3.2 Structures and Materials

Group Leaders: Philippe Geubelle and Keith Hjelmstad

Faculty Investigators: Robert Averback, Armand Beaudoin, Robert Dodds, Philippe Geubelle, Robert Haber, Harry Hilton, Keith Hjelmstad, Dennis Parsons, Petros Sofronis, and Daniel Tortorelli

Research Scientists: Amit Acharya and Nahil Sobh

Postdoctoral Associates: Karsten Albe, Changyu Huang, and Ertugrul Taciroglu

Research Programmers: Scot Breitenfeld and Alireza Namazifard

Graduate Research Assistants: Nathan Crane, Jason Hales, Schalk Kok, Dhirendra Kubair, Scott Meyer, Jayandran Palaniappan, Arun Prakash, Christian Schranz, Lin Yin, and Mariusz Zaczek

Overview

The Structures and Materials group has research efforts in two broad areas—structural analysis and constitutive and failure modeling. The efforts in system simulation concern the development of the basic numerical algorithms for the solid components of the full rocket simulation and the implementation of those algorithms in a finite element code. The efforts in material modeling and failure analysis include atomic scale modeling of material debonding, micro-mechanical modeling of the constitutive behavior of polycrystalline materials, continuum level modeling of viscoelastic materials with damage, and fracture of metals and solid propellant.

Structural Analysis

There are two primary efforts in structural analysis within the Structures and Materials Group. The first, led by Parsons and Hjelmstad, concerns the development of a scalable parallel finite element code that is the basis of *ROCSOLID,* the solid component of the GEN1 rocket code. This code is capable of solving nonlinear transient problems using an implicit time integration scheme. It is based upon a linear multigrid solver and uses an Arbitrary Lagrangian/Eulerian (ALE) formulation to track the burning front between the solid and fluid domains. The second effort, led by Haber and Tortorelli, includes the development of space-time algorithms for modeling the solid (and possibly the fluid) parts of the solid propellant rocket. Space-time algorithms are well suited to problems with moving domains and, while not currently as well developed as the algorithms used in *ROCSOLID*, show promise as an alternative approach to system simulation.

ROCSOLID

Led by Parsons and Hjelmstad, the Structural Analysis team is developing a scalable parallel finite element code as the backbone for structural model development of the solid rocket motor. *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 an implicit Newmark time integration scheme. The linear matrix equations encountered within the Newton iterations at each time step are solved using a scalable parallel multigrid solver. The code is written in Fortran 90 and uses MPI interprocessor communications.

Examination of the multigrid algorithm demonstrates that all of the operations can be performed independently on partitioned domains. In particular, the main component of the algorithm is matrix-vector multiplication that can be efficiently implemented element by element. Interprocessor communications are only required during the matrix-vector multiplications, scalar products, and fine-to-coarse mesh restrictions. Matrix-free element computations reduce the storage and the time requirements of our implementation.

The mesh is partitioned into a number of domains, each with an equal number of elements. The computations, including the matrix-vector multiplications, are done locally on each processor and completed with interprocessor communications, which are performed using non-blocking MPI communications.

Multigrid methods require a hierarchy of increasingly finer meshes. We use *TrueGrid* to produce a sequence of nested, uniformly refined hexahedral meshes. Mesh partitioning is performed on the coarsest mesh using *Metis* to achieve a perfect load balance among the processors. Uniform refinement of the coarsest mesh partitions produces the required partitions for all of the fine meshes. Thus, an excellent element load balance is maintained throughout the mesh hierarchy, though the resulting communication pattern may not be optimal.

ROCSOLID has been benchmarked on several multiprocessor machines including the IBM SP2 (64 processors), the SGI Origin 2000 (124 processors), and the Cray T3E (512 processors). We have observed scalable element computations and dominance of computations over communications. The Cray T3E showed the best scalability. A series of problems was generated that held constant the number of elements (8192) on each processor. These problems were run on different numbers of processors, enabling us to compute the scaled speedups shown in Fig. 3.2.1.

