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Multiphysics Modeling with Aria and SIERRA Mechanics

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Sandia National Laboratories

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ARIA

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Outline & Progress

SIERRA Mechanics Overview

Application Modules Overview

Aria Overview

Aria Development Plans

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Setting the Stage: Today's Large-Scale Engineering Software

- **Today's Needs**
  - Full-system multi-physics
  - Multi-scale : nano to macro
  - *Predictive* capability
    - Uncertainty quantification (UQ)
    - Verification & validation (V&V)
    - Experimental coordination
- **Software issues**
  - Legacy codes
    - Usually single physics
    - Usually fortran 77
    - Need to modernize (language, algorithms, scalability, etc.)
  - Need code-coupling
  - Complexity!

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Today's Software Approaches

- **Modern frameworks & toolkits**
  - Parallel, adaptive, multi-physics
  - Modern software languages (C++, F90, etc.) and software engineering practices
  - The days of one-person, one-code are over

- **Sandia's approach: *SIERRA Mechanics***
  - Large-scale effort funded through DOE's ASC program (formerly ASCI)

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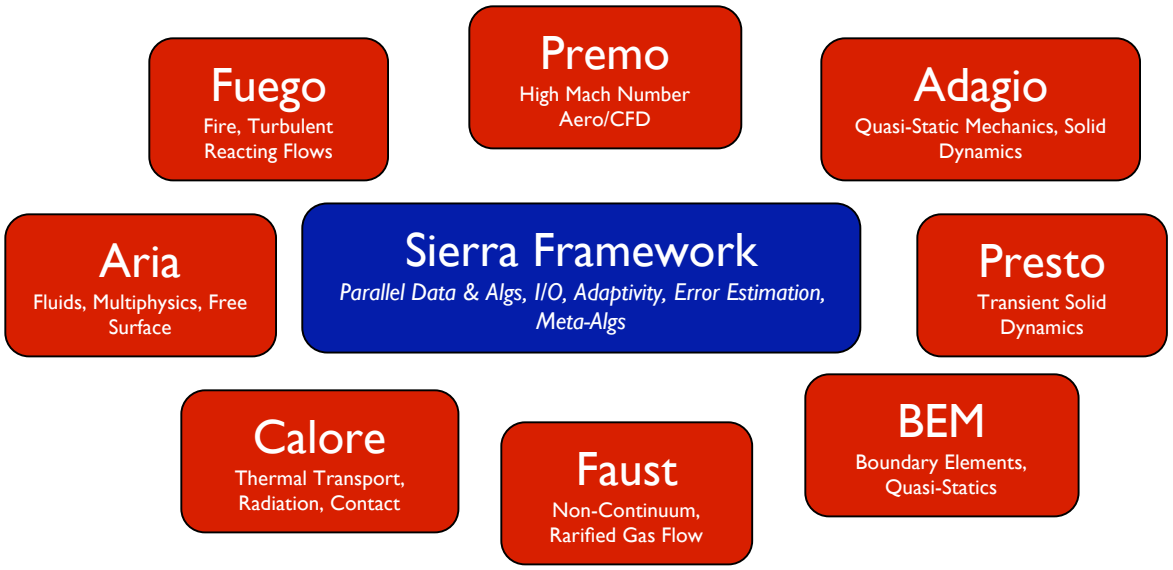
Partial List of Frameworks for Engineering Mechanics

Framework	Institution	Characteristics
SIERRA	SNL	Unstructured, multiphysics, adaptive, C++
Libmesh	UT-Austin	Unstructured, multiphysics, adaptive, C++
SAMRAI and Overture	LLNL	Block structured, overset & embedded meshes, C++
PYRAMID	JPL	Unstructured, F95
Unstructured Grid	Heidelberg Univ.	Unstructured, integrated multigrid solver, ANSI-C
CHARM++ (w/modules)	Univ. of Illinois (UIUC)	Structured and unstructured modules, C++
AMROC	CalTech	Block structured, C++
Uintah	Univ. of Utah	Structured, C++
Cactus	Louisiana State Univ. (LSU)	Block structured, C++ & F90

SIERRA Mechanics & Framework

- **SIERRA Mechanics : mechanics code suite developed on common architecture : SIERRA Framework**
  - Designed to enable versatile single physics capabilities and strongly-coupled multi-physics capabilities
  - Balances need for mechanics-specific algorithms and numerical methods with shared databases and processes
  - Architecture maximizes code re-use in future development efforts



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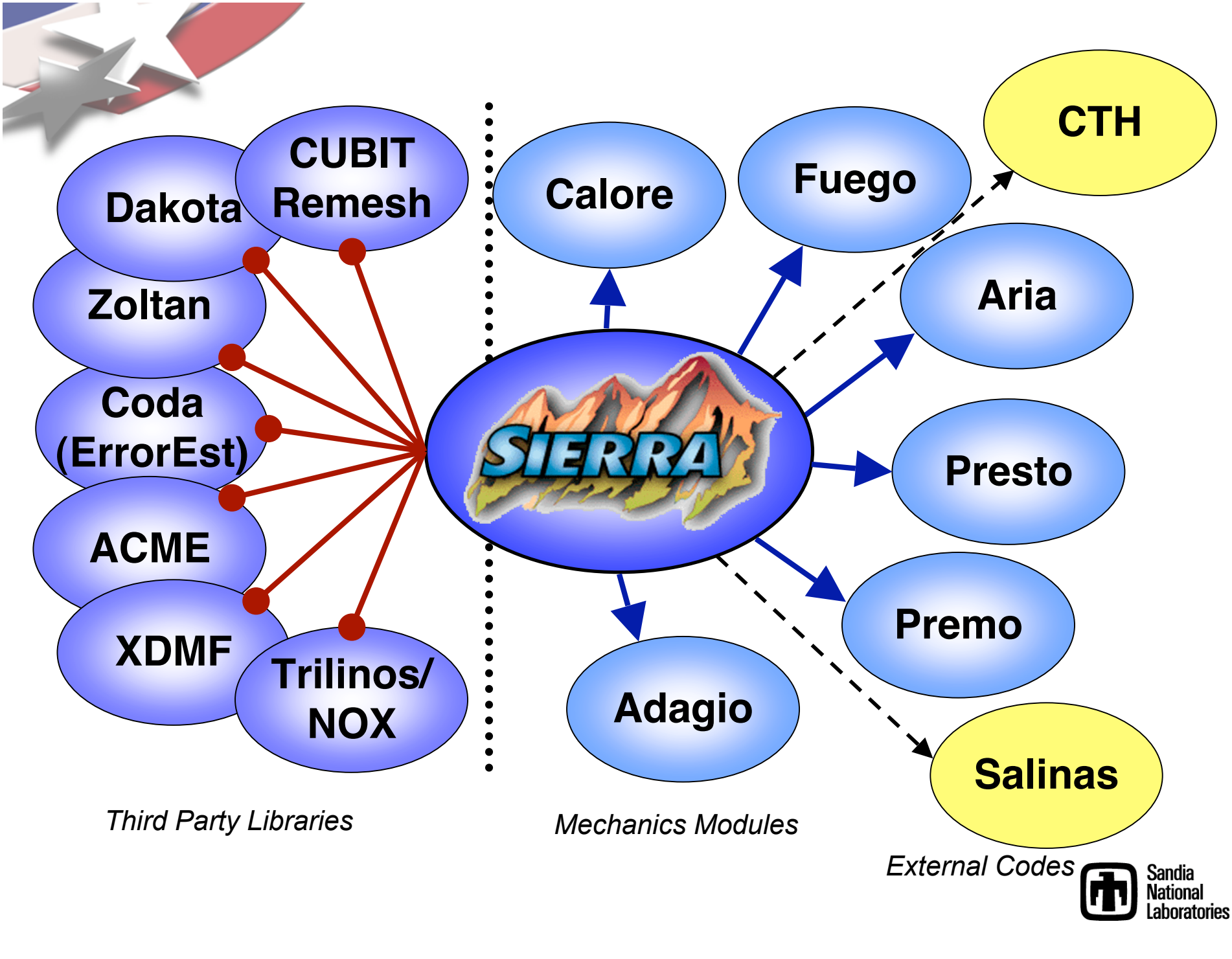
SIERRA Mechanics & Framework

