# 2. Introduction

## DOE ASCI/ASAP Program

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. The specific motivation for ASCI is to ensure the safety and reliability of the Nation's nuclear weapons stockpile in an era when empirical testing of such weapons has been banned by international treaties. Replacing conventional testing by 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 they all 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.

The ASAP centers focus on key multi-disciplinary applications for which the coupling of complex computer-based simulation sequences offer opportunities for major advances in the application domain chosen and support basic and applied science areas important to ASCI and the broader DOE Science-Based Stockpile Stewardship program. The research of the centers is expected to drive advances in critical computer and computational science areas.


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

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.

## Center for Simulation of Advanced Rockets

The goal of the Center is the 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 the ignition and combustion of composite energetic materials; the solid mechanics of the propellant, case, insulation, and nozzle; the fluid dynamics of the interior flow and exhaust plume; the shock physics and quantum chemistry of energetic materials, the aging and damage of components; and the 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.

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. Eight Research Teams have been assembled to address the specific needs of each aspect of the simulation. Five of the research teams operate within the loose bounds of the group structure; three research teams function as crosscutting programs.

Fig. 2.2. NASA Space Shuttle *Discovery*.

## Solid Rocket Fundamentals

The ability to launch payloads into orbit or to escape Earth's gravity entirely, though only about forty years old, is now almost taken for granted. Hundreds of devices now 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.

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 causes 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.

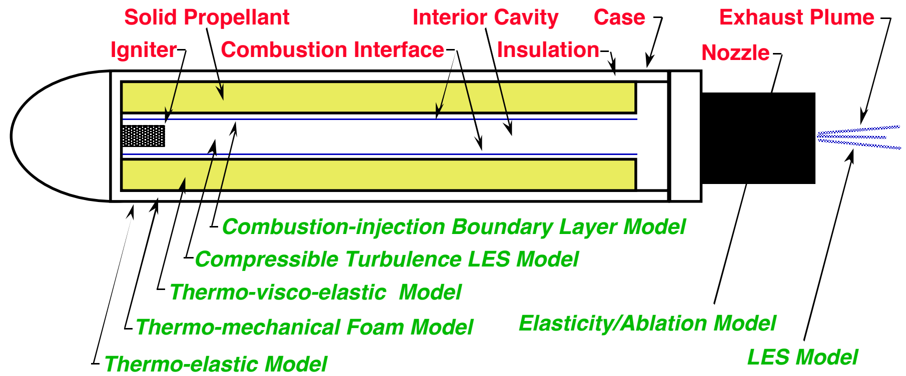


Fig. 2.3. Idealized solid propellant rocket. Major components are indicated in red, initial CSAR simulation models are green.

## Space Shuttle SRB—CSAR Simulation Vehicle

CSAR has chosen the solid rocket boosters (SRB) of the Space Shuttle as the simulation vehicle. The Shuttle SRB is a well-established commercial rocket, is globally recognized, and most importantly, basic design data and propellant configurations are available. NASA-provided[1] system data describe the SRBs:

The two solid rocket boosters provide the main thrust to lift the space shuttle off the pad and up to an altitude of about 150,000 feet, or 25 nautical miles (28 statute miles). In addition, the two SRBs 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 SRBs provide 71.4 percent of the thrust at lift-off and during first-stage ascent. Seventy- five seconds after SRB separation, SRB apogee occurs at an altitude of approximately 220,000 feet, or 35 nautical miles (41 statute miles). SRB impact occurs in the ocean approximately 122 nautical miles (141 statute miles) downrange. The SRBs are the largest solid-propellant motors ever flown and the first designed for reuse.

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

Each is 149.16 feet long 12.17 feet in diameter. Each SRB 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 SRB is approximately 192,000 pounds.

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 mixture in each SRB motor consists of an ammonium perchlorate (oxidizer, 69.6 percent by weight), aluminum (fuel, 16 percent), iron oxide (a catalyst, 0.4 percent), a polymer (a binder that holds the mixture together, 12.04 percent), and an epoxy curing agent (1.96 percent). The propellant is 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.

The SRBs are used as matched pairs and each is made up of four solid rocket motor segments. The pairs are matched by loading each of the four motor segments in 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.

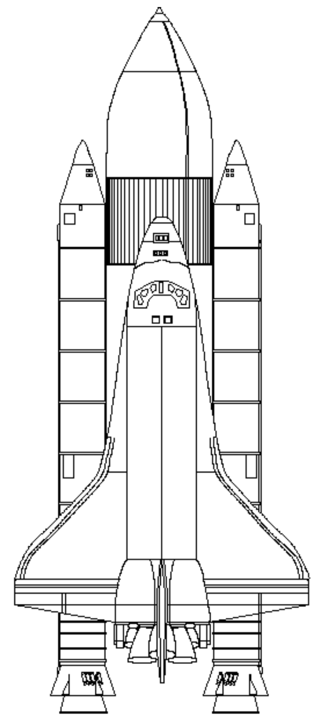

Fig. 2.4. NASA Space Transportation System