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INTEGRATED SIMULATION OF SOLID PROPELLANT ROCKETS

William A. Dick[‡], Robert A. Fiedler[†], and Michael T. Heath^{*}

Center for Simulation of Advanced Rockets
University of Illinois at Urbana-Champaign
Urbana, Illinois 61801, USA

ABSTRACT

This paper presents an overview of research activities at the Center for Simulation of Advanced Rockets (CSAR) at the University of Illinois at Urbana-Champaign. CSAR is one of five university-based research centers funded by the U. S. Department of Energy as part of the Accelerated Strategic Computing Initiative (ASCI). The purpose of ASCI is to advance the state of the art in computational simulation of complex, multicomponent systems and to provide the computational hardware and infrastructure necessary to carry out very large-scale simulations. CSAR is using the solid rocket boosters of the NASA Space Shuttle as the simulation vehicle. Now at the beginning of the fourth year of our ten-year program, the implementation of a fully integrated simulation code is nearly complete and is expected to be finished before the end of 2000. It provides a characterization of various burn scenarios and the onset of potential component failures. Other sub-scale rockets have been simulated to provide verification data for CSAR codes. Refined multiscale component models and advanced system integration concepts based on lessons learned from our current work constitute the key features in the second-generation code targeted for the next few years.

INTRODUCTION

The primary goal of the Center for Simulation of Advanced Rockets (CSAR) is the detailed, whole-system simulation of solid propellant rockets from first principles under both normal and abnormal operating conditions. The U.S. Department of Energy's Advanced Strategic Computing Initiative (ASCI) under the Academic Strategic



Fig. 1: Launch of STS-95, October 1998. CSAR provides whole-system simulation of the NASA Shuttle SRB. (NASA photo.)

Alliances Program (ASAP) funds CSAR. ASCI is a cooperative program among the three DOE Defense Programs National Laboratories—Lawrence Livermore, Los Alamos, and Sandia—to provide leading edge computational modeling and simulation capabilities to support the Strategic Stockpile Program (SSP). The SSP, which is charged with maintaining the safety and reliability of the nation’s enduring nuclear weapons in the absence of underground nuclear testing, requires ASCI’s advanced computational capabilities to shift from nuclear test-based methods to science-based methods.

Replacing conventional testing with computational simulation requires a giant leap in both simulation methodology and computational capacity. Five research centers have been established at major U.S. universities to focus on simulation in the context of real-world physical problems. The ASAP centers share a common theme of integrated, multidisciplinary research. Physical characteristics of an “ASCI problem” include full three-dimensional modeling; coupled physics; diverse length and time scales; high energy densities; reactive, turbulent, and multiphase flows; complex geometries and interfaces; and massive computational requirements. Simulation of solid propellant rockets has all of these features, in addition to being an important problem in its own right.

CSAR is one of the five Centers of Excellence established in September 1997 to perform large-scale, unclassified, integrated, multidisciplinary simulations and to develop the scientific and computational capabilities needed to solve engineering problems of unprecedented complexity. Approximately forty faculty members, thirty professional staff, and forty graduate students from a dozen academic departments participate in CSAR, which also benefits from the guidance of an External Advisory Board composed of representatives from the rocket and computing industries, government laboratories, and academia [Refs. 1,2].

SIMULATION SCIENCE

Safety and reliability remain paramount concerns in rocket motor design because of the enormous expense of rockets and sophisticated payloads. In the spring of 1999, for example, a series of three consecutive U.S. launch failures collectively cost more than \$3.5B. Even if only a small fraction of such accidents could be prevented through science-based simulations, the costs of developing the software and acquiring the computer hardware would be recovered many times over.

The use of detailed computational simulation in virtual prototyping of products and devices has had enormous impact in some industries, for example in the design of automobiles and aircraft, but to date this approach has not made significant inroads in rocket motor design. Computational tools commonly used in the rocket industry are limited to relatively simplified geometries, phenomenological models of material properties, flow fields, burn rates, and the coupling between components. Although simulation may never completely replace empirical methods, it can potentially dramatically reduce the cost of empirical methods by identifying the most promising approaches in advance of building actual hardware.