- ***SIERRA Framework*** **: Suite of libraries that provide mostly computer science services**
  - Unstructured, heterogeneous mesh and fields
  - Physics-independent algorithms, solvers, libraries
  - Dynamic, parallel data management (e.g., adaptivity)
  - Parallel services
  - I/O (ExodusII, XDMF)
  - Code-coupling services (“transfers”)



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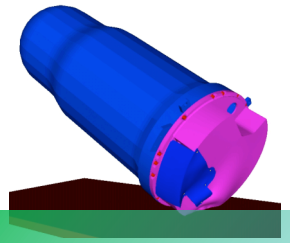
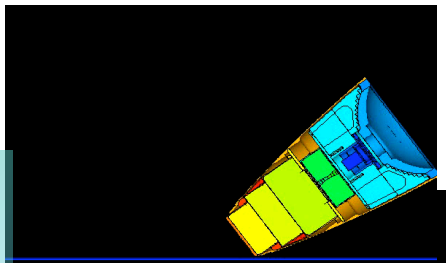
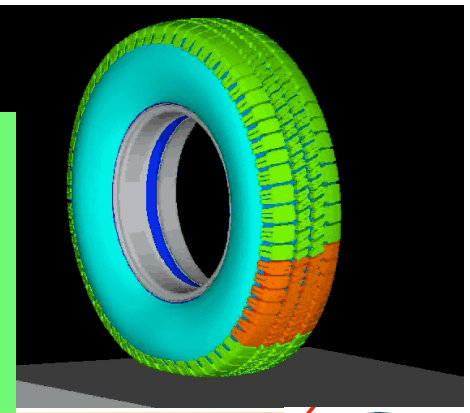
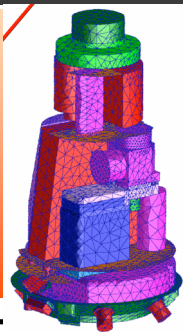
Computational Solid Mechanics and Structural Dynamics









Mechanics complexity

Failure/ fragmentation

Yielding

Contact

Large deformation

Shock

Vibration

Presto (Transient Dynamics)

Adagio/Andante (Nonlinear Implicit Quasistatics/Dynamics)

Salinas (Structural Dynamics)

nano-sec micro-sec milli-sec secs hours

Time Scale

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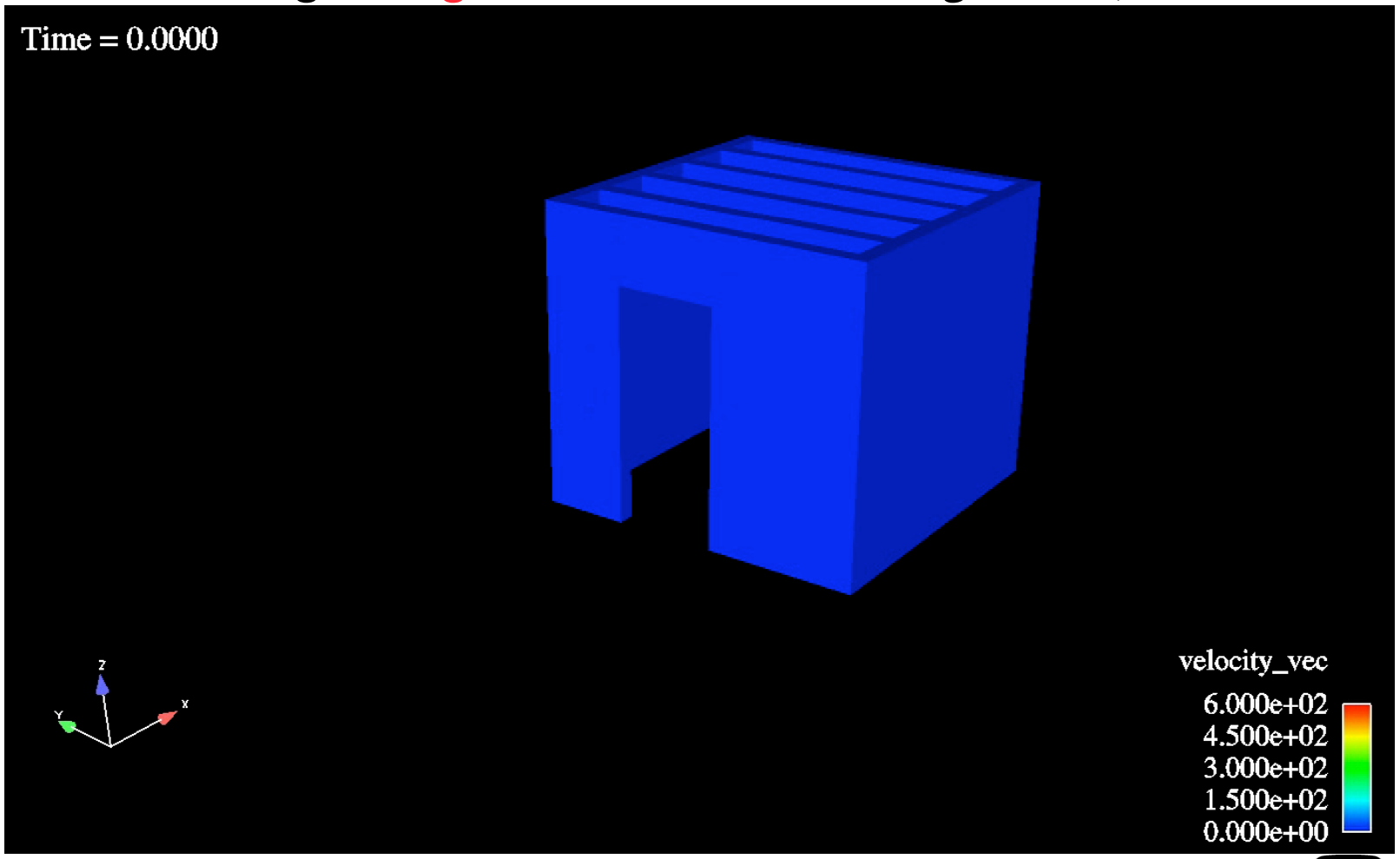
CTH/Presto Coupling Example

- **CTH Loading: 40 kg TNT at *lower left of right wall*, for 2.5 ms**



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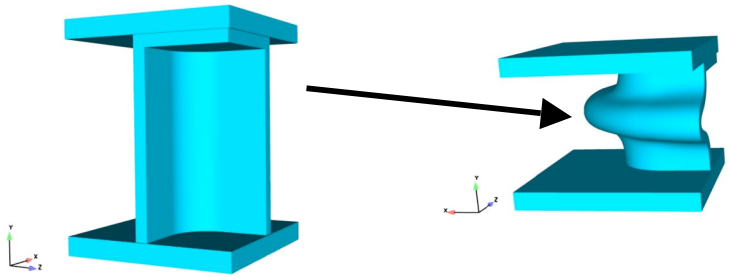
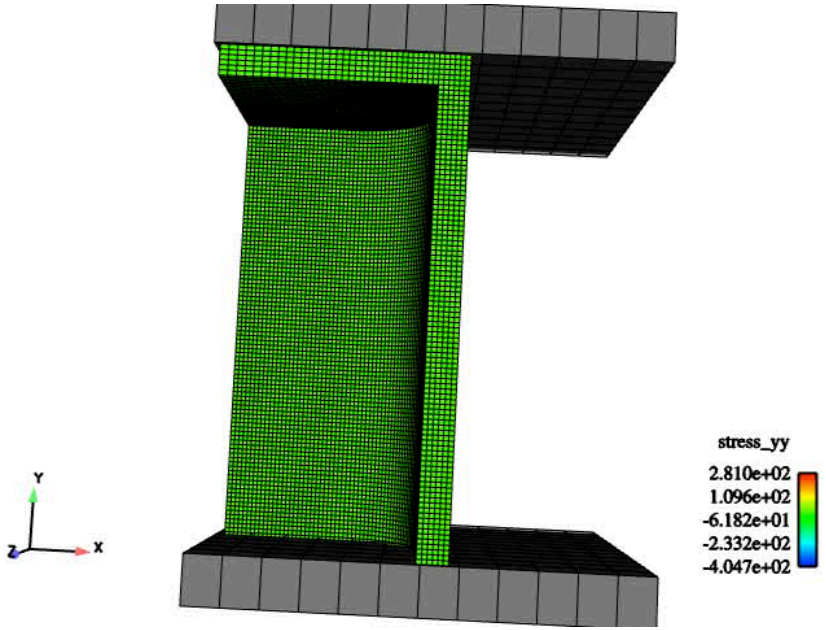
Adagio Example - Quasi-Statics

