SAND2006-7424P

# Radiation Science and Nuclear Engineering Research at Sandia National Laboratories (SNL)

**Presentation at:**

**University of New Mexico**

**November 28, 2006**

**Leonard Lorence, Manager**

**Radiation Transport Department 1341**

**Sandia National Laboratories**

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for the United States Department of **Energy's National Nuclear Security Administration** under contract DE-AC04-94AL85000.



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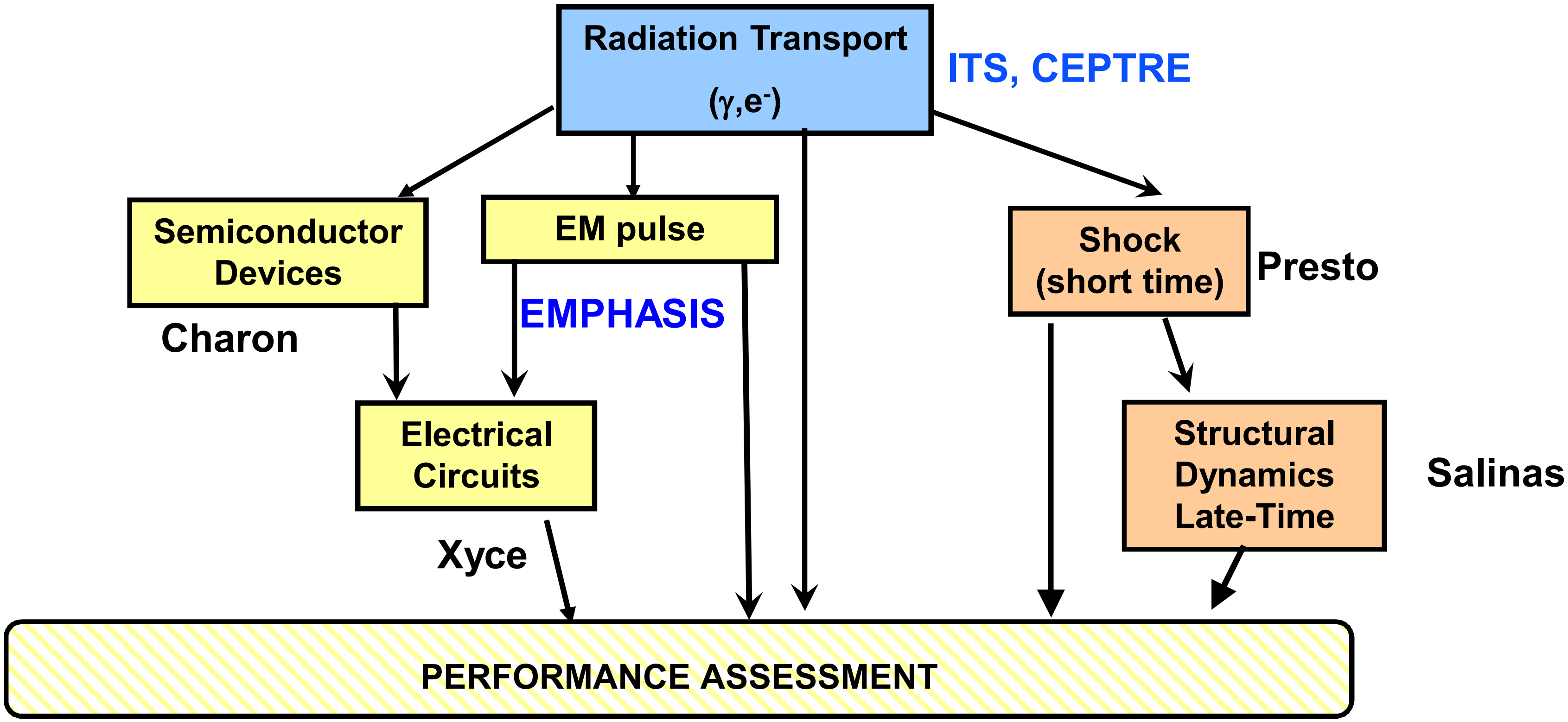
# *Outline*

- **Radiation transport code development**
  - DOE's Advanced Simulation & Computing (ASC) program
  - Coupled electron-photon transport (Monte Carlo, Deterministic)
  - Verification and Validation
  - Coupling to other ASC codes

- **Nuclear Energy Activities**
  - Gen-IV reactors
  - Hydrogen Production
  - Space reactors