Simulating solid rocket motors (SRM) from first principles presents many challenges. Their complex behavior requires fully three-dimensional modeling to capture the essential physics adequately. Examples include combustion of composite energetic materials; turbulent, reactive, multiphase fluid flows in core and nozzle; global structural response of propellant, case, liner, and nozzle; and potential accident scenarios such as pressurized crack propagation, slag ejection,

and propellant detonation. The coupling between components is strong and nonlinear. The geometry is complex and changes dynamically as propellant is consumed. The spatial and temporal scales are extremely diverse.

Modeling and simulating a coupled system is even more demanding, as it requires not only still greater computational capacity, but also that the corresponding software modules interact in a manner that is physically, mathematically, and numerically correct and consistent. When data are transferred between components, physical conservation laws must be honored, mathematical boundary conditions must be mutually satisfied, and numerical accuracy must be preserved, even though the corresponding meshes may differ in structure, resolution, and discretization methodology.

The enormous computational capacity required for integrated, whole-system simulation of an SRM is feasible only through massively parallel computers. Thus, the software integration framework, mesh generation, numerical algorithms, input/output, and visualization tools necessary to support such simulations must be scalable to many processors.

CSAR has taken a staged approach toward developing an application capable of simulating an entire SRM (Figure 2). Within the first few months of CSAR's inception, we simulated a two-dimensional ideal rocket (GEN0) using existing fluid dynamics and structural mechanics codes with limited coupling, primarily as an initial integration exercise. In the following sections of this paper, we summarize more recent results from three-dimensional, fully coupled simulations of an SRM from ignition to normal burn (GEN1) performed at CSAR. We also describe research underway at CSAR toward detailed SRM simulation capability (GEN2).

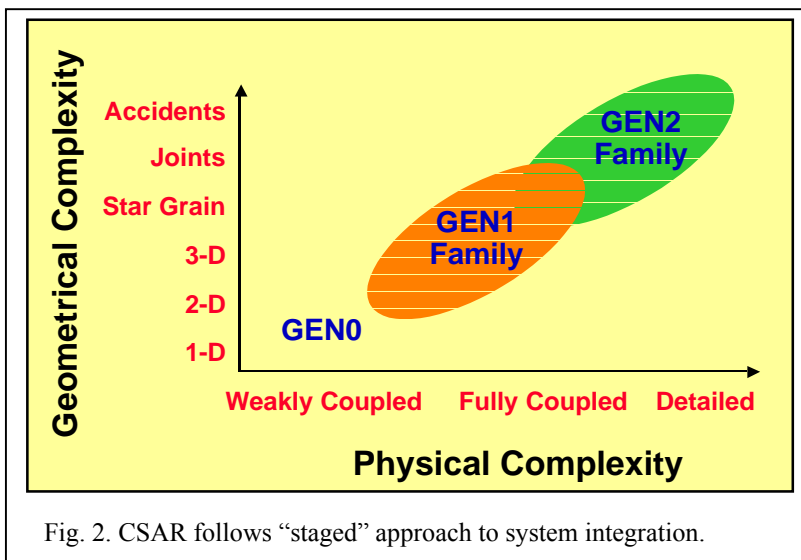


Fig. 2. CSAR follows “staged” approach to system integration.

GEN1 PROGRESS

Our first-generation rocket simulation roadmap is shown in Figure 3. Successively refined treatments of each of the main components of an SRM are represented by a series of overlapping boxes with text summarizing each model. Models in shaded boxes are already incorporated in the current GEN1 system code, while models in white boxes are still under development, with an expected completion date before the end of 2000.

We chose the Space Shuttle RSRM as our initial simulation target for the integrated GEN1 code [Ref. 3]. The geometry is fully 3-D, with specifications gleaned from drawings and other data provided by Thiokol Corporation. Since we currently lack detailed blueprints, the shape of the star grain, joints, and nozzle have been simplified somewhat to ease initial mesh generation.