- **Implicit (quasi-static & dynamic) solid mechanics finite element code**
- **Provides scalable parallel solvers for highly nonlinear problems**
  - Contact
  - Nonlinear material response
  - Large deformation
- **Utilizes services provided by the Sierra Framework to enable**
  - Coupled physics
  - H-adaptivity (under development)
  - Multi-length scale modeling techniques (under development)
- **Design of energy absorbing barrier**
- **Uses multilinear elastic-plastic constitutive model**
- **Demonstrates frictional contact, geometric and material nonlinearities, parallel scalability**





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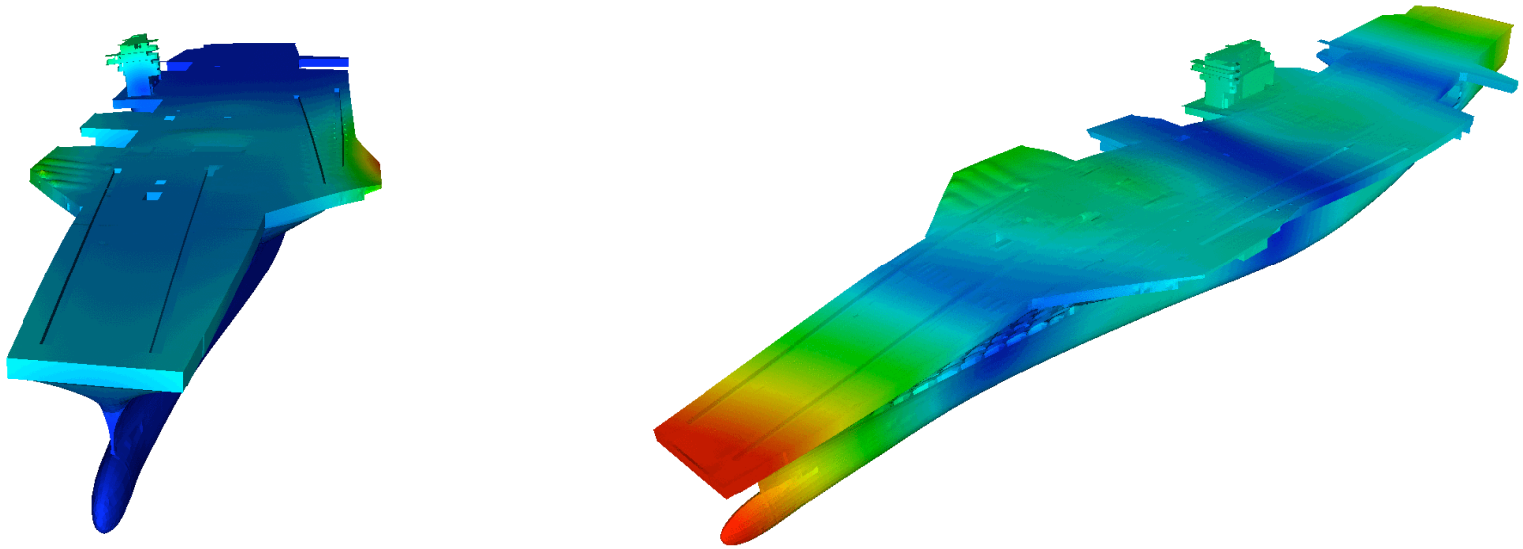
Salinas Example
Modal Analysis of an Aircraft Carrier

- Extremely complex model (1000's of material regions, offset shells and beams)
- 2.0M DOFs, solved on 64 processors



Von Mises Stresses Overlaid on Mode Shapes

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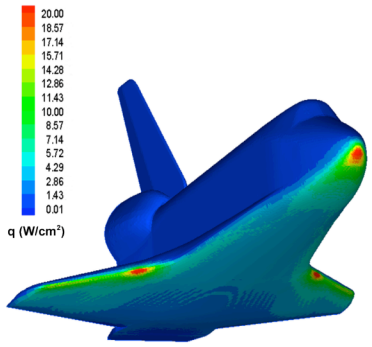
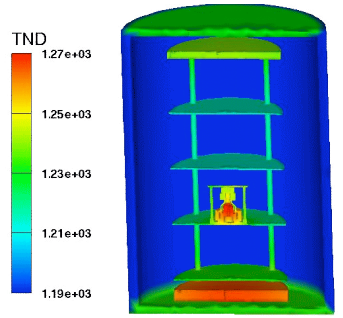
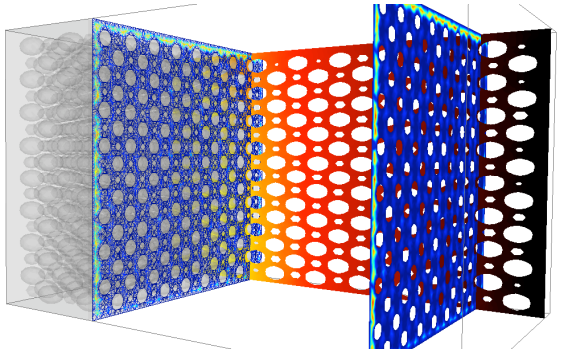
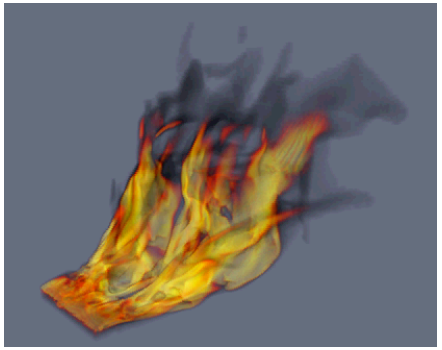
Thermal / Fluids Capabilities

- **Calore** – Heat Transfer, Enclosure Radiation and Chemistry
  - Dynamic enclosures
  - Element birth death
  - Contact
- **Premo** – Compressible Fluid Mechanics
  - Subsonic through hypersonic
  - Laminar and turbulent
  - Unstructured mesh
- **Aria** – Non-Newtonian, Multi-physics, and Free Surface Flows
  - Complex material response
  - Level sets for surface tracking
  - Flexible coupling schemes
- **Fuego** – Low Speed, Variable Density, Chemically Reacting Flows (Fire)
  - Eddy dissipation and mixture fraction reaction models
  - RANS and LES based turbulence models
  - Unstructured Mesh
  - Pressurization models









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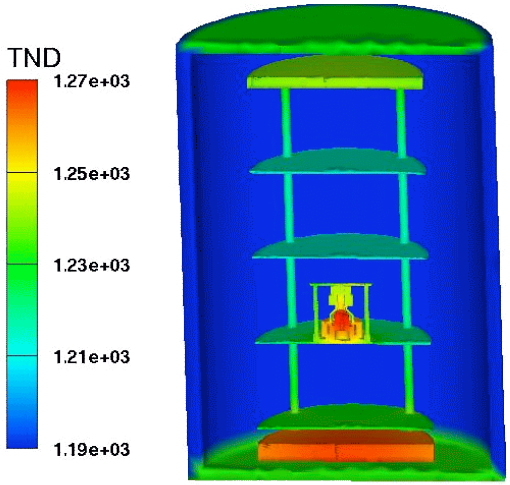
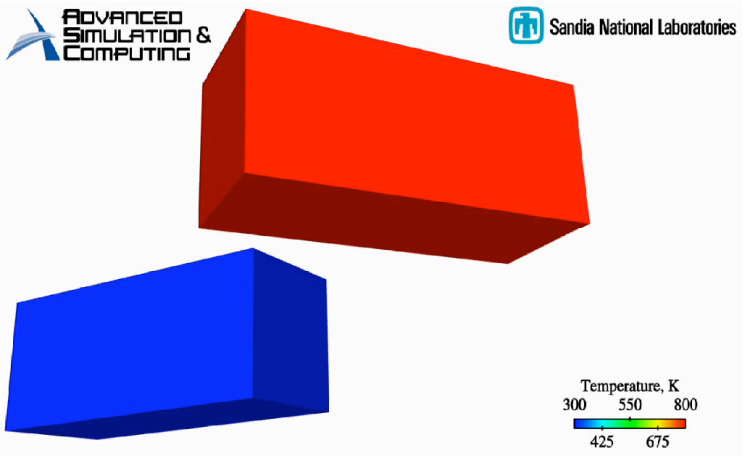
Calore - Heat Transfer

