2 Introduction

DOE ASCI/ASAP Program

The Center for Simulation of Advanced Rockets (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). ASCI is a cooperative technological research program among the three DOE/National Nuclear Security Administration Defense Programs National Laboratories—Lawrence Livermore, Los Alamos, and Sandia—to provide leading edge computational modeling and simulation capabilities to support the Stockpile Stewardship 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- and simulation-based methods.

Fig. 2.1: ASCI Program advances national strengths in computational and simulation science.

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. Replacing conventional testing with computational simulation requires a giant leap in both simulation methodology and computational capacity. Each of the five research centers funded under the Academic Strategic Alliances Program (ASAP) is focused on simulation in the context of a different physical problem, but all share the 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.

The research of the ASAP centers is expected to drive advances in critical computer and computational science areas. The major goals of the Alliance Program are to:

- Solve science and engineering problems of national importance through the use of large-scale, multidisciplinary modeling and simulation.
- Establish and validate large-scale modeling and simulation as a viable scientific methodology across scientific applications requiring both integration across disciplines and complex simulation sequences.
- Enhance overall ASCI efforts by engaging academic experts in computer science, computational mathematics, and simulations in science and engineering.
- Leverage relevant research in the academic community, including basic science, high-performance computing systems, and computational environments.
- Strengthen education and research in areas critical to the long-term success of ASCI and the Stockpile Stewardship Program.

- Strengthen ties among the Defense Programs laboratories and participating U.S. universities.

Center for Simulation of Advanced Rockets

In response to the scientific and technological needs of ASCI/ASAP, the University of Illinois at Urbana-Champaign (UIUC) established the Center for Simulation of Advanced Rockets in September 1997. The outstanding quality of the faculty and staff, facilities, and research infrastructure offered by UIUC have enabled a unique partnership among university researchers and the DOE Defense Program laboratories to advance the state of the art in computational simulation of complex systems. State, regional, and university resources are also supporting the program, and an experienced research team is fulfilling the mission of the Center.

The goal of CSAR is detailed, whole-system simulation of solid propellant rockets under both normal and abnormal operating conditions. The design of solid propellant rockets is a sophisticated technological problem requiring expertise in diverse subdisciplines, including ignition and combustion of composite energetic materials; solid mechanics of the propellant, case, insulation, and nozzle; fluid dynamics of the interior flow and exhaust plume; shock physics and quantum chemistry of energetic materials; aging and damage of components; and analysis of various potential failure modes. These problems are characterized by very high energy densities, extremely diverse length and time scales, complex interfaces, and reactive, turbulent, and multiphase flows.

Fig. 2.2: Launch of STS-100, March 2001. CSAR provides whole-system simulation of the NASA Shuttle RSRM. (NASA photo.)

The whole-system simulation of solid propellant rockets requires the close interaction of the four CSAR Research Groups—Structures and Materials; Fluid Dynamics; Combustion and Energetic Materials; and Computer Science. Nine Research Teams have been assembled to address the specific needs of each aspect of the simulation. Five research teams operate within the loose bounds of the group structure; four research teams function as crosscutting programs.

Solid Propellant Rockets

The ability to launch payloads into orbit or to escape Earth's gravity entirely, though only about forty years old, is almost taken for granted. Hundreds of devices presently in Earth orbit provide global communications, entertainment, and a vast array of scientific data about Earth and the universe beyond. The U.S. Space Transportation System (better known as the NASA Space Shuttle) represents the zenith of this activity, with a 4.5 million-pound vehicle and a crew of seven blasted into orbit routinely on a near-monthly schedule.

Solid propellant rockets perform the "heavy lifting" in the aerospace industry, providing the immense thrust required to launch large payloads into Earth orbit or into outer space. In its brief but fiery lifetime—typically only one to two minutes—the solid booster stage pushes the payload the first thirty miles or so above the Earth, where a more easily controlled liquid-fuel rocket takes over for the final nudge into orbit or beyond.

There is almost universal, if tacit, recognition of the tremendous complexity of rocket systems. Everyone has heard the phrase, “this isn’t rocket science” or “it doesn’t take a rocket scientist to figure that out,” in reference to something that is not overly complicated or difficult. Indeed, some of the world’s brightest minds are involved in the design of solid rocket systems. Nevertheless, the challenge is extreme, failures still occur, and the gap between scientific understanding and hardware design is large. Thus, solid rocket motor design is an ideal focus for research devoted to advancing the state of the art in large-scale computational simulation of complex systems.

