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SAND2008-1093P

A Glimpse of Computational Modeling/Simulation Activities at Sandia's Engineering Sciences Center*

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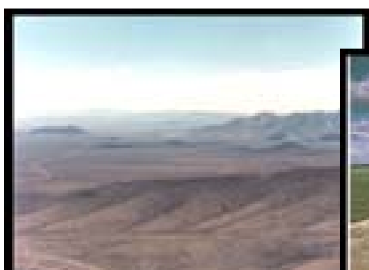
Albuquerque, New Mexico

Kauai Test Facility
Hawaii

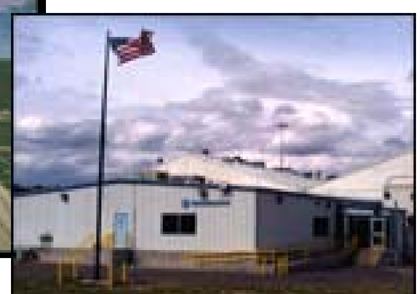
Tonopah Test Range,
Nevada

Livermore,California



Yucca Mountain
Nevada

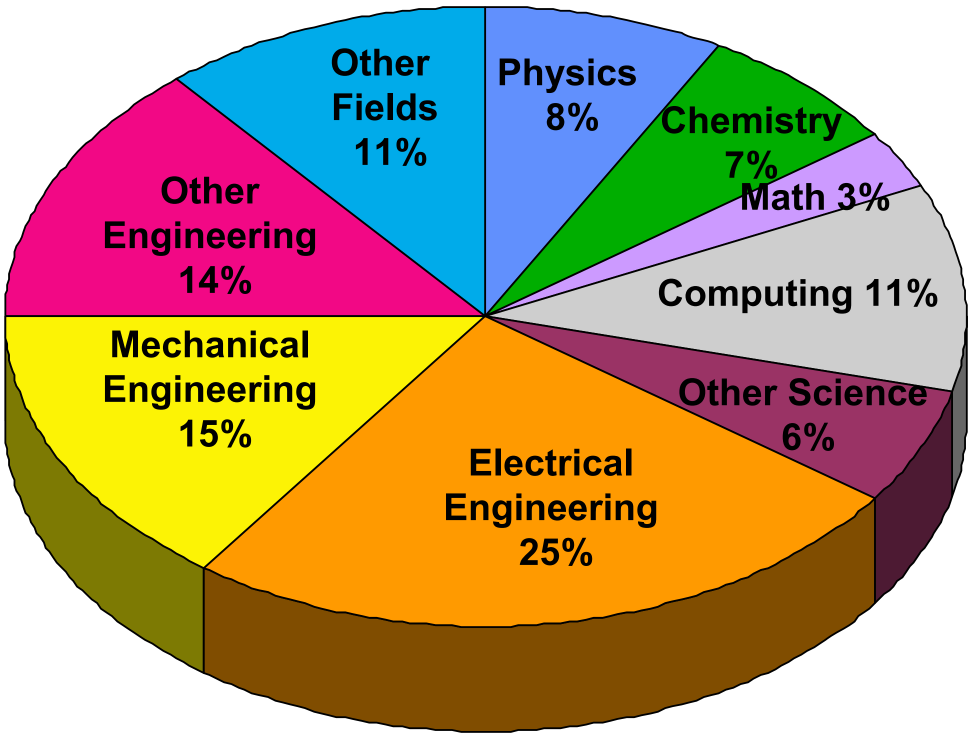
WIPP,
New Mexico

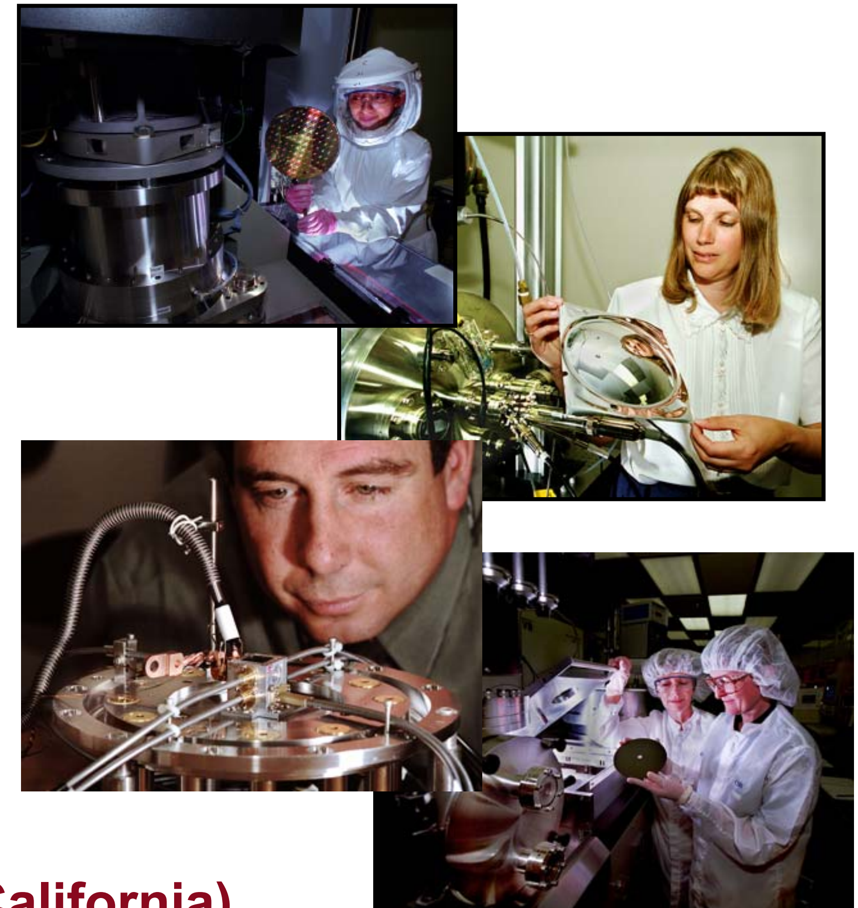


Pantex, Texas

Sandia employs approximately 8,200 employees (plus 2100 on-site contractors)

$ 2.2B Operating Budget FY04





~8,200 full-time employees (~ 900 in California)
1,431 PhDs and 2,235 Masters

Sandia National Laboratories

Student Internship Program at Sandia

- SIP Mission Statement
  - The mission of SIP is to hire the best and brightest students and to provide them with valuable professional and personal development through a variety of experiences and to develop a strategic workforce pipeline.

- Statistics
  - » **Number of Students in SIP >1180**
    - **640 Year-round Students**
    - **35 Telecommuting Students**
    - **~600 Summer-only Students**

Sandia seeks high academic quality in ~11 technical disciplines

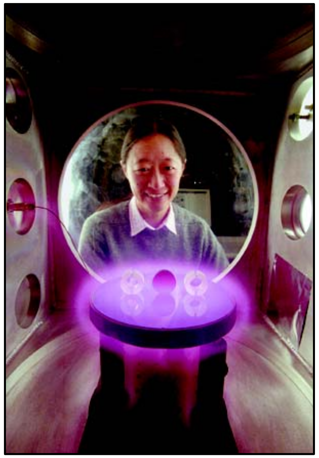
Information Technology
Electrical Engineering
Mechanical Engineering
Chemistry
Physics
Math
Materials Science Engineering
Chemical Engineering
Aeronautical/ Aerospace Engineering
Civil Engineering
Industrial Engineering

Percent of all Hires ***~70% - 75%***

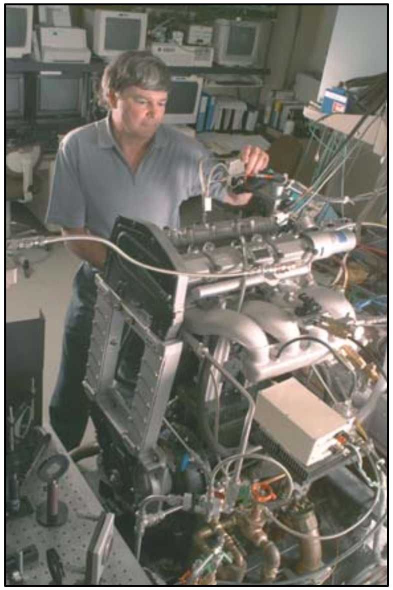
Sandia National Laboratories

Engineering Sciences Center is one of the five Research Foundations at Sandia

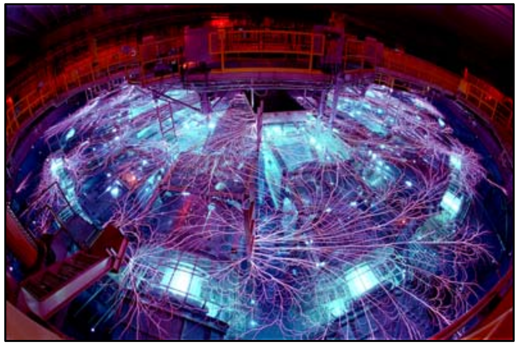
Computational and information sciences



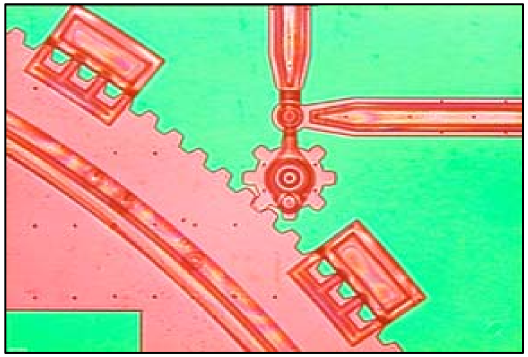
Materials and processes



Engineering sciences



Fusion research



Microelectronics and photonics

Sandia National Laboratories

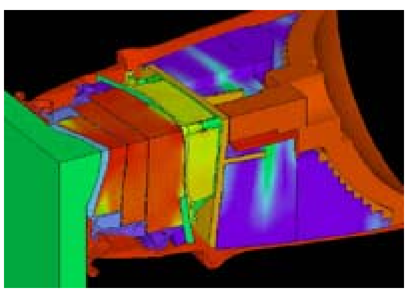
Engineering Sciences Center at Sandia

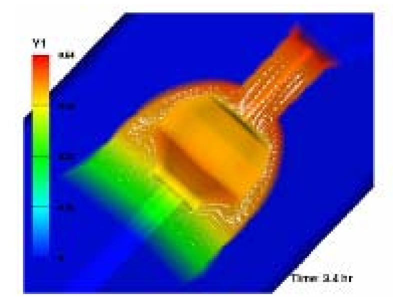
Mission:

Provide Validated, Science-Based, Engineering Solutions Across The Product Life Cycle **to Meet the Mission Needs of Sandia National Laboratories.**

Strategic Intent:

Research to applications… the optimal Engineering Sciences solutions and capabilities, on time, every time.





There are ~300 Engineering Sciences staff and management to meet the research, development and application needs of the Lab and its customers

Sandia National Laboratories

Sandia's Engineeing Sciences Center and NSF have collaborated on a long-standing program to enhance engineering technology

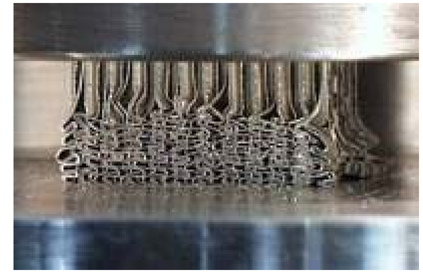
- **Engineering Sciences and the National Science Foundation (NSF) jointly fund $2M/year of university research *(ongoing for 9+ years)***
- **Projects are chosen through the formal NSF review process (***13- new 3-year projects in FY07)*
- **Annual workshops held to exchange information between participants** (*Program review/workshop in October 2007)*
- **Noteworthy outcomes from NSF-Sandia program**
  - *Integrated Atomic and Continuum simulation Studies of Stress-Defect Interactions in Semi-conductors*, **K. Garikipati and M. Falk, University of Michigan:** *resulted in K. Garikipati winning the Sandia sponsored PECASE*
  - *Multiresolution Mechanics for Materials Design,* **W. K. Liu and T. Belytschko, Northwestern University:** *resulted in hiring of Greg Wagner*
  - *Ductile Fracture,* **T. Wierzbicki, MIT: work** *directly complementing ESRF Tech Base work on fracture modeling*

Universities funded under Sandia-NSF Program in FY07

Sandia National Laboratories

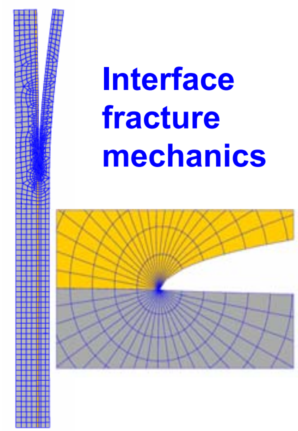
Engineering Sciences provides stewardship of engineering mechanics disciplines at Sandia

- Aerosciences
- Engineering Optimization
- Fluid Mechanics
- Material Mechanics
- Reactive Processes
- Solid Mechanics
- Structural Dynamics
- Thermal Sciences
- Uncertainty Quantification



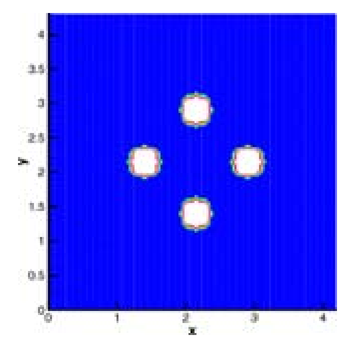
short buckling wavelength

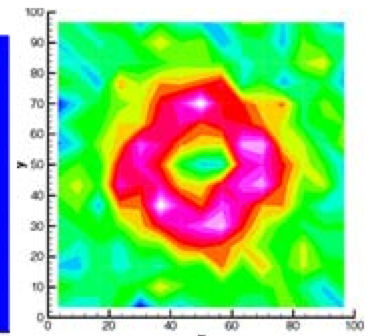
long buckling wavelength



Interface fracture mechanics

Lattice Boltzman





Monte Carlo

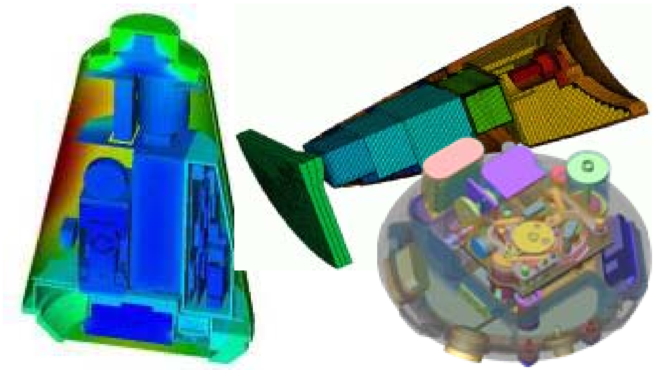
Engineering Sciences Stewardship

- **Assure a sound science-base to meet Sandia's mission goals of today**
- **Develop and nurture future science and technology that Sandia will depend upon to achieve its mission goals of tomorrow.**
- **Provide significant contributions to the leadership of engineering.**