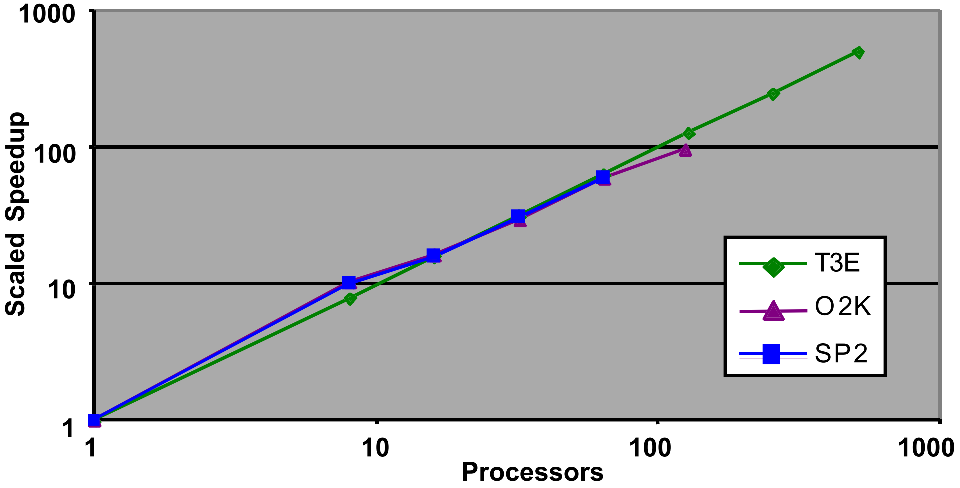

Fig. 3.2.1. *ROCSOLID* scaled problem size speedups

Additional effort has been directed towards developing a formulation capable of correctly modeling the propagation of an interface through a solid. *ROCSOLID* simulates regression of the burning front using an ALE formulation. Implementation of this feature is nearly complete. Nonsymmetric matrix equations are encountered in this formulation and different solvers, including nonsymmetric multigrid solvers, are being tested to see which gives the best performance. Different mesh smoothing techniques can be used to find the location of interior nodes once the interface has moved. This approach has produced a working method that is being verified by solving some 3-D problems with known analytical solutions

Other work has considered advanced solid element formulations (e.g., based on assumed strain methods) and material model development (linear and nonlinear viscoelastic models).

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 rate of the propellant is coupled to the fluid flow via an empirical power law relationship. An interface module takes care of the data transfer across the two codes. All of the components of the GEN1 code are fully parallel and the integrated code has been tested on the NCSA Origin 2000 on up to 124 processors and on the PSC Cray T3E on up to 256 processors. Scalability studies together with preparation and running the validation tests are currently underway.

The *Charm++* environment will be used in *ROCSOLID* to perform dynamic load balancing, which will be needed when other features like adaptive mesh refinement are implemented. A new data object (chunk) is being added to the data structure that will be used by *Charm++* to perform load balancing. A new driving routine is also being written for the code, which will use *Charm++* communication facilities.

Future work on this project includes development of parallel contact procedures for our implicit code, continuing development of the ALE formulation for moving fronts, integration of the solids code into the *Charm++* environment, incorporation of adaptive mesh refinement algorithms, and development of a coupled implicit-explicit time integration scheme.

Space-time Finite Elements

Haber, Tortorelli, and their coworkers have focused on developing novel space-time and discontinuous Galerkin finite element procedures for simulating the response of solid propellant rocket engines. Space-time finite elements provide a natural means for tracking moving boundaries (e.g., a combustion interface or fracture front) as well as topology changes in the analysis domain (as may occur in fracture and other failure scenarios). Discontinuous Galerkin (DG) finite element methods are based on function spaces that admit discontinuities across element boundaries. Relative to conventional finite elements, DG methods offer improved numerical performance, element-wise conservation properties, an intrinsic formulation of physical jump conditions (such as those at combustion interfaces), as well as a number of favorable properties for adaptive algorithms. In the case of hyperbolic problems, DG methods support direct element-by-element solution techniques that offer breakthrough computational efficiency. Thus, combined space-time DG methods appear to be very well suited to rocket simulation.

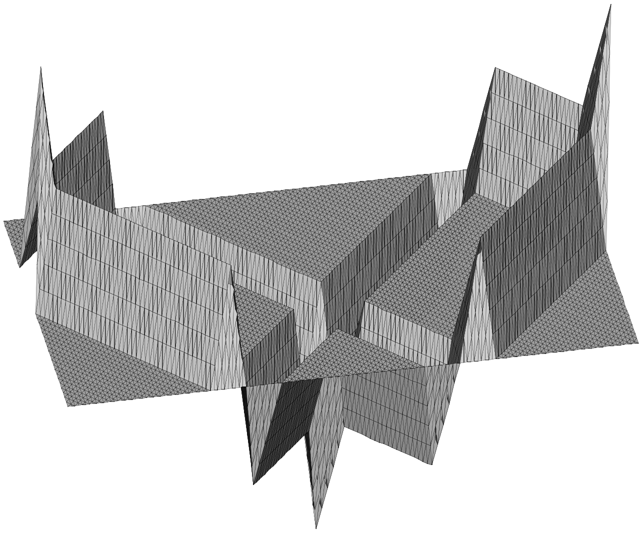

Fig. 3.2.2. Discrete elastodynamic solution for problem with shocks is obtained on characteristic grid with new space-time discontinuous Galerkin formulation. Width of rectangular space-time domain represents space (1-D); length represents time. Height field graphs transient displacement solution. Discrete solution is exact to within machine precision.