The basic idea behind a solid propellant rocket motor is simple: thrust arises from pressurization of a vented chamber by mass injection due to burning of the propellant. Its detailed behavior is quite complicated, however, as the combustion rate depends on the chamber pressure as well as the surface area and storage temperature of the propellant. The particular shape of the solid propellant, called the propellant grain, determines the burning surface area, which in turn affects how the thrust varies over time—progressive, regressive, or neutral profiles are possible. The propellant grain is usually not just a simple cylinder, but often has slots and fins in its interior cavity to increase the surface area. The propellant surface regresses as propellant is consumed, however, so the shape and area of the burning surface change dynamically with time.

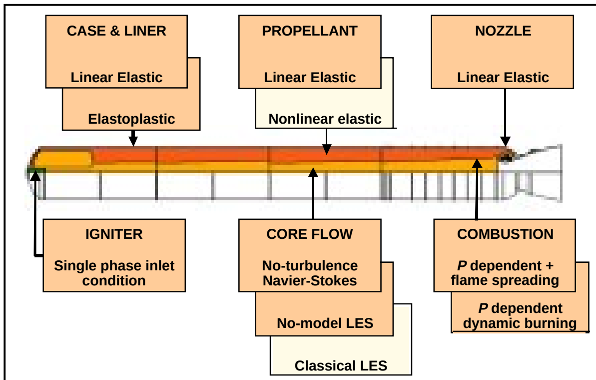

Fig. 2.3: GEN1 Simulation Roadmap provides direction for future research. Shaded boxes show completed tasks.

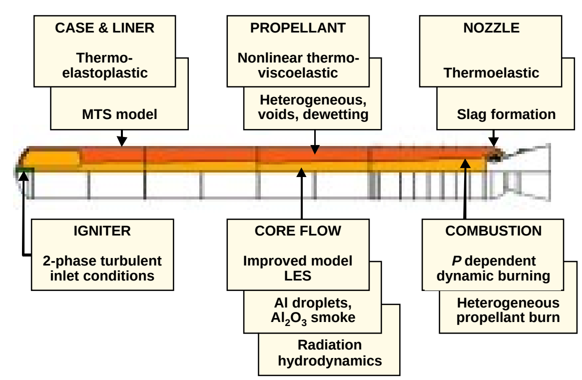

Fig. 2.4: GEN2 Simulation Roadmap.

The coupling and feedback between these variables can lead to instabilities. For example, the burning rate increases with the chamber pressure, and the chamber pressure increases with the burning rate. For this reason, relatively small defects can lead to catastrophic failure. A crack in the propellant, for example, causes an abrupt change in the surface area, and hence in the burning rate, which in turn causes an abrupt change in the pressure. Pressurization of the crack may cause it to grow rapidly, possibly leading to premature burn-through to the rocket casing and catastrophic failure. Yet another potential failure mode is a possible transition from deflagration (normal surface burning) to detonation (explosion), in which, perhaps due to pre-existing damage or compaction of the propellant, energy is released throughout a volume of the propellant, with fatal consequences.

Rocket design is further complicated by manufacturing and transportation constraints. Large boosters are manufactured in segments that are then assembled at the launch site, and the joints between segments are a potential source of failure.

CSAR Simulation Vehicles

Space Shuttle SRB

CSAR has chosen the reusable solid rocket motor (RSRM) of the Space Shuttle as the principal simulation vehicle. Other solid propellant rockets are being used for verification and validation of the CSAR integrated simulation. The Shuttle is a well-established, commercially produced rocket, is globally recognized, and most importantly, basic design data and propellant configurations are available. NASA-provided[1] system data describe the RSRM.