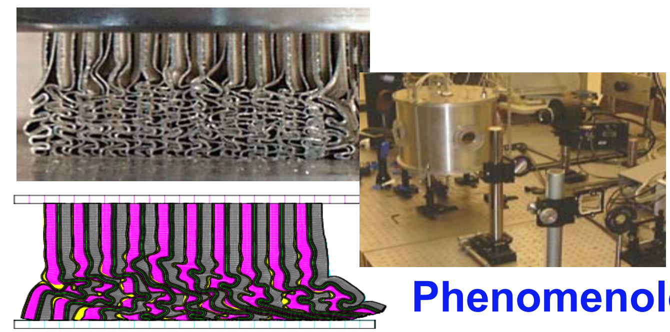
Sandia National Laboratories

Engineering Sciences capabilities span research, development, and application

Engineering Modeling & Simulation

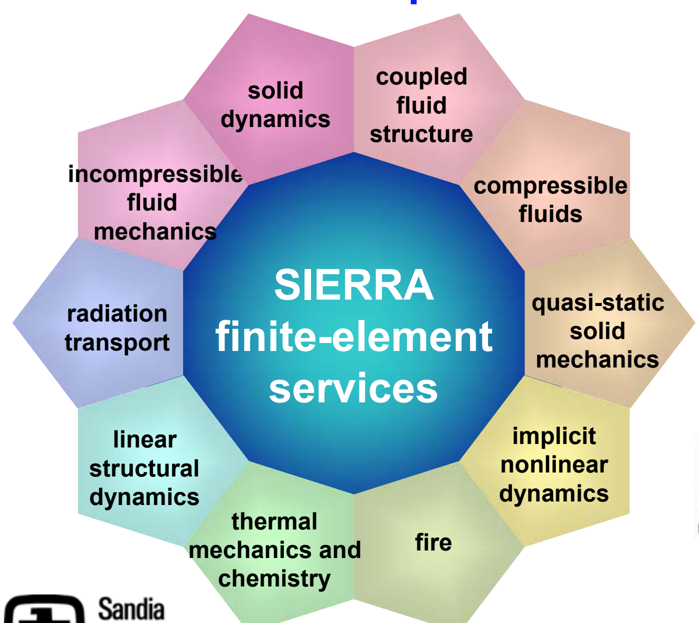


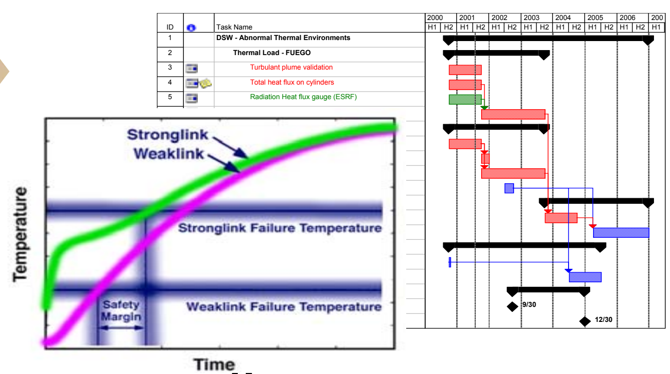
Large-Scale Test /Qualification



Phenomenology & Model Development

Code Development





Uncertainty Quantification, Verification & Validation

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Modeling and Simulation at Sandia's Engineering Sciences Center

- **Full-system multi-physics**
  - » **Physics couplings, e.g.,**
    - **Fluid/Thermal/Solid Mechanics/Blast**
      - **Fire**
      - **Material thermal decomposition**
      - **Structural loading response and failure**

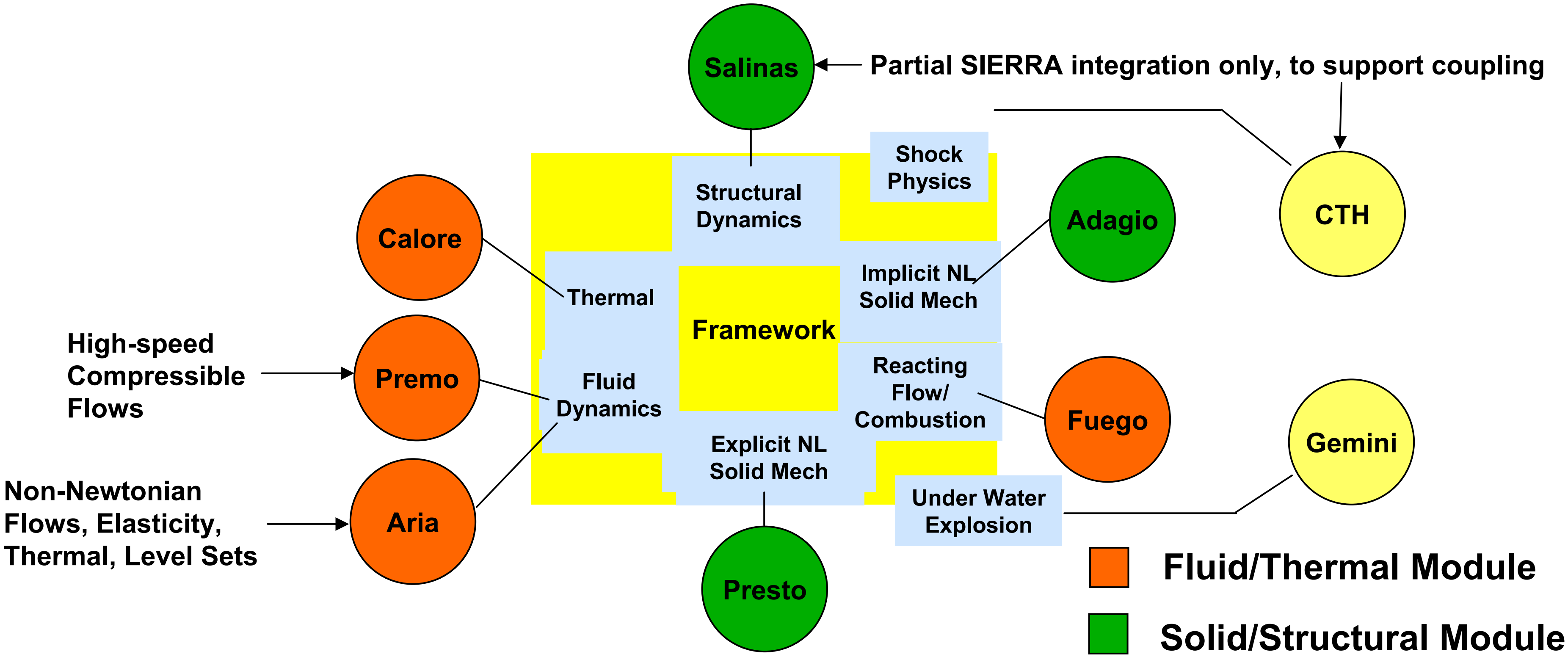
- **Scalable tools**
  - » **From single workstation to 1000's processors**

- **Multi-scale (nano-to-macro scales)**

- ***Predictive* capability**
  - » Uncertainty Quantification
  - » Verification and Validation (V&V)
  - » Modeling and Simulation in conjunction with appropriate experiments

SIERRA Mechanics: The Big Picture

- ***SIERRA Mechanics*** **consists of the following modules:**



- **Modules can readily be coupled for multi-physics applications**
- **Strategic activities underway to combine modules**

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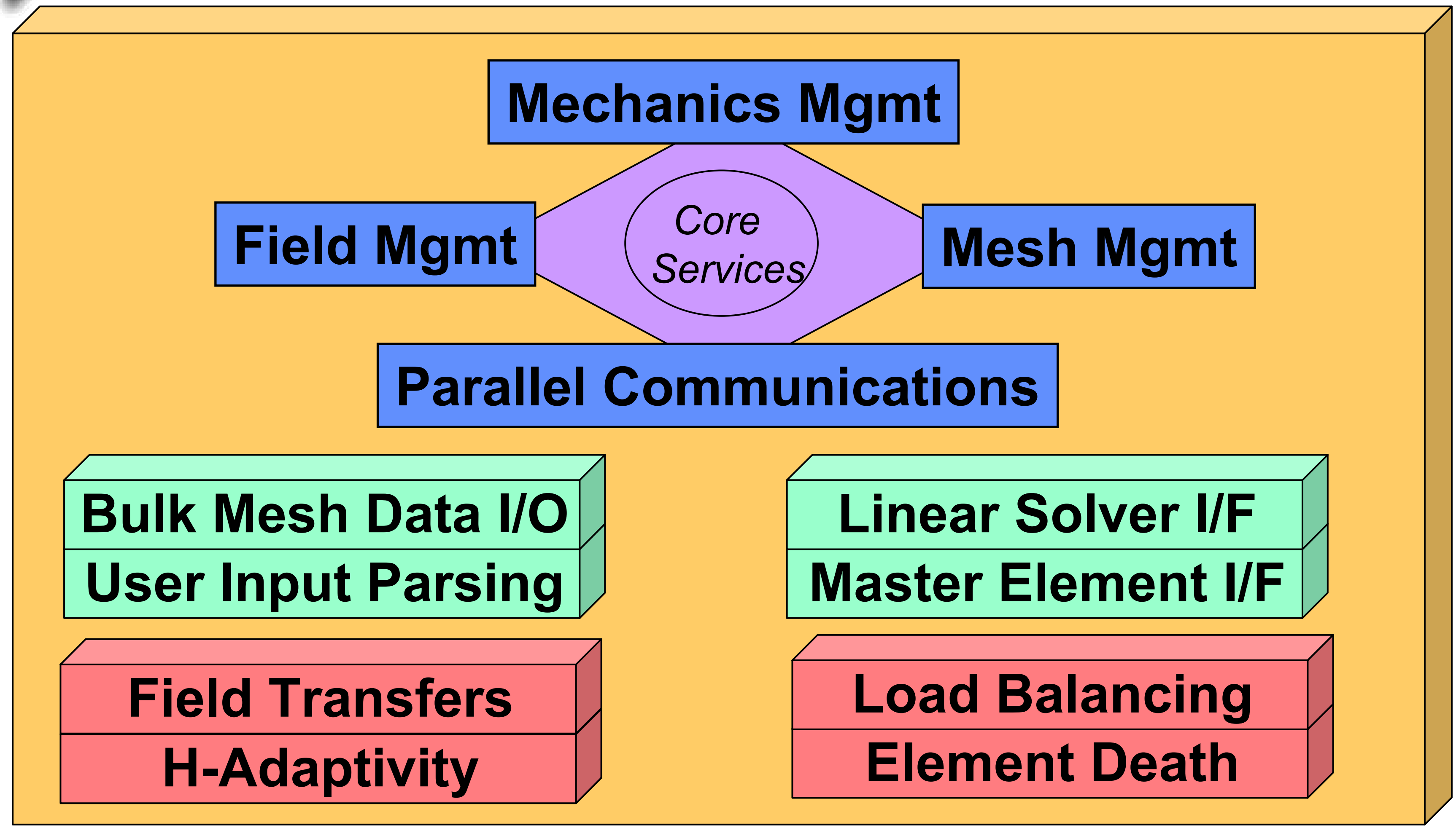
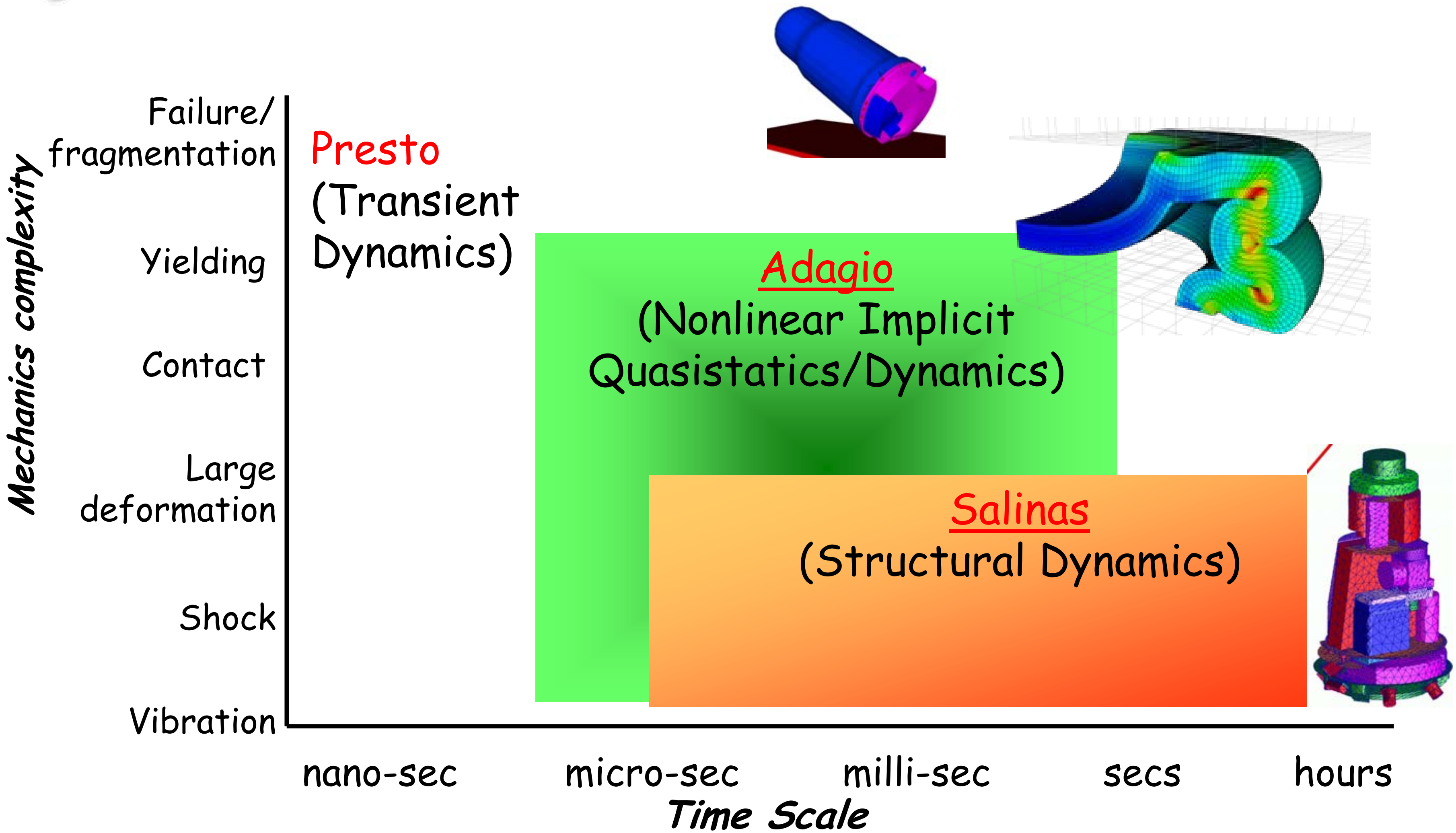
SIERRA Framework Provides Integrating Services



