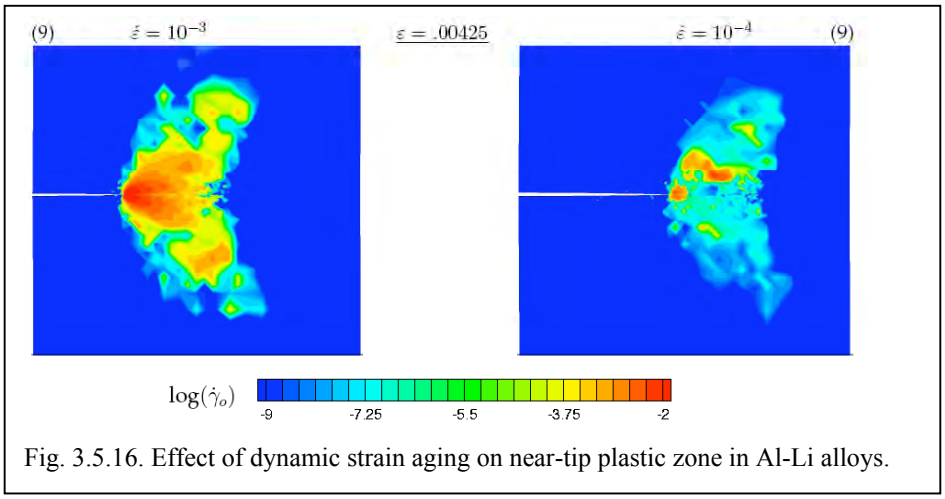

Fig. 3.5.16. Effect of dynamic strain aging on near-tip plastic zone in Al-Li alloys.

In 2003, this CSAR modeling program has been augmented to include an experimental component through an award under the Stewardship Science Academic Alliances Program of the DOE (Prof. I. Robinson, PI). This award complements the simulation component of the mesoscale modeling program with fundamental study on the effect of grain boundaries in metal deformation. Microplastic processes have been observed using *in situ* TEM of polycrystalline Ag, Zr and a Cu-Al materials exhibiting refined microstructures. Based on these experimental observations, a composite grain model has been introduced into a viscoplastic self-consistent model (developed by Carlos Tomé of LANL). This model has in turn been applied to study 75 nm Cu-Nb multilayers through simuation of a rolling process, resulting in a publication co-authored with LANL scientists (AL-

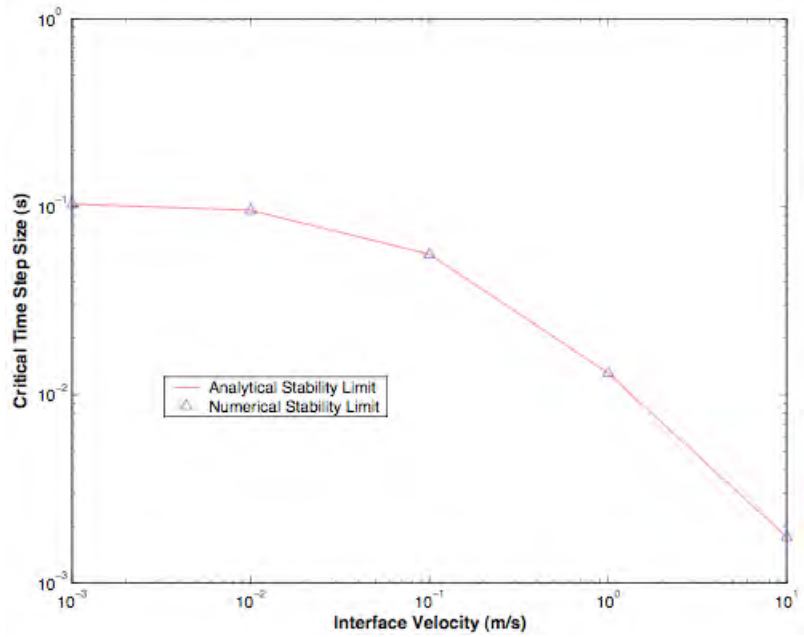

Fig. 3.5.17: Effect of interface velocity on critical time step in coupled thermal simulations. Comparison between theoretical (curve) and numerical (symbols) values.