- 2D/3D massively parallel
- Steady/Unsteady
- Conduction
- Limited Convection
- Chemistry
- Enclosure radiation
- Thermal contact
- Bulk fluid elements
- Coupling to other physics modules
- Error estimation and adaptive mesh refinement
- Dynamic load balancing
- Element birth & death
- User subroutine definition of boundary conditions and material properties



Braze furnace process optimization



Sliding contact with adaptive mesh refinement

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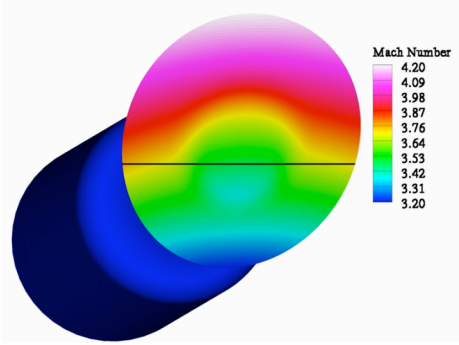
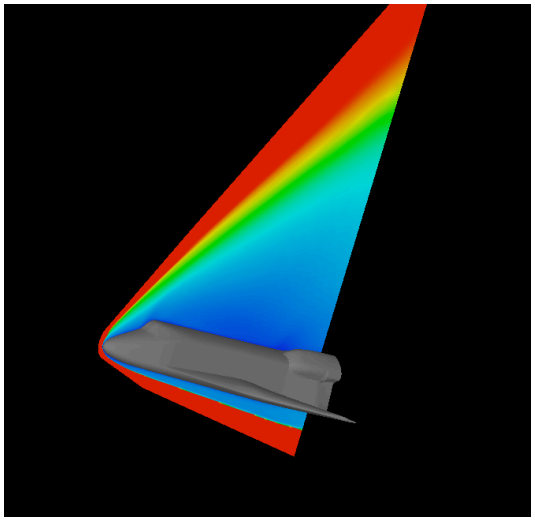
Premo - Compressible Fluid Dynamics

- **Compressible subsonic through hypersonic**
- **Laminar through turbulent regimes**
- **Inviscid and viscous flows**
- **Steady state and transient**
- **Chemically reacting flow**
- **Trajectory analysis**
- **Moving control surfaces**
- **Coupling to other mechanics modules**
  - Aeroelasticity
  - Ablation
  - Aeroheating



Mach contours on the exit of a spin motor



Flow field around a space shuttle during reentry

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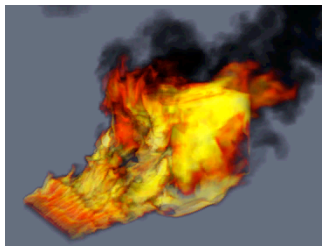
Fuego - Turbulent, Reacting Flow

- **Low Mach number, variable density, unstructured (finite-volume) fluid dynamics**
  - Turbulent reacting flow with coupling to participating media radiation (PMR) and heat conduction
- **RANS and LES-based turbulence models**
  - k-ε, low Re k-ε, v2-f, Ksgs, PANS
- **Reacting flow suite**
  - Eddy dissipation concept, mixture fraction-based models
- **Multiple element types**
  - Hexahedron, tetrahedron, pyramid, wedge
- **Pressurization, low speed compressibility**



Hydrocarbon pool fire

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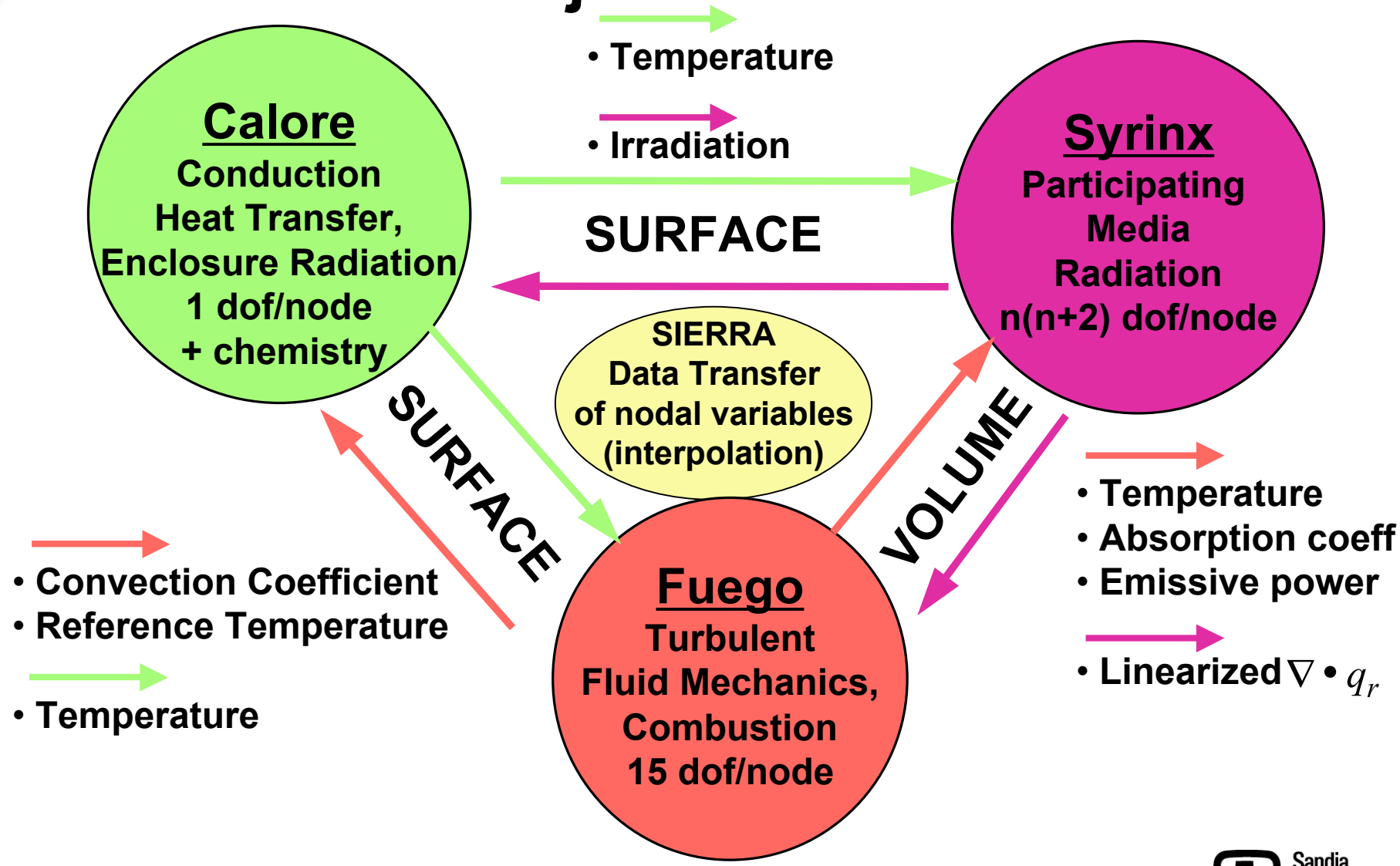
Coupled Code Simulation of Objects in Fire