In creating a single high-performance parallel application, we developed a 3-D fluid dynamics code (*ROCFLO*, [Ref. 4]), a structural analysis code (*ROCSOLID*, [Ref. 5]), and an interface code (*ROCFACE*) to perform the mesh association and interpolation necessary to couple the two mechanics codes together.

ROCFLO solves the Navier-Stokes equations in an Arbitrary Lagrangian-Eulerian (ALE) formulation, which enables its block-structured mesh to move with the propellant surface. This parallel Fortran 90/MPI module uses a second-order upwind TVD finite volume scheme with explicit time stepping. The initial fluid mesh is generated using *Gridgen* from Pointwise, Inc.

ROCSOLID is a finite element code that uses an unstructured hexahedral mesh, a multigrid linear system solver, and implicit time stepping. The Fortran 90/MPI algorithm has recently been extended to an ALE formulation to allow for regression of the propellant. The initial solids mesh is generated using *TrueGrid* from XYZ Scientific Applications, Inc. and partitioned for parallel execution using METIS.

At the boundaries between the solid and the fluid domains, a parallel interface code (*ROCFACE*) efficiently determines which element in the solids mesh is associated with a given point in the fluids mesh. This C++/MPI code also performs interpolation between the two meshes in a locally conservative manner.

For scientific visualization of our 3-D results, we developed *Rocketeer* [Ref. 6]. This C++ application runs on several Unix and Windows platforms and is based on the free Visualization Toolkit (VTK) from Kitware Inc., which uses OpenGL to exploit hardware graphics acceleration. *Rocketeer* supports multiblock structured and unstructured meshes, seamlessly merges data files, and automates the generation of frames for animation.

Our first large Shuttle booster simulation was run on a 256-processor SGI Origin 2000 (Figure 4). There were roughly 4 million fluid cells and 300 000 structural elements. The case and nozzle were taken to be rigid, while the propellant was linearly elastic. The propellant surface was assumed to ignite everywhere at the instant that the simulation begins, acting as a moving mass injection boundary for the fluid. Regression of the propellant due to burning was neglected because of the short physical time reached in this simulation, 100 ms after 10 days of wall clock time.

We have improved our GEN1 simulations in several ways. A fluid mesh that does not over-resolve the flow along the axis of the rocket allows time steps that are 10 times larger than before, speeding up the whole code by nearly a factor of 10. A new ignition and flame spread model [Ref. 7] accounts for transfer of heat to the propellant surface due to exposure to the igniter flow and hot gas from burning propellant until after it reaches the ignition temperature. An algebraic turbulence model that is valid until the boundary layer is blown away by the flow from

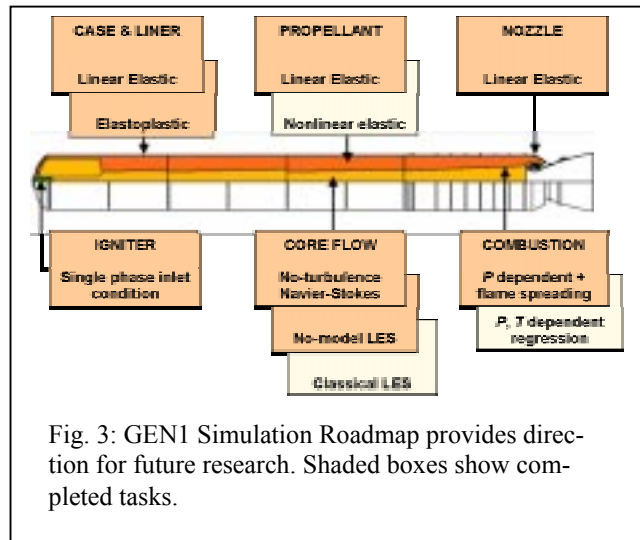


Fig. 3: GEN1 Simulation Roadmap provides direction for future research. Shaded boxes show completed tasks.

burning propellant has been added to *ROCFLO*. Finally, *ROCSOLID* can now treat the case as elastoplastic and the nozzle as elastic.

