# 3 Research Program Accomplishments

## 3.1 Program Overview

The central goal of CSAR is the detailed, whole-system simulation of solid propellant rockets under both normal and abnormal operating conditions. Full simulations (Figure 3.1.1) of such complexity require a sequence of incremental developments—in engineering science, computer science, and systems integration—over an extended period of time. From the outset, however, our emphasis has been on *system integration* rather than separate threads of development that eventually come together at some point in the future. Rapid exploration of critical system integration issues entail the use of simplified—but fully integrated—models and interfaces initially, followed by successively refined models and interfaces as experience is gained (Figure 3.1.2).

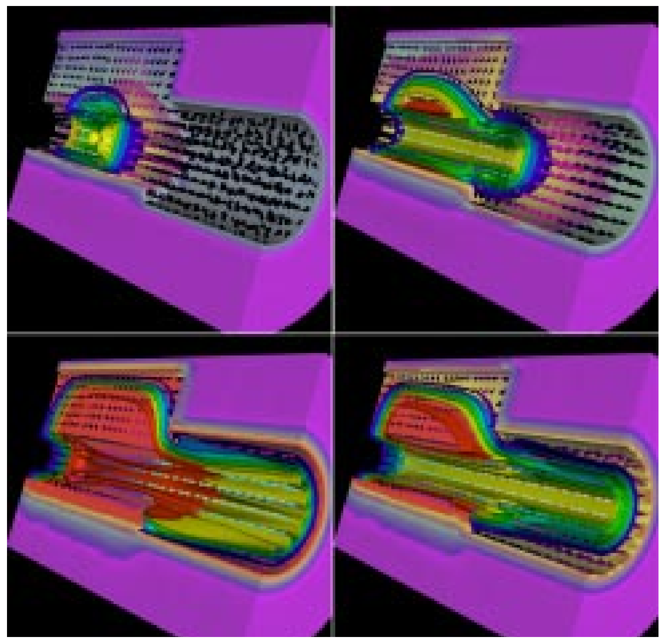

Fig. 3.1.1: Current 3-D fully coupled code includes structural dynamics, combustion, and fluid dynamics simulation modules and ignition model. Images show interaction of solid propellant, combustion layer, and fluid flow following ignition of RSRM (clockwise from upper left: 5, 10, 15, and 20 ms). Colors in solid propellant depict local stress, colored arrows in fluid represent flow direction and speed, and colored isosurfaces in fluid show temperature distribution.

### Simulation Roadmap and Timeline

The CSAR Simulation Roadmap (Figure 3.1.3) depicts the evolution of increasingly sophisticated computational models for the primary rocket components and their interactions. The Project Timeline (Figure 3.1.4) that accompanies the Roadmap indicates the time sequences required for the execution of the technical program. We have been remarkably successful in completing the tasks outlined for Years 1 through 4. Completed tasks are noted on the Timeline.

Our initial implementation of an integrated simulation code (GEN1), expected to be fully operational at the end of 2000, provides a simplified characterization of various burn scenarios. The GEN1 code employs macroscopic models for the separate components to enable a strong focus on the definition and resolution of system integration issues. Refined, multiscale component models and advanced system integration concepts, based on lessons learned from GEN1, constitute the key features in the second generation (GEN2) code—targeted for Years 4-5 and beyond. The refined models also reflect the synthesis of fundamental, subscale studies (bottom right side of Figure 3.1.3), which are critical for detailed simulations of accident scenarios and for reliable simulation of multiscale phenomena such as combustion and turbulence. The code numbers in the diagram indicate dependence of the refined and accident models on the subscale simulations.

The Roadmap also indicates the close coupling among the components; physical quantities such as temperature (T), mass flow ($\dot{m}$), pressure (p), heat flux (q), concentrations ($c_i$), and geometry that must be exchanged between the SRB component models. The computer science integration efforts define the framework for these interconnections and, consequently, their eventual impact on overall code performance. In the right-center box on the diagram, computer science research and development activities are shown that support the SRB simulation through the implementation and optimization of the component models and subscale simulations, the integration of component models and the computational infrastructure required to do large scale parallel computation.