- **Inertial Fusion Energy (IFE) Research**

# *ASC Program : Codes & Effects*



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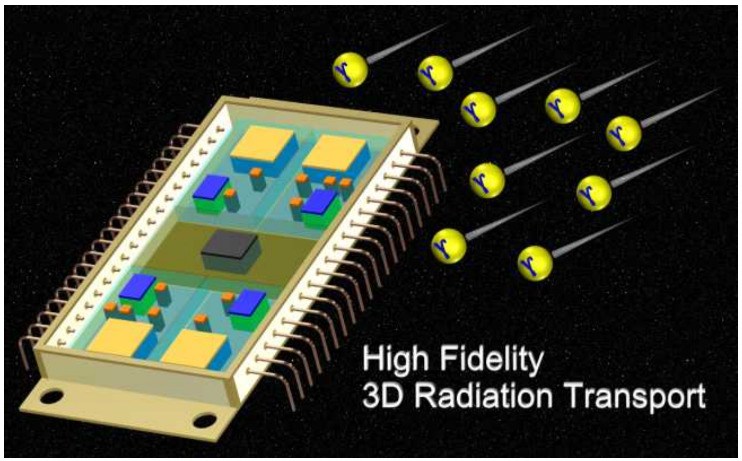
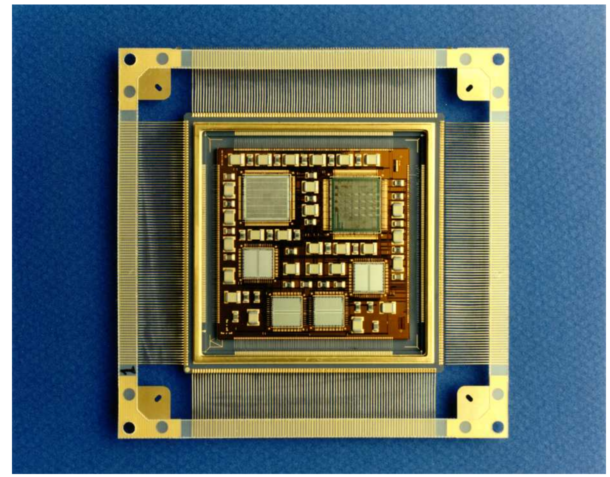
# *Radiation transport is fundamental to understanding the effects produced in nuclear & space radiation environments*

