SAND2006-3074P

ASC Engineering Codes

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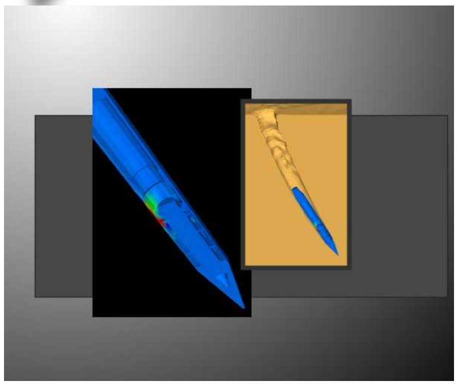
Presented to Northwestern University

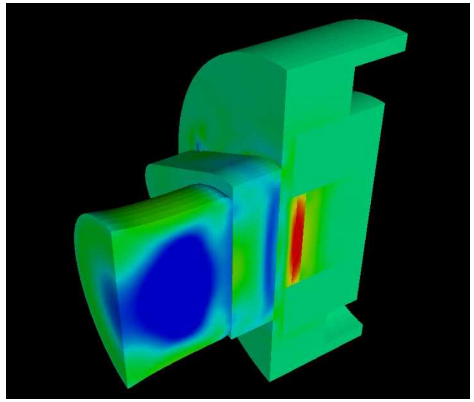
May 2006

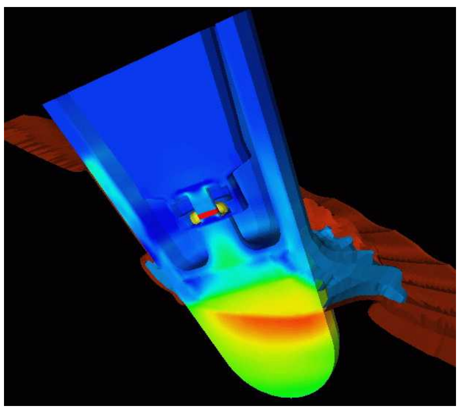
Sandia National Laboratories

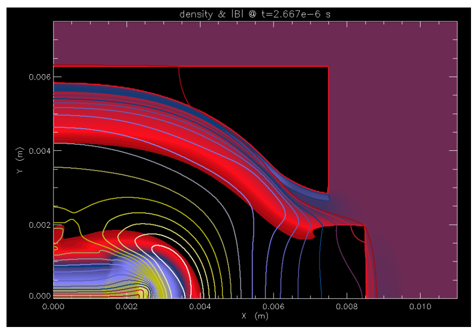
ALEGRA

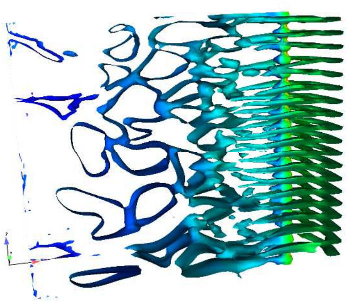
Computational Shock and Multiphysics (1431) *HEDP Theory and ICF Target Design (1674)*

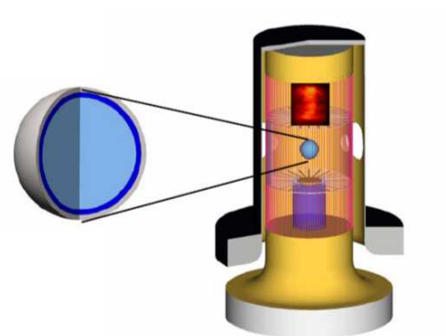












Overview

- The ALEGRA suite of applications model shock and high energy environments for solids, fluids and plasmas using a multi-material arbitrary Lagrangian-Eulerian (ALE) multi-physics methodology.
- The ALEGRA applications run on large parallel message passing architectures in 2D and 3D geometries.

ALEGRA

- Earth Penetration
- Hard Deeply Buried Targets
- Sympathetic Detonation

ALEGRA-EMMA

- Neutron Generator Power Supply
- Contact Fuse
- Fire Set

ALEGRA-HEDP

- Magnetohydrodynamics

ALEGRA-HEDP

- Z-pinch
- Power Flow
- ICE/Magnetic Flyers
- ICF

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SIERRA Mechanics

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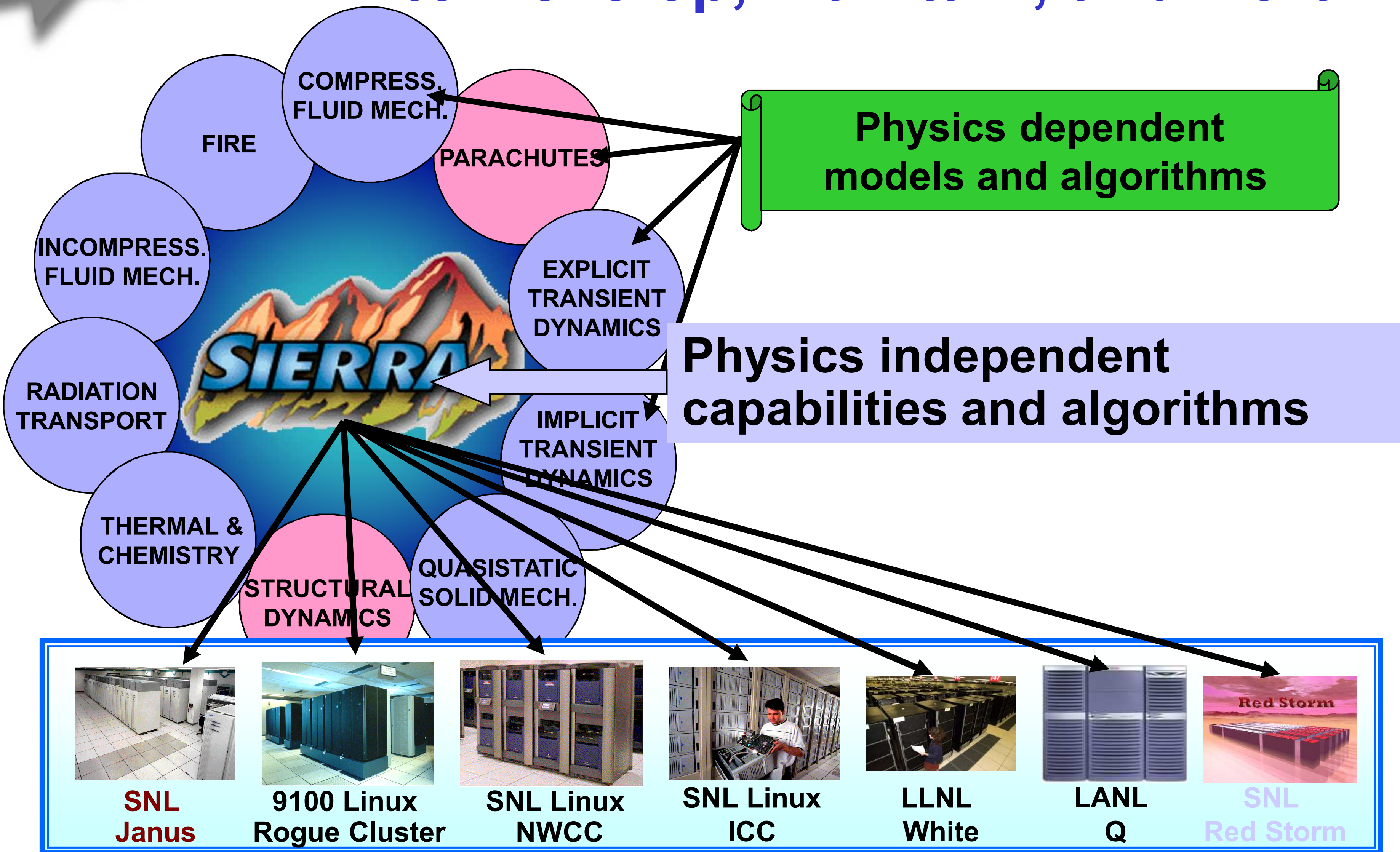
SIERRA Strategy: Minimize Cost to Develop, Maintain, and Port



