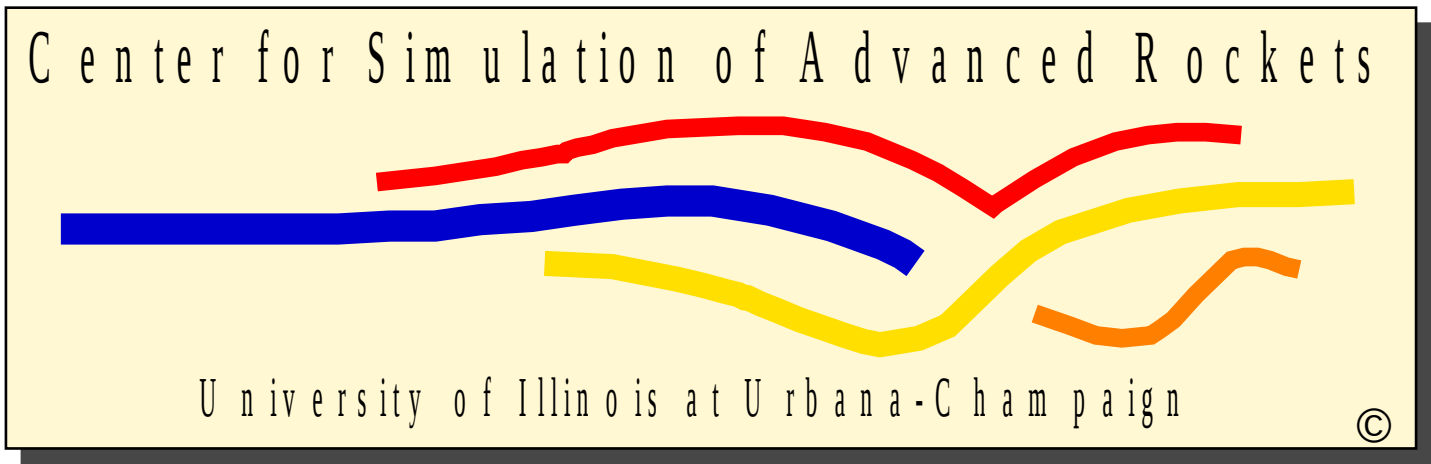




Integrated Simulation of Solid Propellant Rockets

William A. Dick
Managing Director

4 April 2001



Overview

- **Center program goals**
- **US DOE ASCI Program**
- **Research plan and Roadmap**
- **Organization**
- **Progress to date — mostly non-CFD**
- **Future development**

Computational Science and Engineering

Education Program

Computational Science & Engineering Option

12 departments
130 faculty associates
60 students enrolled
10 graduate fellows

Research Program

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DOE funded
\$20 million over 5 years
42 faculty
45 graduate students
25 professional staff

Center for Process Simulation and Design

NSF & DARPA funded
\$2.5 million over 3 years
12 faculty
13 students & staff



US DOE Accelerated Strategic Computing Initiative

- **Response to Comprehensive Test Ban Treaty, 1996**
- **Simulation only — no testing of “strategic stockpile”**
- **Huge computational capability**
 - Sandia — 8000 processor, Intel Pentium
 - Los Alamos — 4000 processor, SGI Origin2000
 - Lawrence Livermore — 1500 x 4 processor, IBM SP2
- **Full 3-D simulation science development**

US Department of Energy

ASCI/ASAP Centers

- Focus on single application that requires an integrated, multidisciplinary approach
- Tackle technical and organizational challenges analogous to those in stockpile stewardship
- Maintain balance among disciplines, especially between science and computation
- Validate!

Accelerated Strategic Computing Initiative
Academic Strategic Alliances Program

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Goals

Overarching Goal: Full 3-D simulation of SP rockets from first principles



- Detailed, whole-system simulation of solid propellant rockets under normal and abnormal operating conditions
- Accurate models of physical components
- Subscale simulations of materials and accident scenarios
- Software framework to facilitate component integration
- Computational infrastructure to support large-scale simulations
- Research collaborations with government laboratories and rocket industry

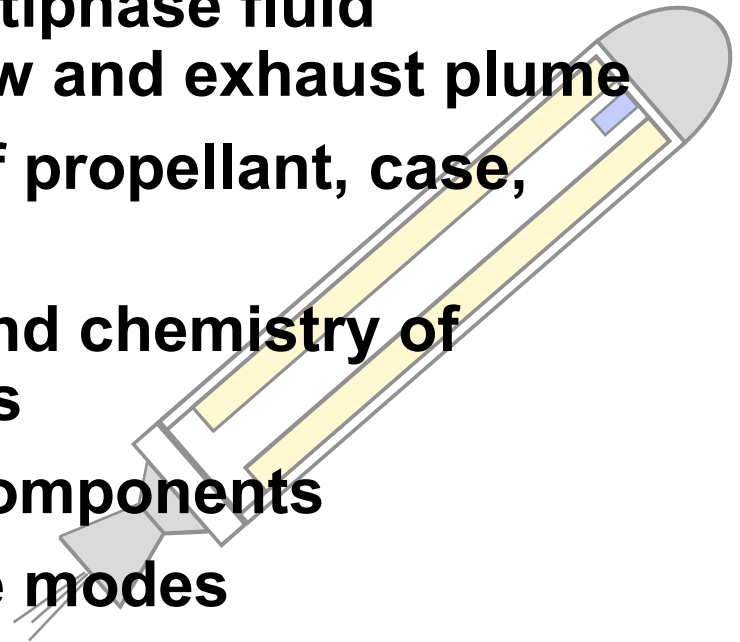
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Research Issues in Rocket Simulation

- Ignition and combustion of composite energetic materials
- Turbulent, reactive, multiphase fluid dynamics of interior flow and exhaust plume
- Structural mechanics of propellant, case, liner, and nozzle
- Fundamental physics and chemistry of materials and processes
- Aging and damage of components
- Various potential failure modes



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Challenges in Rocket Simulation

- Full 3-D modeling essential to capture physics
- Strong, nonlinear coupling among components
- Complex, dynamically changing geometry
- Extremely diverse spatial and temporal scales
- Complex material properties and physical processes
- Enormous computational capacity required for high-resolution simulation of full burn
- Scalability to 1000s of processors essential

Multi-Scale Applications with Common Framework

**Fluid-solid interaction with energy, mass,
and momentum transfer across reactive,
moving interface**

Phenomenon	Overall Scale	Resolution
Global response	10s of meters	cm
Crack propagation	meters	mm
Surface combustion	mm	micron

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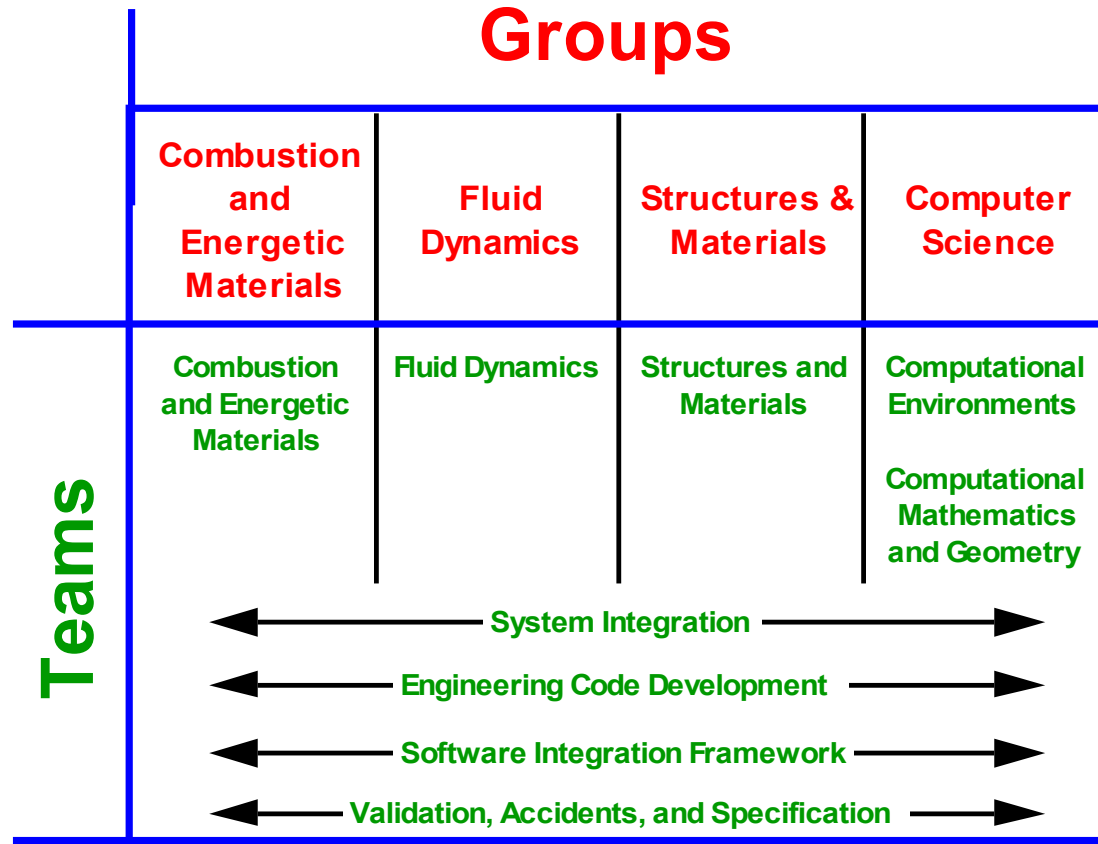