In the past year, we implemented a DG method for thermal advection-diffusion problems that is based on recent work by Baumann and Oden. We formulated a new space-time DG method for elastodynamics that employs a direct element-by-element (EBE) solution procedure. Our initial implementation in one spatial dimension crossed with time delivers the exact solution when the mesh is aligned with the characteristic directions (see Fig. 3.2.2); it also performs very well on general meshes relative to conventional finite element models. The EBE solution technique requires storage for only one element matrix equation at a time, and the computational complexity is linear in the number of elements. We also implemented a space-time DG method for Burger's equation as a preliminary investigation of the applicability of DG methods to compressible gas dynamics.

We are working on enhancements to the DG elastodynamic formulation, which we hope will deliver even better performance on non-characteristic grids. We will undertake a mathematical analysis of the new formulation's stability, convergence, and conservation properties to understand better its numerical performance. Kale and Padua (CS Group) plan to develop parallel implementations of the EBE solution algorithms.

Haber and Tortorelli are working with mesh-generation specialists in CSAR to address the special requirements of space-time DG methods. These include an increase by one in the dimension of the mesh and an extra constraint on the mesh geometry that enables EBE solution methods. DG methods eliminate some of the nettlesome geometric constraints that substantially complicate adaptive algorithms for conventional finite element grids. We are working with CSAR computer scientists to develop special data structures and object-oriented software for adaptive analysis that will exploit this attractive feature of DG models.

Over the next year, meshes in two and three spatial dimensions crossed with time will be generated. This will provide opportunities to test our new formulations in higher dimensions and to test problems relevant to rocket simulation. In the latter context, we are working with Moser (Fluid Dynamics Group) to investigate the feasibility of a full system model—including solid, fluid, and combustion response—based entirely on space-time DG finite element models. If this effort is successful, we plan to apply it to various failure scenarios, such as flame-driven fracture, debonding between the insulation and propellant, and dewetting of particles in the solid propellant.

Constitutive and Failure Modeling

Modeling the constitutive response and failure behavior of various components of the solid propellant rockets is critical to understanding the behavior of the integrated whole. The research activities in constitutive and failure modeling, which are to be integrated in the GEN2 set of codes, involve a wide variety of numerical schemes and length scales.

To improve the constitutive and failure models of the metallic motor case to be used in the GEN2 failure scenarios, Beaudoin, Acharya and Kok are developing a physically-structurally-based model for metal deformation. Although the underlying approach is microstructurally based, special emphasis is placed on linking the resulting model to more conventional continuum formulations to insure that the results will be transferable to full-scale simulations of the rocket motor.

A special emphasis in this research is accurately capturing the dependence of stress response on temperature, strain rate, and grain size. Over the past year, the method has been extended to 3-D, relying on a periodic representation of the granular microstructure (Fig. 3.2.3).

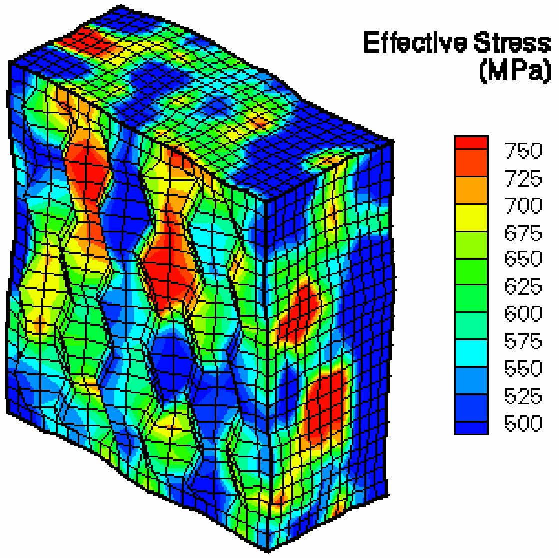

Fig. 3.2.3. Effective stress in metal microstructure arising from grain interaction.