Further improvements are in progress for GEN1. In a real rocket, turbulent vorticity is injected into the core flow by the burning propellant and the igniter. Turbulence must be included in our simulations because it can significantly increase the burn rate and affect the stability of an SRM. To increase the smallest length scale that must be resolved in order to follow a turbulent flow accurately, we have adopted the Large Eddy Simulation (LES) approach.

A serial ALE version of *ROCSOLID* to handle regression is nearing completion, and a parallel multigrid solver for non-symmetric linear systems is under development. A nonlinear elastic constitutive law for the propellant is also being formulated.

A new burn rate module for GEN1 based on the phenomenological Zeldovich-Novozhilov (ZN) approach [Ref. 8] is nearing completion. This model introduces temperature dependence into the burn rate and should allow more accurate simulation of ignition transients.

GEN2 AND SUPPORTING RESEARCH

The second-generation whole-system rocket simulations will be constructed from extended versions of our GEN1 component codes plus new physics modules, which will enable us to include phenomena such as burning aluminum droplets and pressurized crack propagation. Our goals for GEN2 are constrained both by our desire to complete this phase of our project in a two-year time frame and by the wide range of length and time scales that are introduced by some of the more refined models (see Figure 5). Based on our experience with GEN1, a high fidelity simulation of the Space Shuttle booster over the entire two minute burn time would require a prohibitive amount of execution time, even on the largest and fastest platforms available in the near future. Nevertheless, we plan to develop modules to include all of the physics indicated in the figure so that we will have the capability to model normal burn and various accident scenarios in considerable detail. To simulate the entire rocket throughout the full burn, we plan to employ two strategies: “homogenization” of subscale models, and “time zooming.”

Homogenization is a means of extracting essential gross behavior of a subscale model for use in a whole-system simulation. Homogenization may consist of a simplified analytical or numerical model that mimics the solution of the more detailed calculation, or it may involve generating a table of values produced by running the subscale model off-line with various combinations of input parameters. The whole-system code would evaluate these input parameters based

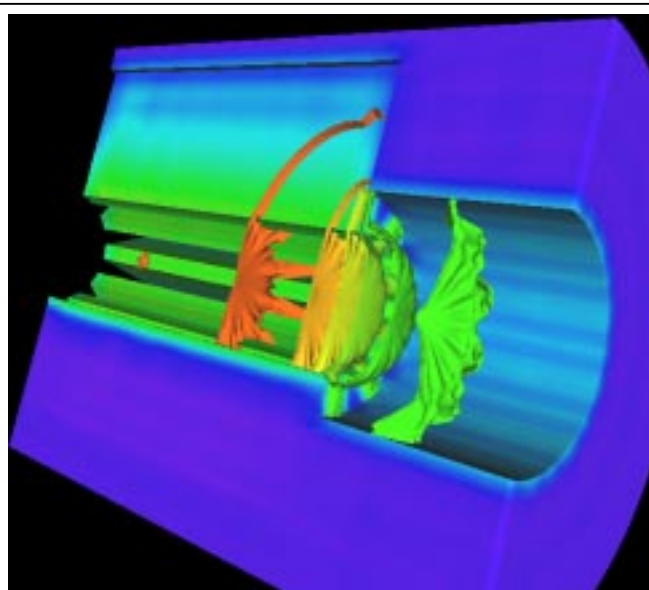


Fig. 4: Full 3-D simulation of star grain in Space Shuttle RSRM showing stress in propellant and gas pressure isosurfaces in slots and core region. Executed on 256-processor SGI Origin2000, visualized with *Rocketeer*.

on the current numerical solution and interpolate between tabulated results from the subscale computations to obtain an approximate solution of the equations governing the subscale model.

The concept behind time zooming is that the details of each physical process are not crucial for computing the long-term evolution of the rocket motor. In such a case it may be possible to run the simulation at full fidelity only for a time sufficient to establish the gross behavior of each subscale model (e.g., statistics characterizing the turbulence), and then take larger time steps over a much longer time interval under the assumption that the gross behavior does not change. After computations for the longer time interval have been completed, the simulation may be run at full fidelity for another short time interval to determine the gross behavior of the subscale models at the advanced time. This concept is a numerical form of homogenization of a subscale model over time, and is somewhat different from “subcycling,” which reduces computational effort by taking short time steps within a subscale module while the whole system is updated using a much longer time step.