Organization

And

Technical Roadmap

CSAR Research Teams



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Participating Units

**Aeronautical and
Astronautical Engr**

Astronomy

Chemistry

**Civil and Environmental
Engineering**

**Computational Science
and Engineering**

Computer Science

**Materials Science and
Engineering**

**Mechanical and
Industrial Engineering**

NCSA

Nuclear Engineering

Physics

**Theoretical and Applied
Mechanics**

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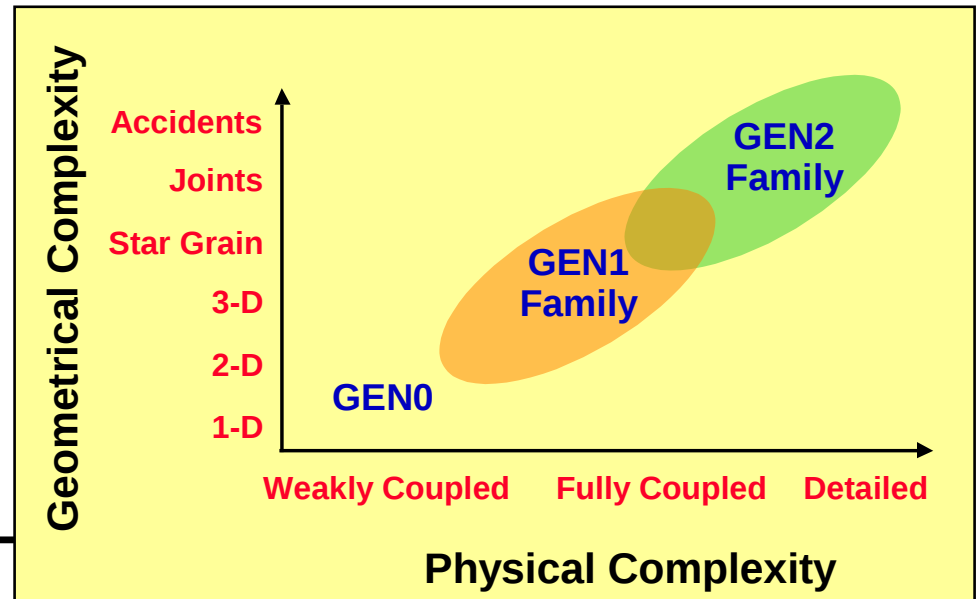
CSAR Staffing

	Current	Projected (FY02)
Senior investigators	40	40
Technical staff	30	32
Administrative staff	3	3
Graduate students	42	40
Undergraduate students	5	10
Total	120	125

Staged Approach

■ GEN0: system integration exercise

- 2-D ideal rocket based on Space Shuttle parameters completed 5/98



■ GEN1: prototype 3-D whole-system simulation code

- Basic component models
- Full component interactions
- Feedback for subsequent design — completed 1/01

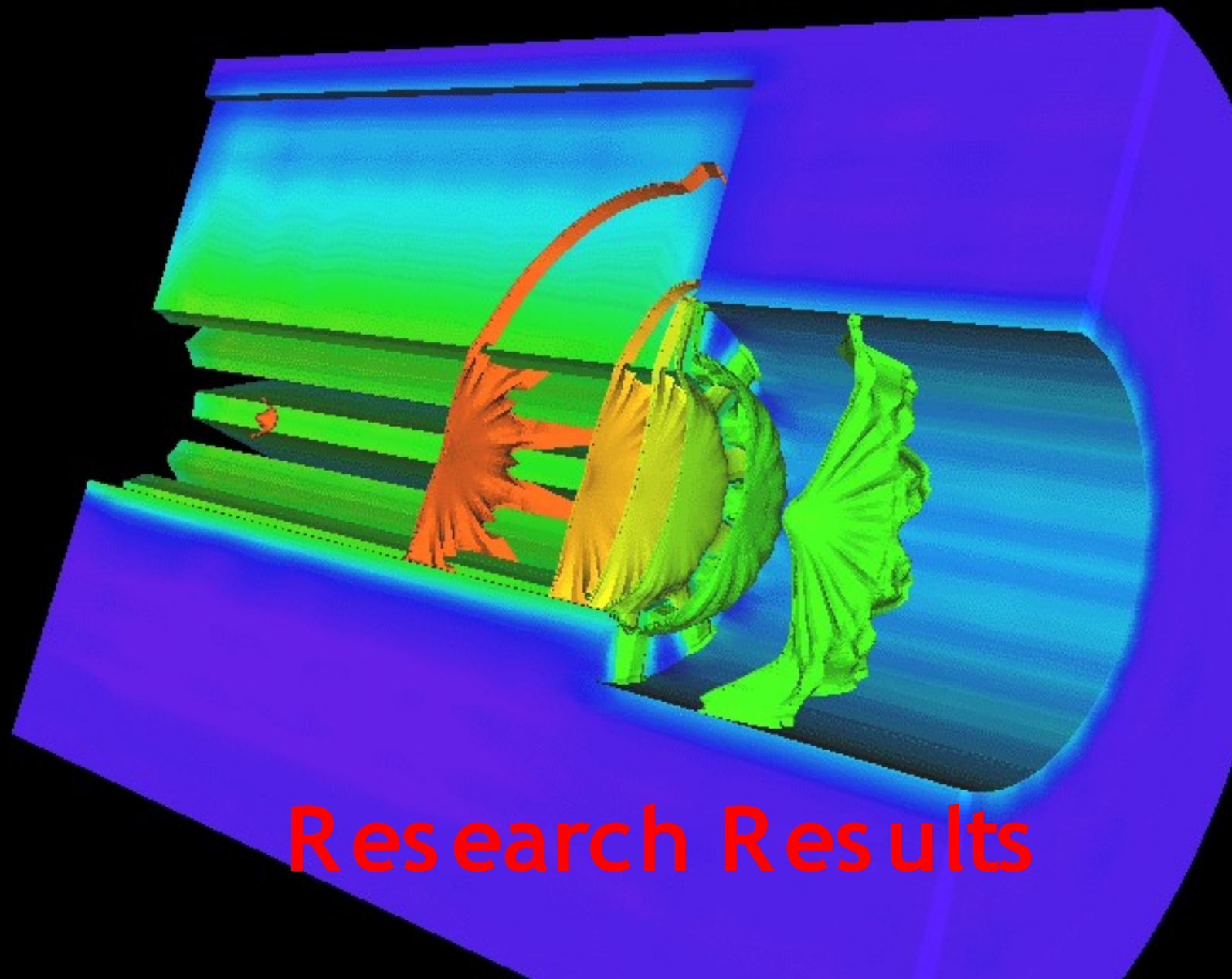
■ GEN2: fully capable rocket simulation tool

- Detailed component models
- Complex component interactions
- Subscale simulations supported