Model validation and extension to a continuum formulation has been achieved through an intensive collaboration with S. R. Chen, D. A. Korzekwa and M. Stout at Los Alamos National Laboratory (LANL). The CSAR model predictions were compared with LANL experimental compression data obtained on various silver samples with different grain sizes and subjected to a range of temperature and strain rate. As shown in Fig. 3.2.4, excellent agreement was obtained between experimental and numerical values. These microscale model results serve as a guide for the development of the Mechanical Threshold Stress (MTS) model to be used at the macroscale level. Recently, LANL researchers have used the results obtained with the microstructural model to introduce a modification to the MTS model that accounts for the effect of grain size. Future plans involve addressing various issues associated with the introduction of the MTS model into the finite element structural code used for the full-scale GEN2 simulations. At the microscale level, Beaudoin and his coworkers plan to introduce damage evolution modeling as well.

The constitutive response of the solid propellant is the focus of Sofronis and Meyer's research activities. Over the past 12 months, they have implemented a 3-D phenomenological model of the viscoelastic response of a particulate composite in an *ABAQUS UMAT* routine, with special emphasis on capturing the dependence on strain rate. To characterize the effect of void-related damage on the constitutive response, a macroscopic potential F has been proposed to relate the macroscopic strains E_{ij} to the corresponding stresses Σ_{ij} as

$$\overline{E}_{ij} = \frac{\partial \overline{\Phi}}{\partial \overline{\Sigma}_{ij}},$$

where the overbar denotes the Laplace transform in the time domain. The resulting prediction for the material dilation under hydrostatic loading has been shown to be in excellent agreement with unit cell finite element calculations of the void effect. Future plans involve extending the potential approach to more complex stress states through the combination of macroscale and unit cell computations. Once the form of the potential for 3-D stress states is established, an overall viscoelastic model accounting for the presence of voids will be available for introduction in the GEN2 structural code. The next step in this research project involves the incorporation of other forms of damage such as particle cracking and dewetting.

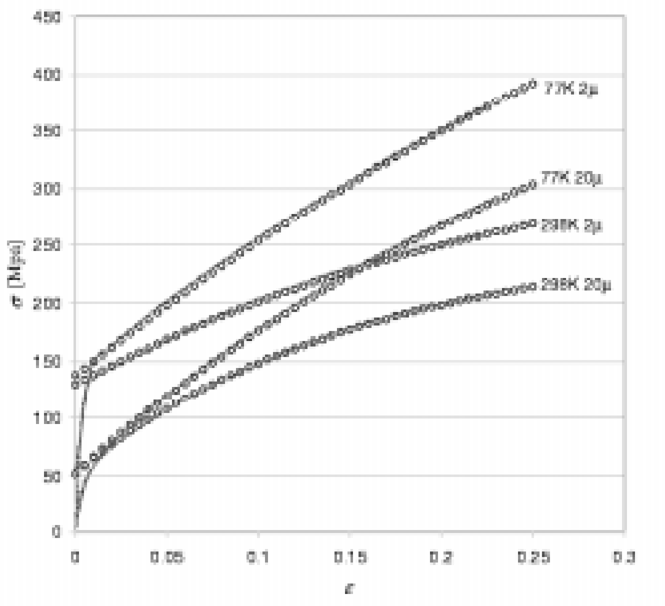

Fig. 3.2.4. Comparison of model predictions (circles) with compression data for silver (lines).

Harry Hilton is working to extend detailed formulations of linear and nonlinear viscoelastic analytical, computational and design structural deterministic and stochastic simulations to achieve proper desired constitutive relations and life cycles of solid propellants. His work is also applicable to liners and filament wound/epoxy matrix composite cases as reliable integrated systems. Nonlinear viscoelastic constitutive relations based on both generalized creep and relaxation functions and on nonlinear Prony series, as well as invariant combined load failure criteria have been formulated and matched to solid propellant experimental data available in the literature. The previously developed efficient serial computational protocols for temporal finite difference and spatial finite elements have been parallelized and applied to deterministic and probabilistic grain analyses. Probabilities of failure of burning propellants are exhibited in Fig. 3.2.5, indicating that it is possible to design motors that survive for a prescribed burning time and failure probability.