SIERRA Solid/Structural Modules Notional Overview



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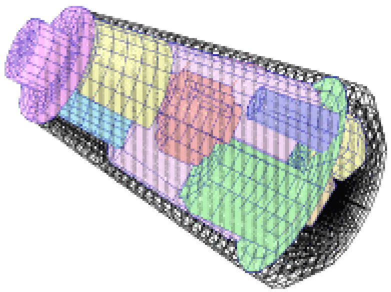
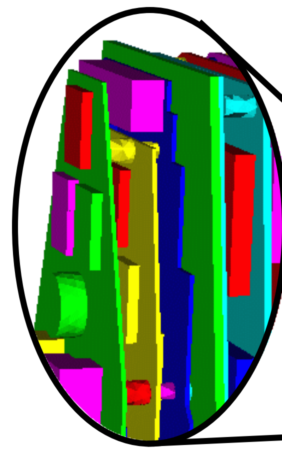
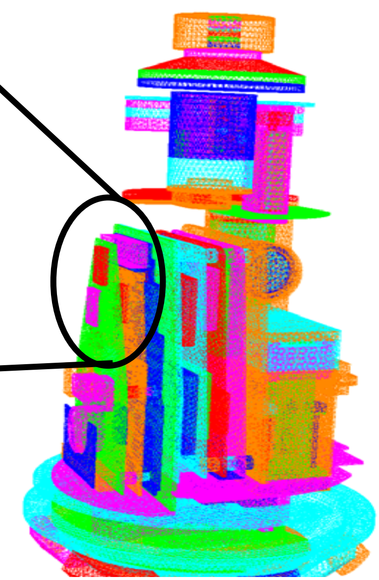
Structural Dynamics - Salinas

- **Predicts the response of a system under dynamic conditions.**
  - **Stresses (particularly in the operating regime)**
  - **Fatigue**
  - **Energy dissipation in joints**
- **Efficient for very large problems**
  - **Many millions of coupled equations**
  - **Serial, direct matrix solutions scale to order N^3**
  - **Parallel, iterative solvers are typically more complex, but scale to the order N**
    - FETI (Farhat)
    - CLIP, CLOP Solvers (Sandia)

Recent Past:
NASTRAN
MC2912
30,000 dof





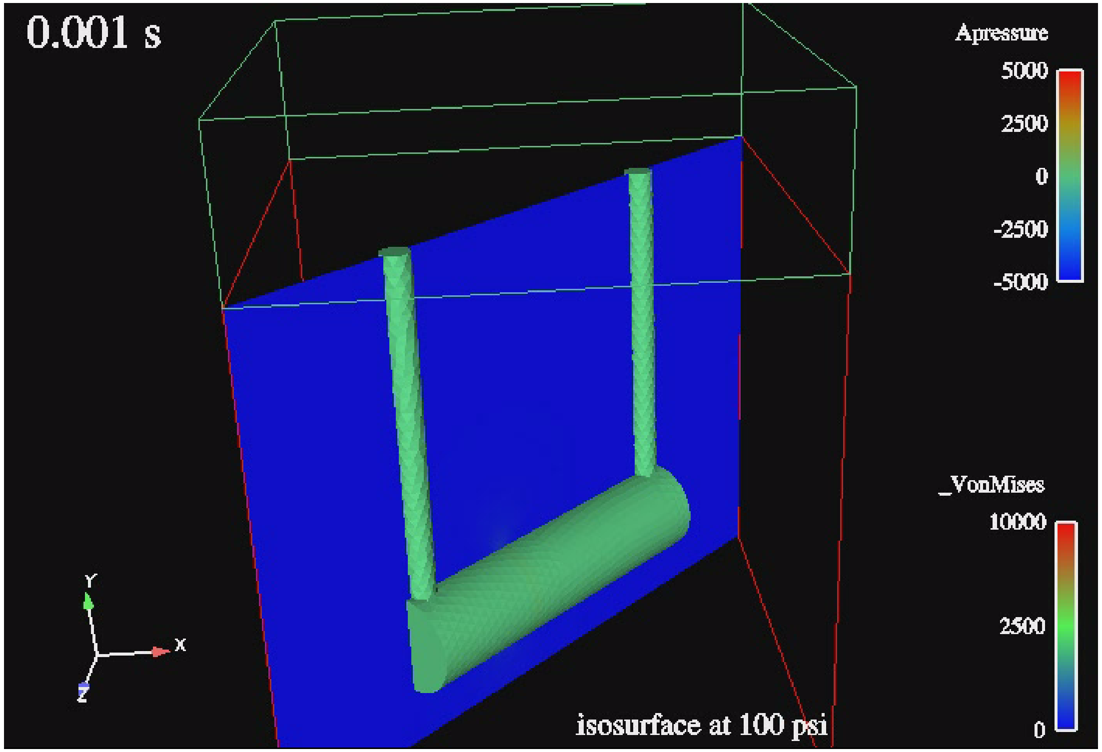


Today:
SALINAS MP
>10M dof

Salinas is scalable and fast, allowing it to handle very large models

Noise Detection in an Underground Bunker

- **Strong coupling between (*nonlinear*) acoustic (air) and structural (soil) fields; absorbing BC's**
- **1.2M DOFs, solved on 80 processors**



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Explicit Dynamics - Presto

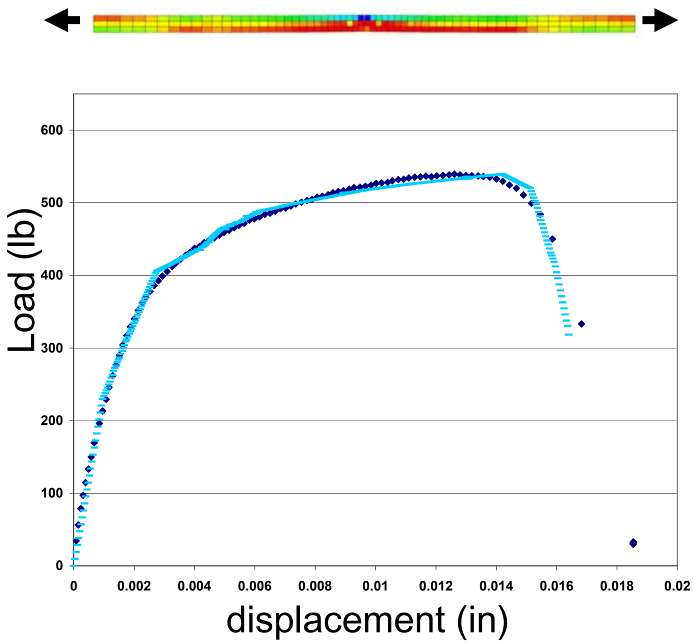
- **Fully Three-Dimensional**
- **Massively Parallel**
  - **Thousands of processors**
- **Finite Elements and Particles**
  - **SPH particles**
  - **Other particle methods planned (e.g., GPA, HPM, RKPM)**
- **Material models: 40+, including energy-dependent materials**
- **Contact: Massively parallel, momentum balance, accurate friction response**
- **Boundary conditions:**
  - **Kinematic and Force**
  - **Specialized: cavity expansion, silent BC**
- **Failure modeling:**
  - **Material failure/element death**
  - **Cohesive zones (elements, contact surfaces)**
  - **Phenomenological models (spot weld, line weld)**

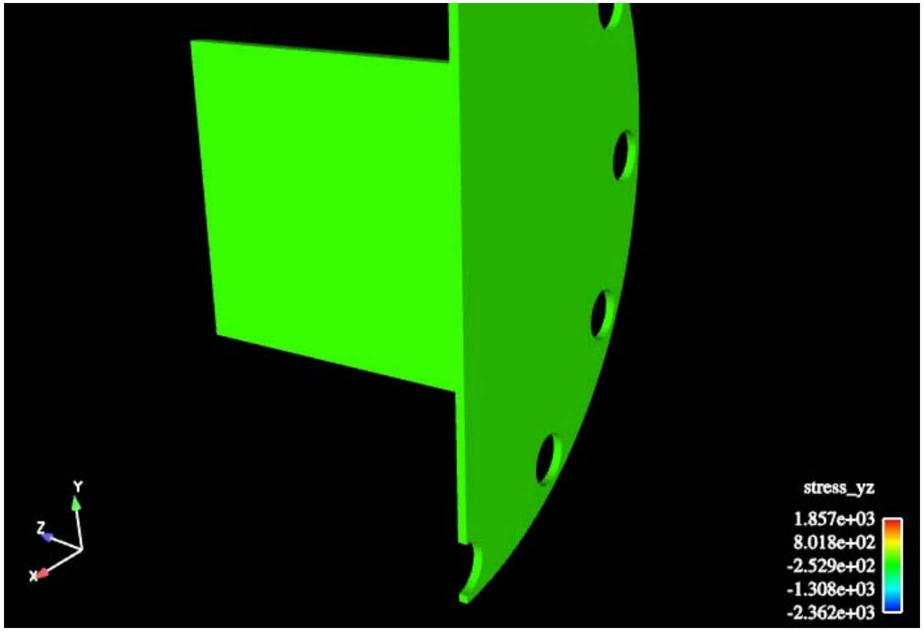
QuickTime™ and a
YUV420 codec decompressor
are needed to see this picture.

Penetration simulation using the node-based tet4 element with re-meshing. This element provides similar accuracy as the hex8.

Weld Failure Under Dynamics Loading

Impact against an unyielding target using spotweld interface model (calibrate against tension test data, validated against cylinder drop test)





Calibration of spotweld model with tensile test data

Validating fitted failure parameters on weld test configuration in cylinder drop test

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Coupled CTH and Presto for Blast

- **Purpose**
  - **To predict the structural response of targets to blast waves**
- **Approach**
  - **A CTH library will be created that will link with Presto**
  - **A SIERRA wrapper will be developed for CTH, which will allow for mapping of CTH’s structured data into SIERRA’s data structures**
  - **SIERRA transfer operators will then be used**
  - **This is an example of how non-Sierra codes are coupled in.**
- **One-way CTH->Presto coupling completed, two-way coupling in progress**

One-Way Coupled CTH/Presto

• **CTH Loading: 5 kg TNT at the *center of room*, for 2.5 ms**

Blast Response

QuickTime™ and a
YUV420 codec decompressor
are needed to see this picture.

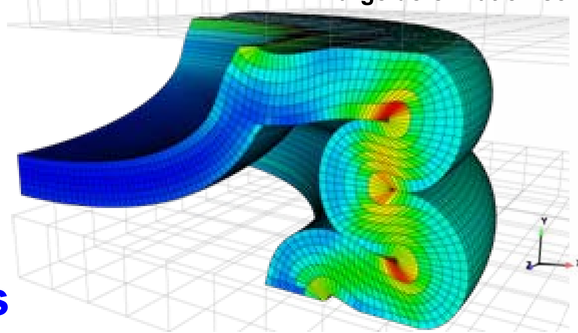
QuickTime™ and a
YUV420 codec decompressor
are needed to see this picture.

Presto Crash Dynamics

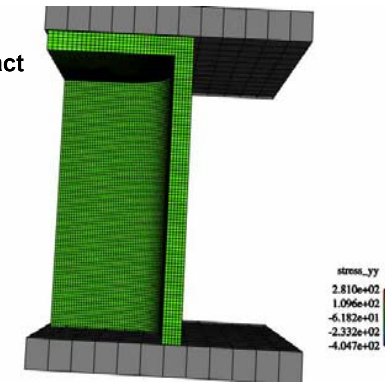
QuickTime™ and a
YUV420 codec decompressor
are needed to see this picture.

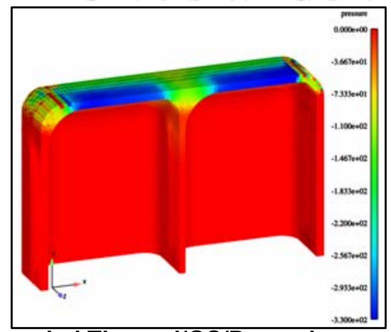
Quasi-static Structural Mechanics - Adagio

- **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)**

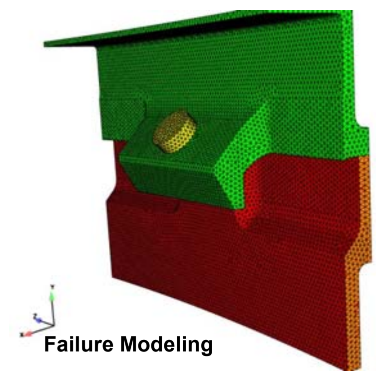


Large deformation/contact





Coupled Thermal/QS/Dynamic



Failure Modeling

- **Design of energy absorbing barrier**
- **Uses multilinear elastic-plastic constitutive model**
- **Demonstrates frictional contact, geometric and material nonlinearities, parallel scalability**

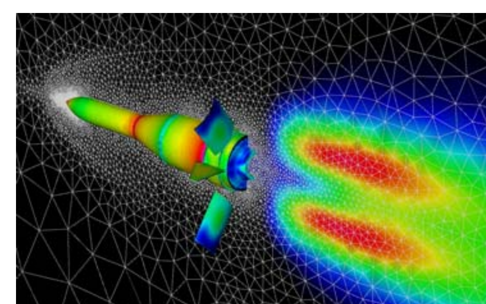
Sierra Thermal/Fluids Capabilities

- **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**

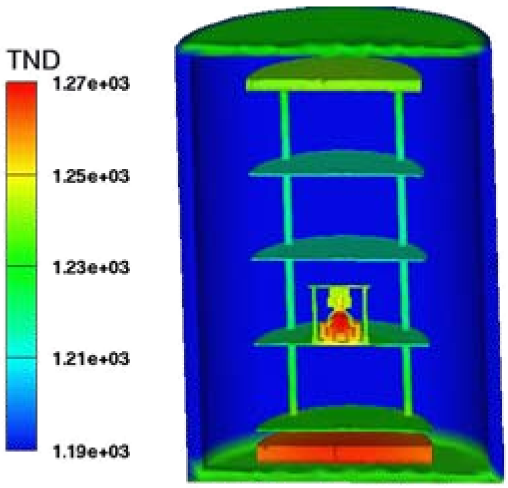
QuickTime™ and a YUV420 codec decompressor are needed to see this picture.