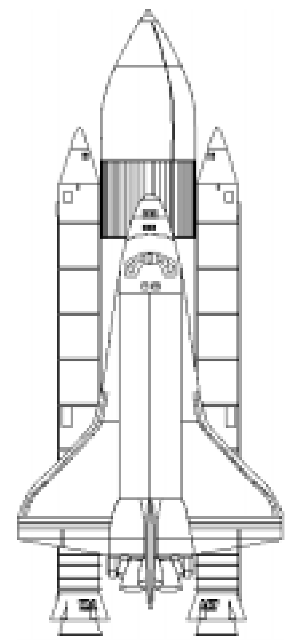

Fig. 2.5: NASA Space Transportation System

The two solid rocket boosters provide the main thrust to lift the space shuttle off the launch pad and up to an altitude of about 150,000 feet, or 25 nautical miles (28 statute miles). In addition, the two RSRMs carry the entire weight of the external tank and orbiter and transmit the weight load through their structure to the mobile launcher platform. Each booster has a thrust (sea level) of 3,300,000 pounds at launch. They are ignited after the three space shuttle main engines' thrust level is verified. The two RSRMs provide 71.4 percent of the thrust at lift-off and during first-stage ascent. Seventy-five seconds after RSRM separation, RSRM apogee occurs at an altitude of approximately 220,000 feet, or 35 nautical miles (41 statute miles). RSRM impact occurs in the ocean approximately 122 nautical miles (141 statute miles) downrange. The RSRMs are the largest solid-propellant motors ever flown and the first designed for reuse. Each is 149.16 feet long 12.17 feet in diameter. Each RSRM weighs approximately 1,300,000 pounds at launch. The propellant for each solid rocket motor weighs 1,100,000 pounds. The inert weight of each RSRM is approximately 192,000 pounds. The propellant mixture consists of ammonium perchlorate oxidizer (69.6 percent by weight), powdered aluminum fuel (16 percent), iron oxide catalyst (0.4 percent), polymer binder that holds the mixture together (12.04 percent), and an epoxy curing agent (1.96 percent).

Primary elements of each booster are the motor (including case, propellant, igniter and nozzle), structure, separation, operational flight instrumentation, recovery avionics, pyrotechnics, deceleration system, thrust vector control system and range safety destruct system. The propellant grain has an 11-point star-shaped perforation in the forward motor segment and a double-truncated-cone perforation in each of the aft segments and aft closure. This configuration provides high thrust at ignition and then reduces the thrust by approximately a third 50 seconds after lift-off to prevent overstressing the vehicle during maximum dynamic pressure.

[1] *NASA Shuttle Reference Manual*, http://shuttle.nasa.gov/reference/, 1998.