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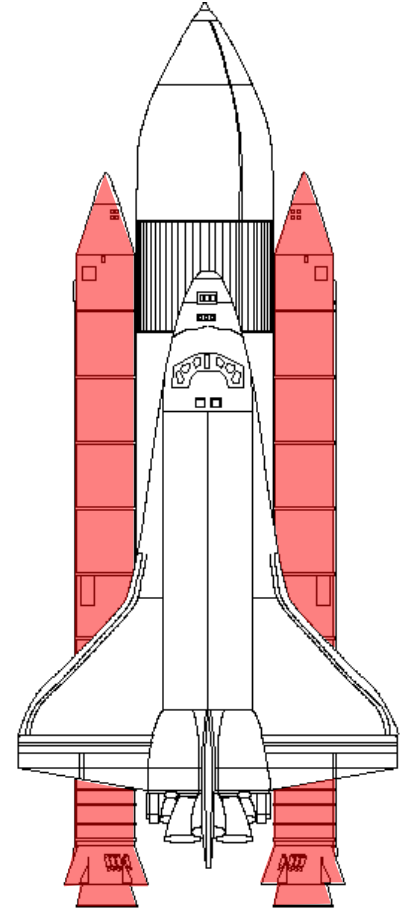
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Research Results

Initial Simulation Target: Space Shuttle RSRM

- Typical modern large solid rocket booster
- Height: 38 m, Diameter: 3.7 m
- Weight: 70 ton empty, 590 ton full
- Manufactured and shipped in four segments
- Aluminized ammonium perchlorate propellant
- Burns for 126 seconds, to altitude of 40 km and speed of 5000 km/h



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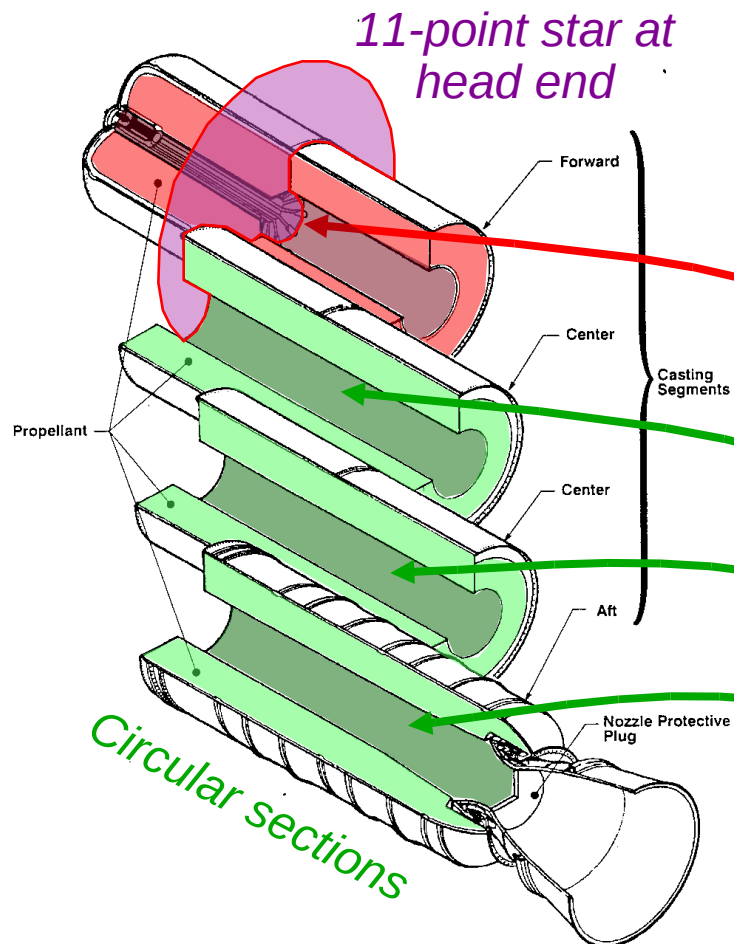


Figure 4.3-1. RSRM Propellant Configuration

A036657a COB

THIOKOL

4-58

930480

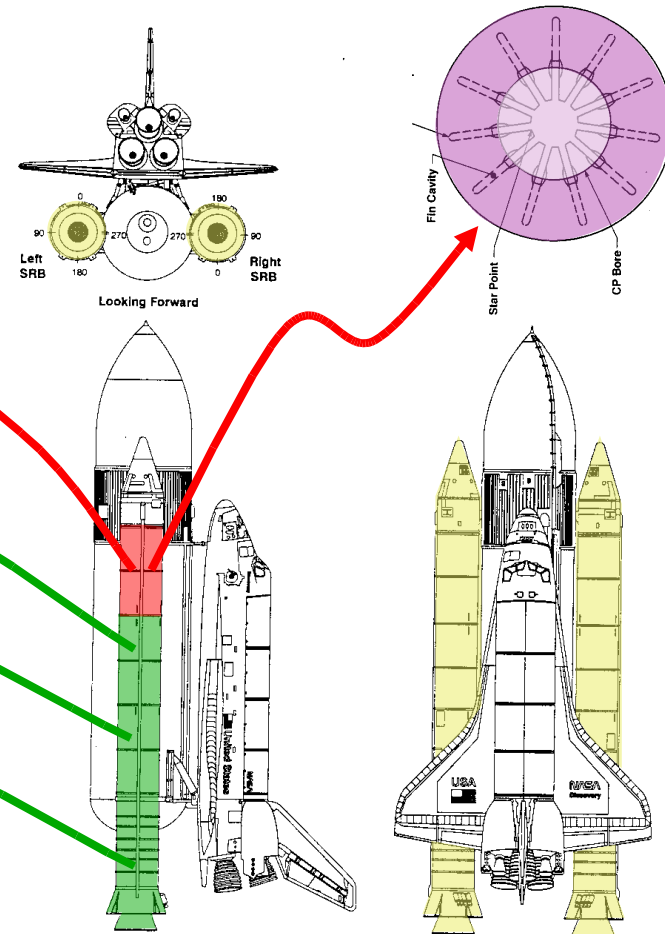


Figure 3.1-1. Boosters Attached to External Tank

A036406a COB

THIOKOL

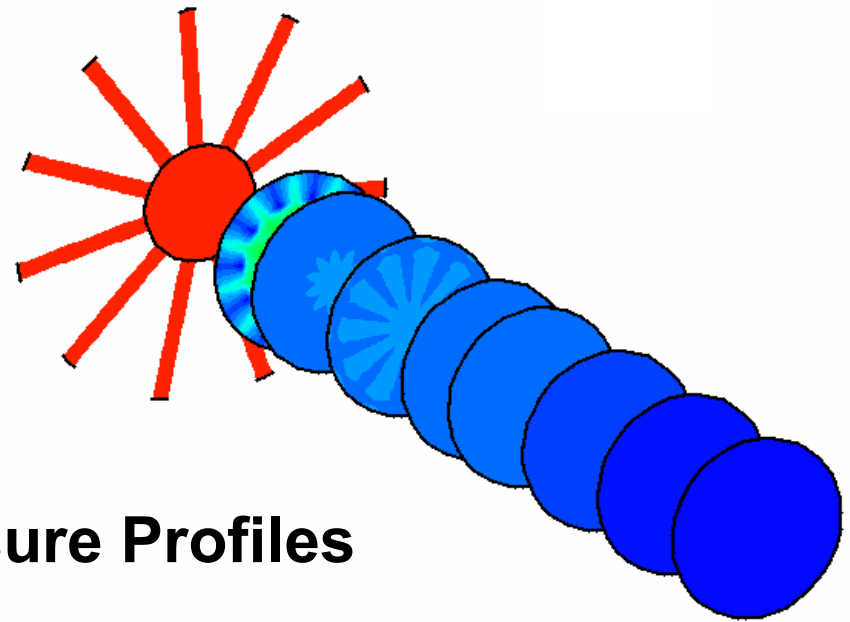
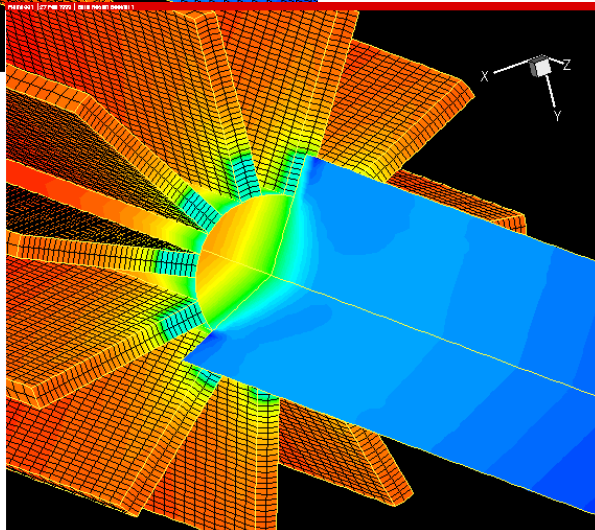
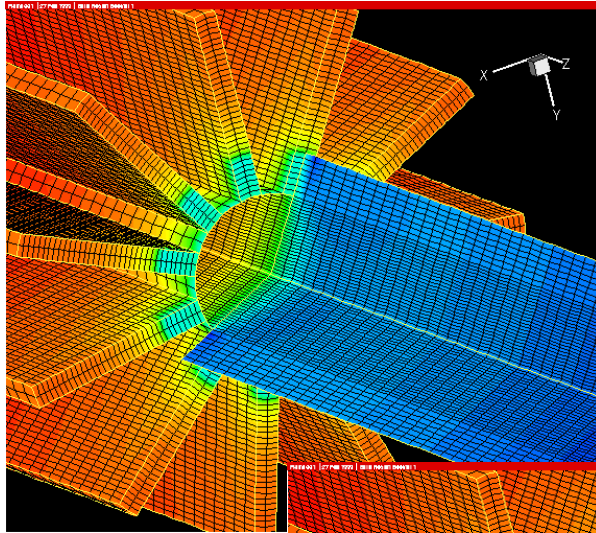
3-2