- **Aria – Non-Newtonian, Chemically Reacting, 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

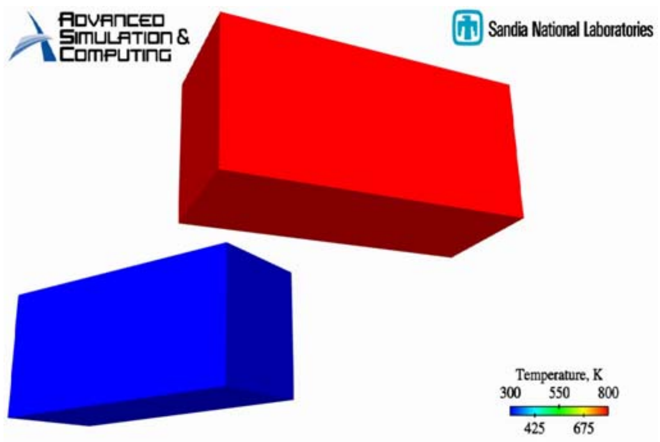


Heat Transfer - Calore

- 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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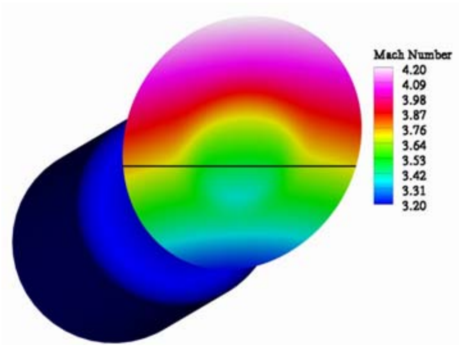
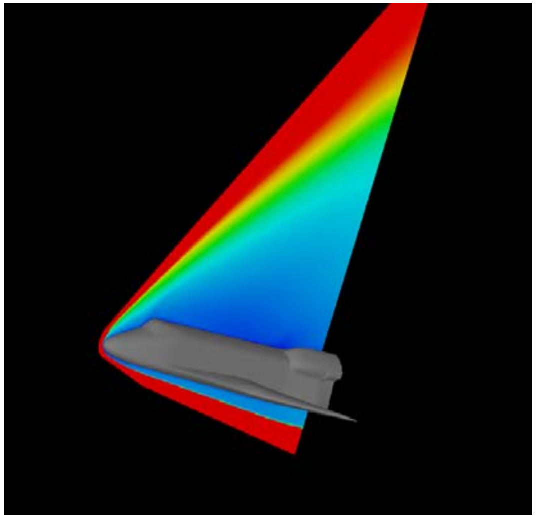
Compressible Fluid Mechanics - Premo

- 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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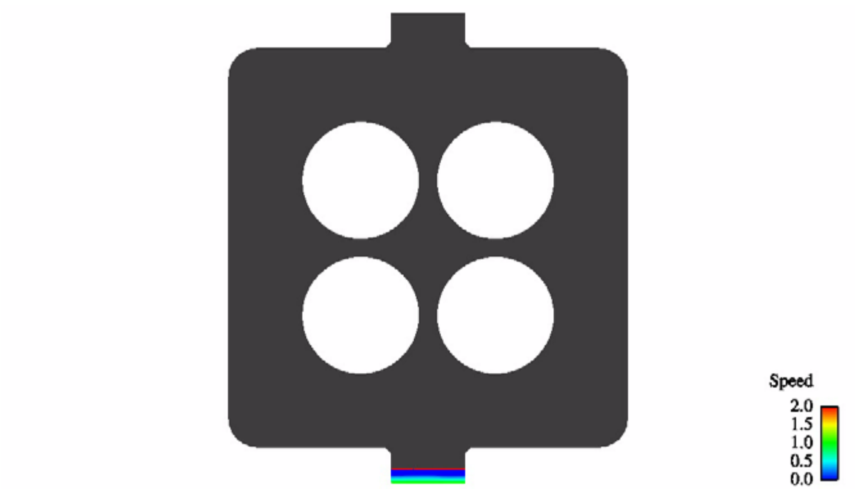
Very Low Speed non-Newtonian Flow - Aria

- Transient & steady; 2D & 3D
- Error estimation and mesh refinements classical ZZ and adjoint-based
- Stabilized Navier-Stokes: PSPG & PSPP
- Front tracking using Level Sets
- Basic Physics
  - Navier-Stokes (variable ρ)
  - Non-Newtonian
  - Energy
  - Species
  - Electrostatics
- Nonlinear Solvers & Coupling
  - Full Newton (analytic)
  - Full Picard
  - Arbitrary loose coupling

QuickTime™ and a
YUV420 codec decompressor
are needed to see this picture.

Liquid dripping into a vessel



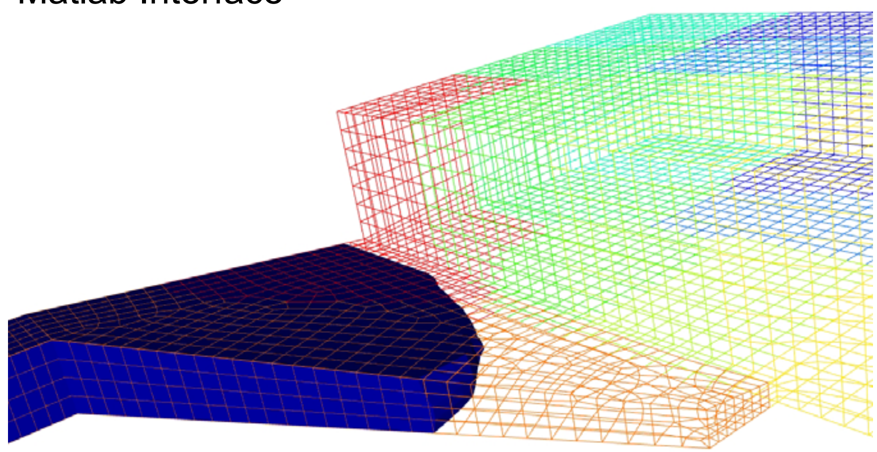
Encapsulation of an electrical component

Aria 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



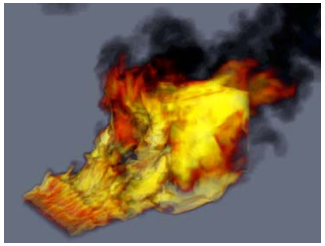
Parallel level set mold filling in Aria

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

Source: Notz (2007)

Fuego Mechanics Module – Overview

- **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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Numerics and Math Models Employed in Fuego

- **Segregated, backward Euler or Crank-Nicholson time solution**
  - **Equal-order interpolation CVFEM technique for low-Mach or acoustically compressible mechanics**
  - **Approximate pressure projection method for continuity/momentum**
  - **Convection operators: Central, pure upwind, skew upwind, MUSCL w/flux limiters (Van Leer, Superbee, etc.)**
- **Basic Favre-filtered equation set (integral form):**

Turbulence closure models required

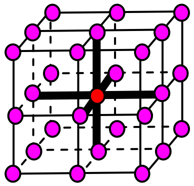
Continuity: $$\int \frac{\partial \bar{\rho}}{\partial t} \mathrm{d}V + \int \bar{\rho}\, \tilde{u}_j n_j dS = 0$$

Momentum: $$\int \frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} \mathrm{d}V + \int \left(\bar{\rho}\, \tilde{u}_i \tilde{u}_j n_j + \bar{p} n_j \delta_{ij}\right) dS = \int \left(\bar{\tau}_{ij} - \tau_{u_i u_j}\right) n_j dS + \int \left(\bar{\rho} - \rho_o\right) g_i \mathrm{d}V$$

Enthalpy: $$\int \frac{\partial \bar{\rho}\tilde{h}}{\partial t} \mathrm{d}V + \int \bar{\rho}\, \tilde{h} \tilde{u}_j n_j dS = -\int \left(\bar{q}_j + \tau_{hu_j}\right) n_j dS - \int \frac{\partial \bar{q}_i^r}{\partial x_i} \mathrm{d}V + \int \left(\frac{\partial P}{\partial t} + \tilde{u}_j \frac{\partial P}{\partial x_j}\right) dV + \int \overline{\tau_{ij} \frac{\partial u_i}{\partial x_j}}\, dV$$

Species: $$\int \frac{\partial \bar{\rho}\tilde{Y}_k}{\partial t} \mathrm{d}V + \int \bar{\rho} \tilde{Y}_k \tilde{u}_j n_j dS = \int \left(\overline{\rho \mathrm{Y}_\mathrm{k} \hat{u}_{j,k}} - \tau_{Y_k u_j}\right) n_j dS + \int \bar{\dot{\omega}}_\mathrm{k} \mathrm{d}V$$

tke: $$\int \frac{\partial \bar{\rho} k_{sgs}}{\partial t} \mathrm{d}V + \int \bar{\rho} k_{sgs} \tilde{u}_j n_j dS = \int \left(\mu + \frac{\mu^T}{\sigma_k}\right) \frac{\partial k_{sgs}}{\partial x_j} n_j dS + \int \left(P_k - \rho\varepsilon\right) \mathrm{d}V$$



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Source: Domino et al. (2007)

Fuego/Syrinx/Calore Example
Design of New Experimental Facility

- **Outdoor Experiment (CFD-based design effort)**
  - **Ten meter hydrocarbon pool fire in strong crosswind**
  - **Object(s) of interest were fully engulfed**
  - **Peak irradiation was measured**
- **Objective**
  - **Replicate peak irradiation that was measured during the outdoor experiment in a [new] indoor facility**

Three design configurations simulated

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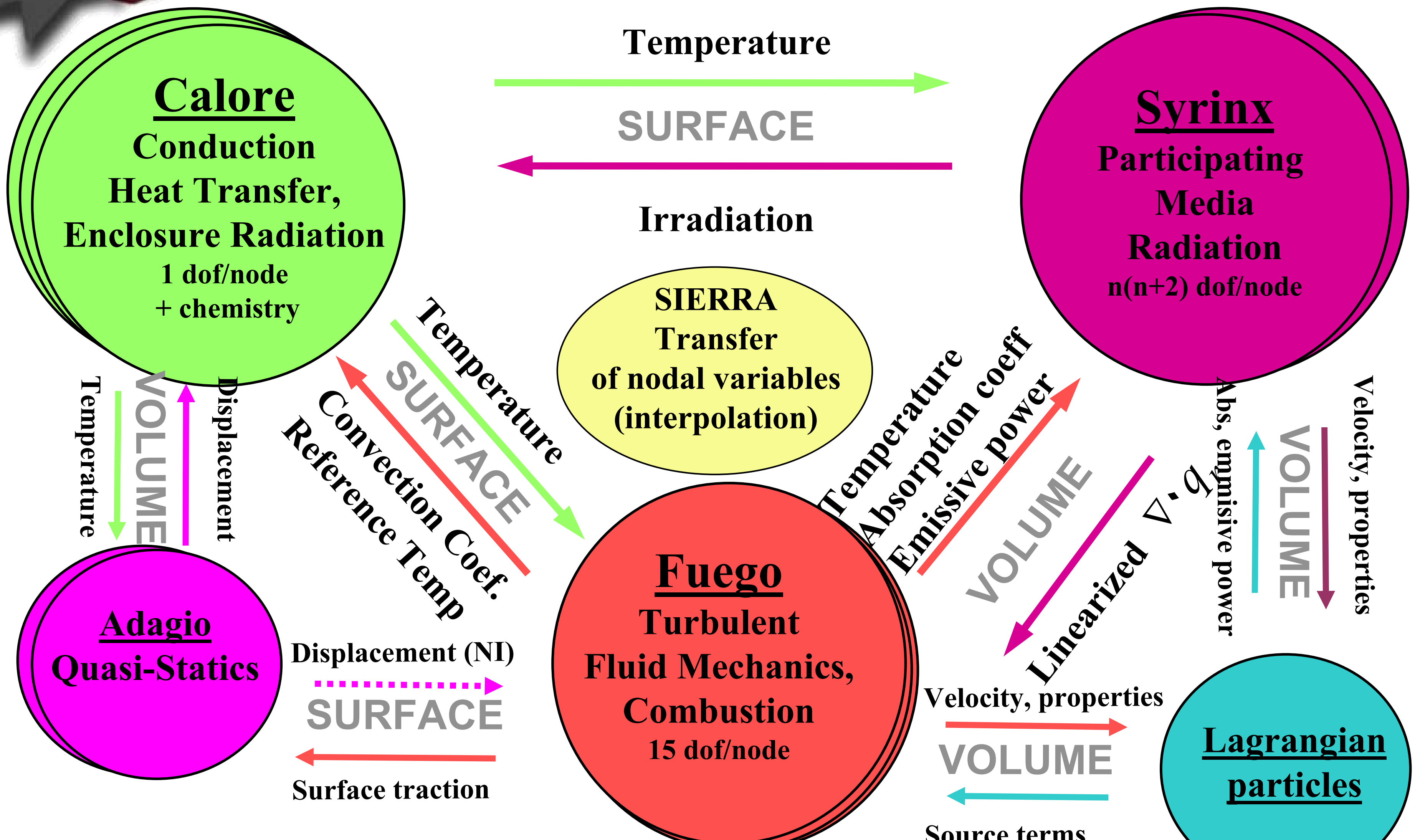
Coupled-Mechanics Object-in-Fire with Structural Response



1:n regions (dynamically created at parsing)

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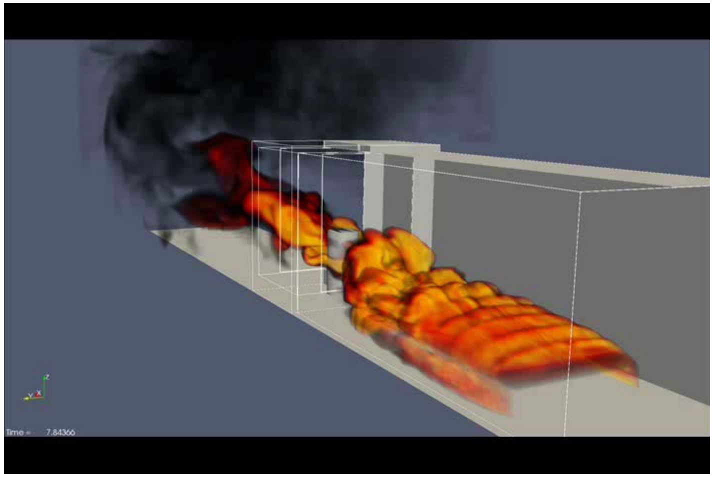
Source: Domino et al. (2007)