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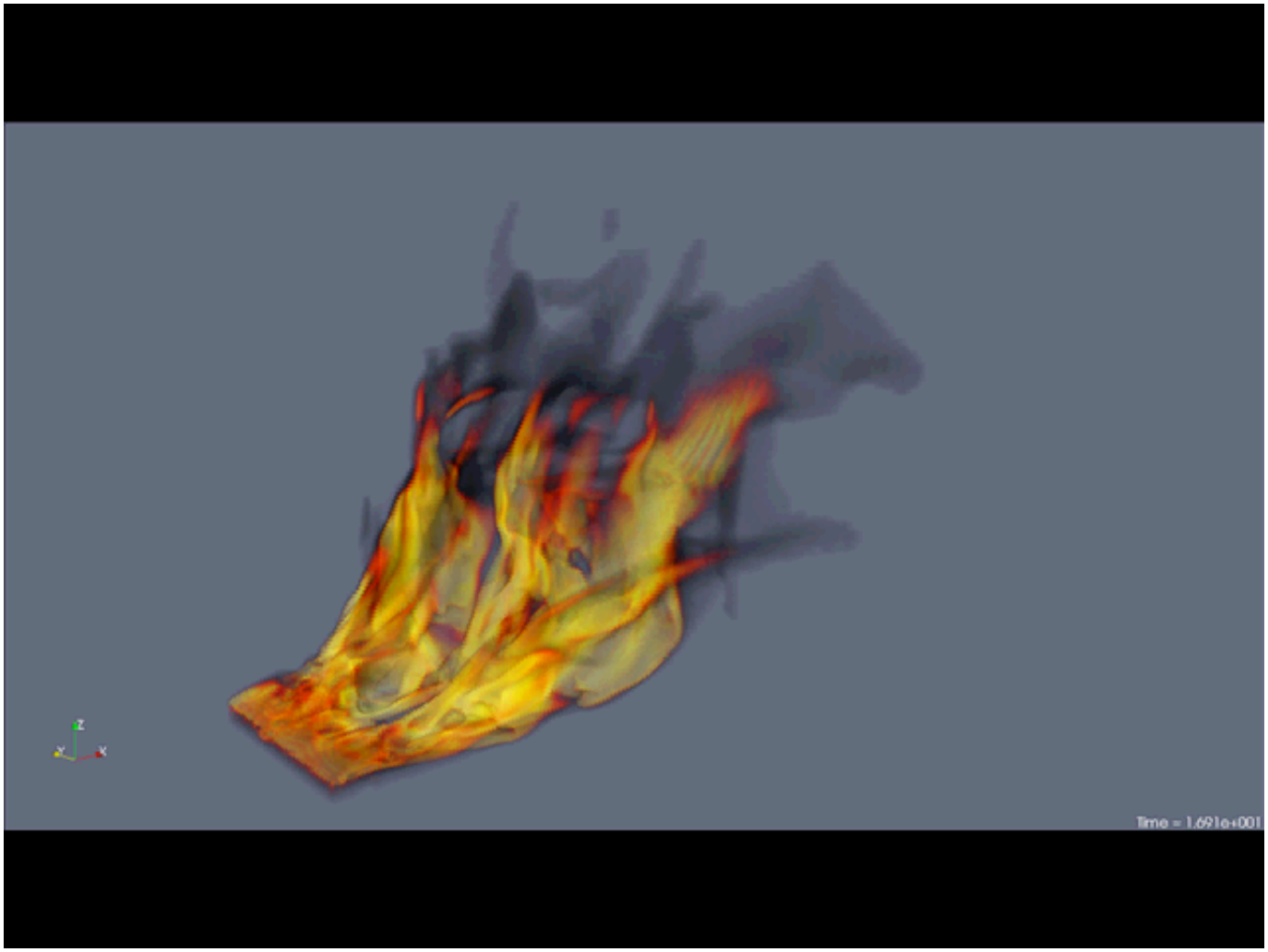
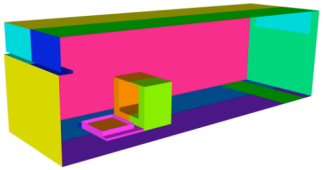
Design of New Experimental Facility for Fire Studies





400M DOFs, 5000 processors on Red Storm

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Aria Overview

Aria Development Plans

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Aria - Incompressible Fluid & Coupled Multiphysics

Inspired by GOMA

Designed for coupled physics

Designed to be extended

Goal : *production computing* & *research platform*

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Feature Summary

Basic Physics

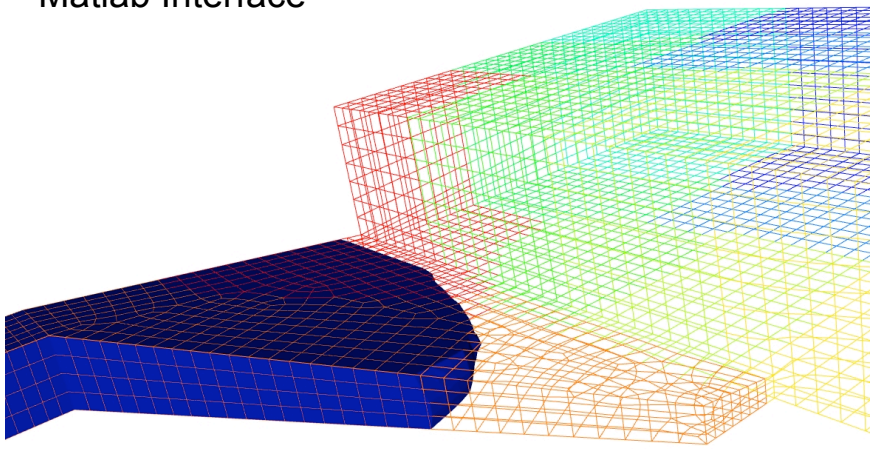
- Navier-Stokes (variable density)
- Energy
- Species
- Electrostatics
- Nonlinear elasticity
- Porous flow (in development)
- Mesh motion (pseudo-solid ALE)
- Level set (diffuse, Krino)

Additional Features

- Transient & steady; 2D & 3D; parallel & serial
- LOCA: Continuation, stability and turning point tracking
- Error estimation
- Mesh refinement: uniform and dynamic adaptivity
- Stabilized Navier-Stokes: PSPG & PPPS
- Initial conditions from existing ExodusII file with interpolation in space and time
- Input fields from and output solutions to different meshes
- Algorithm design via input file
- User plug-ins; user-defined fields
- User/reference manual, ~400 pages, indexed

Nonlinear Solvers & Coupling

- Full Newton (analytic, FD, AD, mixed)
- Full Picard
- NOX: Colored finite difference
- NOX: Matrix free nonlinear
- Arbitrary loose coupling / splitting
- Coupled to Adagio, BEM, Calore, Premo, …
- Matlab Interface