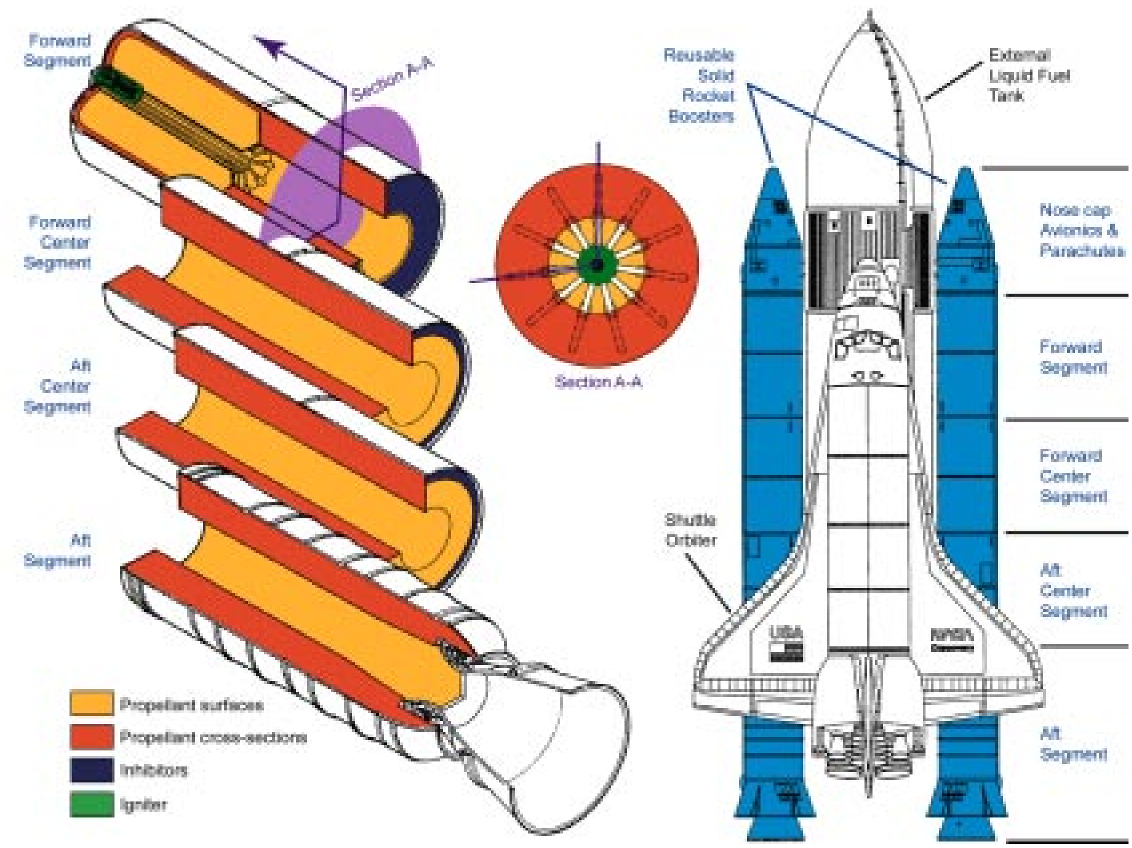

Fig. 2.6: Reusable Solid Rocket Motor (RSRM) is primary booster for NASA Space Transportation System (STS). Section A-A shows eleven-point slot and fin structure in forward segment of RSRM. Propellant in forward-center and aft-center segments form straight-walled cylinders, aft segment propellant tapers outward to submerged nozzle. Inhibitors between segments are asbestos-filled carboxyl-terminated polybutadiene used to tailor burning surface to meet thrust requirements of motor.

The RSRMs are used as matched pairs and each is constructed of four solid rocket motor segments. The RSRMs are matched by loading each of the four motor segments as pairs from the same batches of propellant ingredients to minimize any thrust imbalance. The segmented-casing design assures maximum flexibility in fabrication and ease of transportation and handling. Each segment is shipped to the launch site on a heavy-duty rail car with a specially built cover.

Titan IV Booster Accident Validation

A key goal of the ASCI/ASAP program is to establish and validate large-scale modeling and simulation as a viable scientific methodology across engineering applications. In the case of CSAR, this includes validation of solid propellant rocket simulation codes under normal and abnormal operating conditions. CSAR has chosen a well-documented test-stand failure of a Titan IV rocket booster motor as its full-scale abnormal validation case. A complete description of the CSAR validation simulating this accident appears in Section 3.6, System Integration.

The Titan IV PQM-1 (prequalification motor number 1) SRMU was a solid booster motor developed for the Air Force Space Systems Command by Hercules Incorporated (now AlliantTech Systems, Thiokol Division) under subcontract to the Martin Marietta Corporation.[2] The motor was 126 inches in diameter, 100 feet long, and weighed approximately 778,000 lbs. It had a graphite composite case and contained HTPB propellant. Figure 2.7 is a sketch of the PQM-1 configuration with its forward, center and aft segments, which were assembled in place on the test stand. The forward segment has fin slots, and provided 40 percent of initial burn surface, and the center and aft segments are axisymmetric. Except for a short 6-inch flap near the port of the forward segment, the grain had no inhibitors or other stress relief flaps; rather, stress relief grooves were used at the forward and aft bond terminations of the center segment, and at the forward bond termination of the aft segment.

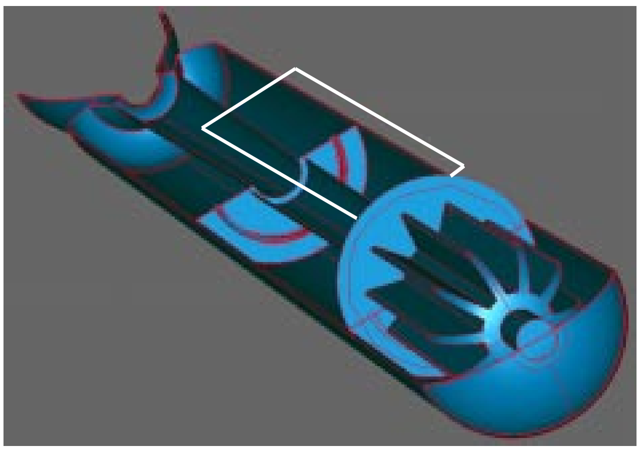

Fig. 2.7: Cutaway drawing of Titan IV PQM-1 motor shows three-segment solid propellant design.

