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 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.

Simulation Roadmap

The CSAR Simulation Roadmap (Figure 3.1.1) depicts the evolution of increasingly sophisticated computational models for the primary rocket components and their interactions. The Project Timeline (Figure 3.1.2) 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 3. 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 3.1.1), 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.

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

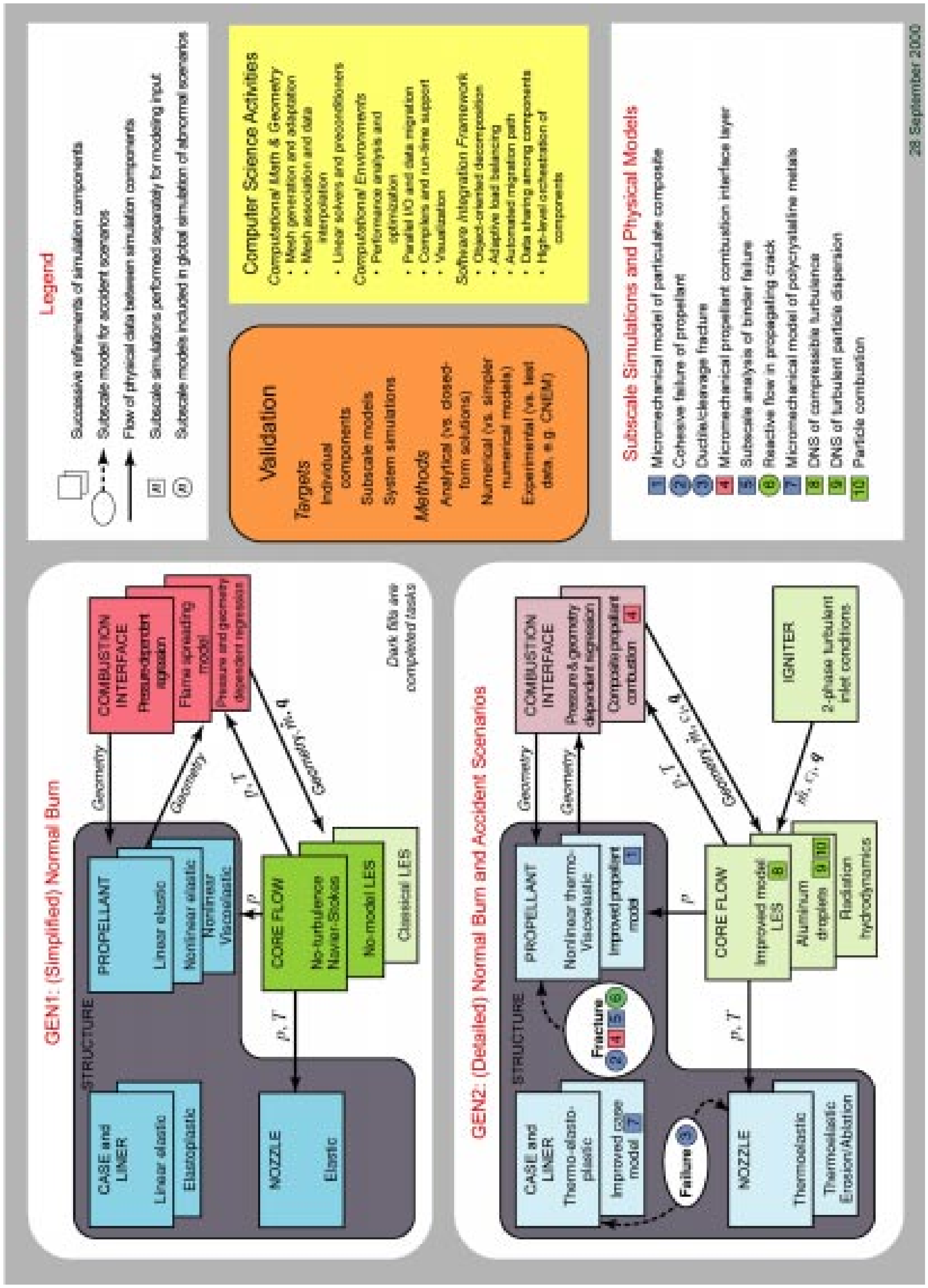

Fig. 3.1.1: CSAR Roadmap showing completed tasks (dark boxes in GEN1) and planned activities for Y4-10.