Parallel level set mold filling in Aria

Element / Topology Types

- Quadratic (Q2), linear (Q1), P0 and P1, MINI
- 2D quad & tri; 3D hex & tet

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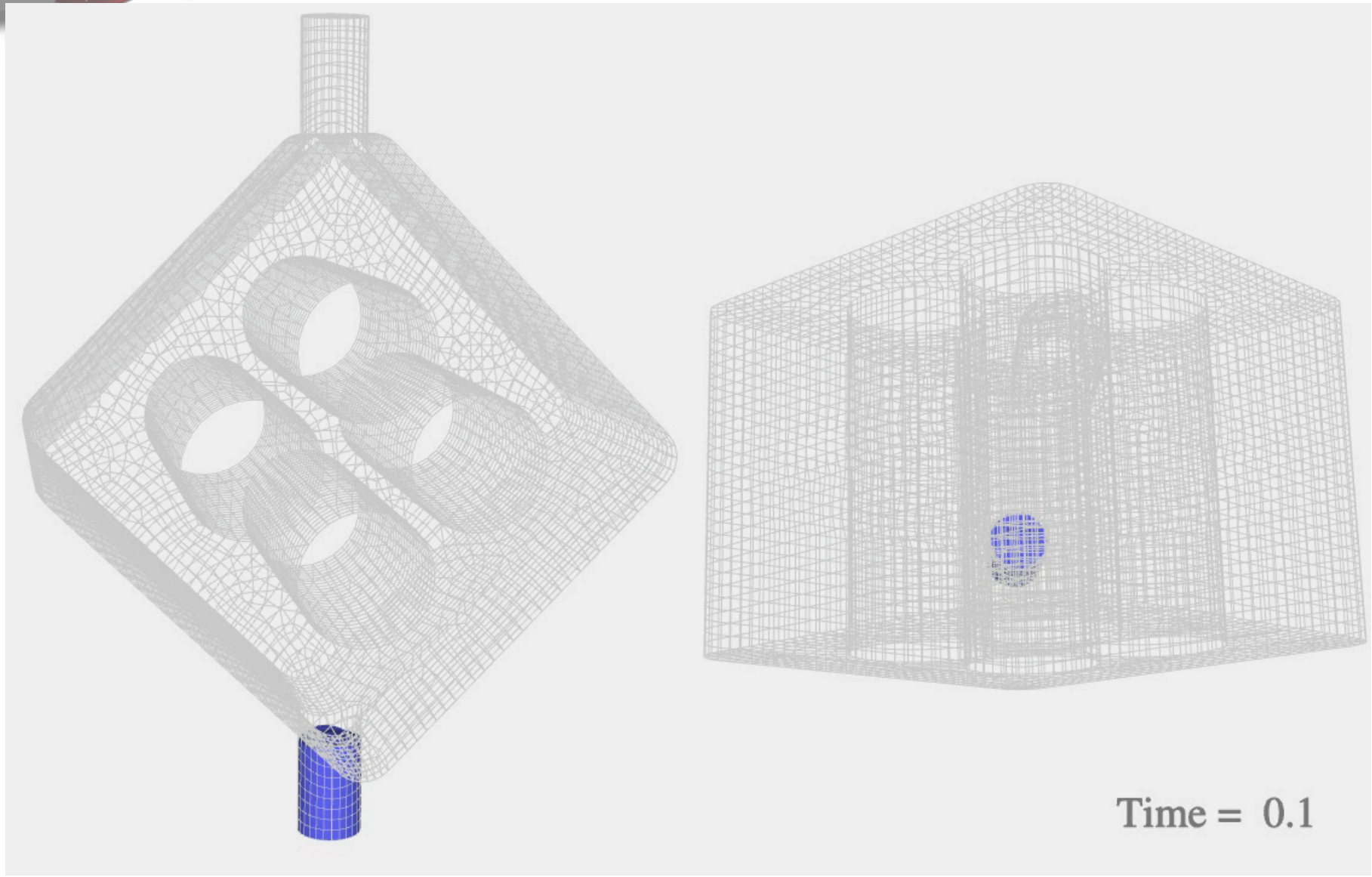
Mold Filling & Encapsulation



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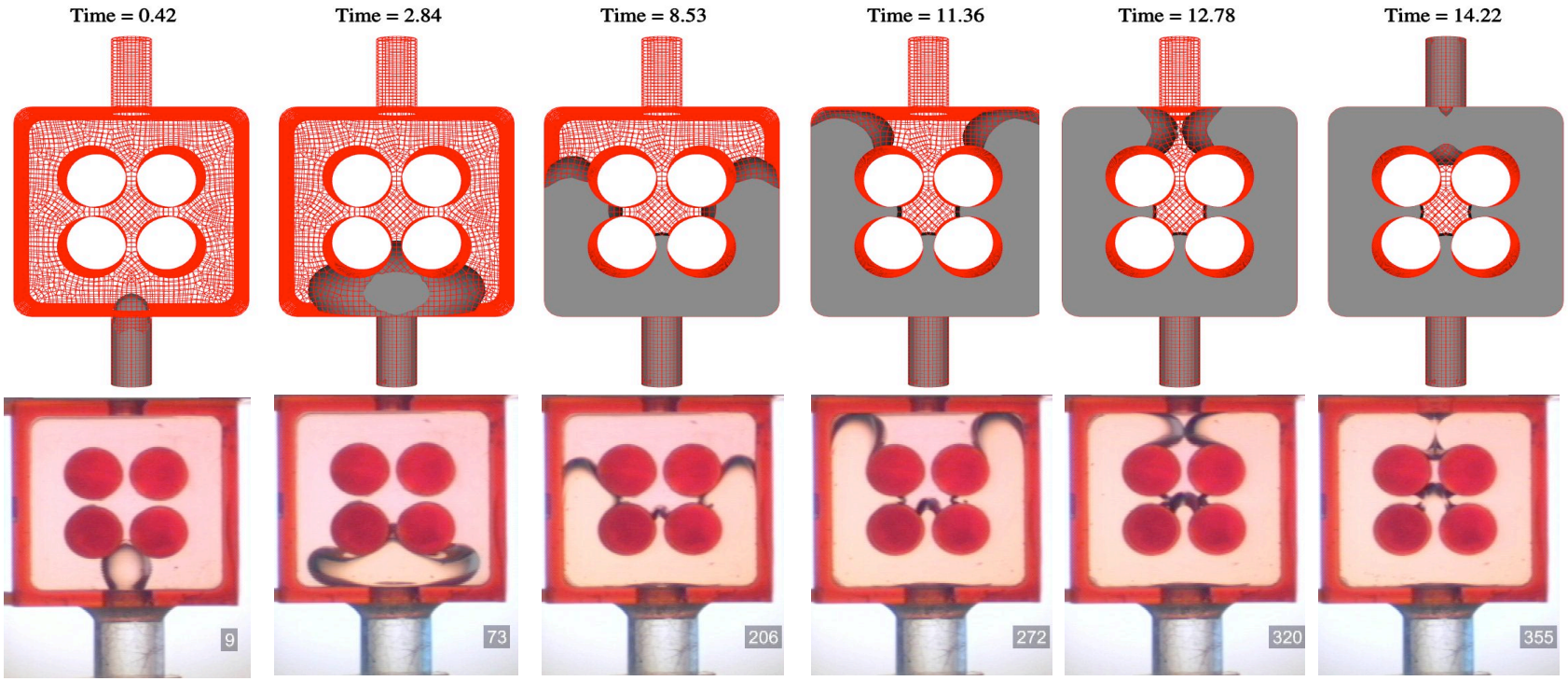
3D Model Matches Experiment Well with Faster Wetting Speed

Model parameters: μ = 390 Poise, θ^{eq} = 39.8°, v_o = 0.0026 cm/s, σ = 42.4 dyne/cm
fill time=14 s



Real parameters: μ = 390 Poise, θ^{eq} = 39.8°, v_o = 0.0013 cm/s, σ = 42.4 dyne/cm
(Ucon 95-H-90000 measured parameters); fill time=12 s

Both: Ca ≅ 20; Re ≅ 0.001

Time*=time/total time

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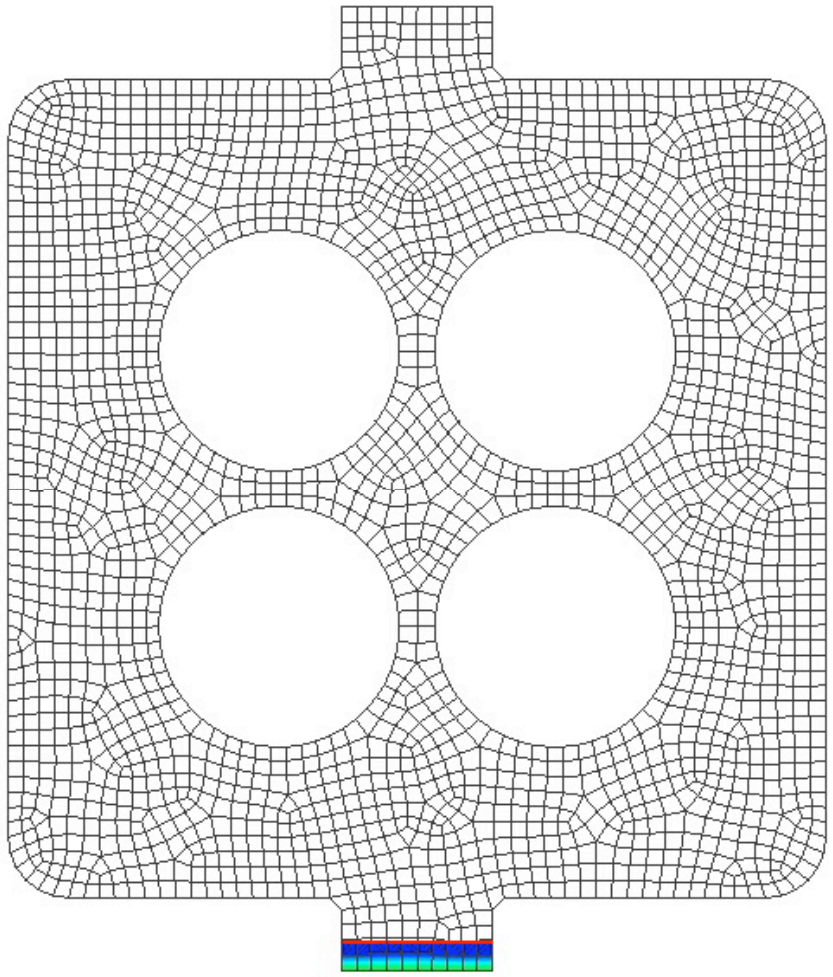
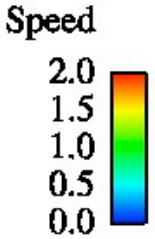
Mold Filling & Encapsulation