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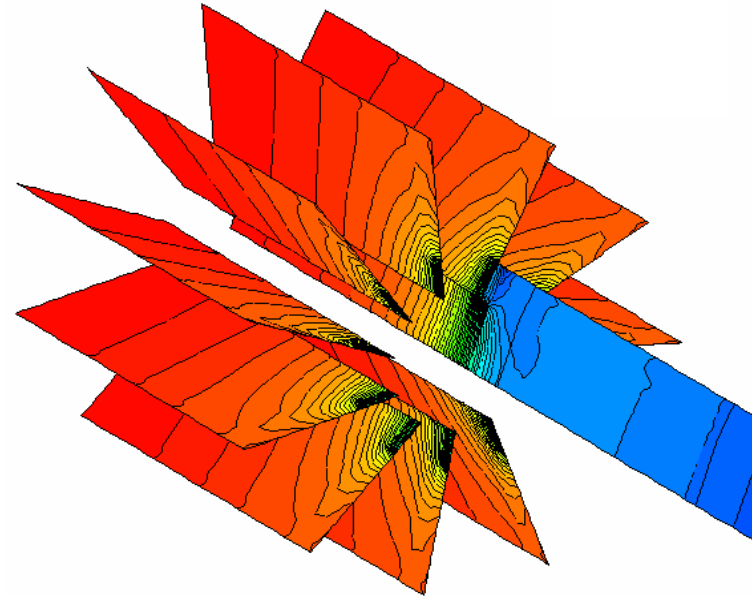
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GEN1 Fluid Axial Profiles



Pressure Profiles



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GEN1 Integrated Results

Stresses in Solid — Pressure in Fluid

QuickTime™ and a
GIF decompressor
are needed to see this picture.

- Fully coupled 3-D simulation of star grain in Space Shuttle RSRM
- Stress in propellant and gas pressure isosurfaces in slots and core region
- Executed on 256-processor SGI Origin2000
- Visualized with CSAR *Rocketeer*

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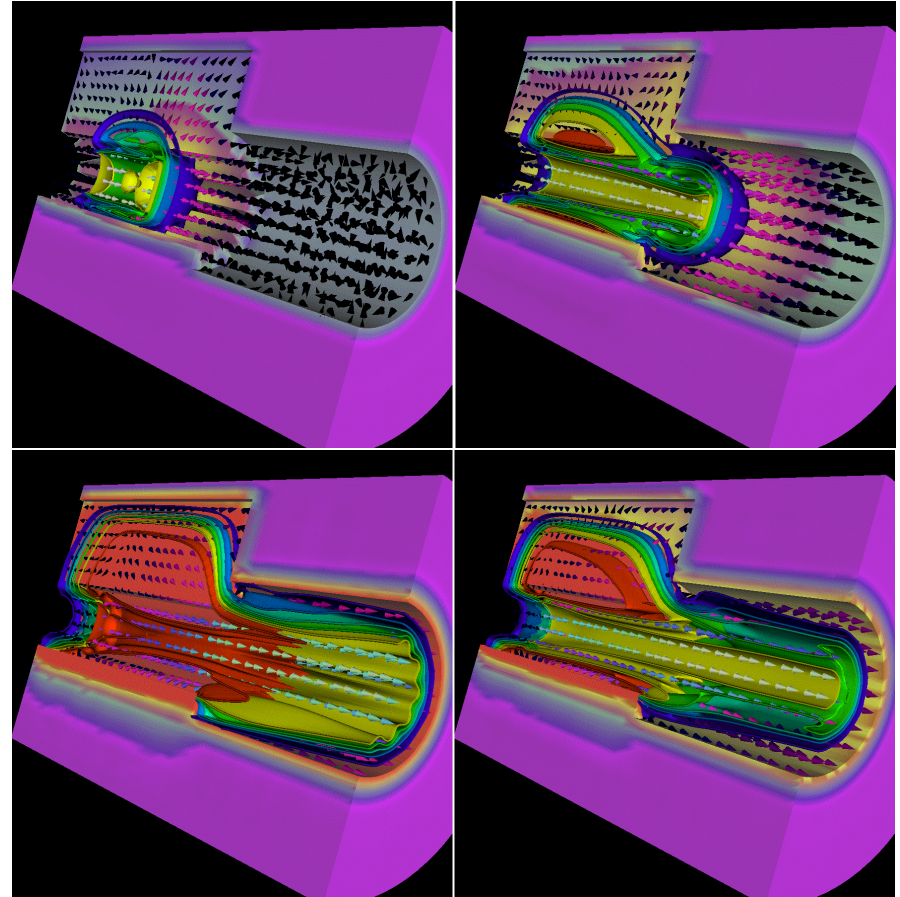


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GEN1 Integrated Results

Ignition Transient with Velocity Vectors

QuickTime™ and a
GIF decompressor
are needed to see this picture.