***(pulsed)***



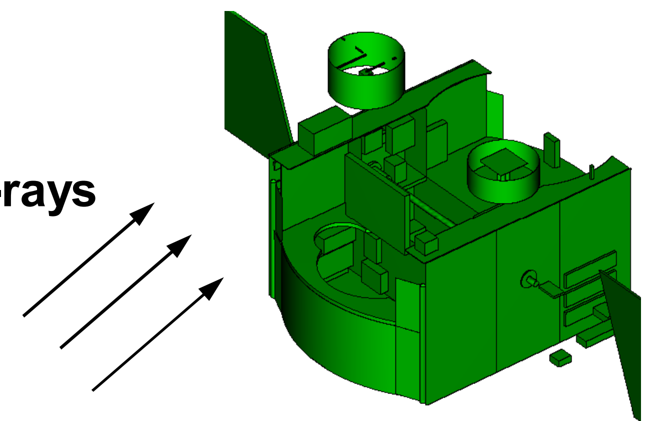

***The transport of coupled photon, electron, and positron radiation from 1.0 keV to 20.0 MeV***



**ICs**

**Goal:** Predict the effect of radiation on electrical components (e.g. ICs, cables)

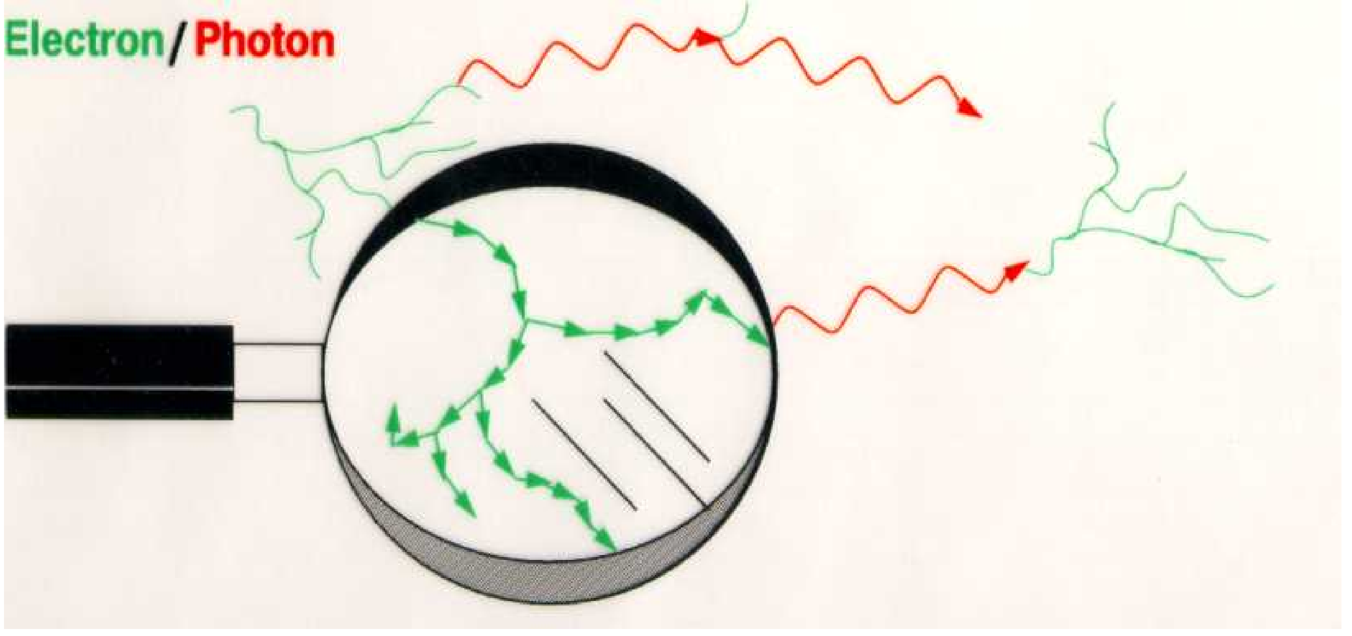
**X-rays**



**Satellite**

**Goal:** Predict the effect of radiation on materials and structures (mechanical effects)

# *Coupled photon-electron particle cascade*




*Electrons and photons have radically different transport scales!*

# Simulation Challenge: Radically different cross sections for electrons and photons

| Particle Energy (keV) | Photon MFP (micron) | | Electron MFP (micron) | |
|---|---|---|---|---|
| | silicon | gold | silicon | gold |
| 100 | 24,000 | 100 | .03 | .006 |
| 30 | 4,000 | 21 | .01 | .003 |

For Monte Carlo, analog simulation of electrons would be prohibitively computationally expensive

- *Solution: Condensed-history models*

For deterministic, proper treatment of electron cross sections would require excessive discretization in energy and angle and would be prohibitively computationally expensive.

- *Solution: Boltzmann-Fokker-Planck (BFP) transport equation*

# Two totally different methods are available in computational physics to model radiation transport

## Monte Carlo Methods (ITS)

*Computer simulation of random walk by statistical sampling*

- Runtime limited
  - Memory not generally a limitation
- Complex 3D modeling capability exists
- Efficient for computing integral quantities
  - Total charge crossing a surface
  - Total dose in a region
- Easily adaptable to parallel computers

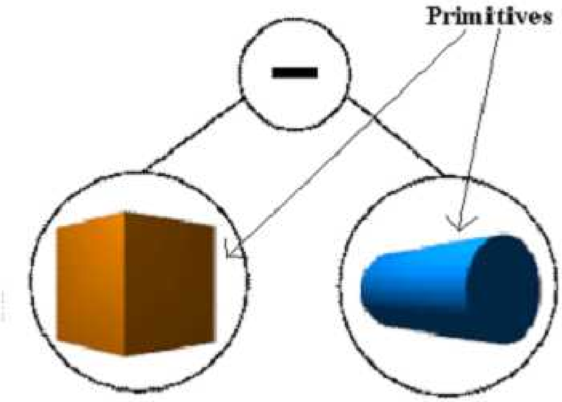
## Deterministic Methods (CEPTRE)

*Numerical solution of the mathematical equation describing the transport*

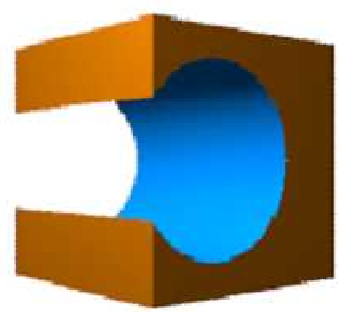
- Memory and/or runtime limited
- Complex 3D modeling capability is being developed
- Essential for computing differential quantities
  - charge deposition distributions
  - energy deposition distributions
  - Space, energy, and angle dependent emission quantities

# ITS Combinatorial Geometry (CG) Legacy approach

- In a CG representation, each model is built from Boolean combinations of primitives
- These combinations form a tree of primitives and set operations such as unions, intersections and subtractions




CG Subtraction



The Resulting Solid



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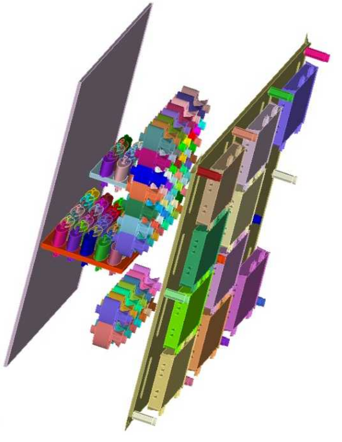
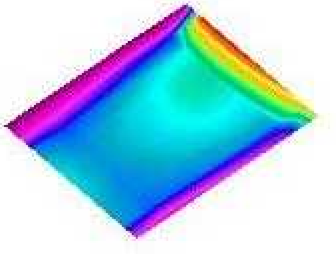
# Ability To Transport on CAD Geometry

- Geometry descriptions in the ACIS® format can be used (separate purchase of ACIS license required).
- The CAD portions of the code are written in C++
- CAD incurs a penalty in computational speed
- Both CG and CAD can be used a single model







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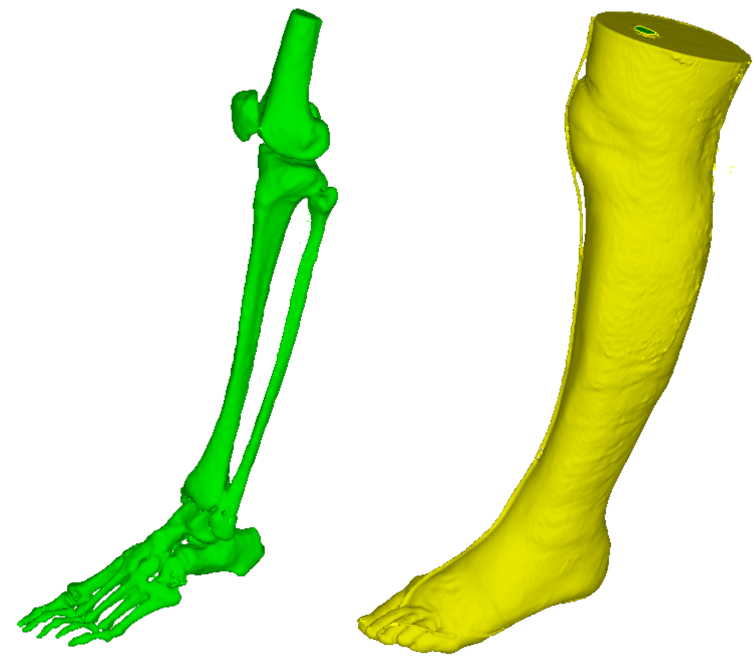
# Use Of Facet-based Geometries