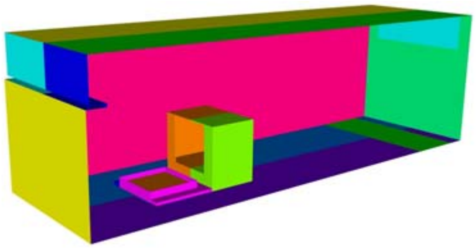
Fuego/Syrinx/Calore Example
Design of New Experimental Facility

- **Configuration 2: Added object container, entrance restricted**
  - Corrected an issue with configuration 1
  - Too low of irradiation on object
  - Experimental fabrication costs very high
- **200 million DOFs; Solved in 2 days using 2048 processors on Red Storm**

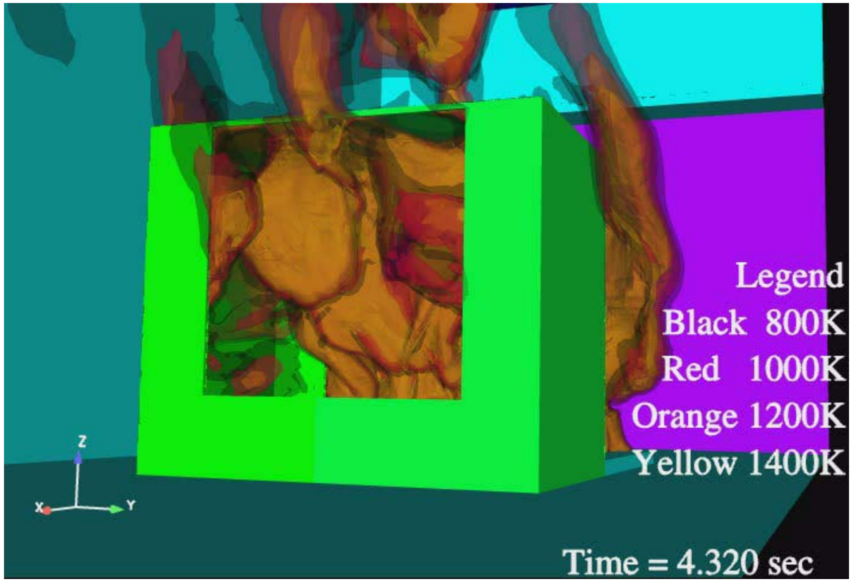


Fuego/Syrinx/Calore Example
Design of New Experimental Facility

- Configuration 3: Issues corrected
- Scoping study (40 million degree-of-freedom) simulation

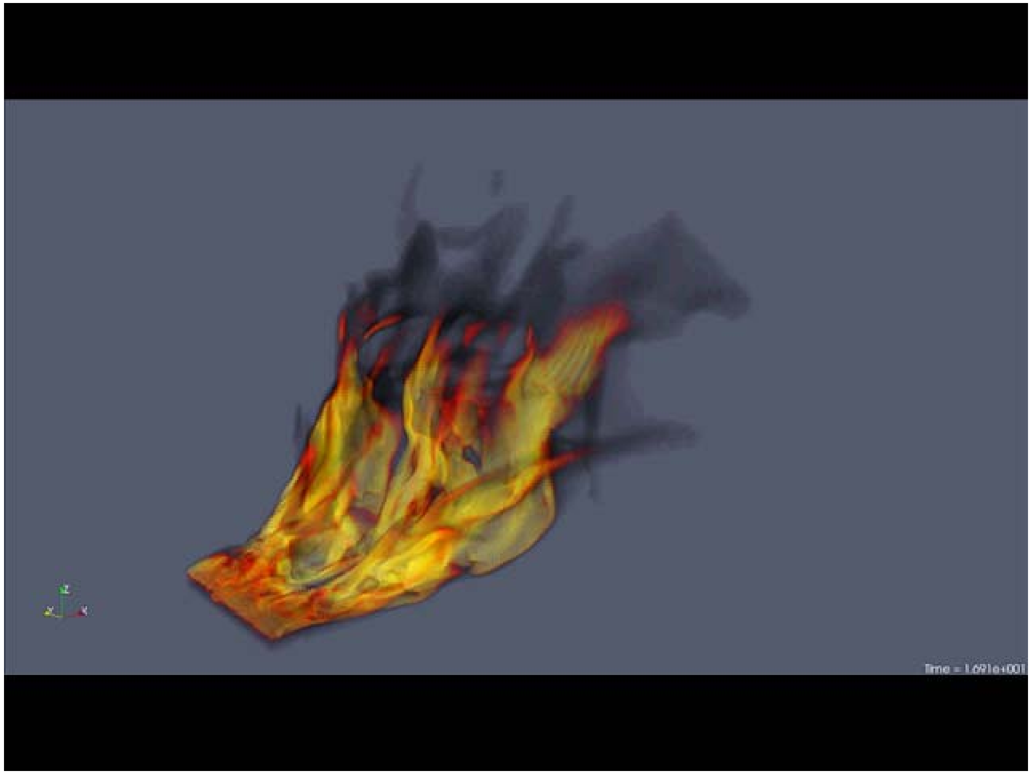


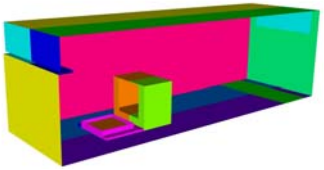
New XTF geometry



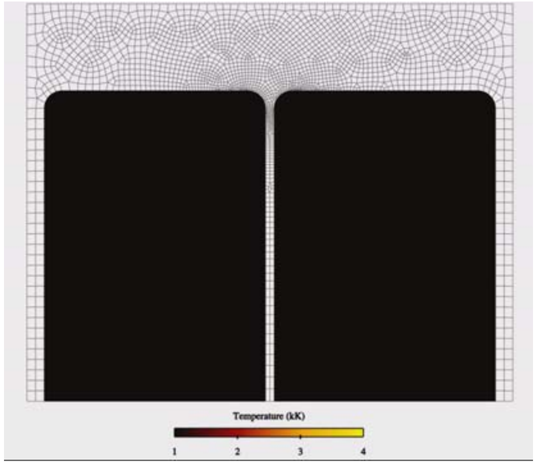
Fuego/Syrinx/Calore Example
Design of New Experimental Facility

- **Solution verification study for Configuration 3**
- **400M DOFs, solved 5000 processors on Red Storm**



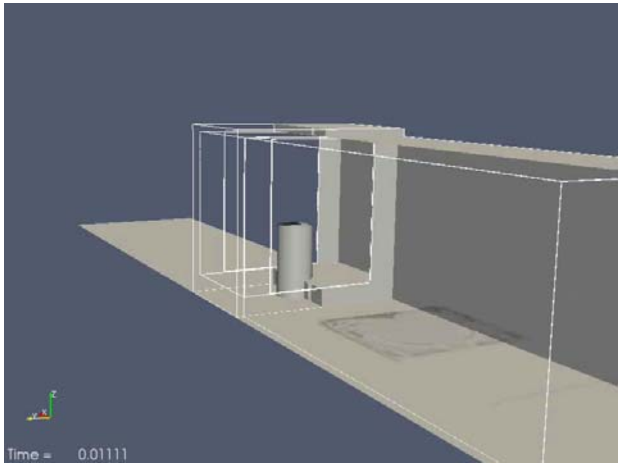


Coupled Physics Examples



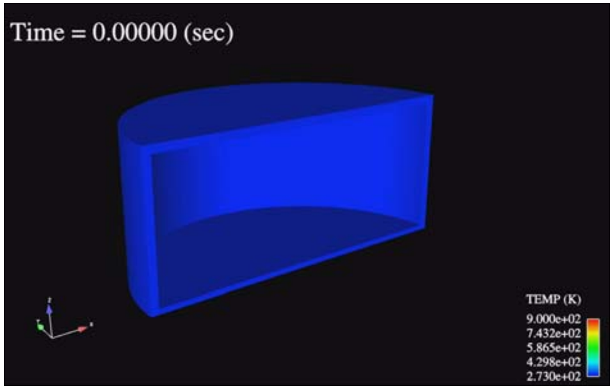
Residual stress prediction for a laser welding process.

Coupled heat transfer, fluid mechanics, quasi-static solid mechanics.



Temperature and internal pressure prediction for an object in a hydrocarbon fire.

Coupled chemically reacting flow, heat transfer, quasi-static solid mechanics.



Internal pressure prediction for a decomposing foam in a thermal environment.

Coupled heat transfer, foam chemistry, quasi-static solid mechanics.

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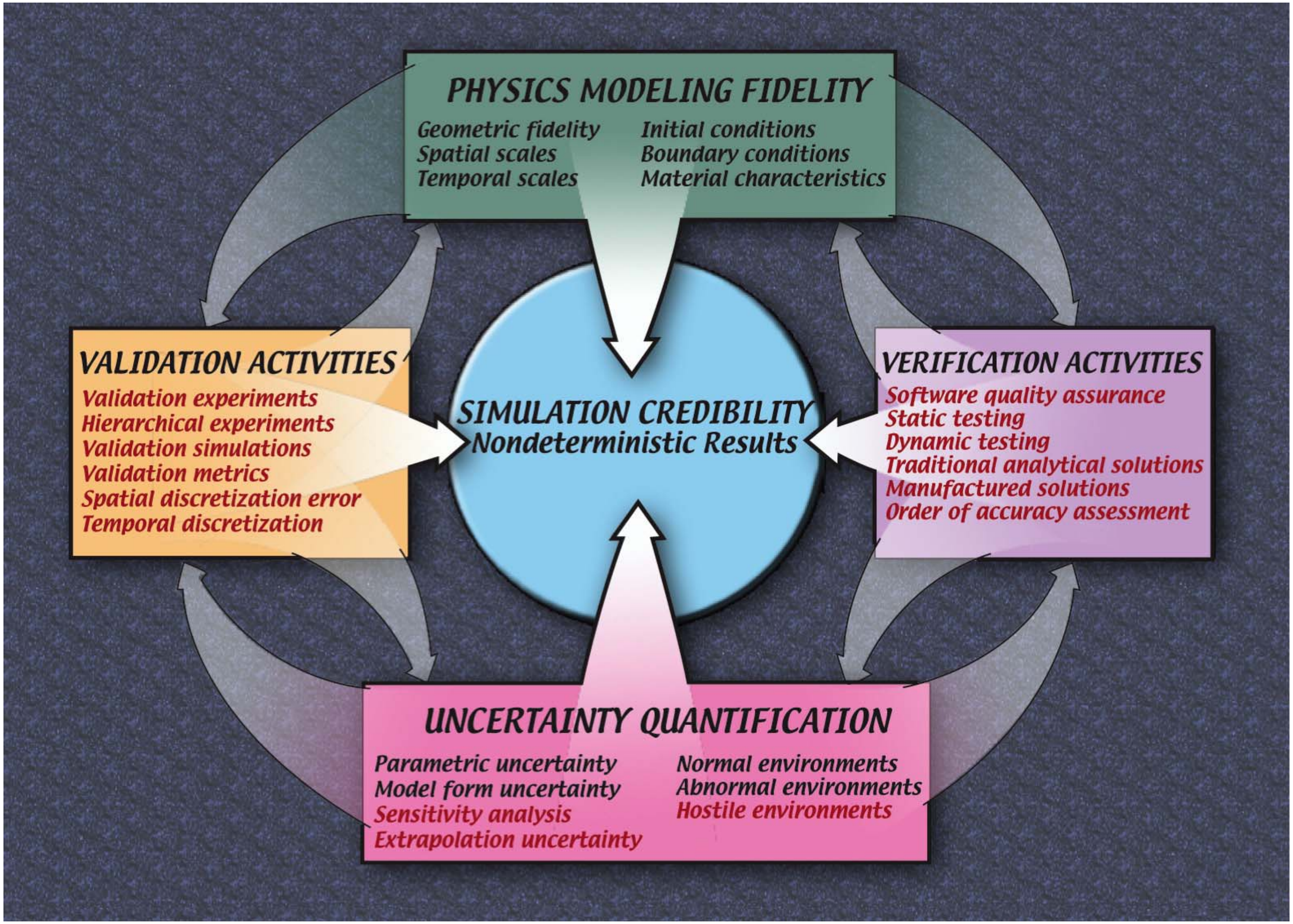
Elements Required in Achieving Credible Simulation and Predictive Capability



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Reference: Oberkampf (2006)

Terminology: Verification

Verification: The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model.

- In computational science and engineering (CSE), two aspects of verification are recognized:
- Code Verification: Verification activities directed toward:
  - Finding and removing mistakes in the source code
  - Finding and removing errors in numerical solution algorithms
  - Improving software reliability using software quality engineering practices
- Solution Verification: Verification activities directed toward:
  - Assuring the accuracy of input and output data for the problem of interest
  - Estimating and reducing the numerical solution error, e.g. error due to finite element mesh resolution

Source: Oberkampf and Giunta (2007)

Terminology: Validation

Validation: The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

- CSE development of V&V methodology and practices:
  - American Institute of Aeronautics and Astronautics published the first engineering standards document on V&V: "Guide for the Verification and Validation of Computational Fluid Dynamics Simulations," American Institute of Aeronautics and Astronautics, AIAA-G-077-1998.
  - American Society of Mechanical Engineers published a recent engineering standard: "Guide for Verification and Validation in Computational Solid Mechanics," ASME V&V 10-2006."
- Important difference in validation methodology between DoD and CSE: **Validation can only be conducted by comparison with experimentally measured data.**

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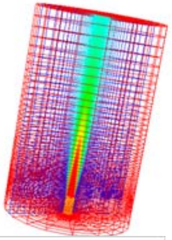
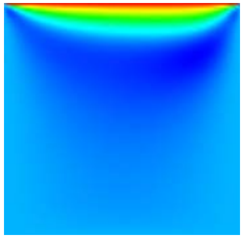
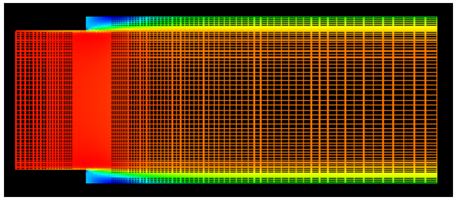
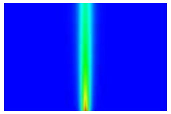
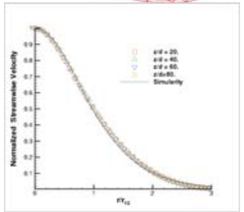
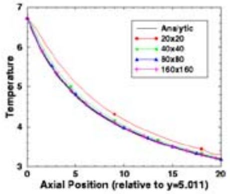
Source: Oberkampf and Giunta (2007)

Verification Test Plan Overview in Fuego/Syrinx/Calore Coupling

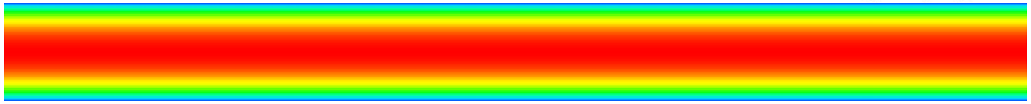
- **First, define and execute single physics verification plan!**
- **Next, define and execute multiphysics verification plan**
- **Combination of all verification tests will range from "Low" to "High" Quality**
  - **Code vs. Code comparisons**