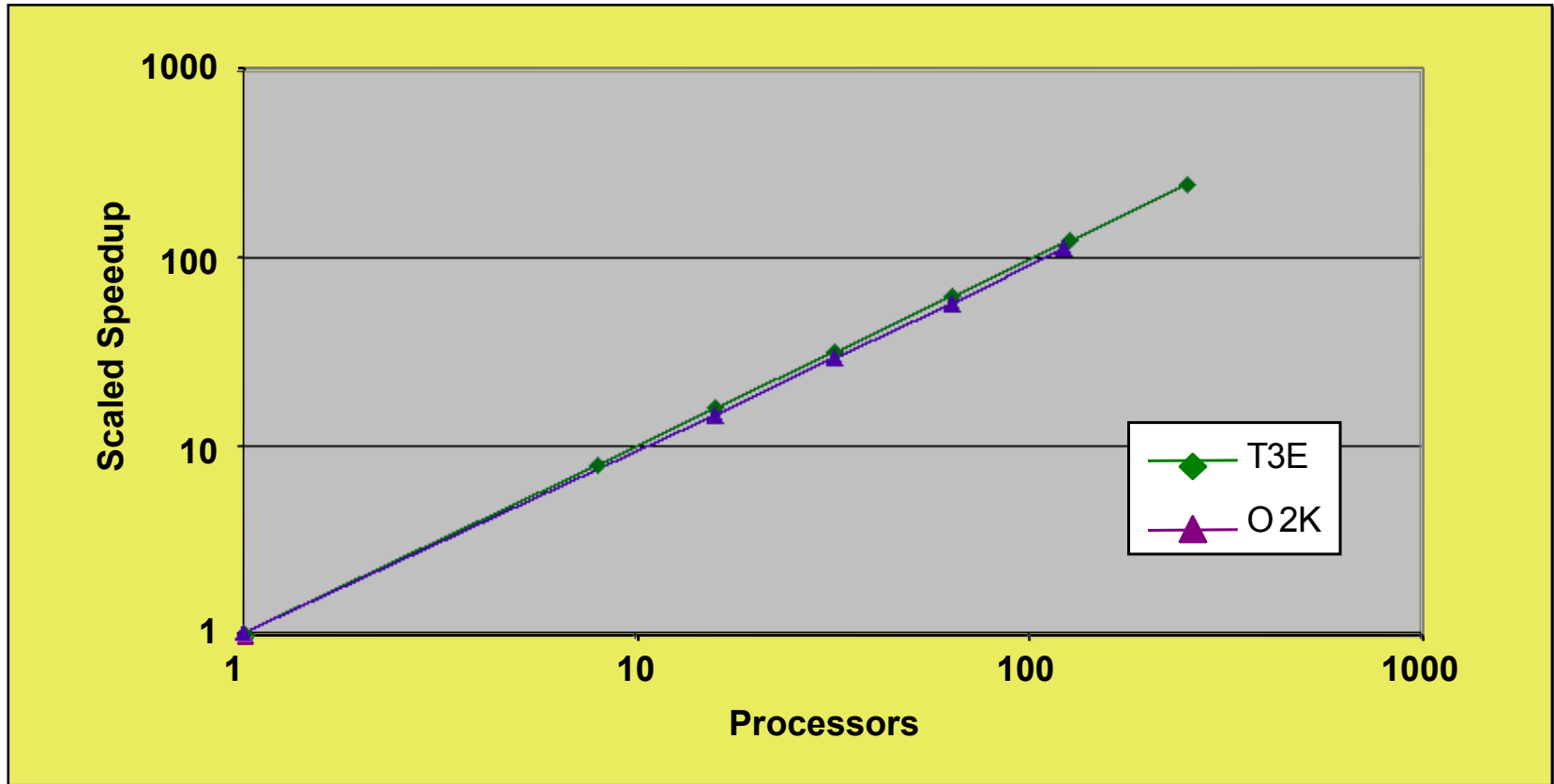


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Scalability of GEN1 for RSRM Problem

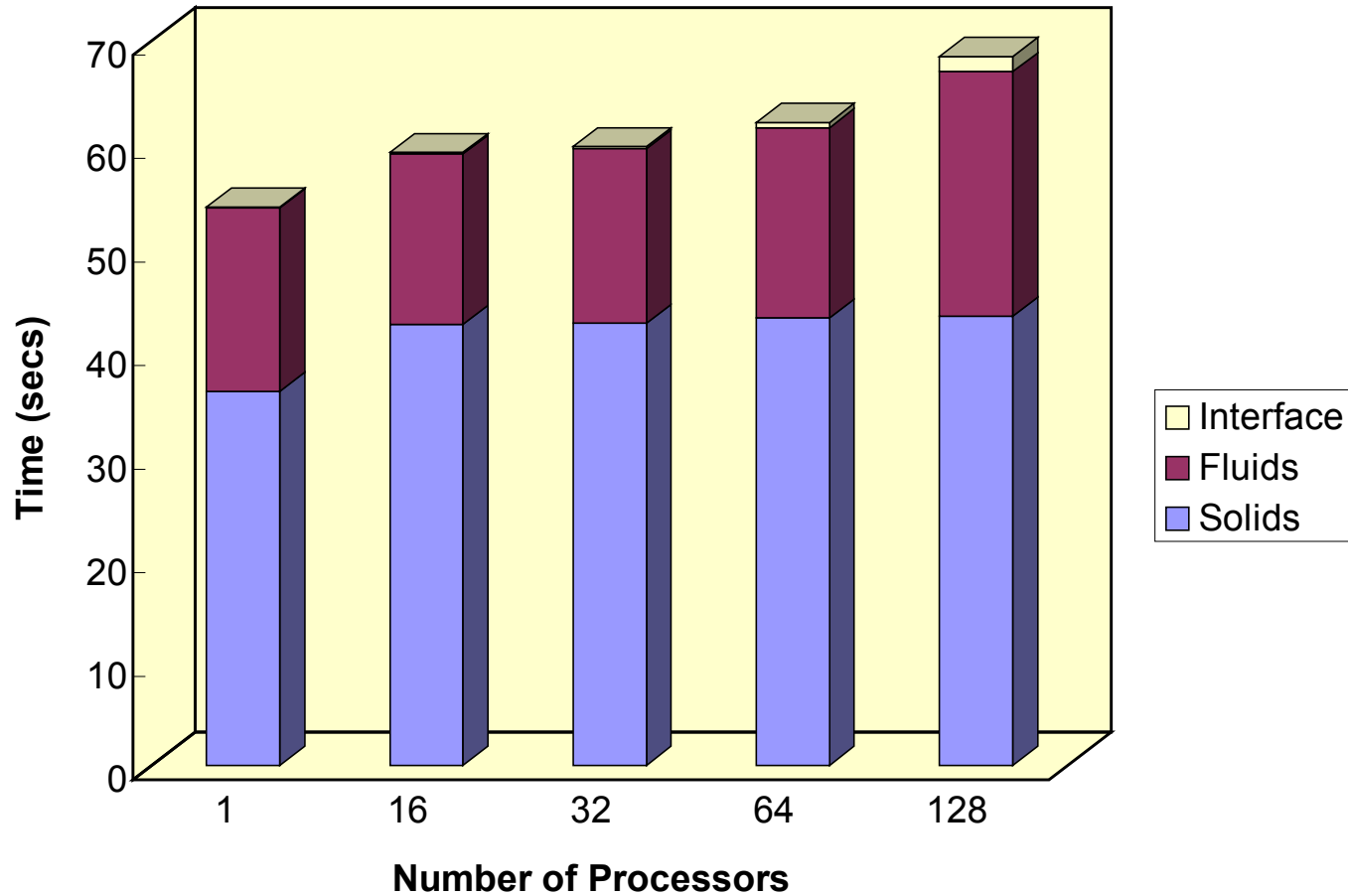


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GEN1 Time Breakdown (SGI Origin)



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Verification and Validation



■ Component codes

- Standard test cases with known solutions
- Data from laboratory experiments at UIUC and elsewhere
- Lab-scale rockets (China Lake, Edwards)

■ Integrated codes

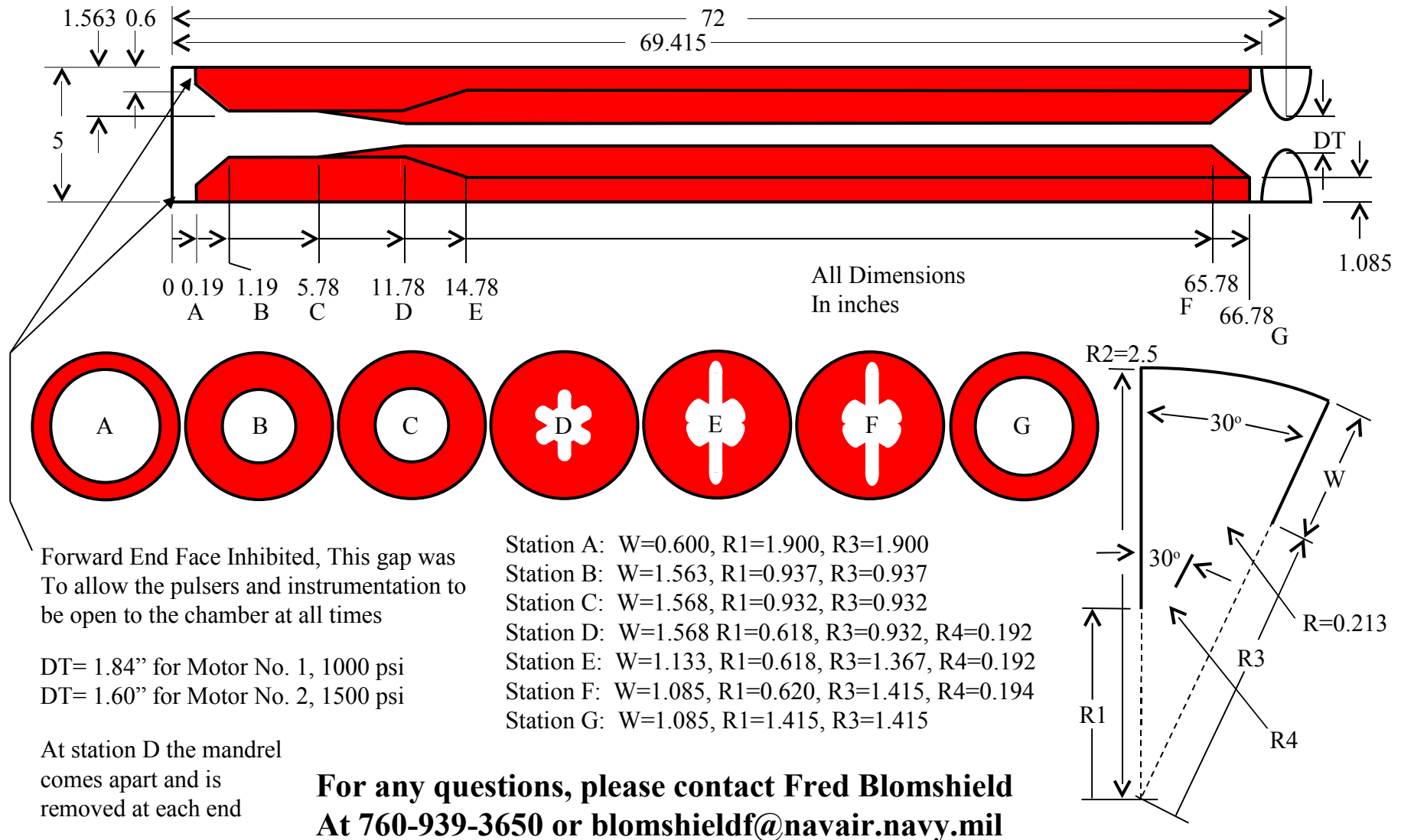
- Flat panel
- AGARD wing
- Shuttle inhibitors
- Titan IV propellant slumping
- Additional normal and accident scenarios for real rockets