Fadhalah *et. al., Phil. Mag*. 2005). Stresses inherent at the Cu-Nb interface have been examined using a parallel code authored by graduate student Satya Varadhan. His program is based on the field dislocation mechanics theory of Acharya (formerly a research scientist with CSAR and presently on the faculty of Carnegie Mellon).

Integrated Multiphysics Simulations

Convective Burning of Cracks in Energetic Materials (Roe, Haselbacher, Massa, Short and Geubelle)

In this project, we are using the integrated multiphysics code to look at the fluid/structure/combustion coupled problem of multiscale modeling of cracks in energetic materials. A major emphasis over the past couple of years has been placed on modifying the fluid and solid solvers to incorporate the necessary physics, i.e., (i) 3D transient thermo-mechanical solver in *Rocfrac*, and (ii) Combustion capability incorporated into *Rocflu*, since some of the assumptions used at the macro-scale ("rocket level") (such as flame sheet model of combustion) are not applicable in the case of very narrow cracks. We have also derived simple stability conditions to characterize the stability of coupled thermal fluid/structure simulations (Figure 3.5.17), with special emphasis on the effect of the interface velocity on the stability of the explicit coupled scheme.

Multiphysics level-set based simulations of burning in damage SP (Srinivasan, Matous, Jackson and Geubelle)

The basic objective of this project is to use novel numerical techniques (such as level-set methods and extended Finite Element Method (XFEM)) to model the propagation of a burning front through a damaged solid propellant. The primary motivation for this work is to eliminate the geometrical complexity associated with the presence of a non-planar burning front and its interaction with voids in the damage composite by using a structured grid approach. In other words, the complexity is moved from the computational geometry to the modeling schemes (Figure 3.5.18). Since the numerical schemes used in this study are quite novel, we have started our analysis in the simpler 1D setting and have investigated the precision and stability of the coupled fluid/solid/thermal scheme through comparison with manufactured solutions.

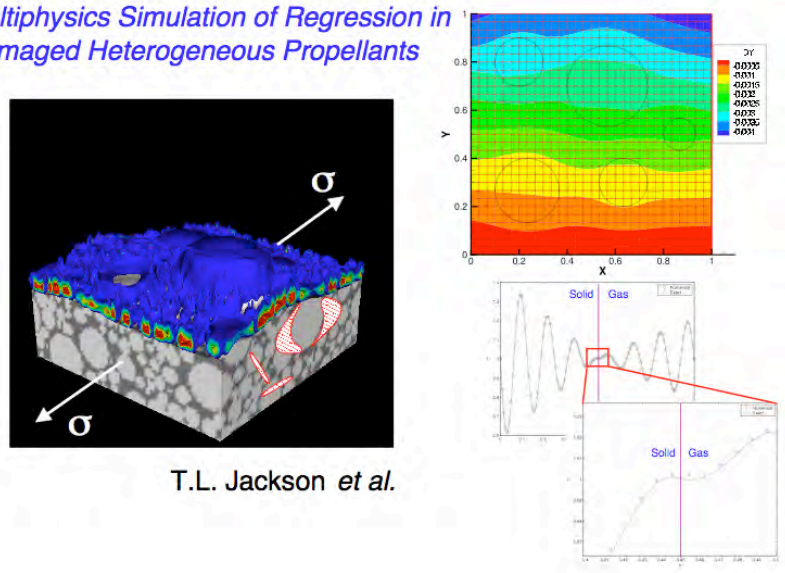

Fig. 3.5.18: Illustration of objective (left), 2D (top right) and 1D (bottom right) implementation of level-set-based numerical scheme. 2D problem shows heterogeneous displacement field (computed with XFEM) present in model particulate composite discretized with uniform grid that does not conform to particle boundaries.