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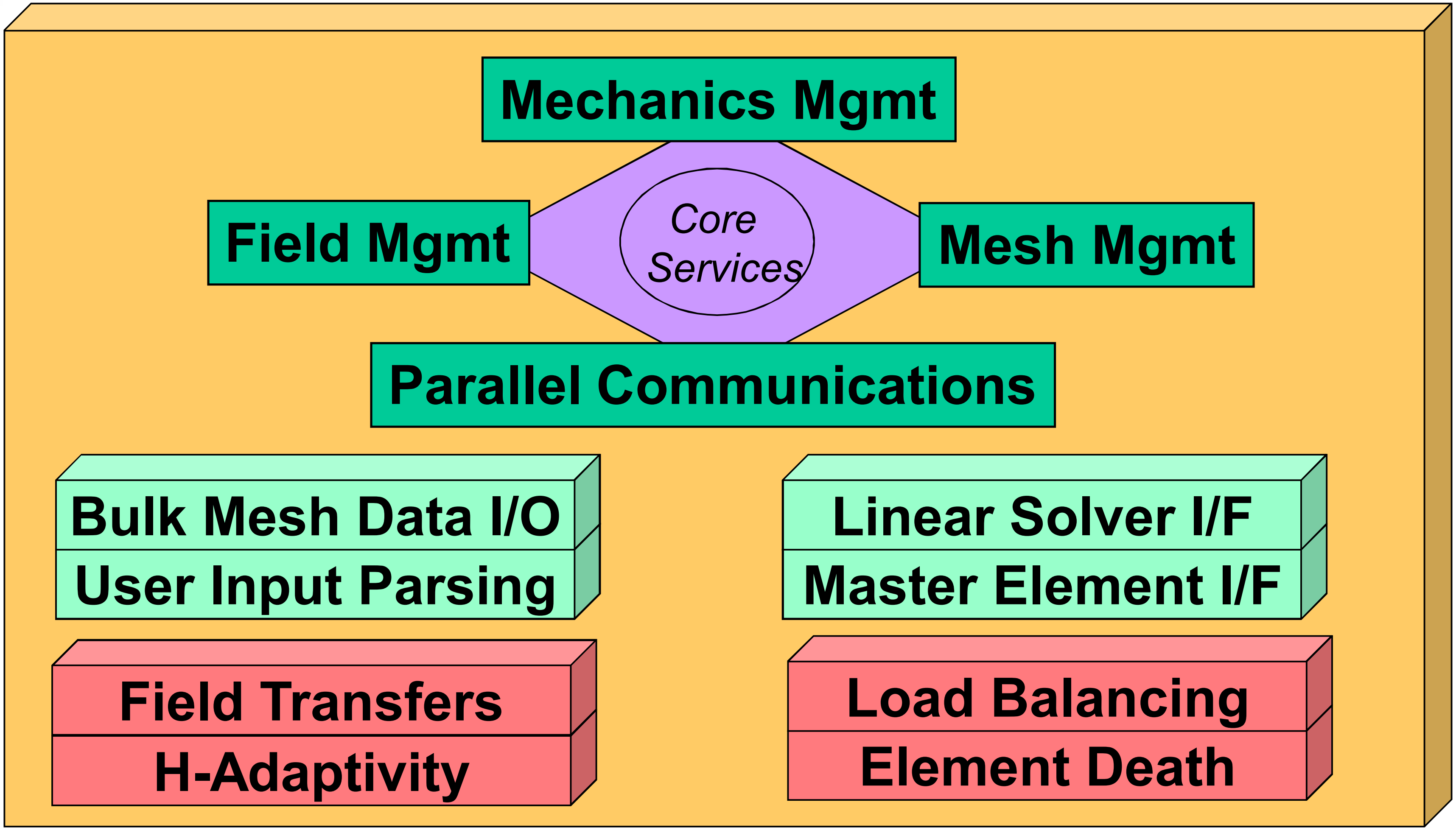
What Does SIERRA Provide?



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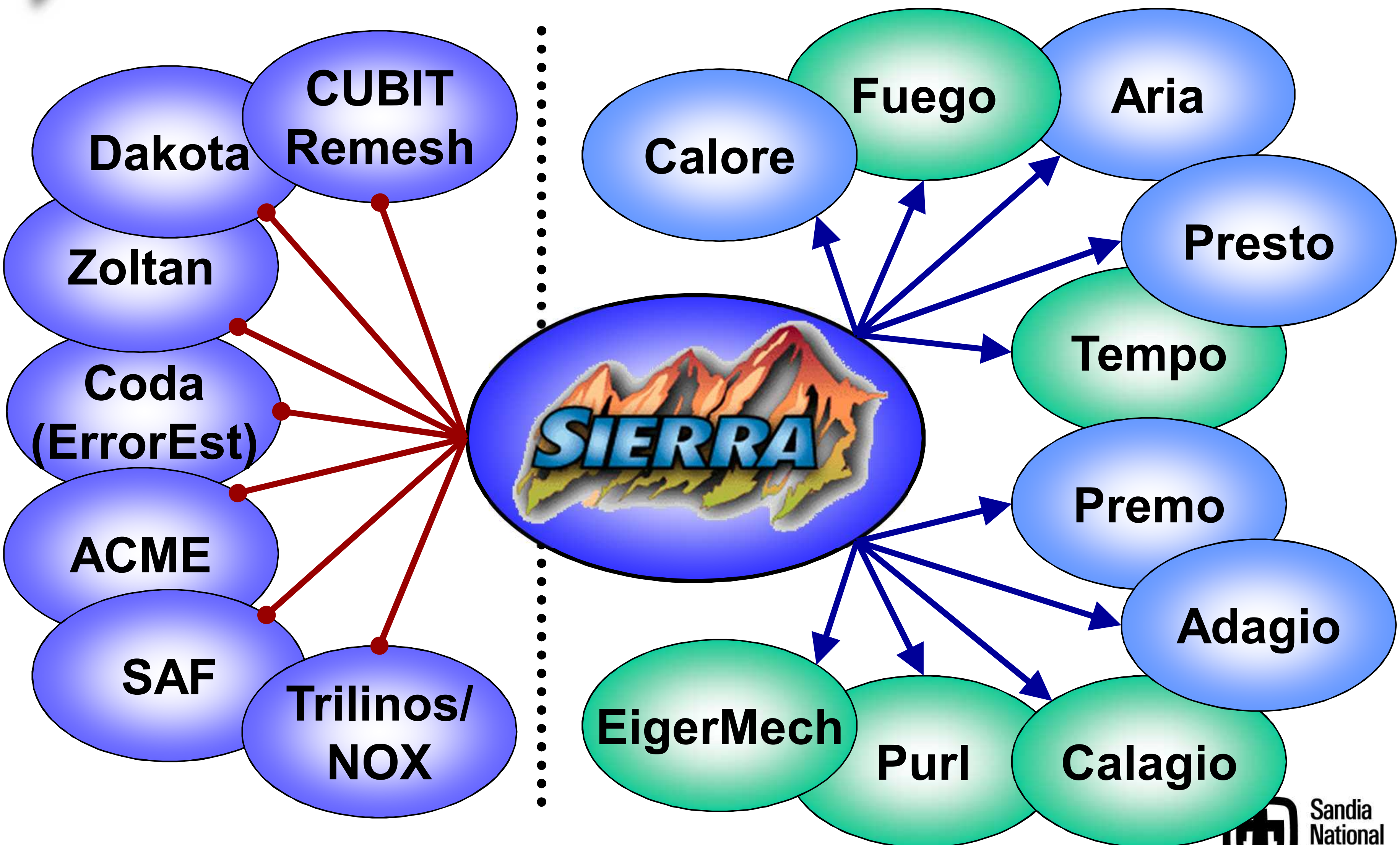
SIERRA Strategy: Integrate {Algorithms} → {Applications}