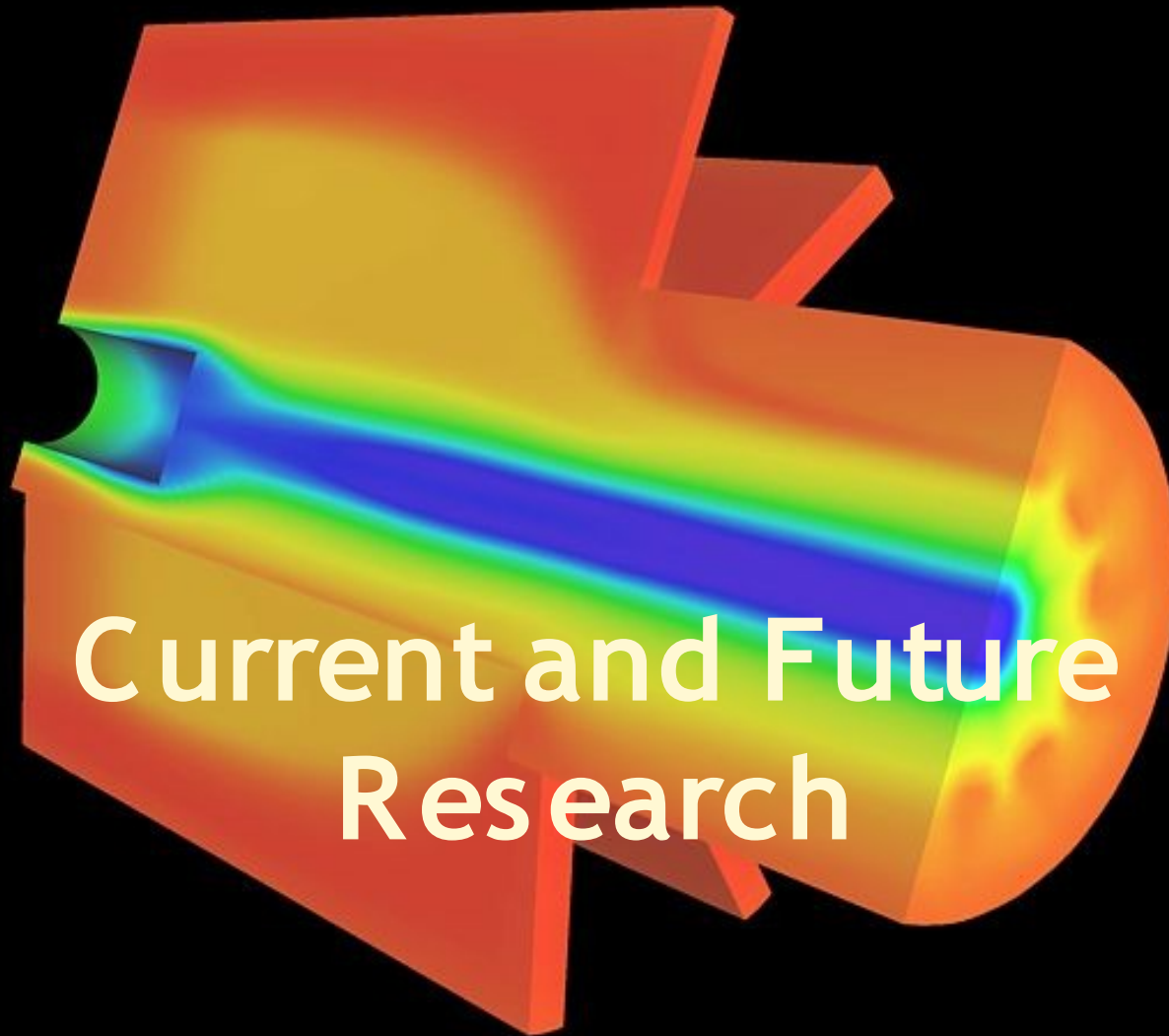
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Motor Geometry for Motors Nos. 1 and 2 (and 3 and 4) Referred to in AIAA Paper No. 98-3557

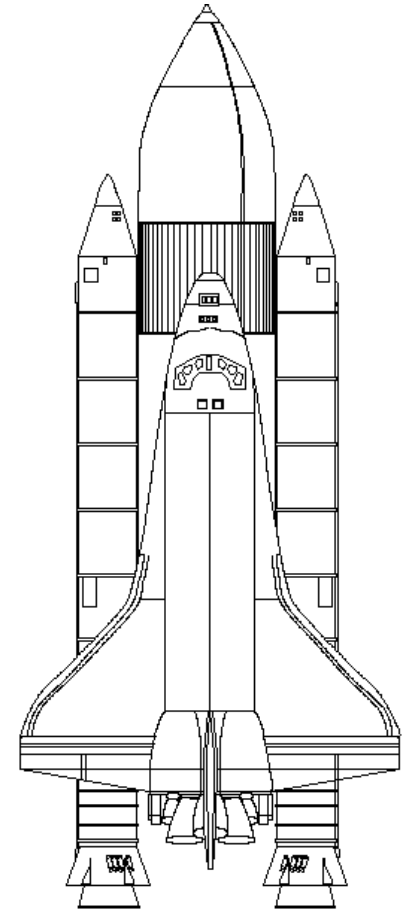




Current and Future
Research

Goals for GEN2

- **Detailed full system simulations of solid propellant rockets**
 - Space Shuttle booster
 - Titan IV
 - Lab scale test motors
- **Keep run times reasonably short**
 - Bridge wide ranges of length and time scales
 - Homogenization of subscale models
 - Sequence of quasi-steady states
 - Advanced capabilities
 - Pressurized crack propagation
 - Joint failure
- **Complete project in ~2 year time frame**