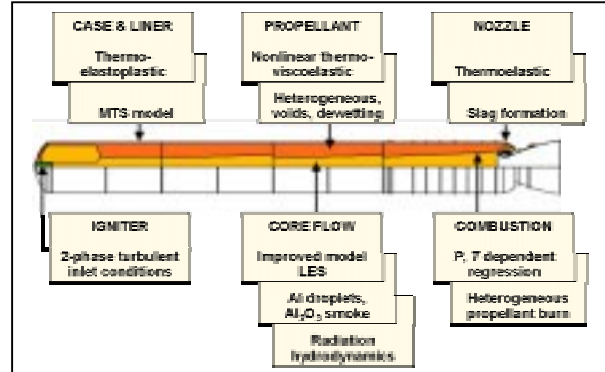


Fig. 5: GEN2 Simulation Roadmap.

GEOMETRY

GEN2 includes greater geometric complexity than the GEN1 system code. The star grain, joints, igniter, and submerged nozzle will be represented more accurately, and flexible inhibitors in the joint slots will be modeled in detail, since they protrude into the core flow after some of the propellant has burned away and are a source of vorticity, which may enhance the burn rate downstream. However, the most significant increase in geometrical complexity will arise when cracks are allowed to form and propagate in the propellant.

STRUCTURES AND MATERIALS

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

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

Modeling inhibitors, propellant slumping, and joint failure require a structural mechanics module that is valid for large deformations. *ROCSOLID* is being extended to handle materials in contact so that joint failure involving gasses escaping past an O-ring can be simulated.

The mechanical properties of heterogeneous propellant will be calculated using a macroscopic constitutive law being developed by Sofronis, et al., which includes the effect of damage (particle dewetting) at the microstructural level. Particle dewetting has a strong temperature and strain rate dependence, so it will be necessary to solve the energy equation to obtain the temperature field throughout the propellant, with initial conditions provided by the ambient temperature and exposure to sunlight at the virtual launch site. We will also allow for variation of propellant properties in different regions to represent inhomogeneity resulting from the casting process of real propellants. Until this heterogeneous treatment is validated and inserted into the system code, we will use a nonlinear viscoelastic model applicable to homogeneous propellants.

Cracks in the propellant will be modeled using the Cohesive/Volumetric Finite Element method [Ref. 9]. We envision either introducing a crack or checking for stresses sufficient to cause a crack at any point within the propellant in the whole-system simulation. A region in the vicinity of the crack will be automatically carved out of the domain computed by *ROCSOLID*, and the crack-propagation module will compute the evolution of the crack and the stress in this region of the propellant. The propellant surface exposed by the crack will begin to burn and a new fluid dynamics module using a 3-D unstructured adaptive mesh to handle the irregular and dynamically changing shape of the crack will determine the evolution of the gas inside the crack.