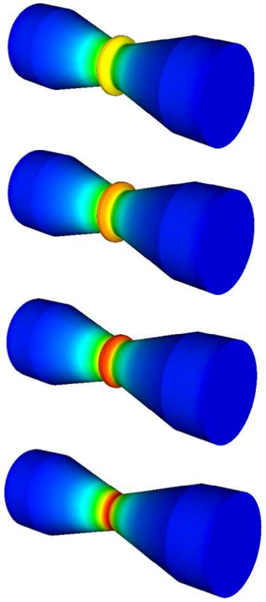
Calore – Thermal Analysis Code

Phenomena:

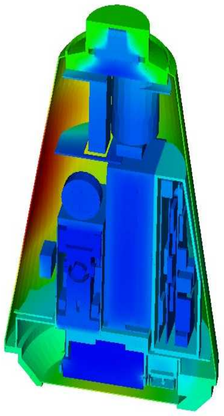
- *Non-linear diffusion, many boundary conditions*
- *Enclosure radiation*
  - *hemi-cube view factor algorithm*
  - *dynamic enclosures*
  - *spatial and temporal emissivity variation*
  - *view factor load balancing*
- *Chemistry (generalized reactions for HE & foam decomposition)*

Algorithms:

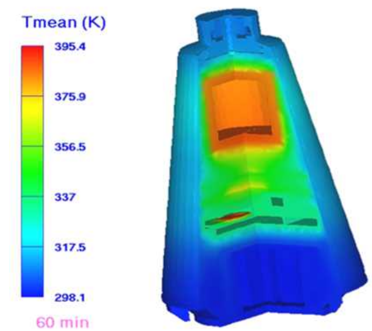
- *h-adaptivity - ZZ error estimation and DLB*
- *Tied contact (MPC) for hex & tet elements (with and without contact resistance)*
- *Element birth/death with inherited boundary conditions*
- *User-subroutine interface for user-specified material properties, boundary conditions, and volumetric heat generation*



e-Calore to Adagio Resistance Weld Sequence



Abnormal Environment Simulation - AF&F



Normal Environment Simulation - Thermal Battery

Couplings:
e-Calore, Adagio, Salinas, and Fuego

Fuego: Fire Modeling – Low Mach No. Variable Density Fluid Dynamics

Numerical Methods:

- *Unstructured mesh, hex/tet/wedge elements*
- *Fuego; turbulent combustion, simple conduction*
    - *Control Volume Finite Element Method*
    - *Approximate projection method with central and upwind (MUSCL) convection*
- *Syrinx; thermal participating media radiation*
    - *Finite Element Method*
    - *Discrete Ordinate; S2-S10 (6-120 DOF)*

Fire Math Models

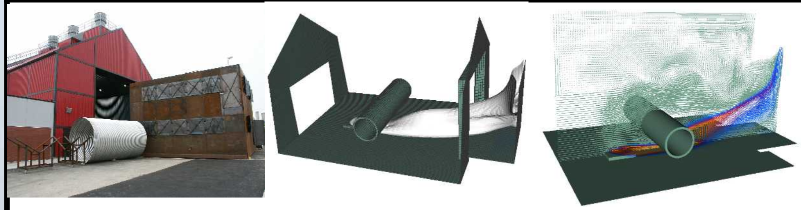
- *Turbulence model*
    - *k-e with Wall Functions, V2f (Durbin)*
    - *k-L; TFNS*
- *Eddy Dissipation Combustion model*
    - *Fuel, O2, CO, CO2, H2, N2, H2O (N-1 PDEs)*
- *Magnussen soot model*
    - *Soot and Nuclei*

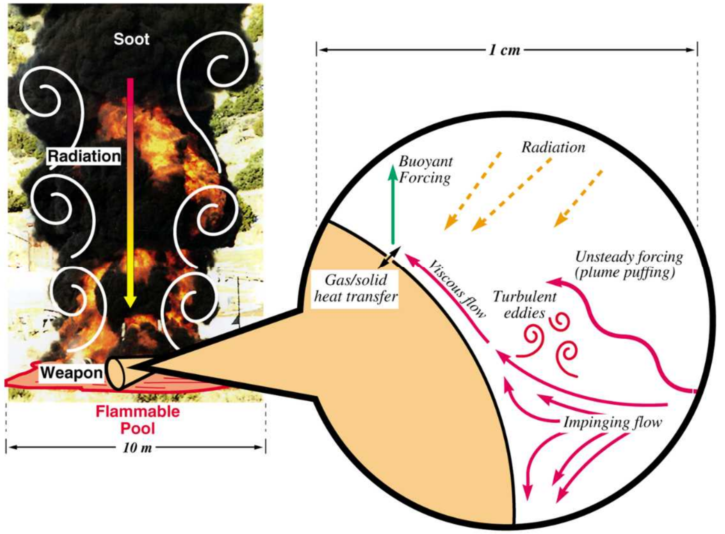
Couplings:

Calore and Adagio

Goal:

- *Model all major modes of heat transfer in hydrocarbon fuel fires that can arise in accident scenarios*





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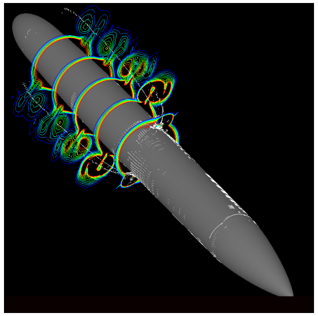
Premo: Compressible Fluids, Aerodynamics, Aerothermodynamics

Capabilities :

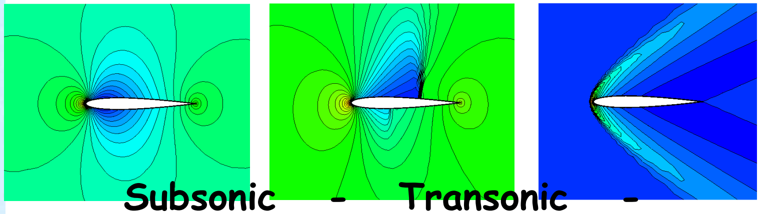
- *Compressible internal/external flow fields*
    - *Subsonic through Hypersonic Flows*
    - *Steady state and transient*
- *Laminar and Turbulent flows*
- *Non-equilibrium reacting gas chemistry*
- *Aeroheating-Ablation boundary conditions*
- *Rotating/Spinning Vehicles - Trajectory analysis – Arbitrary Body Motion*

Solution Strategies:

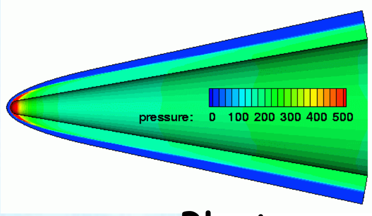
- *Explicit and Implicit*
- *Newton methods (Matrix Free)*
- *Multi-fidelity physics*
- *Adaptivity and Overset meshes*
- *Linear/Nonlinear solvers (NOX)*
- *Time-Integration methods*



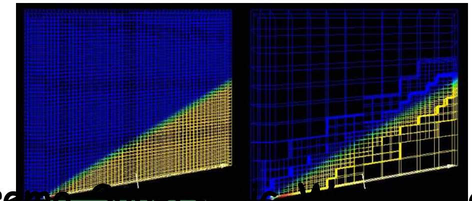
B-61 Spin Motor Vortex-Fin Interaction



Subsonic - Transonic - Supersonic
NACA 0012 airfoil



Mach 14.25 Flow over a Blunt Nose Properties behind normal shock within 5% of analytic solutions