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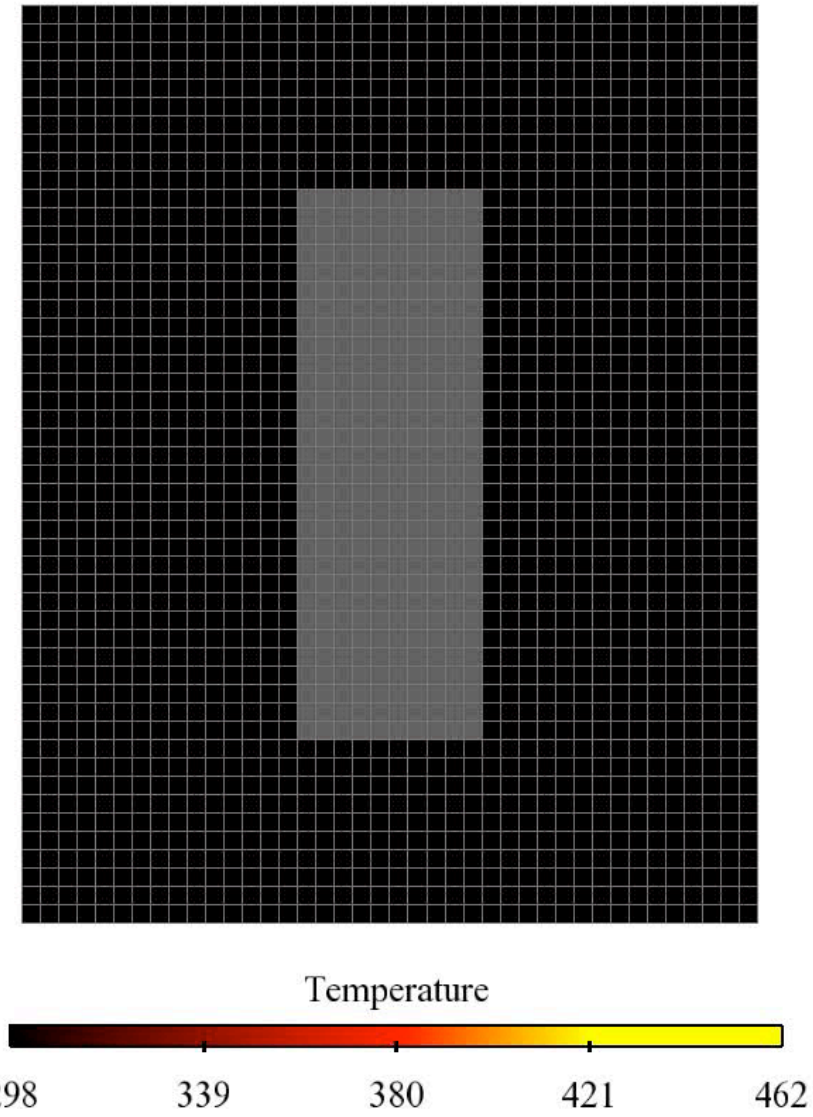
Core Heatup



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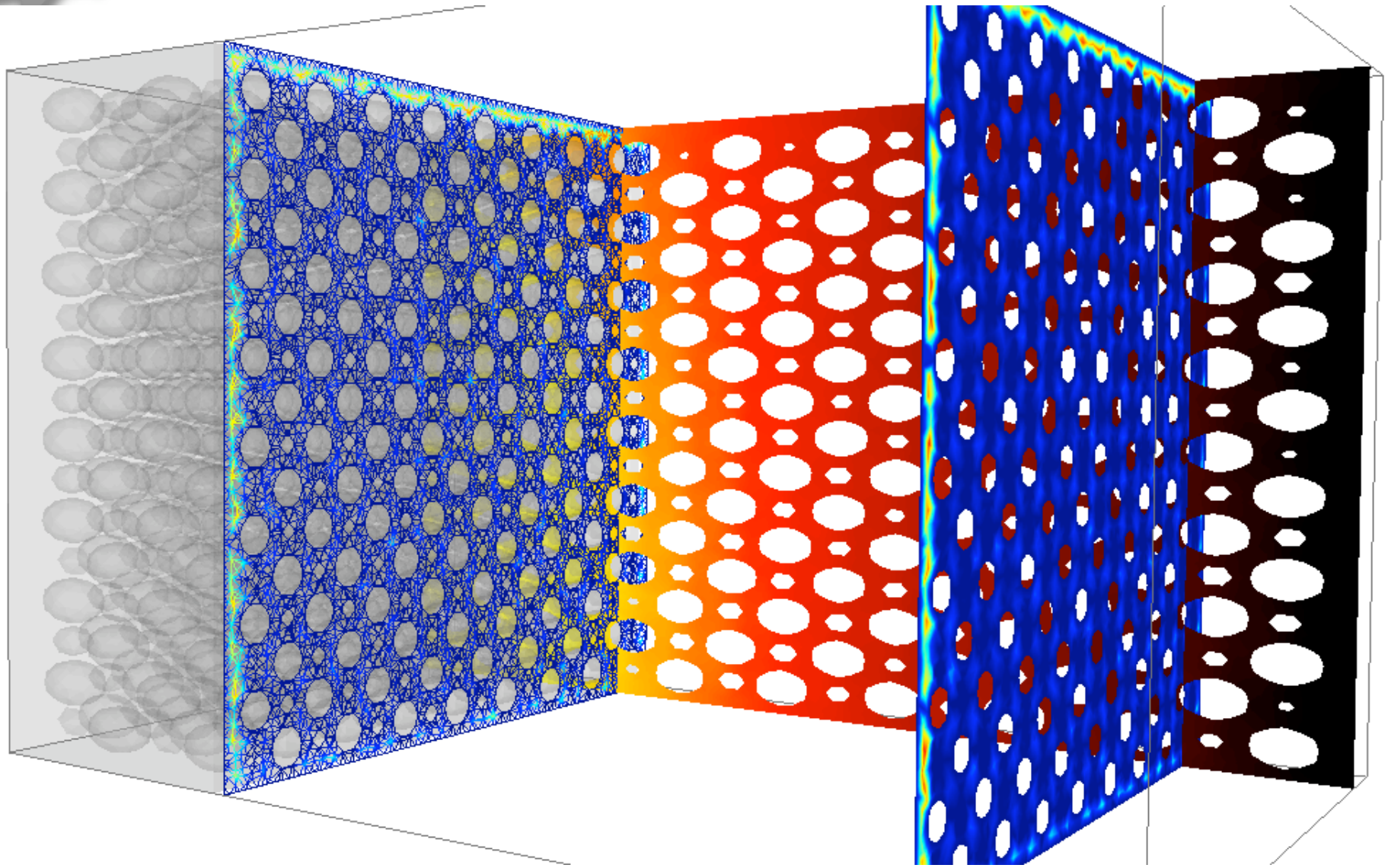
Nano-Particle Flow Solver