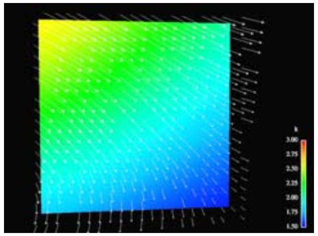
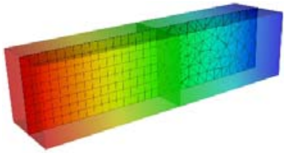
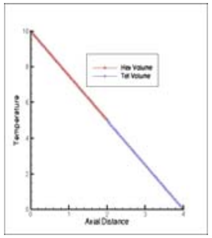
  - **Similarity solutions**

  - **Exact Solutions**



  - **Method of Manufactured Solutions**

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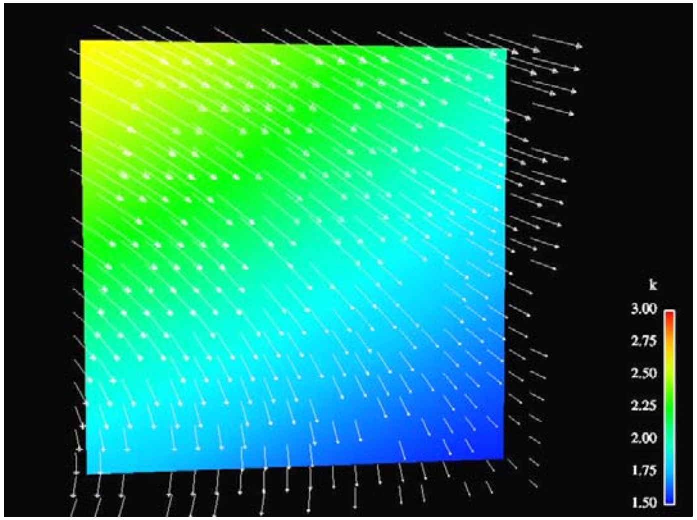
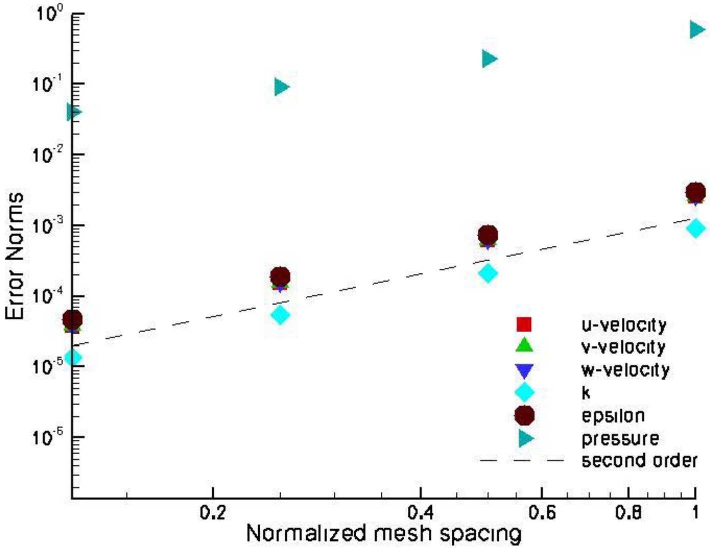
Source: Domino et al. (2007)

Manufactured Solutions for Turbulent Flows



Contour plane of turbulent kinetic energy with velocity vectors of analytic solution

Results – order of accuracy:



- **u, v, w, p, k, and ε are functions of x, y, z. Constant density**
- **Dirichlet boundary conditions. Re ~ 1000**
- **Dimensions of equal extent: Four grids: 10^3, 20^3, 40^3, 80^3**
- **All variables converged to machine tolerance within 1000 iterations**

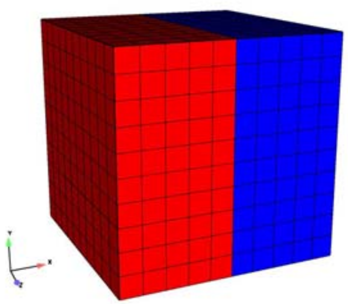
Source: Domino et al. (2007)

Verification of Conjugate Heat Transfer Mechanics

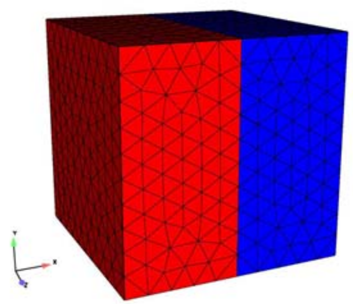
- **Two manufactured solutions solved on cubical domains**

$$T_1(x,y,z) = Ax + By + Cz + D$$
$$T_2(x,y,z) = \sin(A\pi x)\sin(B\pi y)\sin(C\pi z) + D$$

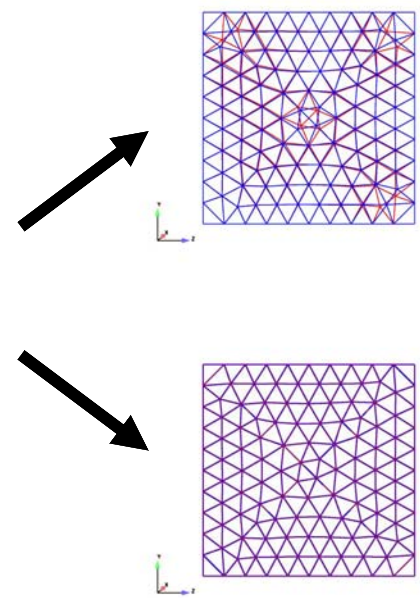
- **Solved on two disparate regions with hex-hex and tet-tet meshes with and without conforming interfaces**



Hex-Hex Mesh



Tet-Tet Mesh

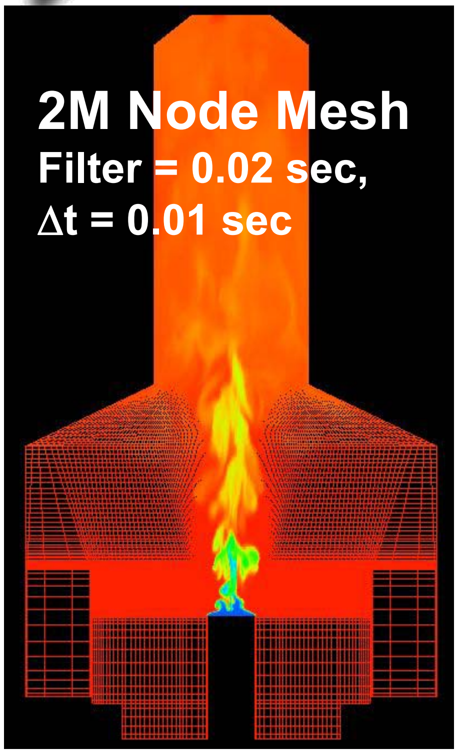


Non-conforming interface

Conforming interface

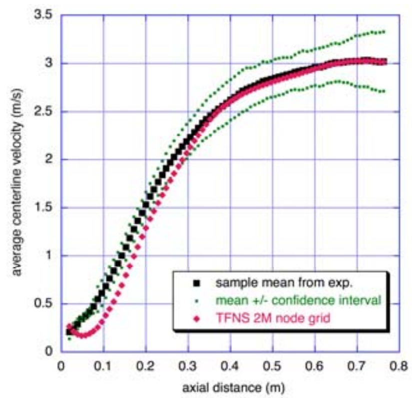
Source: Domino et al. (2007)

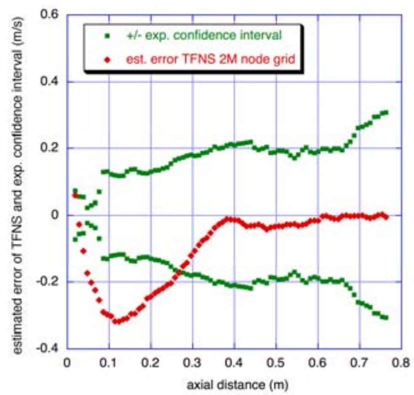
SIERRA/Fuego/Syrinx Subset of Validation Efforts



SIERRA/Fuego 1 meter helium plume validation simulation in FLAME (O'Hern et al)

Metrics

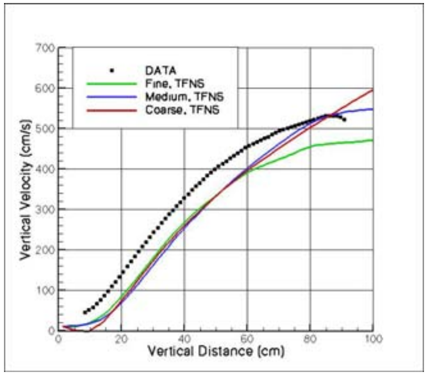




QuickTime™ and a
YUV420 codec decompressor
are needed to see this picture.

SIERRA/Fuego v2-f (TFNS) water channel convection validation simulation (Kearney et al)

QuickTime™ and a
YUV420 codec decompressor
are needed to see this picture.



SIERRA/Fuego/Syrinx 1 meter methane fire validation simulation in FLAME (Tieszen et al)

- 2 meter JP-8 pool fire (Tieszen et al)
- Object in fire (Blanchet et al)

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Source: Domino et al. (2007)

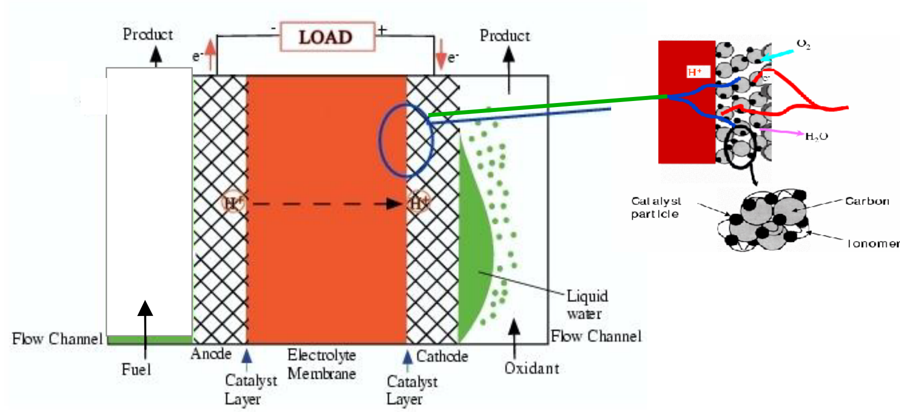
Multi-dimensional finite-element model for simulating PEM fuel cell performance

- **In Flow Channels:**

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \rho \mathbf{u}\mathbf{u} = -\nabla p + \nabla \cdot \mu \nabla \mathbf{u}$$ **(mixture momentum conservation)**

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0$$ **(mass conservation)**

$$\frac{\partial (c_i)}{\partial t} + \nabla \cdot (\mathbf{u} c_i) + \nabla \cdot \mathbf{J}_i = 0$$ **(species mass conservation)**



- **In Gas-Diffusion Layers:**

$$\frac{\partial}{\partial t}\left(\frac{\rho \mathbf{u}}{\varepsilon}\right) + \nabla \cdot \left(\frac{\rho \mathbf{u}\mathbf{u}}{\varepsilon^2}\right) = -\nabla p + \nabla \cdot (\mu_B \nabla \mathbf{u}) - \frac{\mu}{k}\mathbf{u}$$

$$\frac{\partial \varepsilon \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial (\varepsilon c_i)}{\partial t} + \nabla \cdot (\mathbf{u} c_i) + \nabla \cdot \mathbf{J}_i = 0$$

- **In Catalyst Layers:**

$$\frac{\partial}{\partial t}\left(\frac{\rho \mathbf{u}}{\varepsilon}\right) + \nabla \cdot \left(\frac{\rho \mathbf{u}\mathbf{u}}{\varepsilon^2}\right) = -\nabla p + \nabla \cdot (\mu_B \nabla \mathbf{u}) - \frac{\mu}{k}\mathbf{u}$$

$$\frac{\partial \varepsilon \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial (\varepsilon c_i)}{\partial t} + \nabla \cdot (\mathbf{u} c_i) + \nabla \cdot \mathbf{J}_i = r_i$$

- Butler-Volmer kinetics model for HOR and ORR reactions:

$$r_i = \frac{a i_0}{nF}\left(\frac{c_i}{c_{i,ref}}\right)^{\beta}\left[\exp\left(\frac{\alpha_a F}{RT}(\Phi_s - \Phi_e - U_{0,c})\right) - \exp\left(-\frac{\alpha_c F}{RT}(\Phi_s - \Phi_e - U_{0,c})\right)\right]$$

- **Electrical Potentials in Electrolyte & Electrode phases:**

$$\nabla \cdot (-\kappa \nabla \Phi_e) = ai \quad \nabla \cdot (-\sigma \nabla \Phi_s) = -ai$$

where i denotes H_2 and O_2, and $r_{H_2O} \equiv -2 r_{O_2}$

- **Transfer current:**

$ai \equiv 0$ and Φ_s is not defined in membrane region.

$ai = nFr_{H_2}$ in anode catalyst layer with n = 2 $ai = nFr_{O_2}$ in cathode catalyst layer with n = 4

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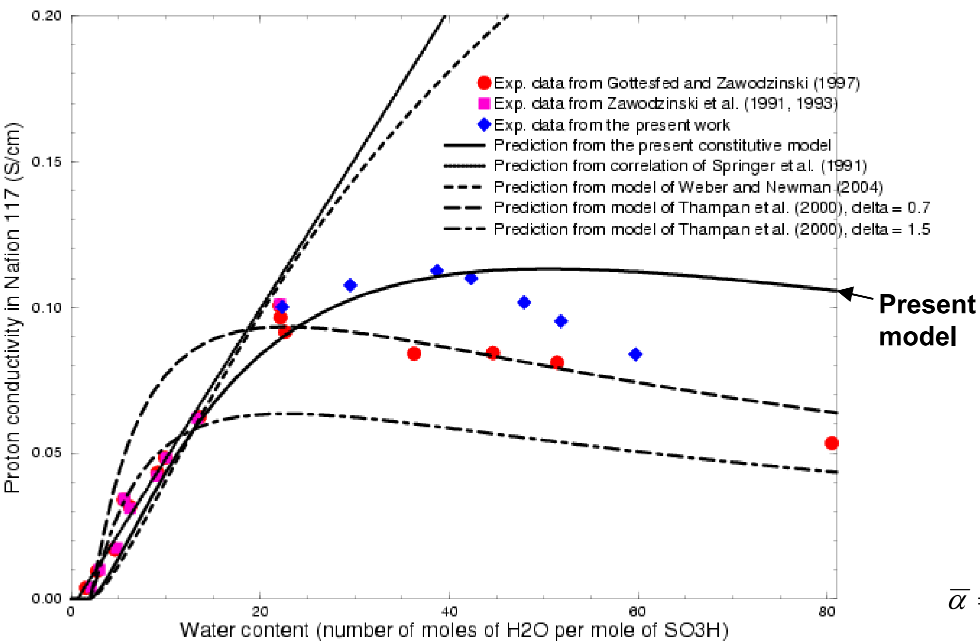
Reference: Chen et al., Sandia Technical Report, SAND2006-6964.