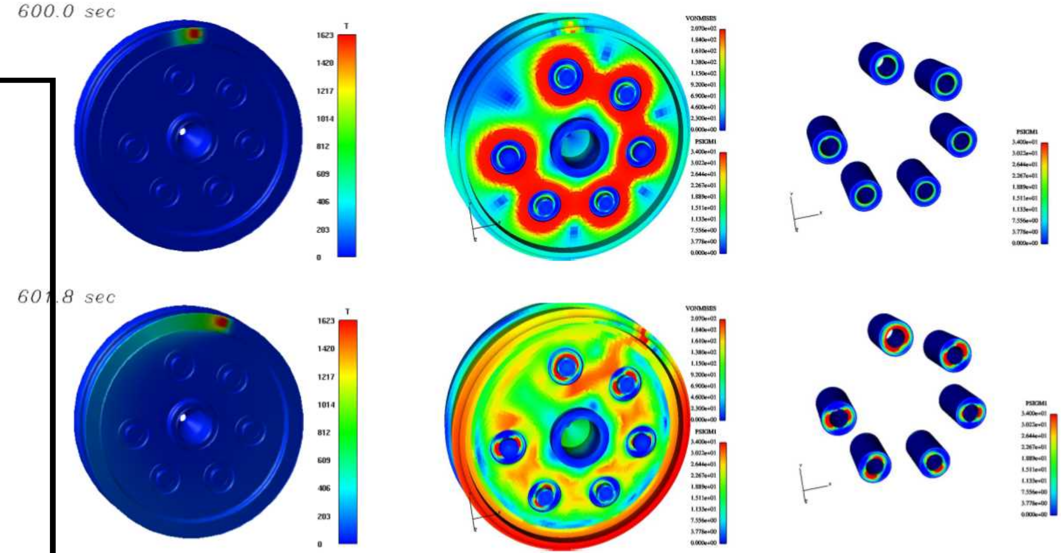


Premo Supersonic Wedge Flow
3 level h-adaptive 2D Mach 2.5 10 deg wedge Density Gradient Error Estimator

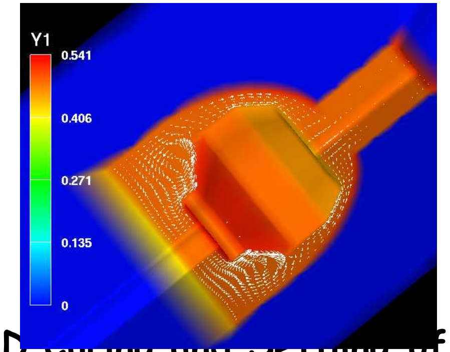
Aria: Coupled Physics Analysis

Coupled Multi-Physics:
- *Fluid Dynamics with Free and Moving Boundaries*
- *Solid Mechanics*
- *Thermal / Energy*
- *Chemical Species*
- *Electrostatics*
- *Non-Newtonian Rheology*

Versatile Algorithms:
- *Transient and Steady State*
- *Newton and Picard Methods*
- *Tight and Loose Coupling*
- *Flexible User Defined Models*
- *2D and 3D Cartesian*
- *Quad/Tri and Hex/Tet Elements*



Laser-Welding Induced Warpage of a Firing Set Bracket (Goma/Jas3D)



3D Curing and Settling of Particle-Laden Epoxy in Neutron Generator Geometry (Goma)

Aluminum Aeroshell Melt & Relocation (Goma)

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BEM – Boundary Element Code

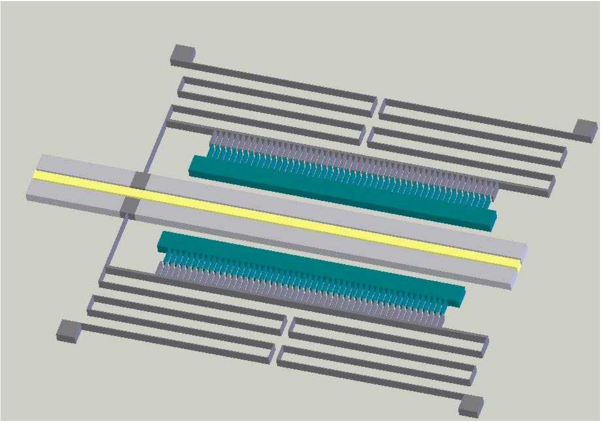
Capabilities :

- *Electrostatics*
- *Stokes Flow*
- *Solid Particle Transport*
- *Acoustics*
- *Conduction Heat Transfer*
- *Potential Flow*

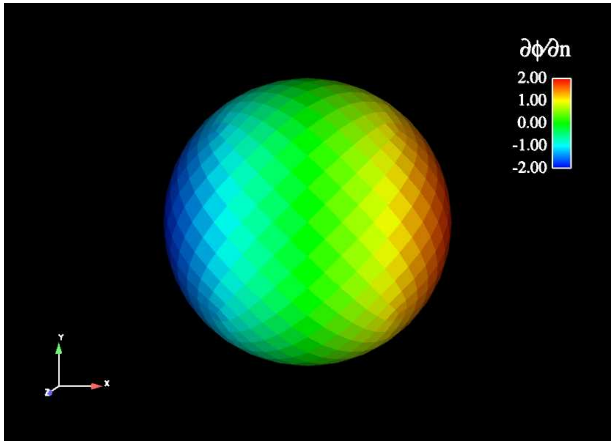
Applications :

- **Coupled electrostatic structural simulation of microsystems:**
  - **acceleration switches**
  - **non-volatile memory**
  - **micro-firesets**
- **Manufacturing Processes**
  - **filled epoxy potting**

Couplings:
Adagio



MEMs electrostatic switch



Electrically conducting sphere
in a uniform e-Field

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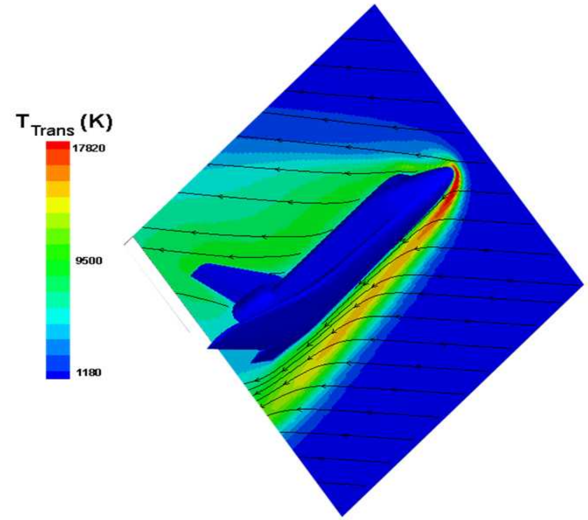
Faust – Particle Simulation Code

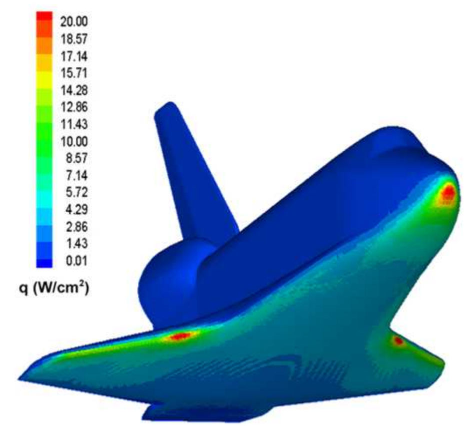
Capabilities :

- ***3D Transient/Steady state non-equilibrium, rarefied flow. (implemented)***
- *Chemistry: Atmospheric chemistry, Silicon species chemistry.*
- *Self-induced electrostatic fields.*
- *Surface chemistry modeling, Feature scale modeling.*
- *Thermal and Infra-Red Radiation.*

Applications

- ***Reentry Vehicles: thermodynamic and chemical non-equilibrium flows.***
- ***Signature prediction: non-equilibrium radiation from plumes and shock layers.***
- ***Microelectronics manufacturing: plasma processing, etching.***
- ***MEMS: micro-scale flows.***
- ***Particle Transport: Brownian motion, thermophoretic transport for EUVL contamination,_soot motion, and species detection applications.***
- ***Physical/Chemical Vapor Deposition (CVD, PVD):surface_evolution.***





Shuttle Re-entry simulations

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Presto: Transient Dynamics
(Large Deformation, Contact & Failure)