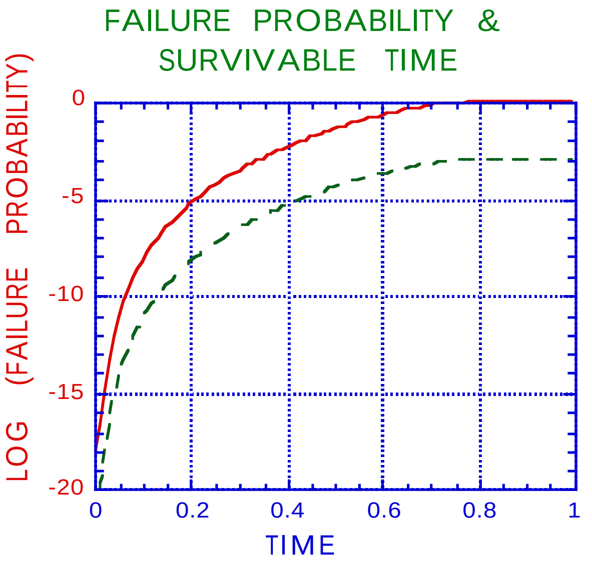

Fig. 3.2.5. Life cycle prediction model for solid propellant for prescribed burning time and failure probability.

The atomic scale modeling being performed by Averback and

Albe will provide insight on the constitutive and failure properties of a solid/soft interface. They are using a massively parallel molecular dynamics (MD) simulation code with atomistic force fields as the only input. For the large-scale simulations of interest here, these force fields are derived from computationally efficient classical potentials, which deliver an analytical approximation of the energy hypersurface and allow MD simulations of millions of atoms. During the past year, they have focused on the development of classical potentials for multicomponent systems in order to simulate real heterophase interfaces. To test the computational approach, a potential for the niobium-sapphire interface has been developed. In addition to being a system of technological importance in its own right, the niobium-sapphire combination provides an excellent illustration of the mechanical behavior of an interface between a hard and a soft material. (Among others, solid propellant rocket examples include the case-liner interface and the aluminum particle-polymer matrix interface.) The modified embedded atom method was used to derive the potential. Due to the lack of necessary experimental data, the team has performed fully self-consistent total-energy calculations within the density functional theory on thermomechanical and elastic properties of pure niobium and aluminum, their oxides, and Al-Nb. This database has then been used for simultaneous fitting of the adjustable potential parameters.

Averback and Albe's plans for the next year are threefold. First, they will perform large scale MD simulation of the failure of interfaces and refine the polymer-metal potential by an ansatz that integrates the underlying bond-order-theory and the embedded-atom method. Their second goal is the implementation of the parallel replica scheme and the hyper-molecular dynamics method developed by Art Voter at LANL. These techniques have the potential to enhance greatly the efficiency of their MD-calculations and to narrow the gap between real time scales in burning rocket fuels and their simulation times. Finally, they will implement an FEM-method where classical potentials replace the phenomenological constitutive laws, enabling them to deal with real-size systems while using the most accurate information from the atomistic force fields.

At the macroscale continuum level, Geubelle and his co-workers have continued the development of an explicit cohesive-based finite element scheme to investigate failure of the solid propellant. The emphasis over the past year has been placed on two aspects of the problem. First, Breitenfeld and Geubelle have been developing a 3-D version of the cohesive/volumetric finite element (CVFE) code. The method is based on a combination of conventional (volumetric) elements with interfacial (cohesive) elements. The latter elements are introduced along the boundaries of the volumetric elements to simulate fracture surfaces in the structure. Large deformation kinematics has been introduced to account for the possible large rotations associated with the propagation of cracks. Due to the very large number of degrees of freedom involved in this type of simulation, an MPI parallel version of the CVFE code has been implemented.

A joint effort involving Hwang, Acharya, and Geubelle (Structures and Materials Group), together with Liou and Balsara (Fluid Dynamics Group), aims at developing a computational tool to model crack propagation in the solid propellant and along the propellant/liner/case interface. This project, which is first being developed in a simpler 2-D setting, has recently focused on the interaction between the core flow and the reactive gas flowing out of a radial crack. Details on the CFD aspects of this study are provided in the Fluid Dynamics section of this report. The solid mechanics component of the subproject is a 2-D version of the explicit CVFE scheme described above. A nonlinear Arruda-Boyce elastic model has been implemented to describe the constitutive response of the volumetric elements and to account for the large deformations involved in this type of problem, where the applied pressure may be as much as five times larger than the material stiffness. An illustration of the evolution of the crack shape is shown in Fig. 3.2.7.