- Added facet-based geometry ability to deal with some CAD inefficiencies
  - Spline surface replacement
- Can combine all three geometries types in a single calculation
- Use the best representation for each part of the geometry



Computed Tomography Isosurface
Data from Visible Human Project™



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# Ongoing ITS Development Efforts

- **Efficiency improvements.**
- **Generalized Boltzmann-Fokker-Planck (GBFP) moment-preserving transport of electrons.**
- **Extending some photon transport capability to sub 1-keV energies.**
- **Doppler broadening of Compton electrons.**
- **Implementation of the random hinge algorithm in ITS.**
- **Improvements in external electric and magnetic field descriptions.**

# Generalized Boltzmann-Fokker-Planck

**Ongoing ITS Development Efforts**

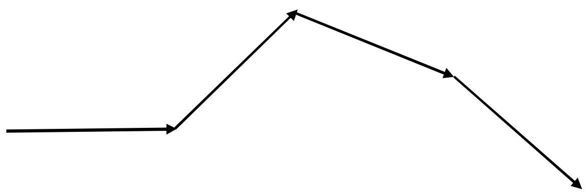
- A computationally efficient single-event method of Monte Carlo transport.
- Analog cross sections for electrons are converted into corresponding discrete cross sections that exactly preserve low order moments of the cross sections.
- Alleviates boundary crossing problems of condensed history.
- Will be offered as an alternative to conventional condensed history in a future version of ITS.

# ITS Research: Alternative Algorithms for Electron Transport

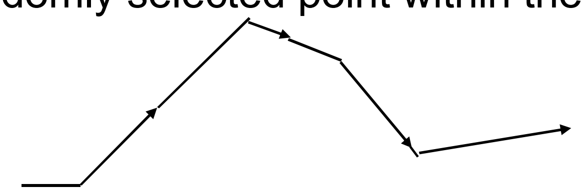
## Conventional Condensed History

**Apply an infinite medium angular solution and algorithmically approximate the spatial displacement.**

- ETRAN, ITS, MCNP model: particle scatters at the end of the step



- Random Hinge model: particle scatters at a randomly selected point within the step

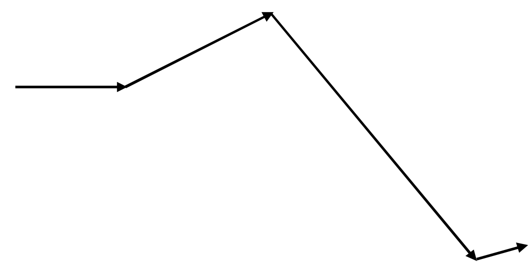


- Angular sampling from a multiple-scattering distribution

## GBFP: Transport-like Condensed History

**Solve an approximate Boltzmann transport equation.**

- Random distance-to-collision is sampled from an exponential distribution
  - Reduce the simulated interactions



- Angular sampling from analytical, multiple-scattering, discrete, or other distribution
  - *Promising results with discrete-angle and discrete-energy representations*