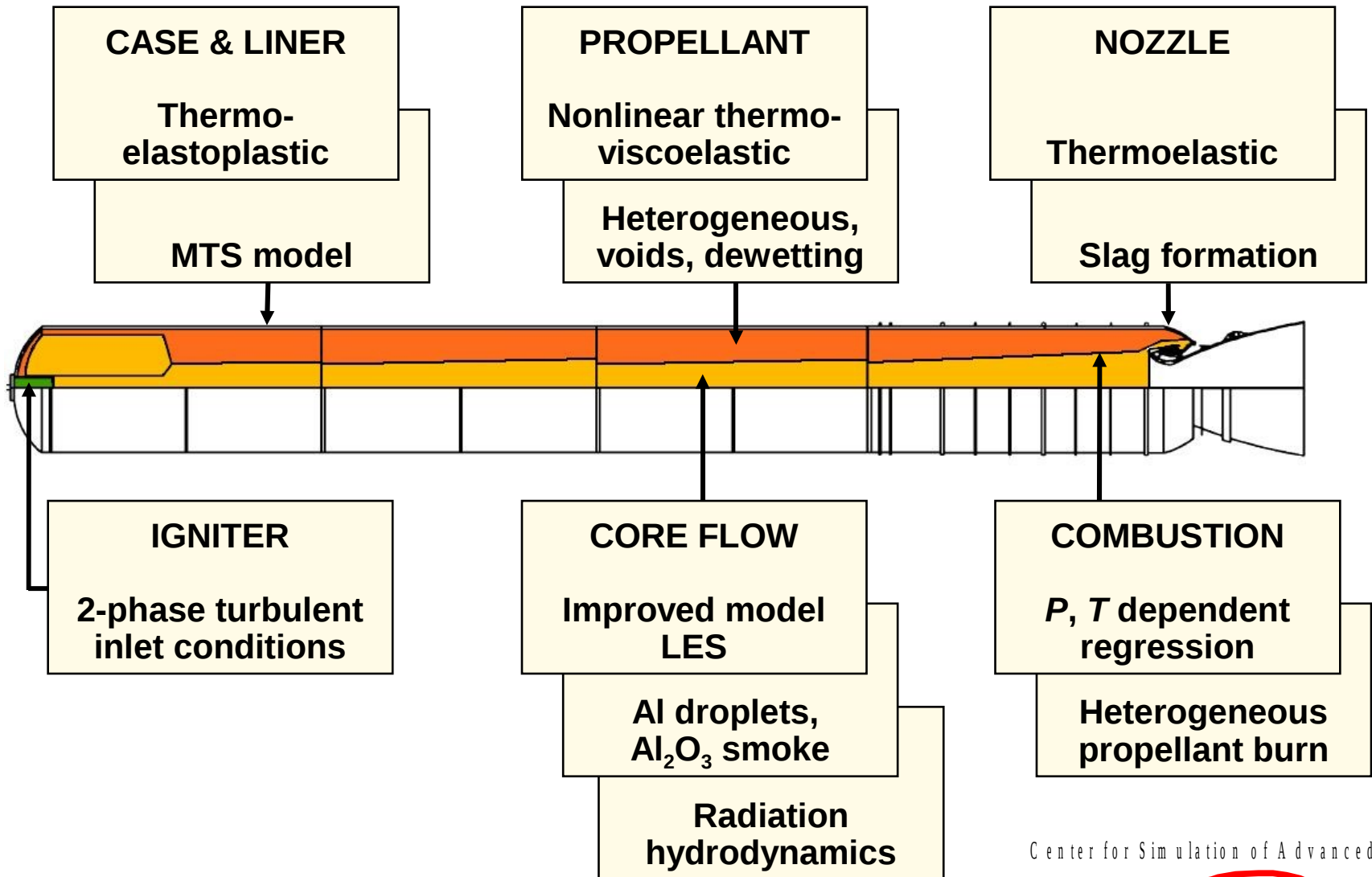


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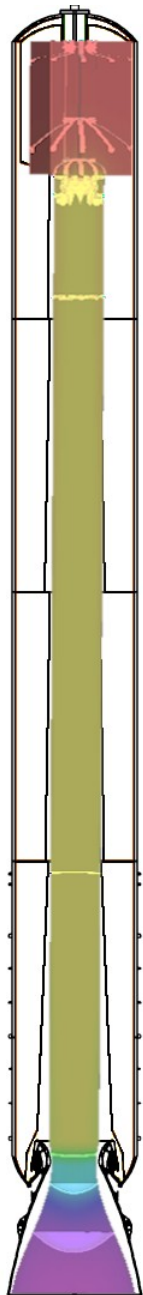
GEN2 Roadmap



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GEN2 Geometry

■ Whole system simulations

- Full 3-D, no symmetry
- Star grain at head end
- Joints
- Inhibitors
- Igniter
- Submerged nozzle

■ Capabilities

- Crack propagation
- Joint failure
- Plume

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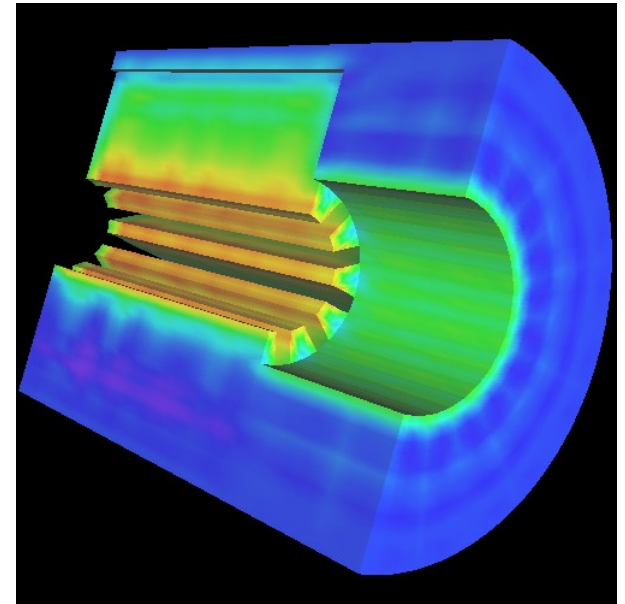
Structures & Materials

■ Physics (*Rocsolid* extensions)

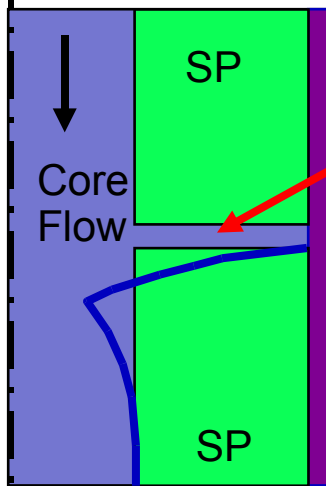
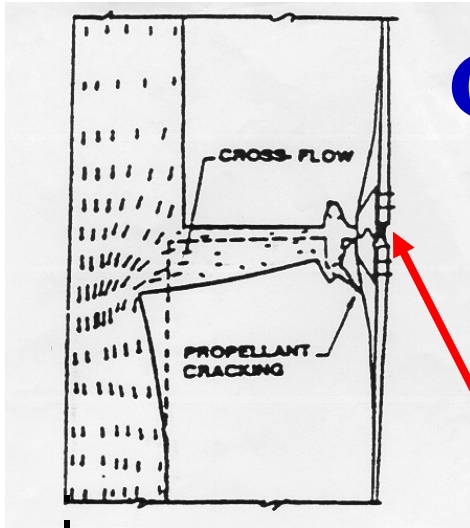
- Large deformations
- Materials in contact
- Temperature throughout propellant
- Material properties
 - Propellant: non-linear visco-elastic, heterogeneous
 - Case: Mechanical Threshold Stress model