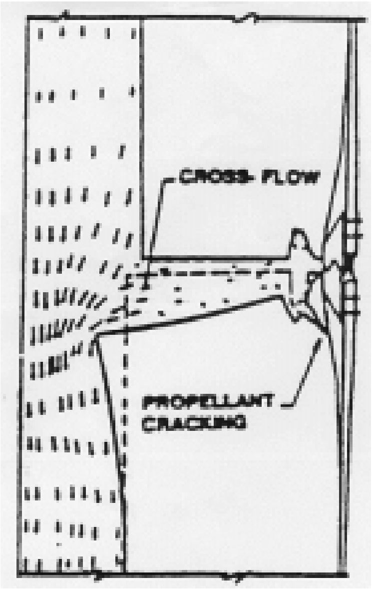

Fig. 3.2.6. Grain failure due to propellant deformation in Titan IV.

The results clearly show the opening of the pressurized crack and the creation of a high-pressure region on the leeward face of the crack and a low-pressure region just downstream of the crack. This combined effect causes substantial deformation that is reminiscent of the grain collapse accident that occurred on a Titan IV SRMU in 1991 (Fig 3.2.6). In that accident, the deformation of the propellant grain due to a similar aeroelastic effect caused a catastrophic failure of the motor. The modeling of that accident constitutes one of our main objectives for the next few months. Also on our agenda are the introduction of a viscoelastic constitutive model and the simulation of crack propagation along the case/liner/SP interface, which is a likely accident scenario to be simulated in GEN2.

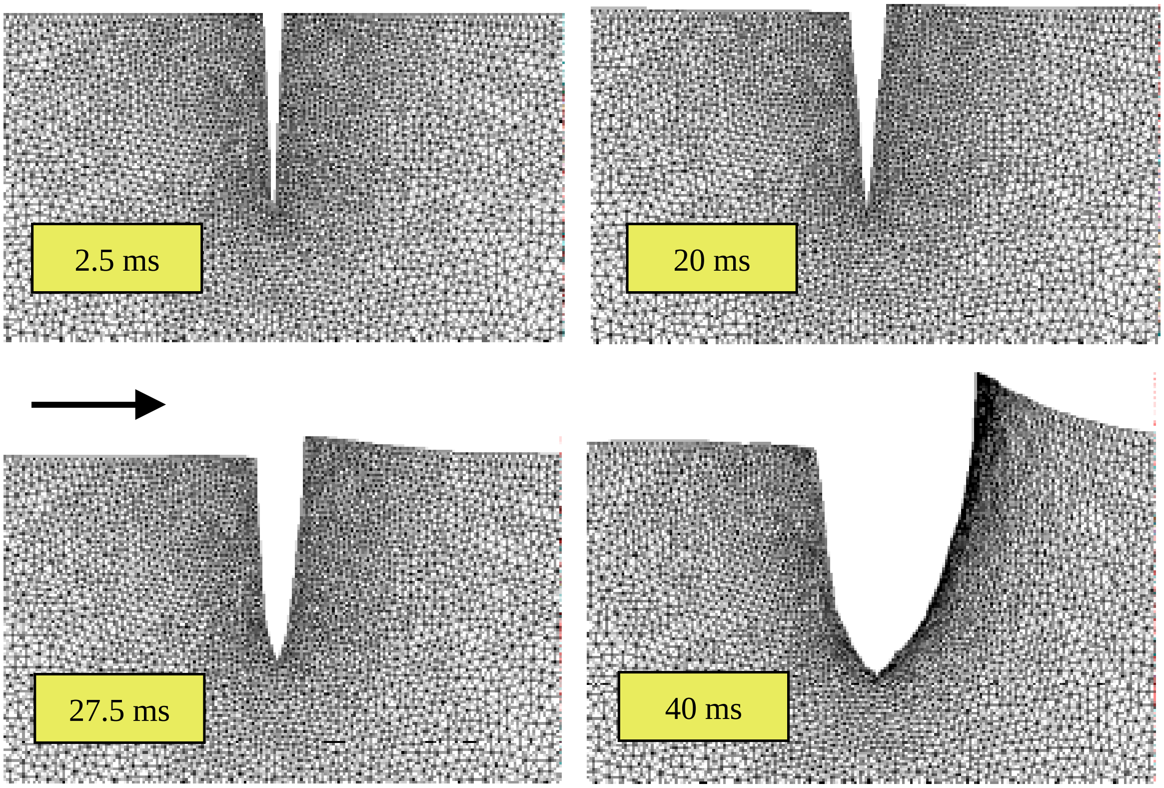

Fig. 3.2.7. Evolution of shape of non-propagating radial crack pressurized by reacting gas. Arrow indicates direction of core flow (Mach 0.25).