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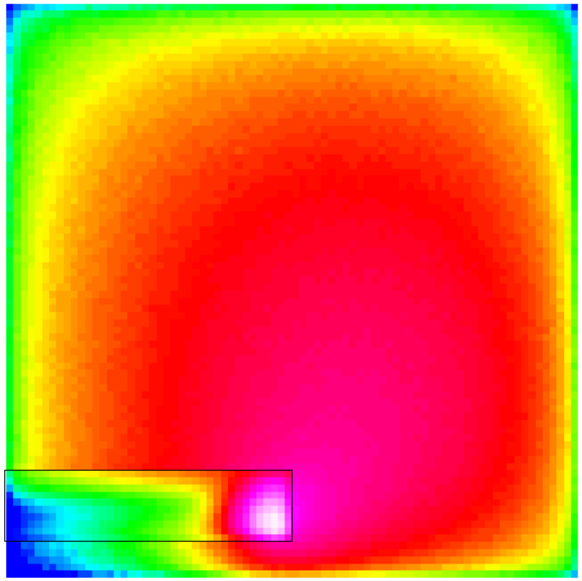
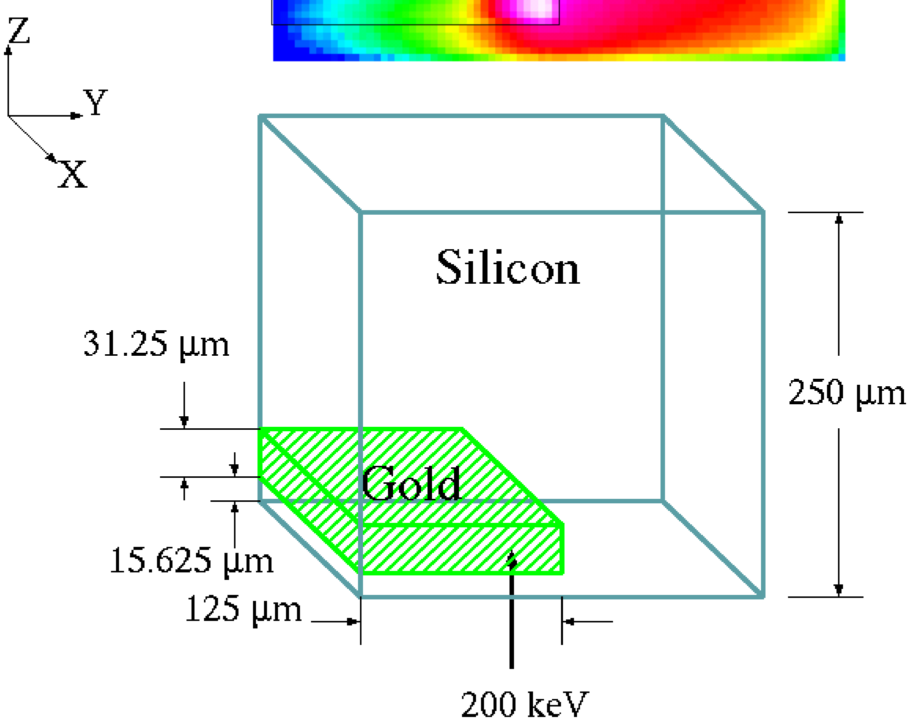
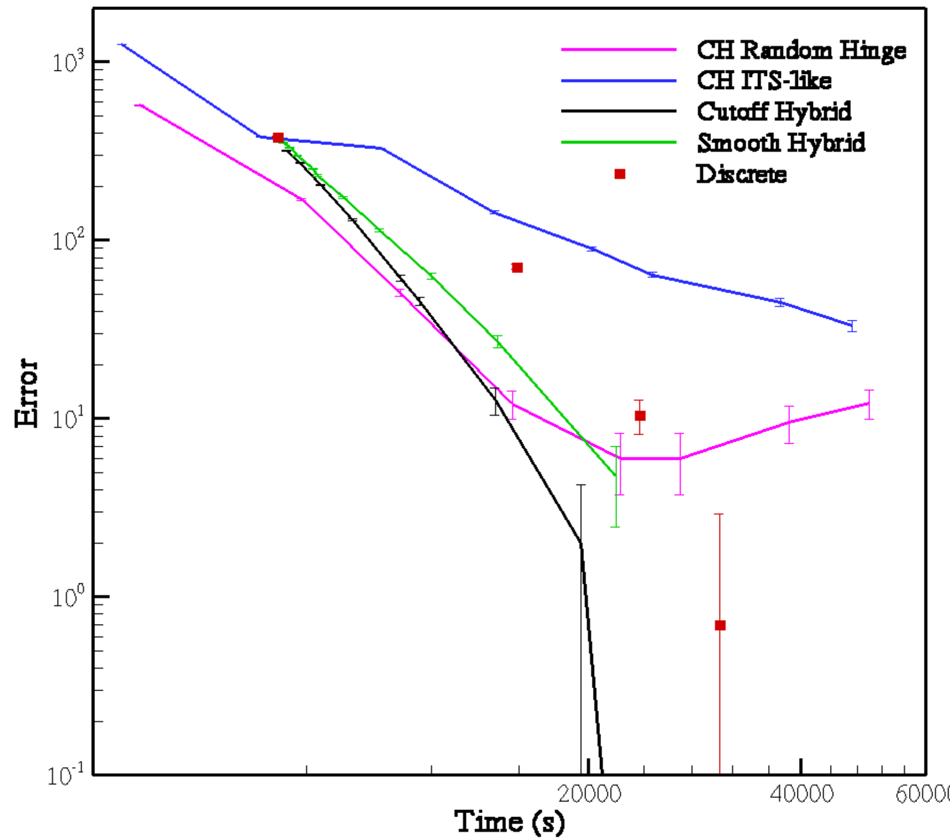
# GBFP Results

**Analog Benchmark Dose**






See Franke and Prinja, "Monte Carlo Electron Dose Calculations Using Discrete Scattering Angles and Discrete Energy Losses", NSE 149, 1–22 (2005) for a detailed discussion of this method