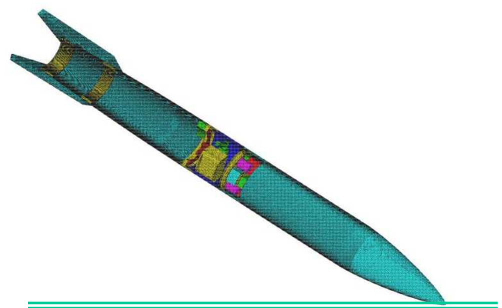
Mechanics:

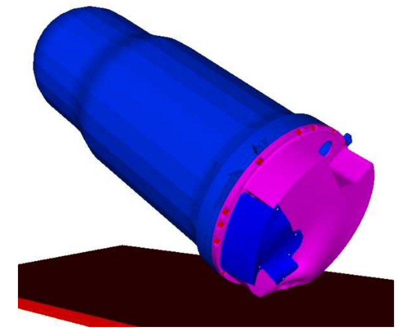
- *Large deformations*
- *General contact w/friction laws*
- *Elasticity, plasticity laws*
- *Wide range of materials (metals, foams, composites ceramics, geologic)*
- *Energy dependent material models*
- *Cohesive and adhesive interfaces*
- *Smooth particle hydrodynamics*
- *Cavity Expansion*
- *Energy Deposition*
- *Spot weld failure models*

Algorithms:

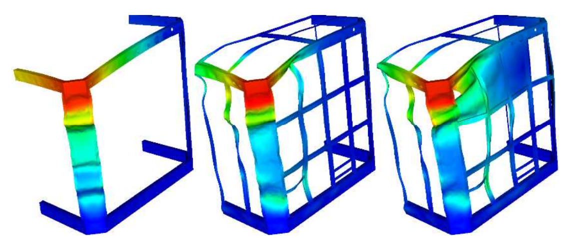
- *Explicit central difference time integrator*
- *Iterative exact contact enforcement*

Normal Environments:
B61 Laydown Simulation





Abnormal Environments:
W80 Accidental Drop



Transportation Safety:
Tractor/Trailer Crash

Adagio/Andante: Nonlinear Implicit Solid Mechanics Simulation

Mechanics:

- *Large deformations*
- *Contact w/coulomb friction*
- *Elasticity, plasticity laws*
- *Wide range of materials (metals, foams, composites)*

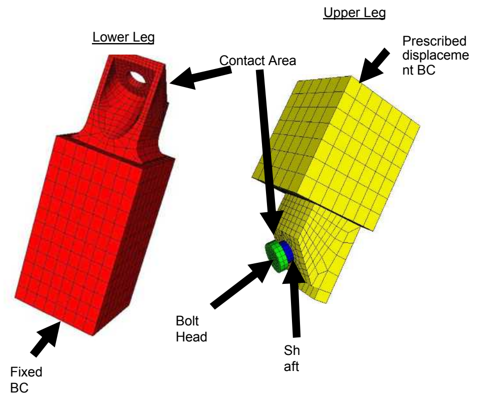
Algorithms:

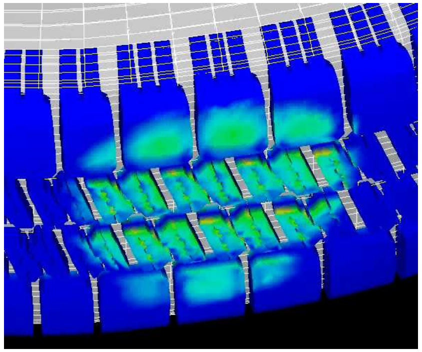
- *Nonlinear preconditioned conjugate gradient solver with control levels*
- *Implicit time integrator w/damping*
- *Nested parallel linear solvers*

Coupling:

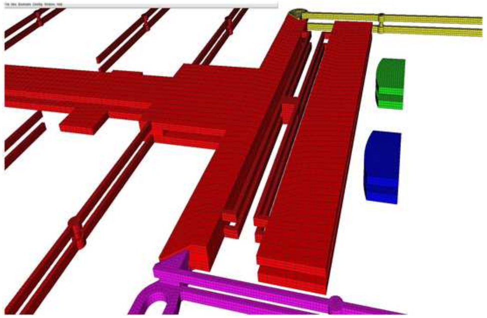
- *Tempo (Preload to Presto)*
- *Calagio (Adagio/Calore)*
- *E-Calagio (ElectroThermalMechanical)*
- *Adagio/Aria: Melt relocation*

Normal Environments: Joint Microslip Simulation





Goodyear CRADA: Tire Mechanics



MEMS Simulation: Nonvolitile Memory Device

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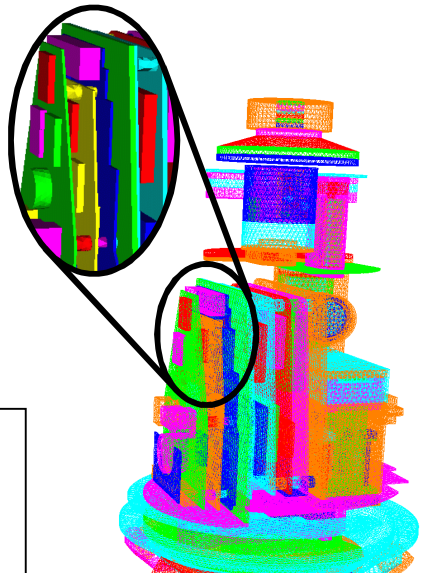
Salinas: Structural Dynamics
(System-level Shock and Vibration Response)

Mechanics:
- *Small Deformation*
- *Linear Elasticity*
- *Linear Viscoelasticity*
- *Frictional Microslip*
- *Acoustical fluid*

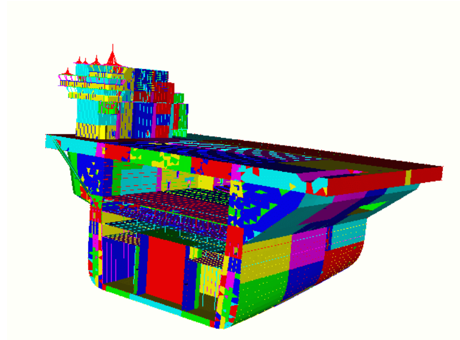
Solution Procedures:
- *Linear Statics*
- *Vibration Eigen-Analysis*
- *Implicit Dynamics*
- *Frequency-Domain Methods*
- *Nonlinear Statics/Dynamics*
- *Structural Acoustics*

Numerical Algorithms:
- *Parallel Iterative Solvers (FETI-DP, Prometheus)*
- *Tied Constraints*



Impact on M&S:
4 orders of magnitude increase in model fidelity in 15 years

Accomplishments:
2002 Gordon Bell Award for Innovative Techniques to Produce New Levels of Performance on a Real Application



DoD Applications:
NNS - Carrier Models

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Coupled Application Examples
SIERRA Applications

- Calagio = Calore (thermal) + Adagio (quasistatics)
- Calore/Fuego = Calore + Fuego (Low-Mach Number fluids)
- Tempo = Adagio + Presto (explicit dynamics) + Andante (implicit dynamics) + ...
- Arpeggio = Aria (arbitrary Lagrangian-Eulerian non-Newtonian fluids) + Adagio

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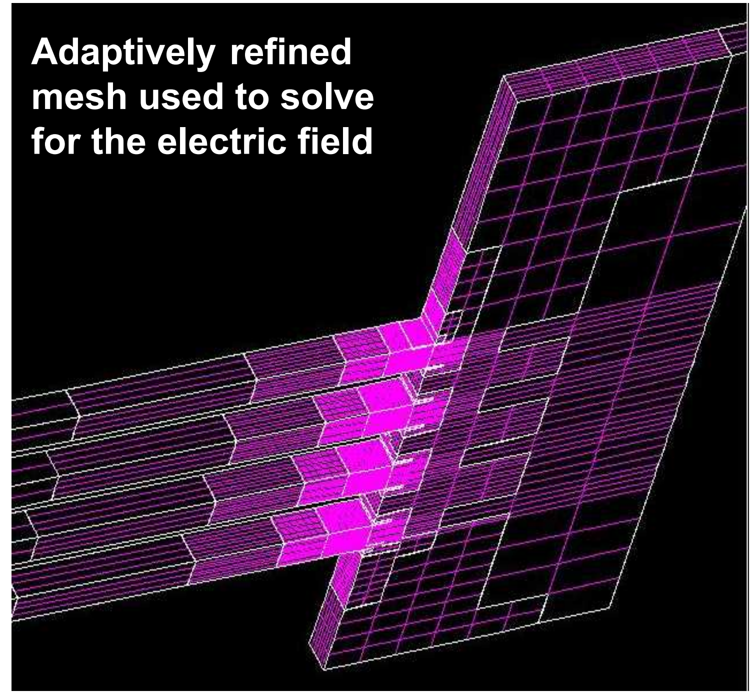
Micro Actuator Simulation with Calagio

Adaptive Mesh Refinement

The adaptive mesh requires approximately 1/6 the CPU time as the manually refined mesh for the same global accuracy.