A new constitutive model relating proton conductivity to membrane water content

The new constitutive model is based on Faraday's law and Nernst-Einstein Equations and relates proton conductivity to membrane water content and temperature:

$$\kappa = \frac{F^2}{RT}\frac{D^0{}_{H^+,w}}{\overline{V}_m(1+\alpha\lambda)}\left(\frac{\alpha\lambda}{1+\alpha\lambda}-0.06\right)^{1.5}\exp\left[1137\left(\frac{1}{303}-\frac{1}{T+273}\right)\right] \quad \text{where} \quad \alpha = \frac{\overline{V}_w}{\overline{V}_m}$$

Proton conductivity as a function of water content: comparison of present model with models from literature and experimental data



- Springer et al. (1991)'s empirical correlation:

$$\kappa = (0.005193\lambda - 0.00326)\exp\left[1268\left(\frac{1}{303}-\frac{1}{273+T_{cell}}\right)\right]$$

- Weber and Newman (2004)'s semi-empirical model:

$$\kappa = 0.5\left(\frac{\alpha\lambda}{1+\alpha\lambda}-0.06\right)^{1.5}$$

- Thampan et al. (2000)'s constitutive model (4 adjustable parameters):

$$\kappa = \frac{F^2}{RT}\frac{D^e{}_{12}}{(1+\delta)}\frac{1}{\lambda\overline{V}_w}\overline{\alpha}\left(\frac{\alpha\lambda}{1+\alpha\lambda}-f_{v0}\right)^{1.5} \quad \text{where}$$

$$\overline{\alpha} = \frac{(\lambda+1)-\sqrt{(\lambda+1)^2-4\lambda(1-1/K_{A,C})}}{2(1-1/K_{A,C})}, \quad K_{A,C} = K_{A,C,298}\exp\left[-\frac{\Delta H_0}{RT}\left(\frac{1}{T}-\frac{1}{298}\right)\right]$$

- **The present constitutive model yields good agreement with experimental data over a wide range of water content: from $\lambda = 1.5$ to $\lambda \sim 45$.**

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Reference: Chen and Hickner, in ASME Proceeding IMECE2004, #60848 (2004)

Numerical Solution Methods

- Finite element discretization with structured or unstructured meshes.
- Galerkin weighted residuals with quadratic basis function for velocity components, species concentrations and electrolyte potential, and linear basis function for hydrodynamic pressure.
- Fully-coupled implicit solution scheme via Newton's method.
- Second-order accurate predictor-corrector time-integration scheme with adaptive time-step control (Adams-Bashforth predictor, Moulton corrector).
- Goma as the solution platform; Goma is a multi-dimensional, multi-physics, finite-element computer code developed and currently being enhanced by Sandia National Laboratories; Goma can be run on parallel computing environments.

More Details on Solution Methods

1. **Represent nodal unknowns (velocity, concentrations, potential, etc.) in terms of finite-element basis functions and nodal unknown coefficients:**

$$\mathbf{u} = \sum_{j=1}^{9} \mathbf{u}_j \psi_j \qquad c_i = \sum_{j=1}^{9} c_{i,j} \psi_j \qquad \Phi_e = \sum_{j=1}^{9} \Phi_{e,j} \psi_j \quad ,etc.$$

2. Form residual equations by weighting the overall governing equations over the entire domain with basis function chosen as weighting functions:

$$R^M{}_k = \iint (\nabla \cdot \rho \mathbf{u}\mathbf{u} + \nabla p - \nabla \cdot \mu \nabla \mathbf{u}) \psi_k dA \quad ,etc.$$

$$R^S{}_{i,k} = \iint (\nabla \cdot \mathbf{u} c_i + \nabla \cdot \mathbf{J}_i) \psi_k dA \qquad R^\Phi{}_k = \iint [\nabla \cdot (-\kappa \nabla \Phi_e) - ai] \psi_k dA$$

3. Solve the nonlinear algebraic equations by Newton's method with an initial guess of the solution vector, $U^{(0)}$:

$U^{(k+1)} = U^{(k)} - J^{-1}(U^{(k)}) R(U^{(k)})$ **or** $J \, \Delta U^{(k+1)} = -R(U^{(k)})$, $\Delta U^{(k+1)} = U^{(k+1)} - U^{(k)}$

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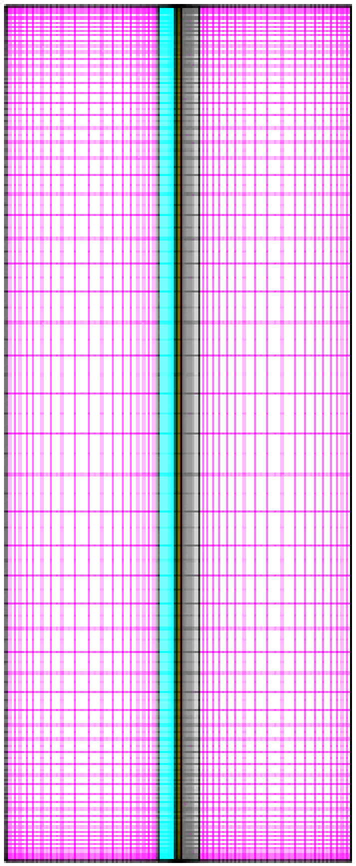
Sample predictions computed from 2-D FEM model: finite-element mesh, velocity field, pressure contours

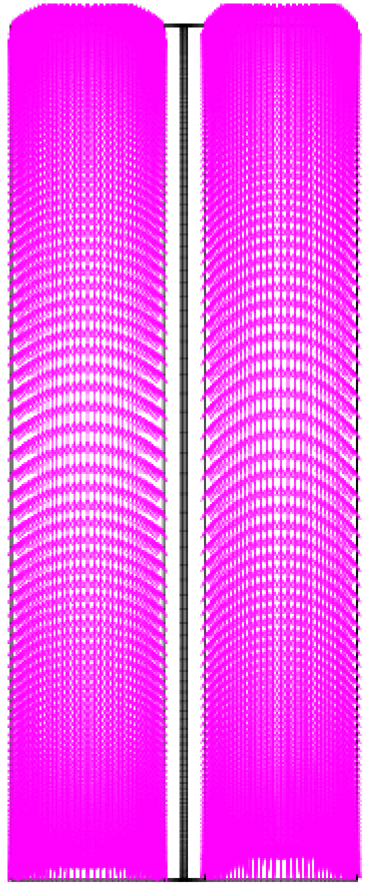
(cell thickness is magnified by a factor of 5 to improve visual effect)

Finite-element mesh



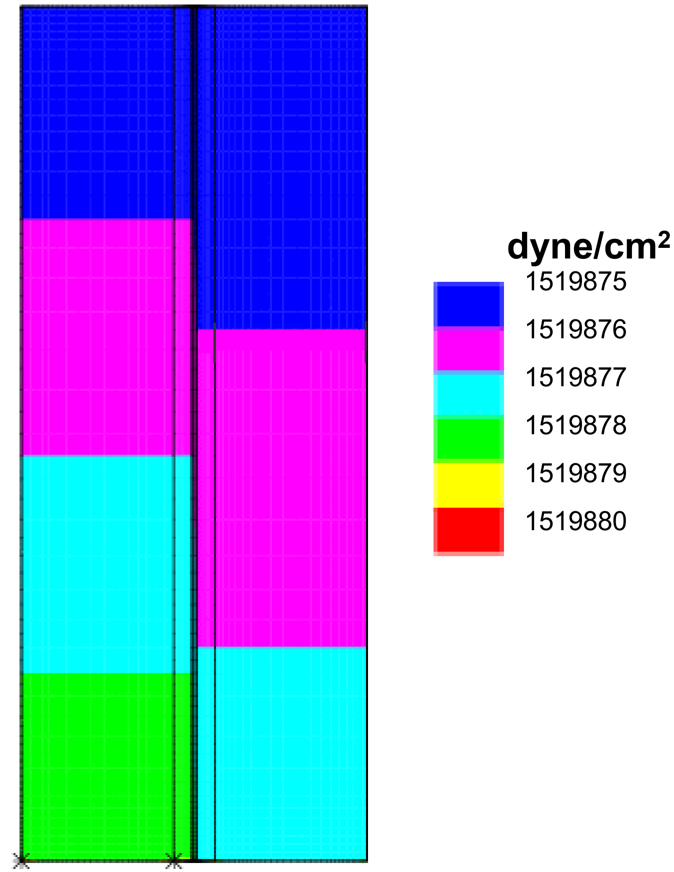
22,743 nodes
5,610 elements
127,590 unknowns

Velocity field



Anode inlet velocity: 10.02 cm/s
Cathode inlet velocity: 14.54 cm/s
(plug flows at inlets)

Pressure contours



Anode back pressure: 1.5 atm
Cathode back pressure: 1.5 atm

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Cell length: 7.112 cm, total cell thickness: 0.5751 cm, gas channel width: 0.254 cm,

GDL thickness: 295 μm, membrane thickness: 51 μm, catalyst layer thickness: 15 μm

Cell geometry, operating conditions and transport properties in base-case study

Cell geometry:

Cell length: 7.112 cm,

Total cell thickness: 0.5751 cm,

Gas channel width: 0.254 cm,

GDL thickness: 295 μm,

Membrane thickness: 51 μm,

Catalyst layer thickness: 15 μm .

Operating conditions:

Cell voltage: 0.7 V

Cell temperature: 80° C

Relative humidity at inlets: 100%

Anode inlet: 1.5 atm, 2.5 stoic @ 0.75 A/cm2.

Cathode inlet: 1.5 atm, 2.0 stoic @ 0.75 A/cm2.

Electrochemical & Transport properties:

Transfer coefficient for HOR: $\alpha_a = \alpha_c = 1$

Transfer coefficient for ORR: $\alpha_a = \alpha_c = 1$

Exchange current density:

$aj_{0,a} = 1000\ A/cm^3$, $aj_{0,c} = 0.0025\ A/cm^3$

Gas diffusion layer porosity*: 0.7*

Gas diffusion layer permeability: $1.12\times10^{-10}\ cm^2$

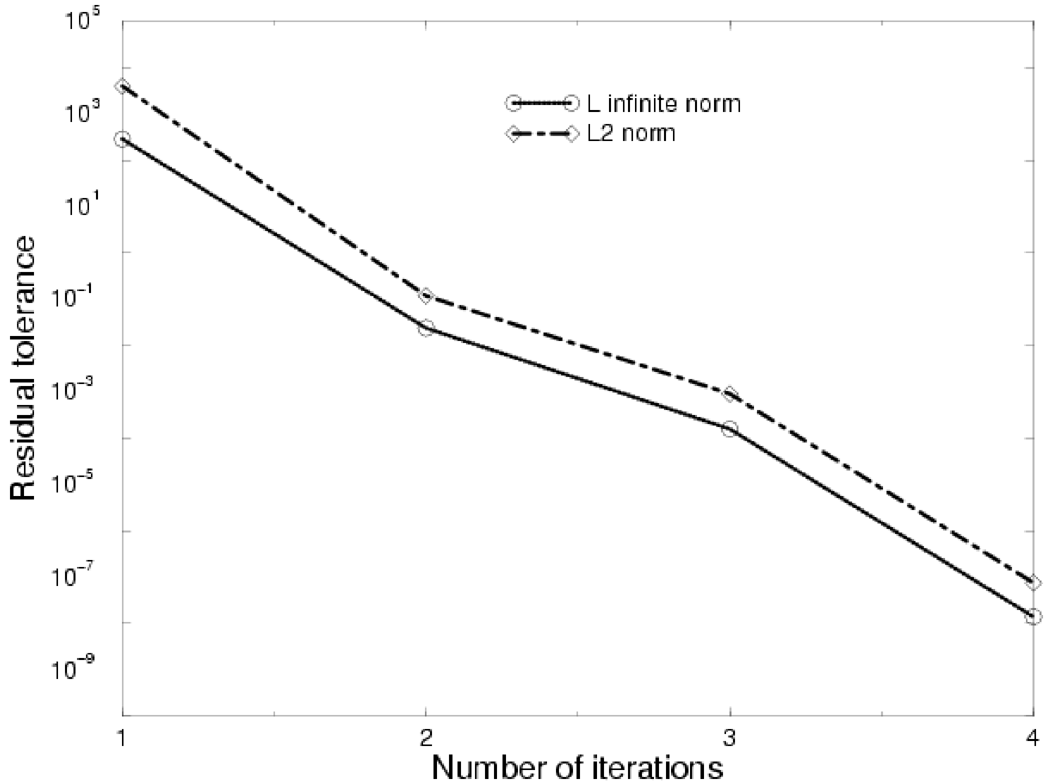
H_2 diffusivity in anode gas channel: $1.1\ cm^2/s$

H_2O diffusivity in anode gas channel: $1.1\ cm^2/s$

O_2 diffusivity in cathode channel: $0.0324\ cm^2/s$

H_2O diffusivity in cathode channel: $0.074\ cm^2/s$

Sample convergence history:
Error norms vs. number of iterations



- **Both error residual norms show quadratic convergence.**
- **It took around 10 minutes of CPU time on a 3.6 GHz hp workstation xw8200 to converge in 4 iterations with 127,590 unknowns.**