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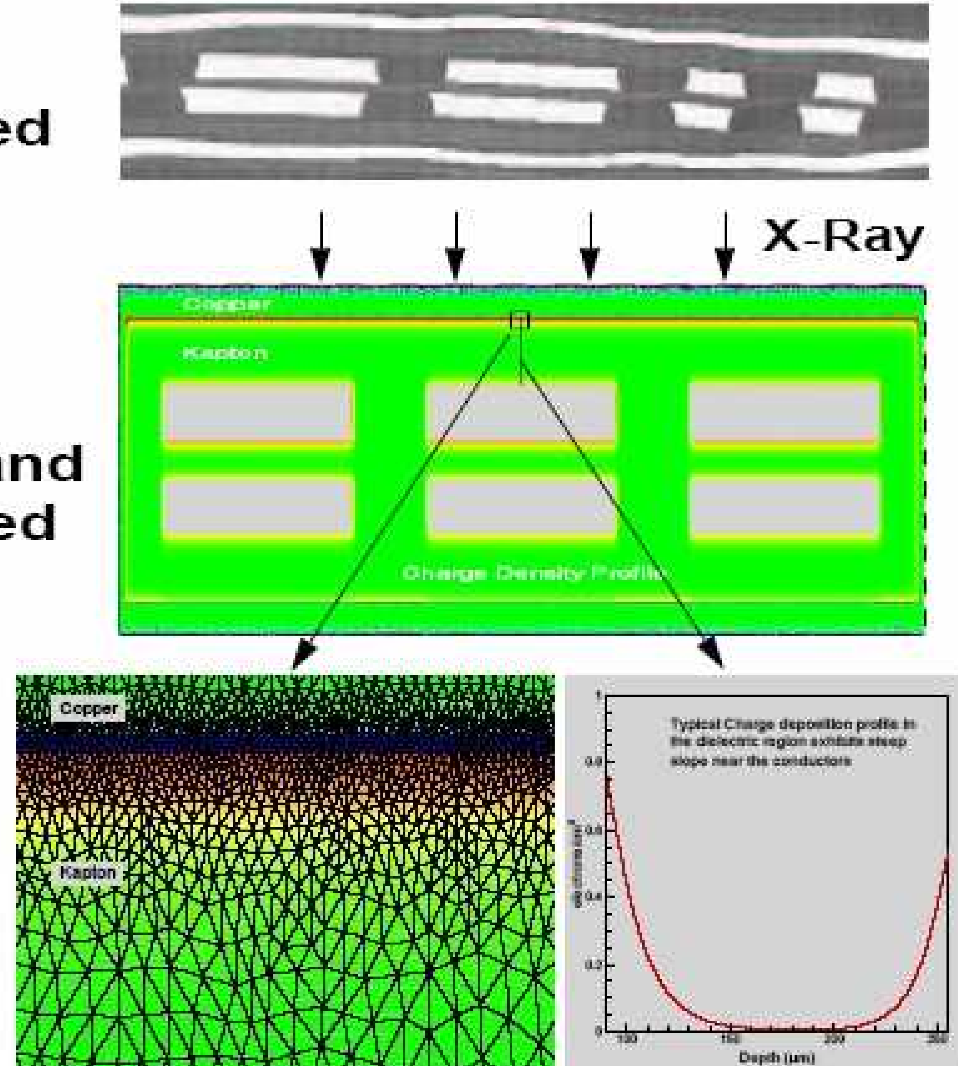
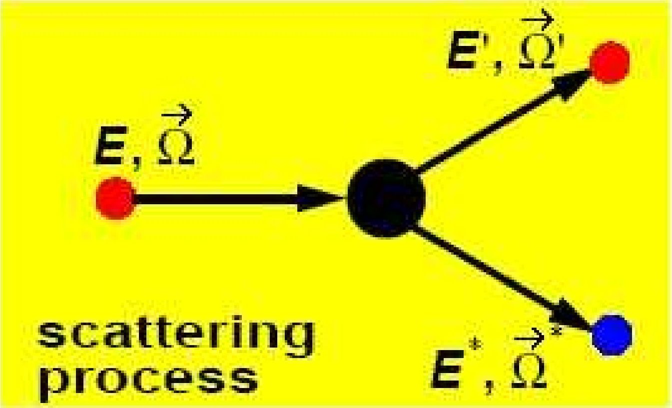
# *CEPTRE : Deterministic Radiation Transport*

- **Time-independent, deterministic, coupled electron-photon transport code on unstructured mesh**
- **Provides energy deposition, current and charge profile induced by radiation**
- **Extremely small mesh cells near the material interfaces are needed to resolve charge profile**



# Deterministic Radiation Transport

- Numerical solutions to the Boltzmann transport equation which describes the particle distribution in phase space $(\vec{r}, E, \vec{\Omega})$




- Physics of particle-media interaction properly characterized by cross sections

- Discretization of Phase Space
  - *Multigroup* approximation in energy along with Legendre expansion of scattering cross sections
  - *Discrete-Ordinates* approximation in direction
  - *Finite-Element* approximation in space

- Symmetric Positive-Definite Forms

# CEPTRE Utilizes A Unique Iterative Solution Strategy

- Slow convergence rate for electron transport
- Low parallel efficiency due to coupling in directions from scattering

**Conventional Source Iteration**


- Fast convergence rate for electron transport
- Good parallel efficiency
- Large storage requirement

**CEPTRE**

# Iterative Solution Algorithm

- Preconditioned Conjugate-Gradient method with domain decomposition and extensive use of the AZTEC libraries
- Slow convergence rate for photons due to the small mesh size (90% of run time)
- Diagonal-Block preconditioner has been implemented and shown to be effective in reducing both the iteration counts and run times
- The preconditioning matrix could also be ill-conditioned and require another level of preconditioning