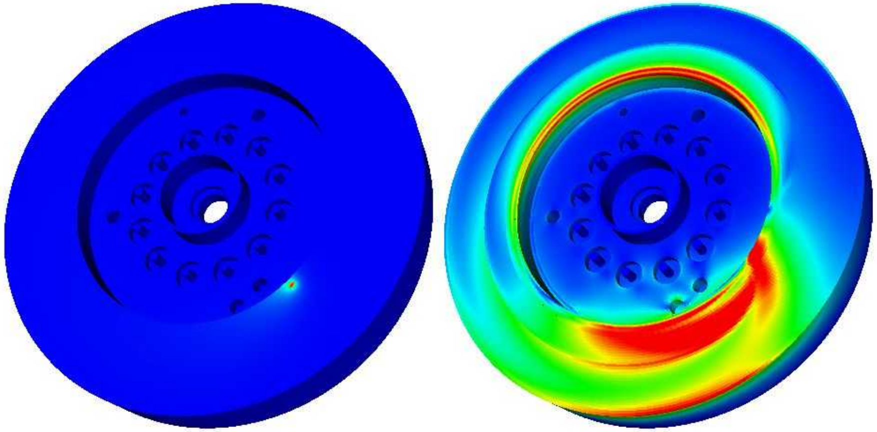


Adaptively refined mesh used to solve for the electric field

	0x Unif	1x Unif	2x Unif	3x Unif	Adapt	Adapt	Adapt
H_1 EST	**14.50 %**	**8.70%**	**5.30%**	**3.10%**	**8.70%**	**5.30%**	**3.10%**
CPU (s)	**0.3**	**4**	**42**	**678**	**1.4**	**7.1**	**115**

Laser Welding with Arpeggio

- Weld induced distortion can destroy critical seals in components
- Currently Aria solves for temperature and Adagio solves for displacement and stress
- Will add phase change (melting) and fluid flow to simulation



Temperature Von Mises Stress

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Coupled Application Examples

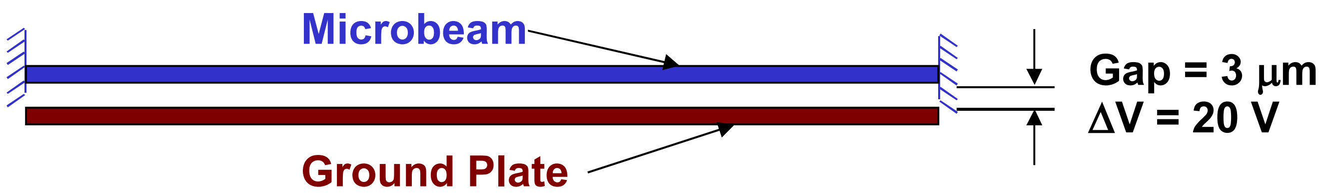
SIERRA and Non-SIERRA Applications

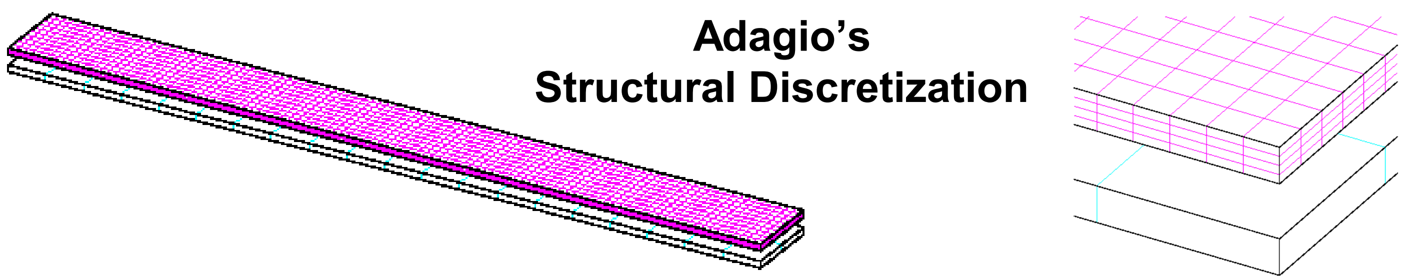
- Eigermech = Adagio + Eiger_S (electrostatics)
- Purl = Presto + Vipar (fluid - 3D vortex)
- Tempo = Adagio + Presto + Andante
  + Salinas (structural dynamics)
- Presto + CTH (planned – not yet named)

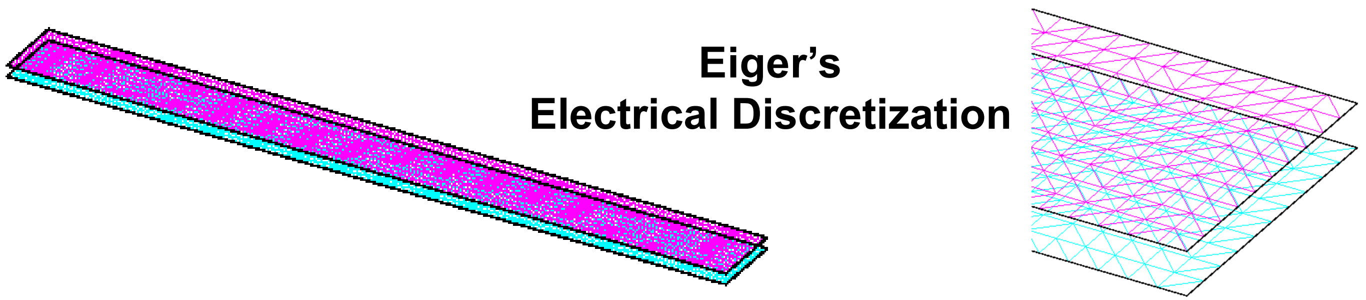
Microbeam Simulation with Eigermech, Electrostatic Loading

Microbeam:

Length = 200 μm
Width = 20 μm
Thickness = 2 μm
E = 160 GPa







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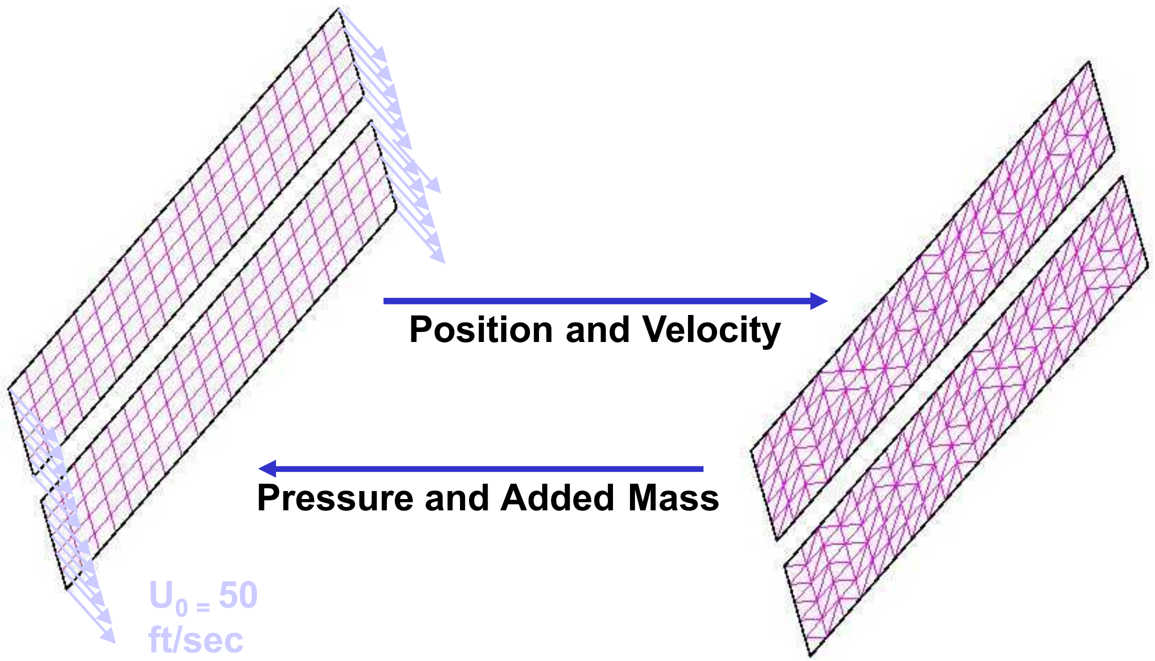
Parachute Simulation with Purl (two ribbons)



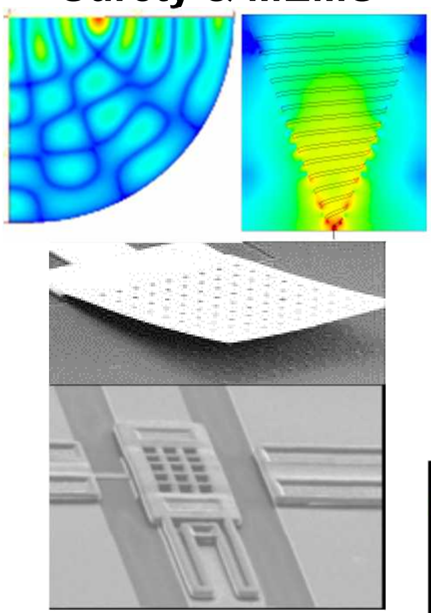
Shell Mesh for Presto Structural Simulation

Boundary Mesh for Vipar Fluid Simulation

Electrical Simulation for STS Environments

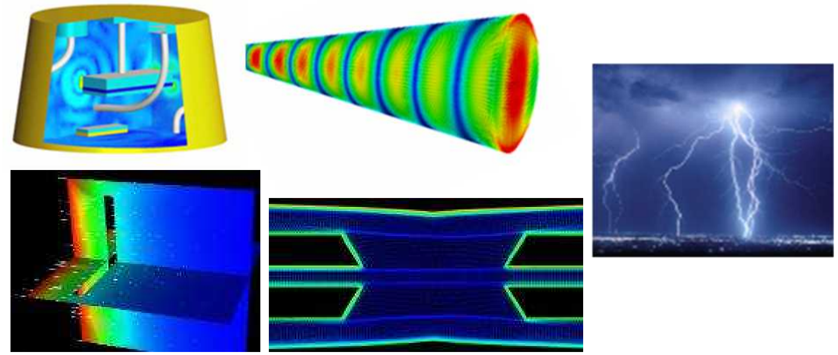
ASC EMPHASIS: Validated, High-Physical Fidelity, 3D Electromagnetics (EM) & Plasmas

Transformational Surety & MEMS



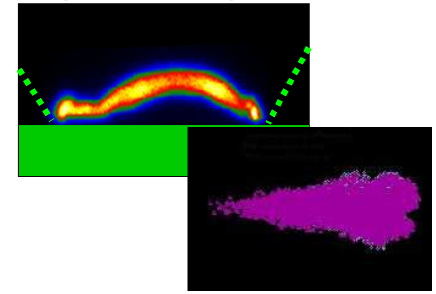
High-Frequency Cavity/Aperture Response, Advanced Antennas, RF-MEMS devices

NW System Response to Normal & Abnormal EM and Hostile (SGEMP) Environments



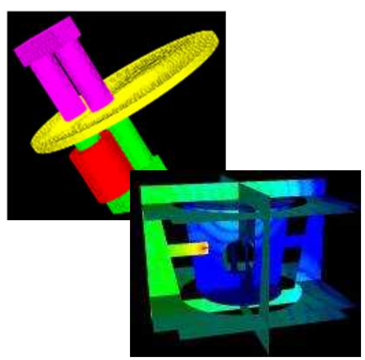
Includes Refurbishment & Dismantlement

High Voltage Science



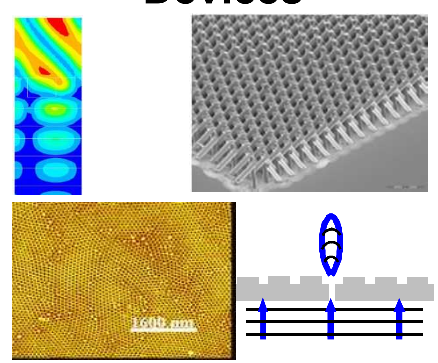
HV Standoff, Arcing, Leakage Currents, Electrostatic Discharge

NW Components



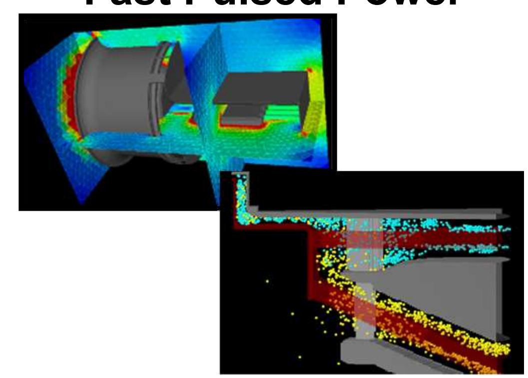
Stronglinks, Radar, Firesets, Neutron Tubes

Advanced Devices



EM/Photonic Band-gap Devices; Plasmon Structures, Micro/Nano

Fast Pulsed Power



Z-pinch apps for NW, Mat'l Dynamics, Fusion Energy

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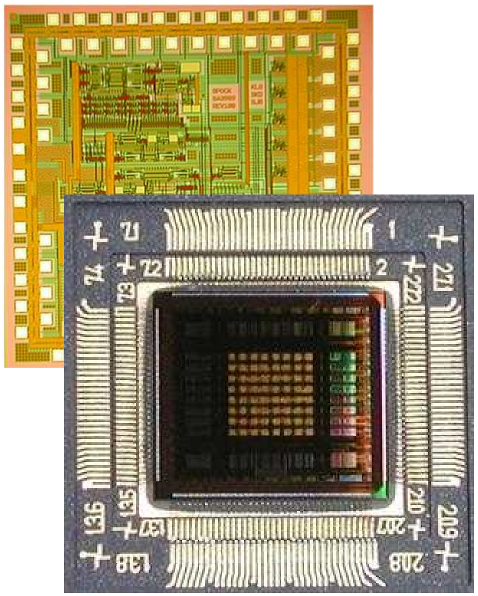
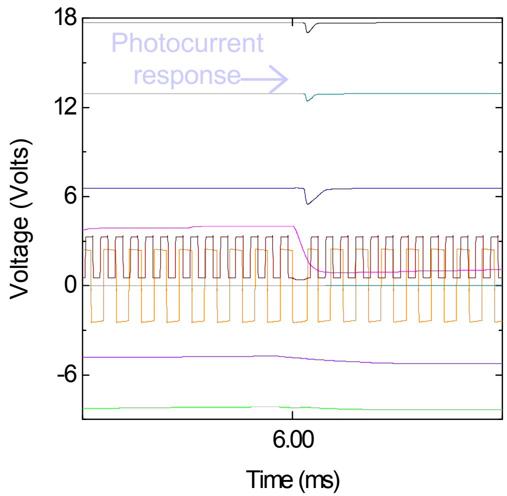
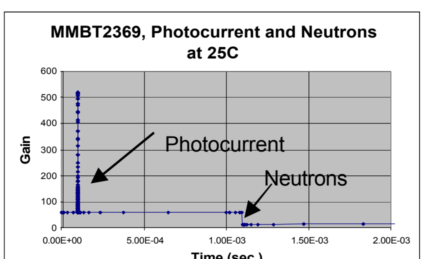
Xyce: Parallel Analog Circuit Simulator