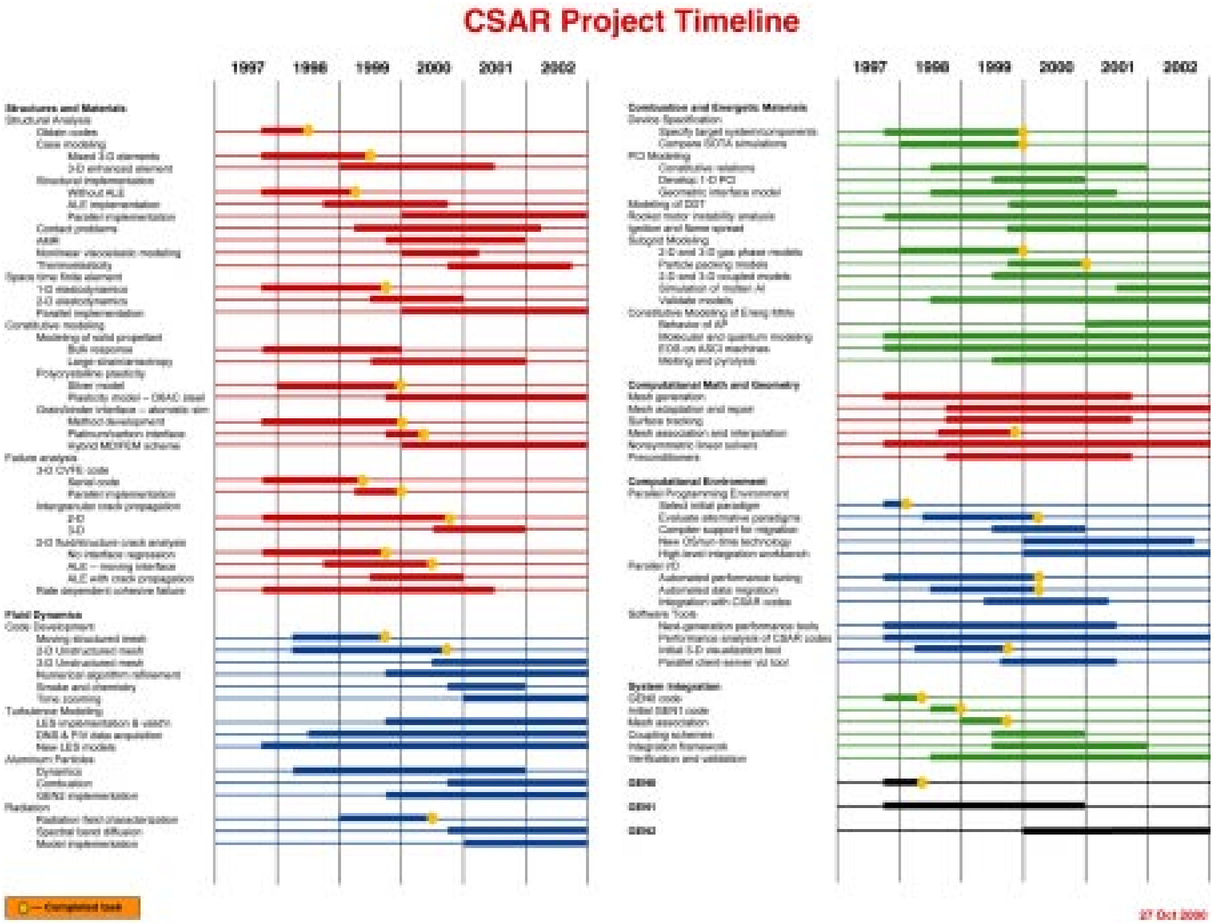

Fig. 3.1.2: CSAR Project Timeline shows completed tasks and future activities.

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 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.

Integrated Simulation Components

The ASCI Alliance Strategy Team (AST) and the DOE-DP Tri-lab Support Teams (TST) identified a need to establish early and periodic prototypes of the integrated simulation capabilities (ISC) of each of the five university-based ASAP Centers. The goal for "ISC99" was a fully 3-D, coupled, integrated solid/fluid code, employing MPI parallelism on the ASCI machines. This goal was achieved in September 1999. Key tasks for Y3 and Y4 were identified following the completion of ISC99. Table 3.1.1 presents the goals and specific tasks for each research group.

Table 3.1.1: Key Simulation Tasks for Y3 and Y4

CSAR Goal	Fully 3-D, coupled, integrated solid/fluid code, employing MPI parallelism on ASCI machines.
Structures and Materials	• 3-D enhanced element completed • ALE structural implementation completed, begin parallel implementation • Contact problems continued • AMR continued • Nonlinear viscoelastic modeling completed • Space-time finite element for 2-D elastodynamics completed • Constitutive modeling continued • 2-D intergranular crack propagation completed, begin 3-D • 2-D pressurized crack ALE completed
Fluid Dynamics	• Fully 3-D, including star grain, flow in head-end slots simulation completed • Code development for 2-D unstructured mesh completed, 3-D mesh continued • Al smoke and chemistry component modeling begun • Time zooming studies begun • Turbulence modeling and experiments continued

	• Al particle dynamics and combustion modeling continued • Radiation: spectral band diffusion model begun
Combustion and Energetic Materials	• 1-D propellant-combustion interface (PCI) model implemented • Geometric PCI model completed • Instability model enhanced • Improved ignition and flame spread model installed • Subgrid models: particle packing model completed, simulation of molten Al particles begun • Constitutive modeling of AP begun
Computer Science	• Surface tracking modules completed • Mesh adaptation and repair continued • Preconditioner development continued • Initial software framework implemented • Compiler support for migration completed • Parallel I/O tools integrated with CSAR codes • Next-generation performance tools implemented • Parallel client-server visualization tool implemented • Performance results and scalability studies on local and ASCI machines continued
System Integration	• GEN1 simulation completed • Coupling schemes implemented