FLUID DYNAMICS

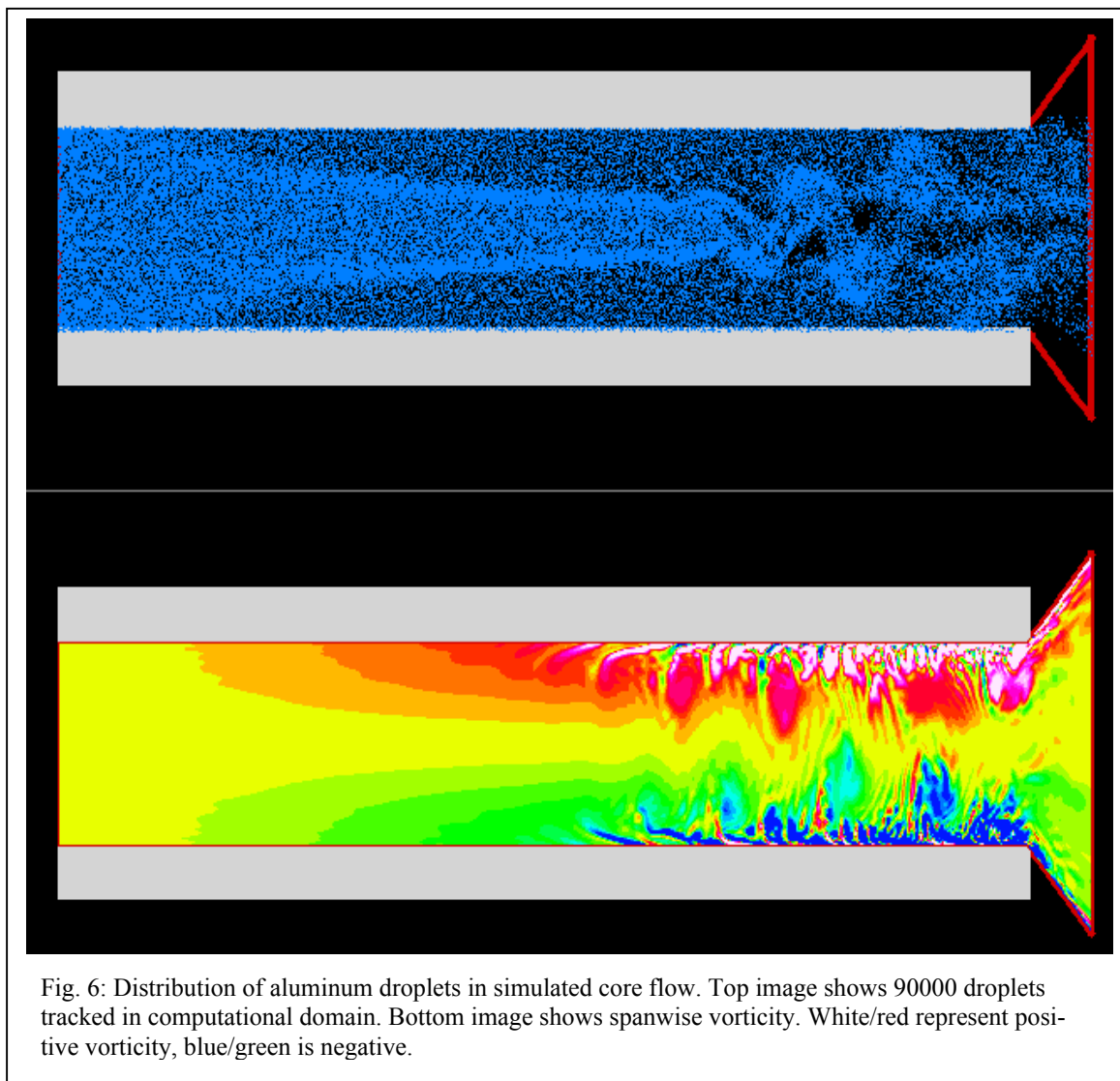
There are four primary research and development activities being pursued in the Fluid Dynamics Group. These are the development and testing of the primary GEN1 fluid dynamics code, *ROCFLO*; two-phase flow simulation and modeling to represent aluminum and aluminum oxide particles; turbulence simulation and modeling through large-eddy simulation; and modeling and simulation of radiative heat transfer. All of these activities are directed toward the requirements of the GEN1 and GEN2 simulation requirements for the core flow.

ROCFLO is being extended to handle two-phase flows arising from burning aluminized propellants. As the propellant burns, aluminum particles melt and form pools on the surface. The aluminum droplets are carried into the core flow region by the stream of hot gasses emitted from the propellant surface. Najjar, et al., are modeling the injection and subsequent motion of aluminum droplets in the flow (Figure 6) [Ref. 10], and Rani and Vanka are studying turbulent flow with particles [Ref. 11]. Balachandar, et al., are developing an accurate force law for particles in rocket flows and a continuum model for efficiently computing the evolution of aluminum oxide smoke particles in the core flow [Ref. 12]. Incorporating aluminum will allow us to predict the details of energy release within the core flow as well as the formation of slag near the submerged nozzle.