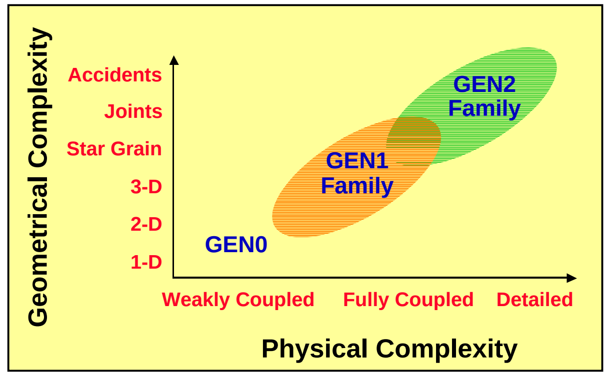


Fig. 3.1.2: CSAR follows "staged" approach to system integration.

Finally, the central placement of validation efforts in the diagram highlights the priority assigned to this activity. Each subscale, component, and integrated simulation must be validated against existing analytical, numerical, and experimental data available in the open lit-

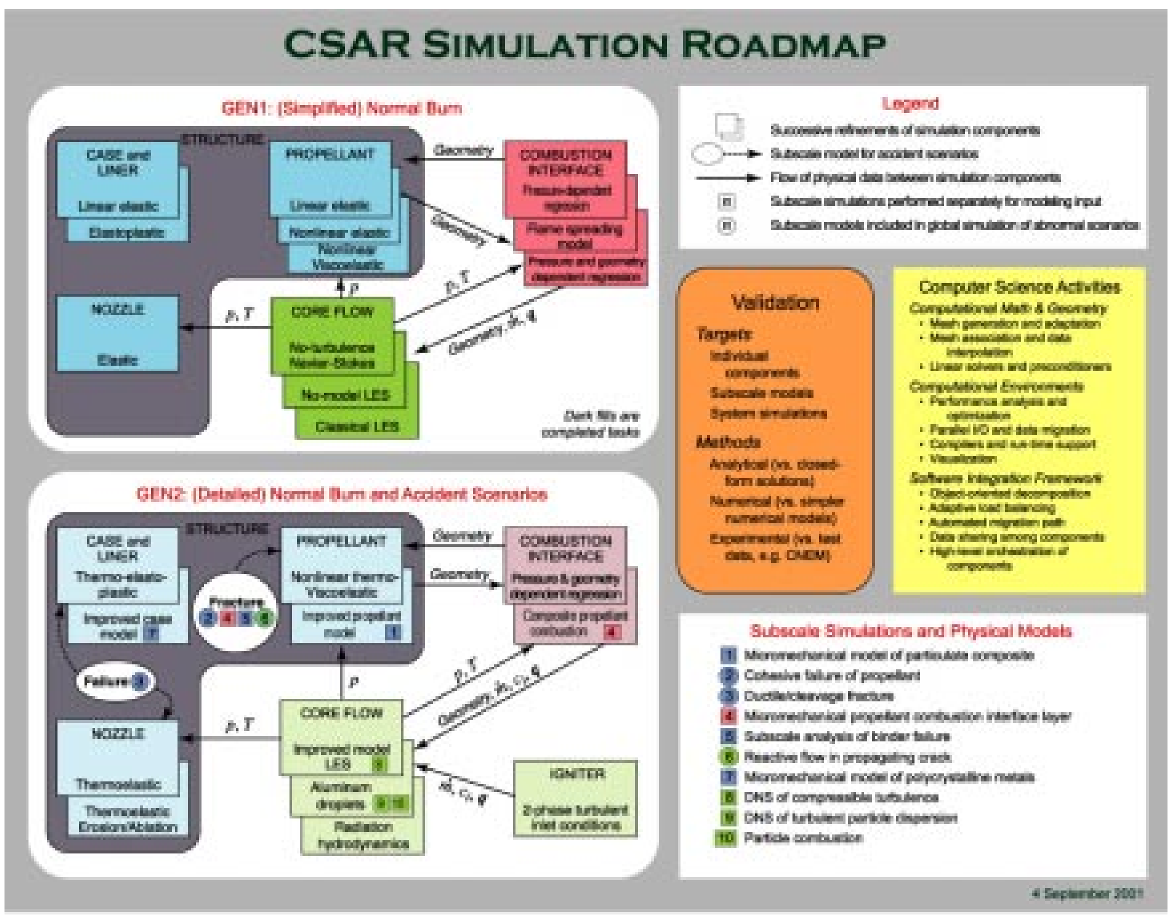


Fig. 3.1.3: CSAR Roadmap showing completed tasks (dark boxes in GEN1) and planned activities for Y4-10.

erature or obtained from our sister Center for Novel Energetic Materials (CNEM).