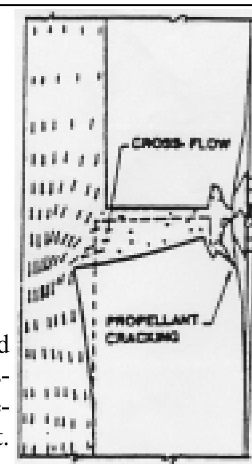

Fig. 2.8: PQM-1 failed due to excessive pressure drop and grain deformation near aft slot.

The first static test unit under the Titan IV SRMU development program, motor PQM-1, was fired vertically at Phillips Laboratory, Edwards AFB, California on 1 April 1991. The motor case ruptured at 1.58 seconds due to over pressure. The three-segment motor ignited normally in the predicted 0.6 sec interval, but forward pressure was approximately 130 psi higher than the predicted 1140 psi. Forward pressure rose gradually until 1.2 sec, at which time it began to rise at an increasing rate until the case ruptured at approximately 1840 psi, the expected hydroburst level. Aft pressure (nozzle region) was increased though the test period as expected until 1.5 seconds when it began to decrease. Long-wire strain gages on the individual segments indicated that a large pressure drop, on the order of 600 psi, developed in the vicinity of the radial slot between the center and aft segments.

Several failure analysis boards concluded that failure was caused by excessive pressure drop and grain deformation near the aft radial slot (Figure 2.8). It was determined to be a grain stability failure in which the higher-than-predicted pressure drop caused excessive constriction of the aft centerport, which, in turn, aggravated the pressure drop. Grain redesign activities involved chamfering of the forward ends of the center and aft segments. Extensive flow and grain deformation modeling activities were validated through subscale testing.

[2] This description of the Titan IV PQM-1 failure is taken liberally from: Wilson, W. G., J. M. Anderson, and M. Vander Meyden, “Titan IV SRMU PQM-1 Overview,” AIAA 92-3819, AIAA/SAE/ASME/ASEE 28th Joint Propulsion Conference and Exhibit, 6-8 July 1992.

Other ASCI/ASAP Centers

As is the case with CSAR, the focus of effort at each ASCI/ASAP center leads to revolutionary advances in physical and engineering sciences and in mathematical and computer sciences, to the benefit of the SSP and the nation. Of significant value to ASCI is the experience acquired by faculty and students using massively parallel computers. Each center supports about 70 full-time people per year. The total number involved is considerably larger due to the broader involvement of the scientific community as well as individual transitions in and out of the centers.

At the California Institute of Technology, the Center for Simulating the Dynamic Response of Materials is developing simulation codes for a virtual shock physics test facility (VTF). The VTF allows researchers to simulate numerically strong shock and detonation waves that collide with solid or fluid targets. The goal is to compute the subsequent dynamic response of the target materials and to validate these computations against experimental data. Demonstrating the capability of the simulation codes to model the dynamic response of materials addresses a key technical issue for ASCI. *http://www.cacr.caltech.edu/ASAP/*

Fig. 2.9: ASCI/ASAP centers are located at five major research universities.

The goal of the ASCI Alliance Program at Stanford University's Center for Integrated Turbulence Simulations is to build a detailed computational simulation of a gas turbine. This requires modeling the key engine components, including the compressor, combustor, and turbine. The resulting integrated models examine many characteristics, including turbine blade vibrations, rotating stall in the compressor, instabilities as fuel burns in the combustor, and heat transfer from the hot combustion products to the first rows of blades in the turbine. *http://cits.stanford.edu*

Researchers at the University of Chicago Center for Astrophysical Thermonuclear Flashes study the physics of thermonuclear explosions, which appear in a wide range of astronomical phenomena. The required high temperatures and densities are found in compact stars such as white dwarfs or neutron stars. *http://www.flash.uchicago.edu/*

The focus of the Center for Simulation of Accidental Fires and Explosions (C-SAFE) at the University of Utah is to provide science-based tools for the simulation of accidental fires and explosions, especially in the context of handling, transporting, and storing highly flammable materials. These simulations will help to evaluate the risks and safety issues associated with preventing and controlling fires and explosions in the aerospace, chemical, and petroleum industries. *http://www.csafe.utah.edu*