CSAR researchers are developing improved LES models [Ref. 13] based on direct numerical simulations (DNS) of turbulent flows in geometries similar to those inside rocket motors. These calculations are validated by comparison with experiments.

Since radiative heating of the propellant surface can increase the burn rate significantly, we will also add to *ROCFLO* the implicit radiation hydrodynamics module developed by Hayes and Norman. The simplifying assumption of flux-limited diffusion will be adopted to prevent calcu-

lation of the 3-D radiation field from dominating the run time. The strong dependence of optical properties on frequency will be approximated through use of a multigroup scheme.



COMBUSTION AND ENERGETIC MATERIALS

Reproducing the ignition transients, erosive burning, and instabilities present in real rocket motors requires detailed knowledge of how heterogeneous solid propellants burn. CSAR researchers are working toward detailed subscale simulations of a small 3-D section of burning heterogeneous propellant that include a non-planar burning surface, unsteady heat conduction in the solid, the influence of an unsteady chamber flow field, complex reaction kinetics, the melt layer, aluminum particles, and radiation. This subscale model is by itself an ASCI-scale problem, and a staged approach is being taken to solve it.

Knott and Brewster have modeled 1-D periodic heterogeneous propellant combustion including fully coupled gas and solid phases, steady-state free surface regression, and a double flame reaction mechanism [Ref. 14]. Jackson, et al., studied the effect of the imposed fluid flow

for two-dimensional flames on a 1-D periodic heterogeneous propellant. This work has recently been extended to 2-D heterogeneous propellant with random packing of two sizes of AP particles and non-planar surface regression [Ref. 15]. In support of these calculations and their extension to 3-D, a realistic model of particle packing in 3-D heterogeneous propellants has recently been developed by Knott, Buckmaster, and Jackson (Figure 7). They have already computed 3-D flames arising from a flat surface obtained by slicing through 3-D periodic heterogeneous propellant at various depths. Until the 3-D flame models are completed, we will continue to use a burning rate law based on ZN theory.

Tang and Brewster have simulated nonlinear combustion and bulk-mode (L^*) chamber gas dynamics. Their results suggest that the spike in the pressure observed during ignition of SRMs may be due to nonlinear dynamic (but quasi-steady) burning rather than erosive burning [Ref. 17].

Surzhikov, Krier and Murphy have developed a 2-D flame simulation model that includes various reduced kinetic schemes, is fully coupled with the solid, and may include the effect of external radiation [Ref. 18].

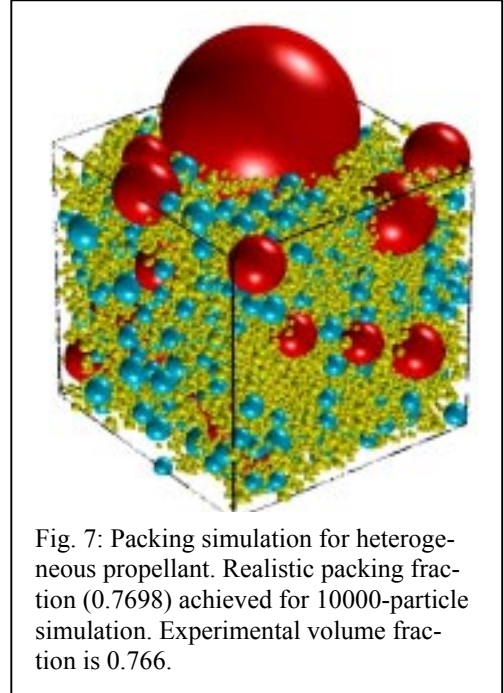


Fig. 7: Packing simulation for heterogeneous propellant. Realistic packing fraction (0.7698) achieved for 10000-particle simulation. Experimental volume fraction is 0.766.

COMPUTER SCIENCE AND VISUALIZATION

Integrating the component modules and subscale models in the GEN2 code without sacrificing performance or scalability requires a sophisticated software framework. *ROCFACE* and the time-stepping scheme described for the GEN1 system code form part of this framework, but GEN2 requires a more flexible and intelligent interface for mediating communication between component modules. For example, if a crack appears, the crack propagation module will take over a portion of the solid propellant domain and an unstructured mesh fluid dynamics code will compute the flow inside the crack. These modules are to be inserted automatically, and the time-stepping scheme and communication pattern must both be updated automatically.