■ Subscale models/capabilities

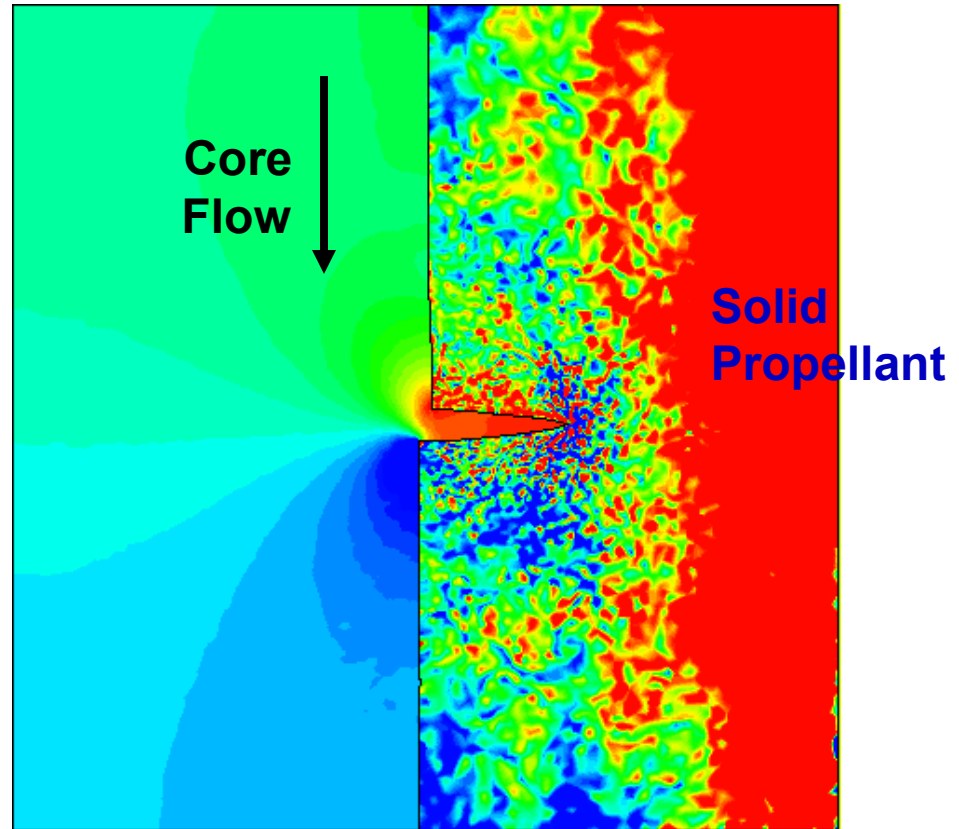
- Crack propagation (cohesive finite elements for solids, unstructured mesh for fluids)
- Joint failure
- Constitutive relations



Simulation of Titan IV Grain Collapse Accident (1991)



Grain
Joint



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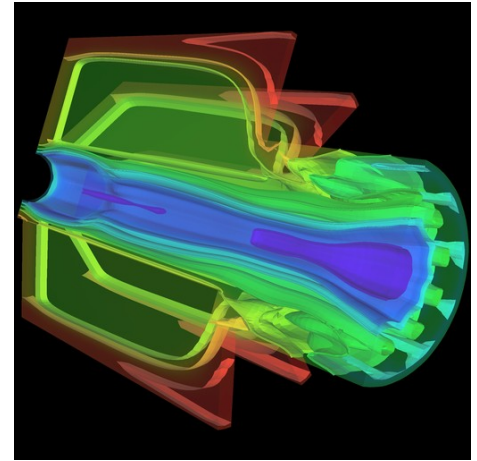
Fluid Dynamics

■ Physics (*Rocflo* extensions)

- Burning Al droplets (Lagrangian superparticles)
- Al_2O_3 smoke (Fast Eulerian)
- LES turbulence (higher spatial order?)
- Radiation (diffusion, multigroup)
- Slag formation

■ Subscale models/capabilities

- Crack propagation (Unstructured AMR)
- Direct Numerical Simulation of turbulence
- Chemical reactions
- Plume



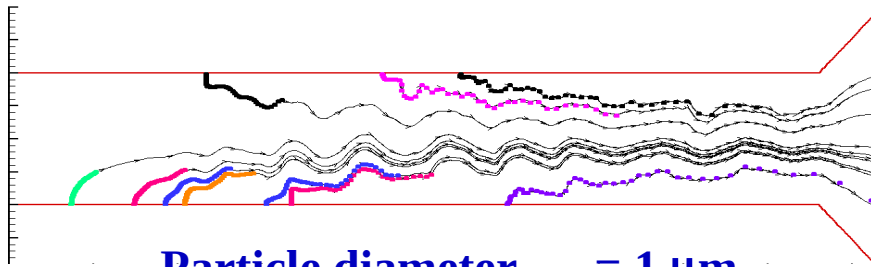
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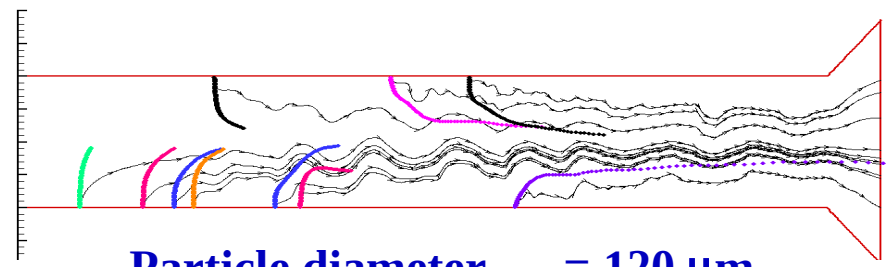


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2-D Aluminum Particle Flows



Particle diameter_{mean} = $1\ \mu\text{m}$



Particle diameter_{mean} = $120\ \mu\text{m}$

QuickTime™ and a
BMP decompressor
are needed to see this picture.

Particle diameter_{mean} = $35\ \mu\text{m}$; $t = 3.0\text{ms}$

Aluminum Particle Flows

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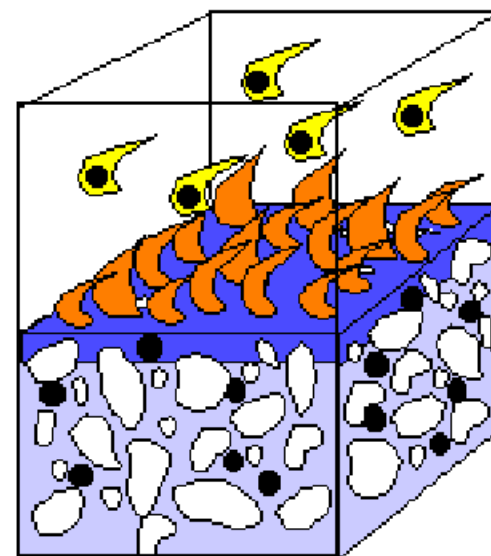
Combustion & Energetic Materials

■ Physics (derived from subscale models)

- Unsteady burn rate
- Burning Al droplets
- Erosive burning
- Heterogeneous propellant (rough surface)
- Realistic reaction kinetics
- Turbulent inlet boundary conditions (based on particle packing)

■ Subscale models/capabilities

- Combustion interface propagation (level sets, marker particles)
- 1-D and 3-D flame models
- Detailed reaction kinetics
- Plume (chemistry, radiation)



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2-D Model of Burning Propellant

QuickTime™ and a
GIF decompressor
are needed to see this picture.

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Research in Computer Science

■ Computational Mathematics and Geometry

- Linear solvers
- Mesh generation and adaptation
- Interface propagation and interpolation

■ Computational Environment

- Software integration framework
- Parallel I/O and data migration
- Performance tools and techniques
- Computational steering
- Visualization

Computer Science/System Integration

■ Algorithms

- Characterize/compare temporal coupling schemes
- Multigrid method for non-symmetric system
- Mesh adjustment and adaptation

■ Software Integration Framework

- Library for communication, mesh association, interpolation
- Coding style specification for MPI codes
- Automatic conversion tools for adding modules
- Flexible orchestration
- Automatic load balancing (Charm++)
- Interactive steering (Autopilot)
- Performance monitoring (SvPablo)



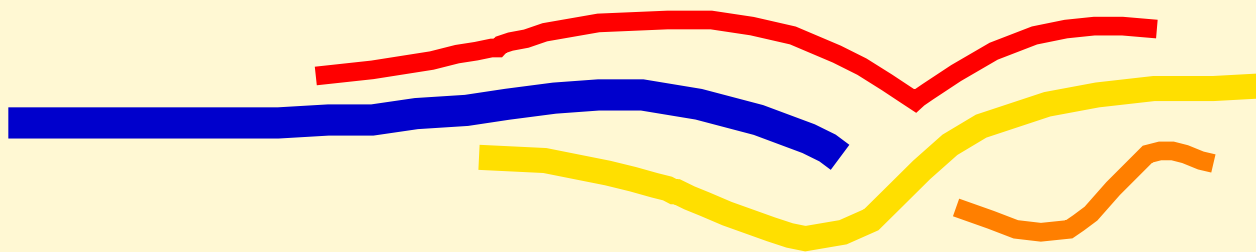
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C e n t e r f o r S i m u l a t i o n o f A d v a n c e d R o c k e t s



U n i v e r s i t y o f I l l i n o i s a t U r b a n a - C h a m p a i g n



<http://www.csar.uiuc.edu>

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