**SCEPTRE Development:**

- **First-order $S_n$ for photons coupled to second-order Sn for electrons**

# Availability of ITS Version 5 and CEPTRE

- Currently ITS version 5* and CEPTRE are only available for government use.
  - Contact Ron Kensek (rpkense@sandia.gov) or its-support@sandia.gov for license application procedures.
- We are pursuing, for ITS5 and SCEPTRE:
  - Licensing for universities and research partners.
  - Distribution through RSICC (at Oak Ridge National Laboratory)

* Version 3 available thru RSICC w/o restriction

# *V & V: Validation and Verification*

- **<u>VERIFICATION:</u> The process of determining that a computational software implementation correctly represents a model of a physical process - (solving the equations right)**

- **<u>VALIDATION:</u> The process of determining the degree to which a computer simulation is an accurate representation of the real world for a specific application - (solving the right equations)**



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# Method of Manufactured Solutions

- **Exponential spatial dependence in x, y and z**
- **Linear/quadratic angular dependence**
- **Expected convergence rates for the $L_2$ norm:**
  - **2 for linear elements**
  - **3 for parabolic elements**
- **L2 norm computed with high-order quadrature integration**

$L_2$ norm: $$\|u - u_h\|_0 = \left( \iint \left| \phi(\mathbf{r}, \mathbf{\Omega}) - \phi_h(\mathbf{r}, \mathbf{\Omega}) \right|^2 d\mathbf{\Omega} d\mathbf{r} \right)^{1/2}$$

# 3D Manufactured Problem

Boltzmann Transport Equation:

$$\mu_x \frac{\partial \phi}{\partial x} + \mu_y \frac{\partial \phi}{\partial y} + \mu_y \frac{\partial \phi}{\partial y} + \phi = \frac{1}{4\pi} \iint \left( \frac{1}{2} + \frac{\mu_0}{2} \right) \phi(\mathbf{r}, \mathbf{\Omega}') d\mathbf{\Omega}' + Q$$

Analytic Solution:

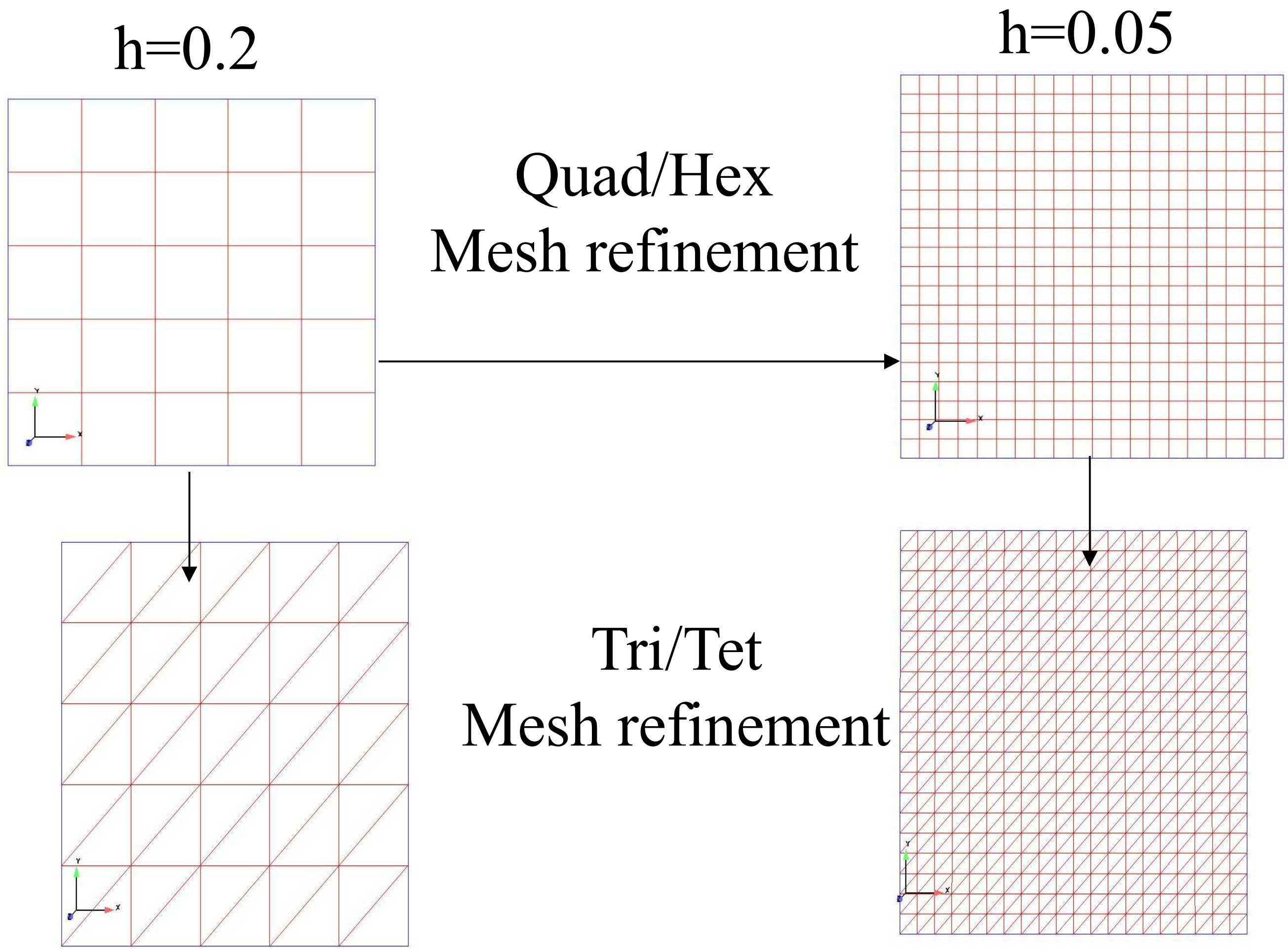
$$\phi(x, y, z, \mu_x, \mu_y, \mu_z) = e^{-x} e^{-y} e^{-z} (1 + \mu_x + \mu_y + \mu_z)$$