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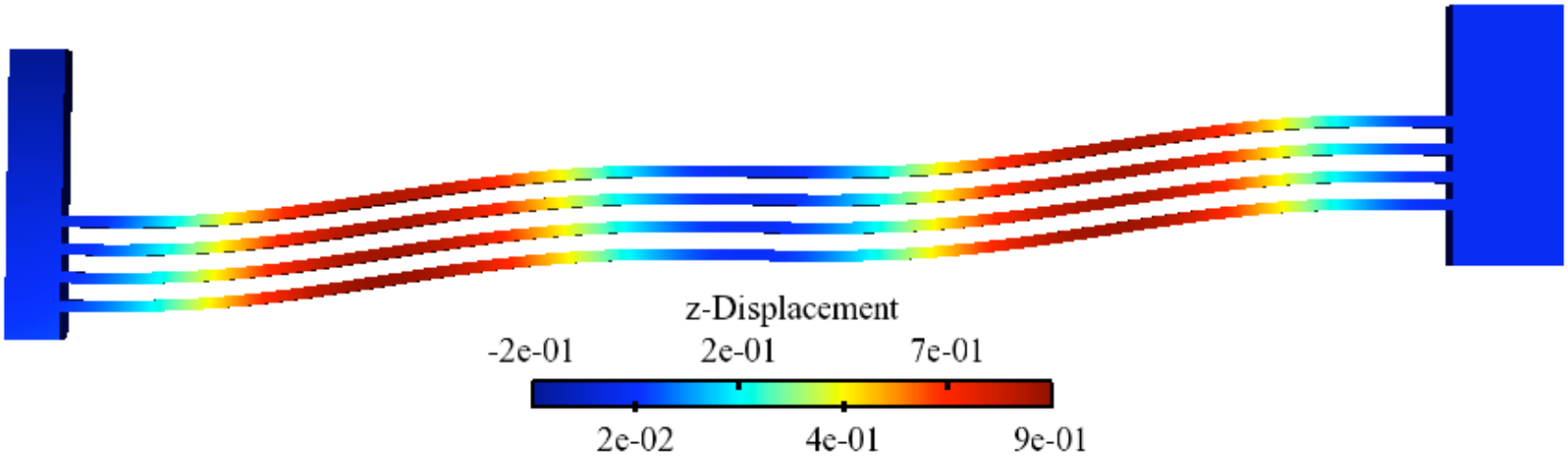
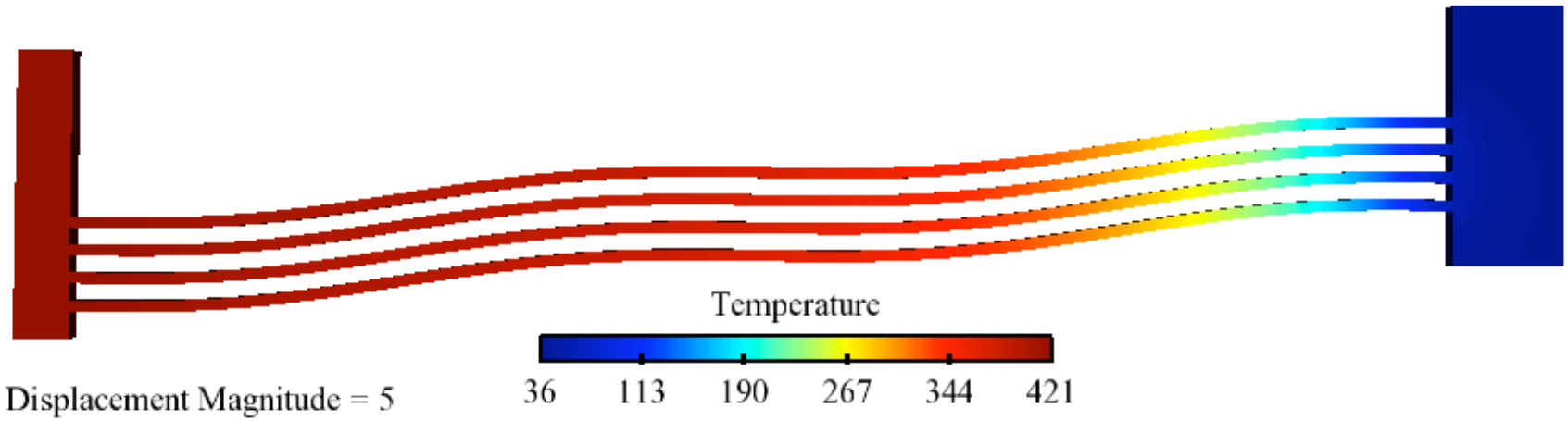
Electro-Thermal Actuation of a MEMS Device





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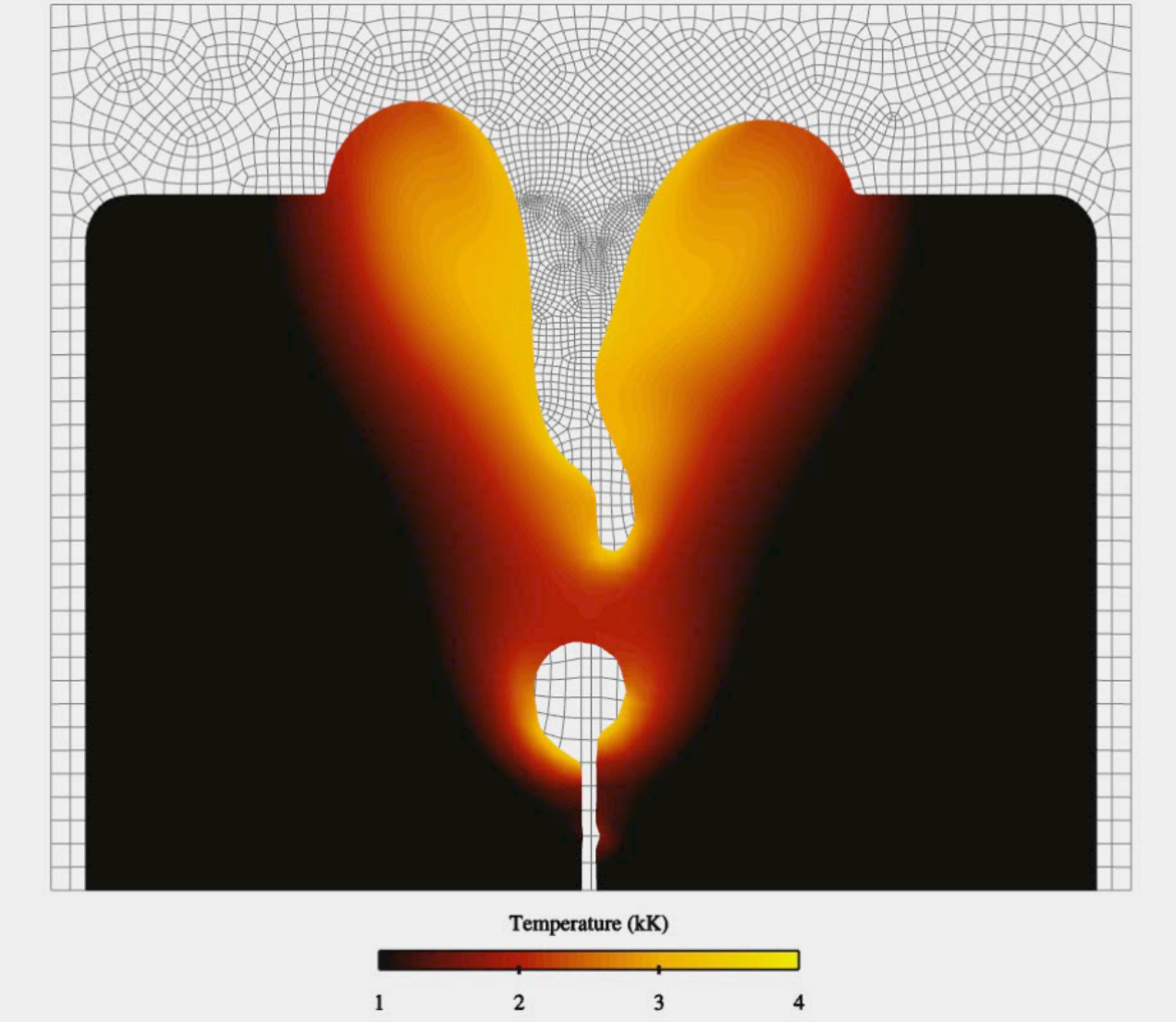
Thermal-Fluid Analysis for Welding



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Development Plans

Balance *performance* & *rapid development*

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Large-Scale, Free-Surface Flows

3D, transient (10k time steps), multiphysics

Explicit, semi-implicit methods under study

Specialized preconditioners

Improved pressure stabilization

Loose coupling where it makes sense

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Advanced Capabilities

Enclosure radiation

Thermal contact

Porous flow (fully & partially saturated)

Adaptivity

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Rapid Development & Agility

User plugin models (IC, BC, materials, etc.)

User plugin equation systems

Mixed sensitivities: analytic, automatic, finite difference

Advanced level-set based algorithms

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