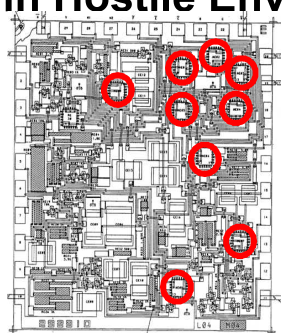




High Density ASICS in Hostile Environment

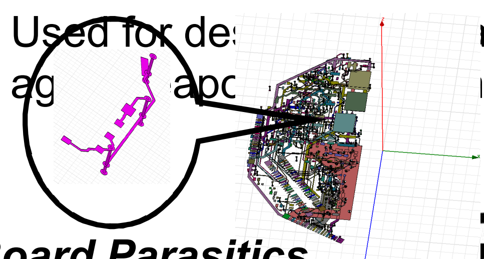


Combined Effects Devices



Subsystem Circuit Analysis

- Distributed memory parallel analog electrical circuit simulator
- Includes large set of models used in SNL weapon electrical system designs
- Specialized Sandia physics based predictive device models
  - radiation, temperature and age aware
  - combined effects (2 and 3 environmental effects)
- Can use environmental data from ITS and Nuget for hostile environment circuit performance calculations
- Used for des… analysis of ag… apc… .



Board Parasitics

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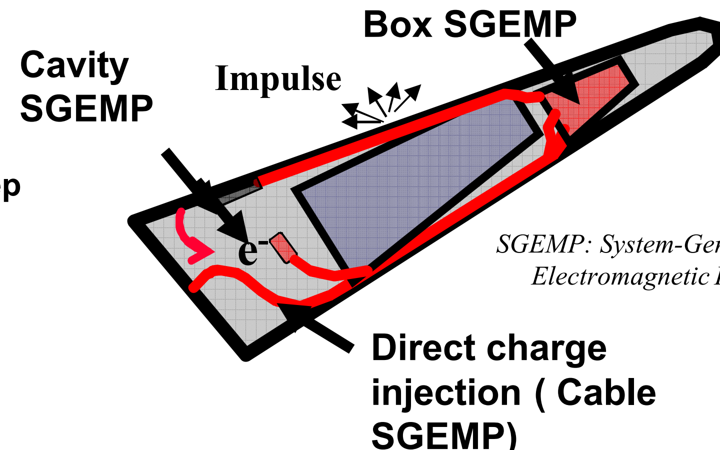
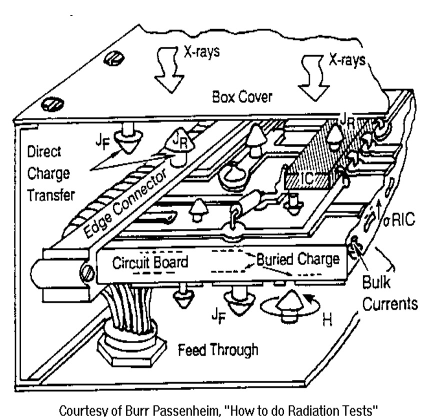
CEPTRE : Deterministic Electron-Photon Radiation Transport

- **Coupled electron and photon transport**
  - **Unstructured finite element mesh**
  - **Multigroup in energy**
  - **2^{nd}-order Boltzmann transport solution**
  - **Hybrid transport solver under development (1^{st}-order sweep for photons coupled to 2^{nd}-order transport solver for electrons**

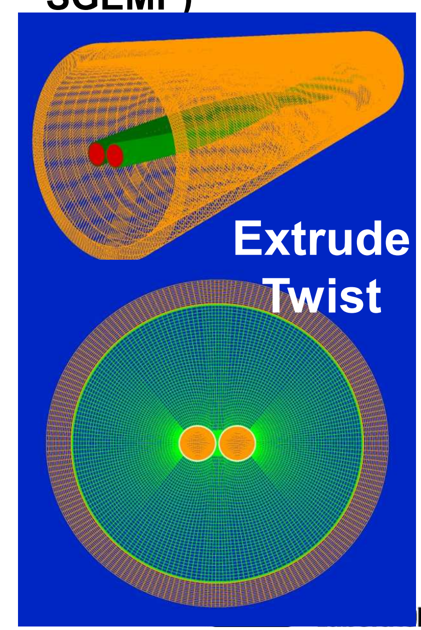
- **Applications (Hostile STS: Electrical response to x-ray radiation and Impulse)**
  - **CABLE SGEMP: Charge deposition output can be used by electromagnetics code (e.g. EMPHASIS) to predict cable electrical response to x-rays**
  - **BOX SGEMP: Photo-emission and charge deposition output can be used by EMPHASIS to predict SGEMP electrical response**
  - **IMPULSE: Radiation transport coupled to hydrodynamics code (e.g. ALEGRA) to predict blow-off and associated impulse loads**



SGEMP: System-Generated Electromagnetic Pulse

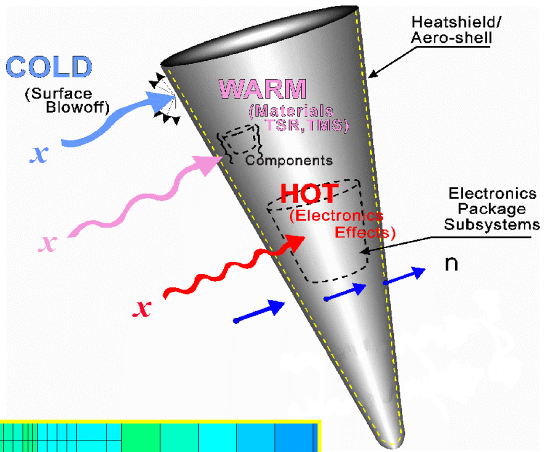


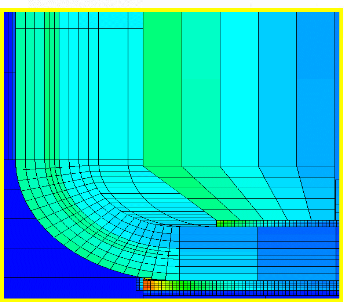
Box SGEMP



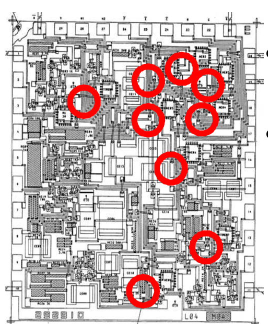
Electrical Cable Cross Section and Mesh

ITS: Monte Carlo Electron-Photon Radiation Transport





3D dose spatial profile to drive mechanical response



Dose-rate on board to drive circuit response

- **Fully coupled particle cascade including positrons from 1 keV to 100 MeV**
- **System-level radiation transport on CAD geometry for STS Hostile (x-rays) and STS Normal (INRAD)**
  - W76-1 AF&F
  - Replacement neutron generators for W76-1 and W78
- **Worst-case exposure angle analysis using inverse (adjoint) transport**
- **Dose output can be used by shock physics code (e.g. PRESTO) to predict thermo-mechanical shock (TMS) and thermo-structural response (TSR) from x-rays.**
- **Dose-rate output can guide design, or be used with Xyce circuit code to predict transient electrical response to x-rays.**
- **Photoemission output can be used by electromagnetics code (EMPHASIS) for cavity SGEMP response to x-rays.**
- **Modeling of electron beam transport and bremsstrahlung production can be used for design of AGEX experiments.**

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