System integration involves two major tasks to ensure the physical, mathematical, geometric, numerical, and software compatibility of the component models and the codes implementing them. The first task is providing information transfer across component boundaries. Boundary conditions for the component models must be compatible mathematically (e.g., an outflow from one component becomes an inflow for a neighboring component). The discretizations of neighboring components must fit together geometrically. Different spatial resolutions and discretization methodologies must be reconciled via interpolation where necessary.

The other major task is temporal coupling of the components so that the whole system is evolved in a self-consistent manner. Different components may have very different time step sizes due to the choice(s) of algorithm(s) (e.g., explicit vs. implicit methods), spatial resolution, and/or the physics of the subproblem that the module solves. The computational cost of forcing each module to take a time step determined by the module requiring the shortest step is often prohibitive. We continue to investigate multiple strategies for coupling modules requiring different time step sizes while maintaining the accuracy of the overall simulation.

Our approach to system integration has been to develop a single executable code containing modules for the various components and the interface code for tying them together. We are following an object-oriented design methodology that hides the data structures and

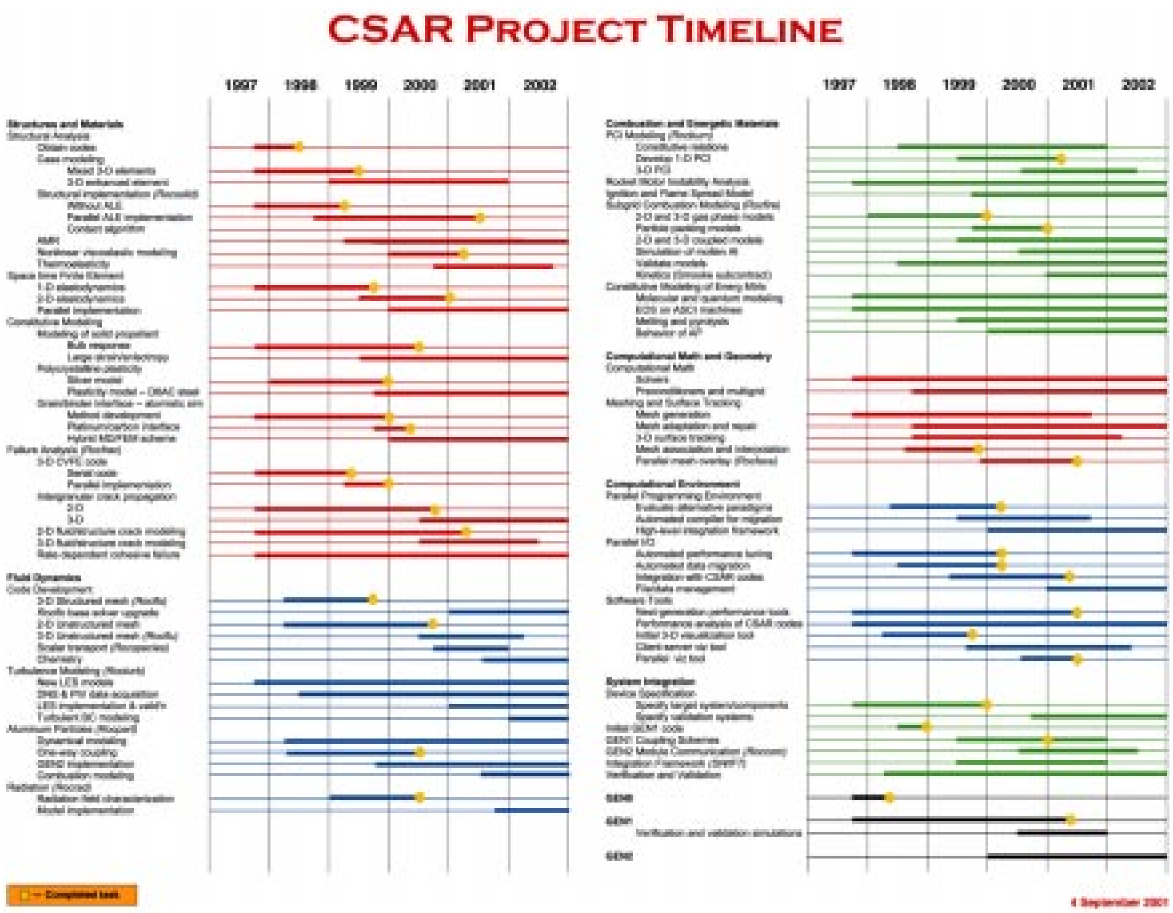


Fig. 3.1.4: CSAR Project Timeline shows completed tasks and future activities.

other internal details of the individual component codes. This simplifies development and maintenance of the interface code and the component codes, and also makes it easier to swap different versions of the same component—a critical capability for determining the most efficient algorithms and implementations.