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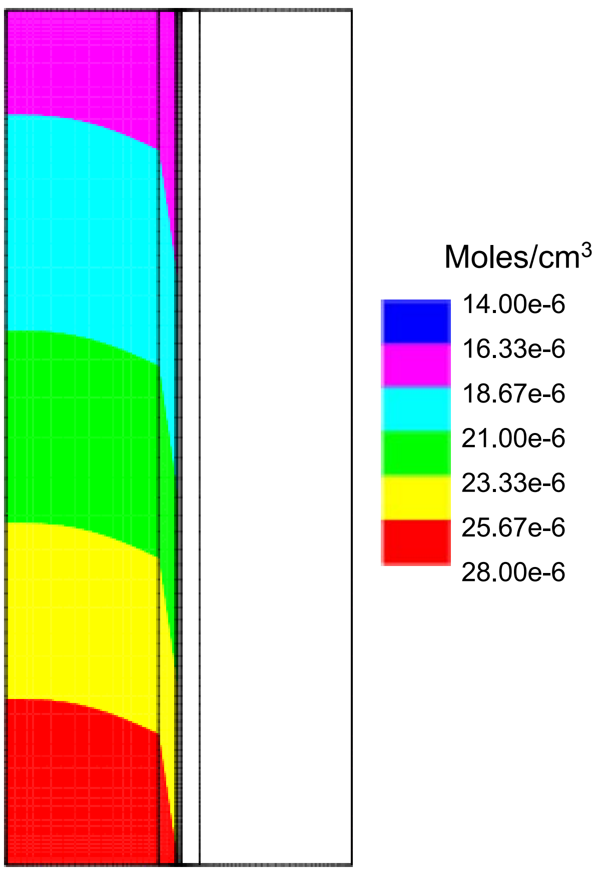
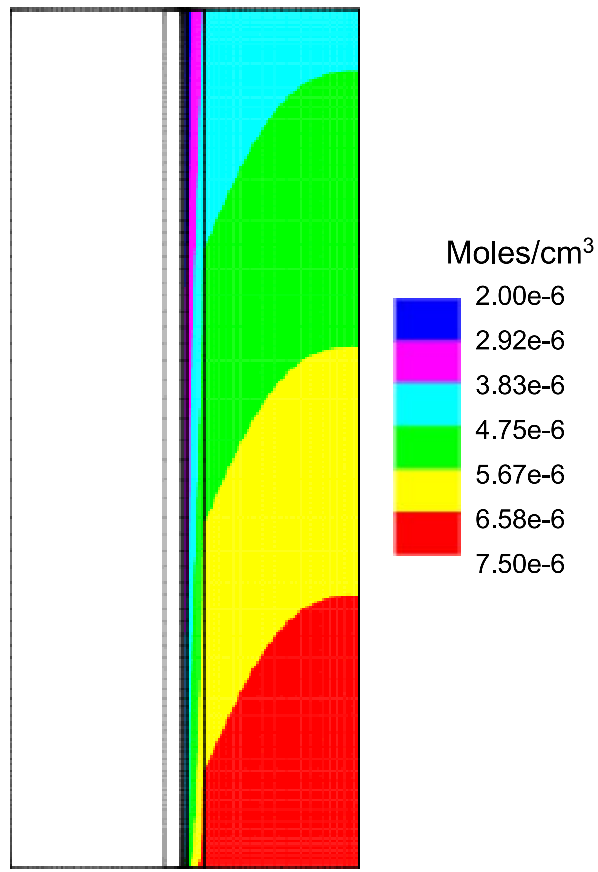
Sample predictions computed from 2-D FEM model: contours of H_2, O_2, and H_2O concentrations

(cell thickness is magnified by a factor of 5 to improve visual effect)

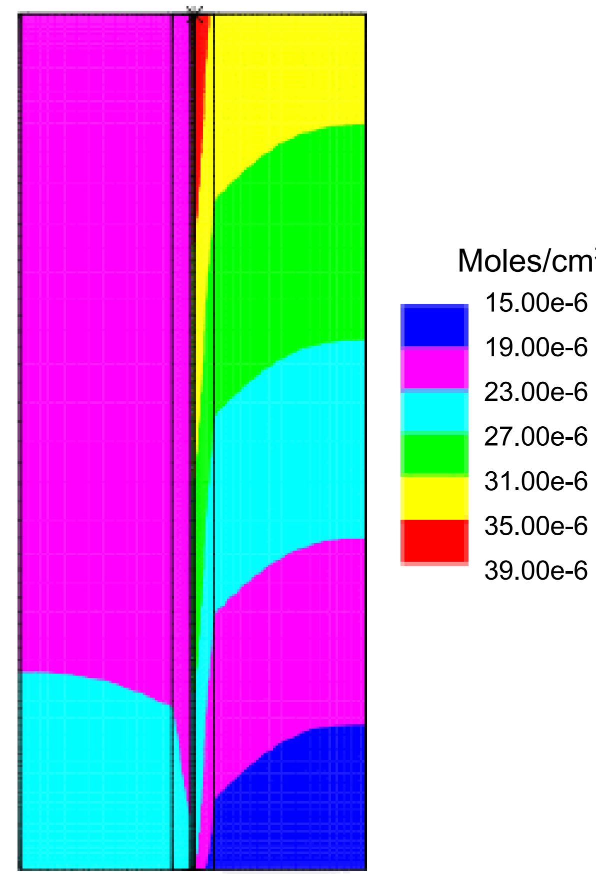
H_2 concentration



O_2 concentration



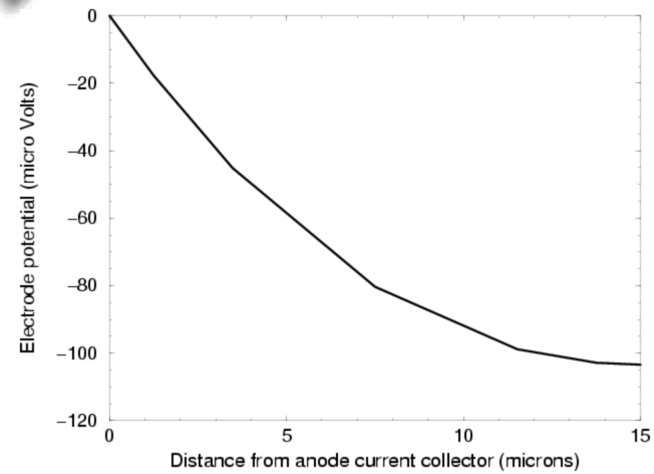
H_2O concentration



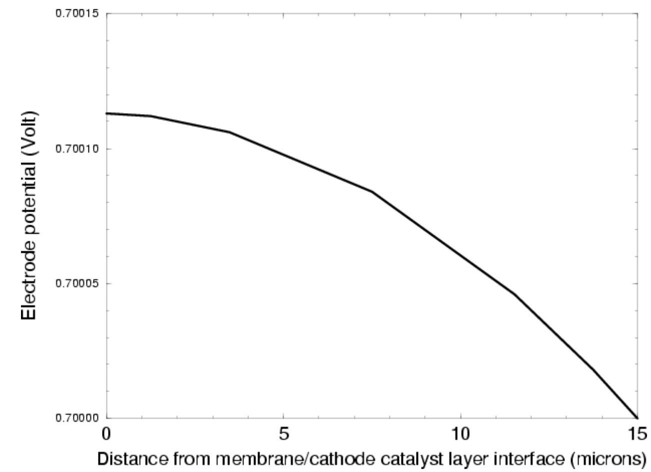
- **H_2 molar concentration decreases along anode channel due to HOR, which consumes H_2 .**
- **O_2 molar concentration decreases along cathode channel due to ORR, which consumes O_2 .**
- **H_2O concentration drops along anode channel due to electro-osmotic drag of H_2O from anode to cathode.**
- **H_2O concentration rises along cathode channel due to electro-osmotic drag & ORR, which generates H2O .**

Sample computed model predictions: electrode and electrolyte potentials
(at mid-channel location, cell voltage = 0.7 V)

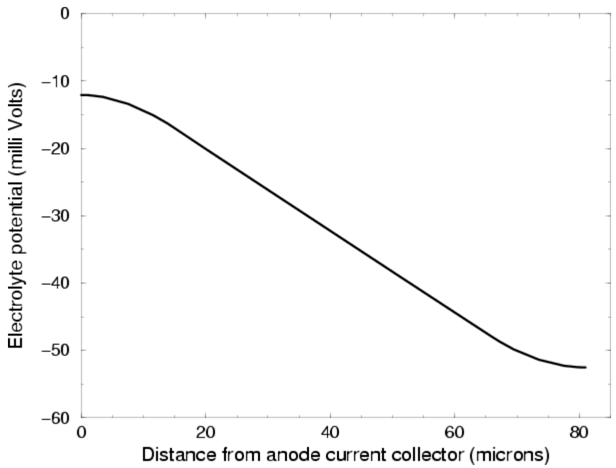
Electrode potential across anode catalyst layer



Electrode potential across cathode catalyst layer



Electrolyte potential across MEA



- **Slopes of electrode potential at ACL/membrane and membrane/CCL interfaces vanish, as expected.**
- **Drops in electrode potential across the anode and cathode are on the order of 100 micro-volts, as expected.**
- **Slopes of electrolyte potential at both the anode and cathode current collectors vanish, as expected.**
- **Drop in electrolyte potential across MEA is on the order of tens of milli-volts, as expected.**

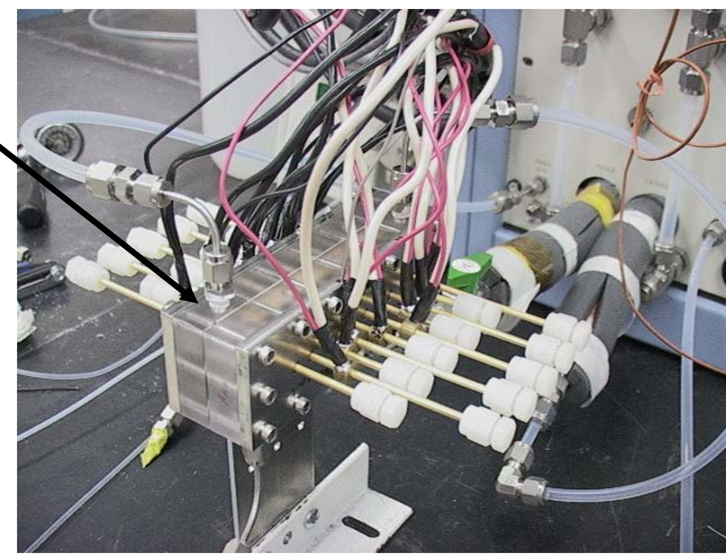
Current distribution measurements via segmented cell diagnostics

Arbin multichannel poteniostat with computer data acquisition

segmented cell

Fuel cell test stand – controls cell temperature, gas flow rates and humidity, and cell pressure

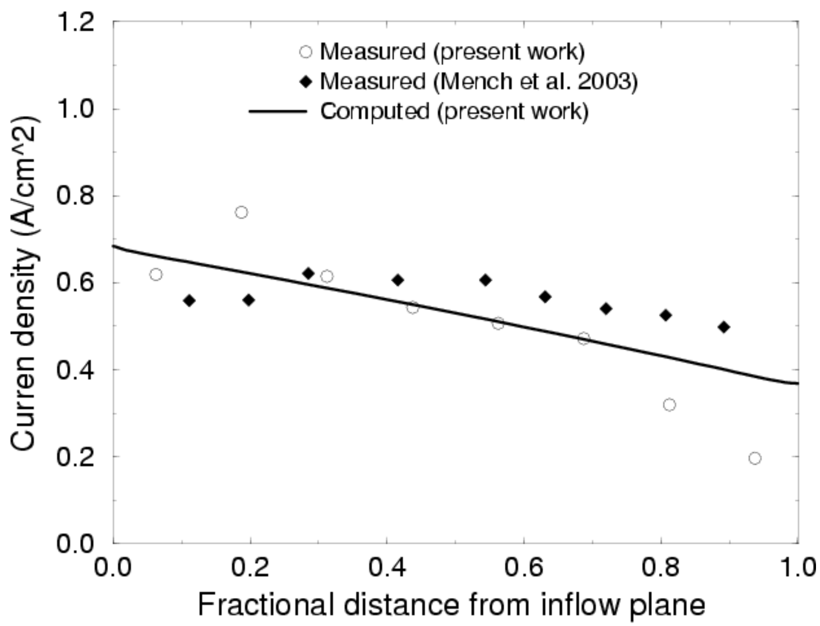
Segmented cell connected to an Arbin multichannel potentiostat for current distribution measurements and fuel cell test stand for gas inlet humidity and cell temperature control. Gas sample ports capped.



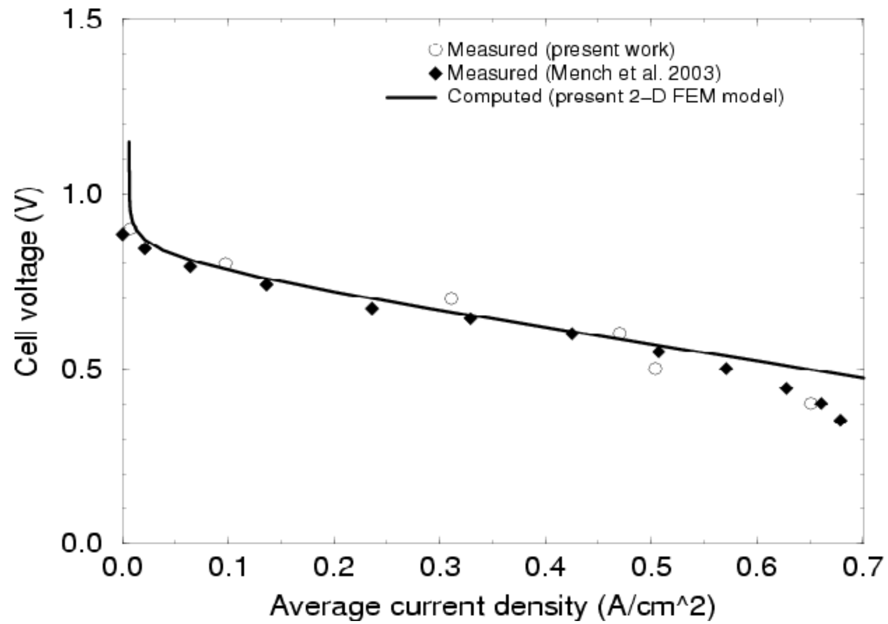
Model validation: computed & measured current distributions and overall polarization curves

Comparison between Computed and Measured Current Distributions & Polarization Curves

Computed and measured current distribution along flow channel direction



Computed and measured overall polarization curves



- **Comparisons between computed and measured current distributions and polarization curves show reasonably good agreements.**
- **Discrepancies do exist, particularly near the entrance and exit of the cathode inlet and outlet.**
- **Model improvement and more experimental data are needed.**

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Reference: Chen et al., Sandia Technical Report, SAND2006-6964.

Summary

- An overview of computational modeling and simulation activities at Sandia's Engineering Sciences Center was given.
- My presentation has focused on SIERRA and demonstrating its applications. SIERRA is an object-oriented framework that enables diverse computational mechanics (versatile single-physics or strongly-coupled multi-physics) applications.
- My presentation also discussed the V&V (Verification & Validation) efforts being carried out at Sandia's Engineering Sciences Center.
- Lastly, our specific effort on modeling the performance of PEM (polymer electrolyte membrane) fuel cells using the finite-element method and a fully-coupled implicit solution scheme via Newton's method was reported.