A number of frameworks for building complex parallel applications have been designed and implemented, but none has a large user base. The primary reason for this seems to be that these frameworks require potential users to make many changes to their existing applications. CSAR has therefore proposed a framework that requires a minimal number of changes in order to plug in a module. Substantial progress has already been made in constructing a prototype framework. For modules that use the MPI library to pass messages between chunks, most of the commonly used MPI routines are simply replaced by CSAR-developed versions [Ref. 19].

A client/server version of *Rocketeer* is under development to visualize the enormous data sets that will be generated by GEN2 and some of our subscale models. The server part will run in parallel on a large remote system where the data are stored, while the client will control graphics operations and render images on a local graphics workstation. Large speedups are possible when generating frames for animation from a series of output dumps, since they can be processed in-

dependently once we specify the data range, camera position, and sequence of graphics operations to be performed.

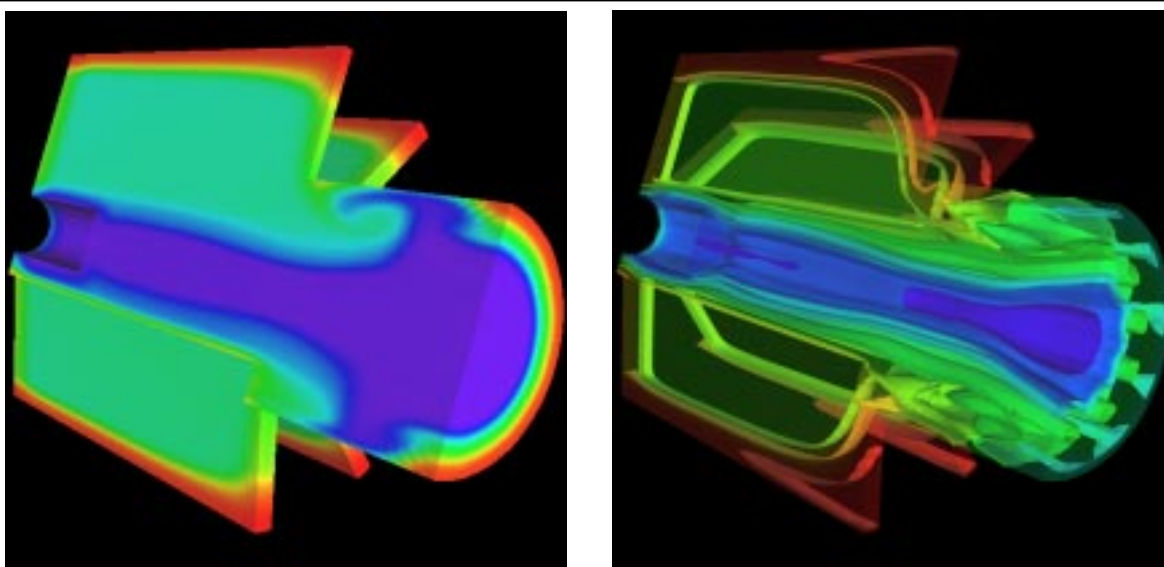


Fig. 8: Gas temperature computed by *ROCFLO* in star grain region of Space Shuttle RSRM near onset of steady burning, visualized by *Rocketeer*. Values range from 3364 K (magenta) to 3392 K (red). Temperature is represented as tint on interior surface of propellant (left image) and as series of translucent colored isosurfaces in interior at slightly later time (right image). Rocket has been cut in half along lateral axis to improve visibility.

CONCLUSIONS

CSAR will soon have the capability of producing the most detailed and accurate simulations ever undertaken of solid propellant rockets, thanks to the dedication of many individuals from numerous departments and disciplines at the University of Illinois, along with collaborators from industry, government laboratories, and other universities. The techniques used to advance the state of the art in rocket simulation will be applicable to many complex engineering problems.

ACKNOWLEDGEMENTS

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