## Key Project Milestones for FY02

### Scalar Transport Model Implemented in Rocflo — 1Q02

Implementation of the scalar transport model, *Rocspecies*, will enable the simulation of various chemical species and $Al_2O_3$ smoke in the core flow. Rocspecies implements a technique called the Equilibrium Eulerian method that was developed at CSAR. The new simulation method evolves the velocity field directly from the fluid flow information, rather than requiring a separate velocity flowfield. The new module will interface with *Rocflo*.

### 3-D Surface Tracking Module Developed — 2Q02

*Rocface* will be extended to include a new 3-D surface tracking module. A more general interpolation method is being developed to replace the current implementation. The new module will construct an intermediating mesh, whose elements are nested in an element of both fluid and solid input meshes. The data are then interpolated through this intermediate mesh and local conservation is enforced on the elements of the intermediate mesh.

### 3-D Unstructured Fluid Dynamics Module Implemented — 2Q02

A new fluid dynamics solver, *Rocflu*, will be implemented in the coming year. The new module is an unsteady, viscous, compressible flow solver that employs adaptive, mixed, unstructured 3-D meshes. It is being developed as a complement to *Rocflo*, CSAR's existing structured 3-D flow solver.

### GEN2 Simulation Implemented — 3Q02

Our second-generation whole-system rocket simulation includes many new physics modules that supplement and extend those in GEN1. The extensions enable us to include phenomena such as burning aluminum droplets and pressurized crack propagation.

### 3-D Propellant Combustion Interface Model Developed — 4Q02

The combustion region at the interface between the chamber flow and the propellant is thin, on the order of tens of microns. In contrast, the overall dimensions of solid rocket motors are often measured in meters. Hence, the integrated system code must treat the combustion layer as an interface across which mass, momentum, and energy are given in terms of jump conditions. There are a number of strategies of varying sophistication with which to generate these conditions. The most detailed approach is the generation of a complete sub-grid combustion model (*Rocfire*), a three-dimensional unsteady simulation of the propellant flames, the thermal layer in the solid, and the unsteady nonuniform regression of the solid surface.

Table 3.1.1: Key Thrust-level Tasks and Accomplishments for Y4 and 5

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|---|---|
| Structures and Materials | • 3-D enhanced element for case modeling completed<br>• Parallel implementation of implicit structural analysis code (*Rocsolid*) completed<br>• Contact algorithm completed<br>• AMR continued<br>• Parallel implementation of space-time finite element for 2-D elastodynamics completed<br>• Constitutive modeling continued<br>• 3-D fluid/structure burning crack simulation continued<br>• Parallel implementation of explicit structural analysis code (*Rocfrac*) completed |
| Fluid Dynamics | • Code development for 3-D unstructured flow solver completed (*Rocflu*)<br>• Scalar transport (smoke and chemical species) model implemented (*Rocspecies*)<br>• Turbulence modeling and experiments continued<br>• Al particle dynamics module implemented (*Rocpart*)<br>• Radiation model begun (*Rocrad*) |
| Combustion and Energetic Materials | • 3-D propellant-combustion interface (PCI) model implemented (*Rocfire*)<br>• Nonlinear dynamic burning model implemented (*Rocburn*)<br>• Improved ignition and flame spread model installed<br>• Ignition pressure spike simulated<br>• Parallel particle packing module completed<br>• Kinetics models developed<br>• Constitutive modeling of AP continued |
| Computer Science | • Parallel 3-D interface module implemented (*Rocface*)<br>• Mesh adaptation and repair continued<br>• Preconditioner development continued<br>• Automated compiler for applications migration completed |

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|---|---|
| | • Parallel I/O tools for massive file/data management developed<br>• Performance results and scalability studies on local and ASCI machines continued |
| System Integration | • GEN2 simulation implemented<br>• GEN1 verification and validation studies continued<br>• New coupling schemes implemented (*Roccom*)<br>• Parallel client-server visualization tool implemented (*Rocketeer*)<br>• New solid rocket validation systems selected |