Even-Odd Parity Distributed Source Terms:

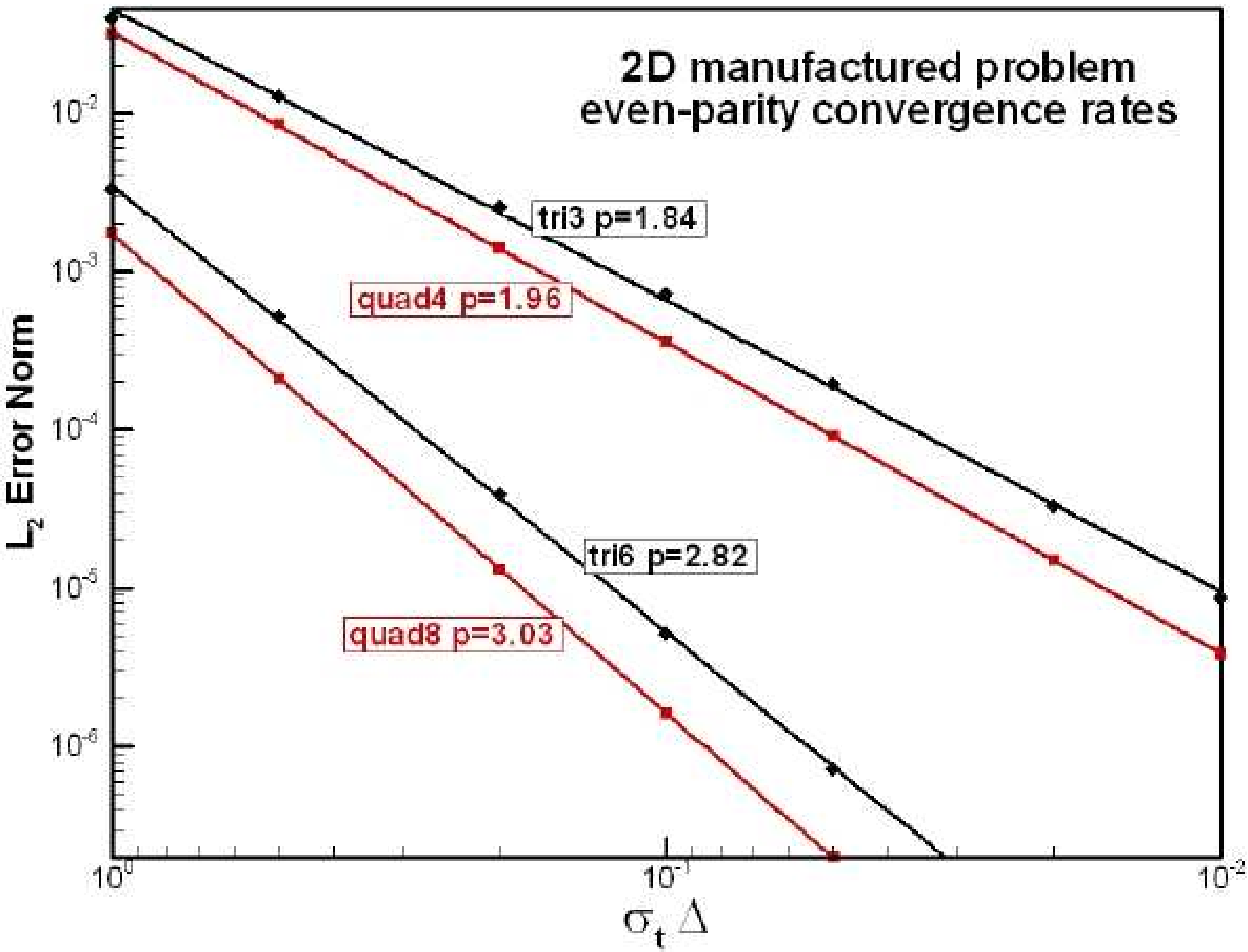
$$Q^+(x, y, z, \mu_x, \mu_y, \mu_z) = e^{-x} e^{-y} e^{-z} \left[ (1 + \mu_x + \mu_y + \mu_z)(1 - \mu_x - \mu_y - \mu_z) - \frac{1}{2} \right]$$

$$Q^-(x, y, z, \mu_x, \mu_y, \mu_z) = -\frac{1}{6} e^{-x} e^{-y} e^{-z} (\mu_x + \mu_y + \mu_z)$$

# *Mesh-Refinement Convergence Studies*



# 3D Even-Parity Results



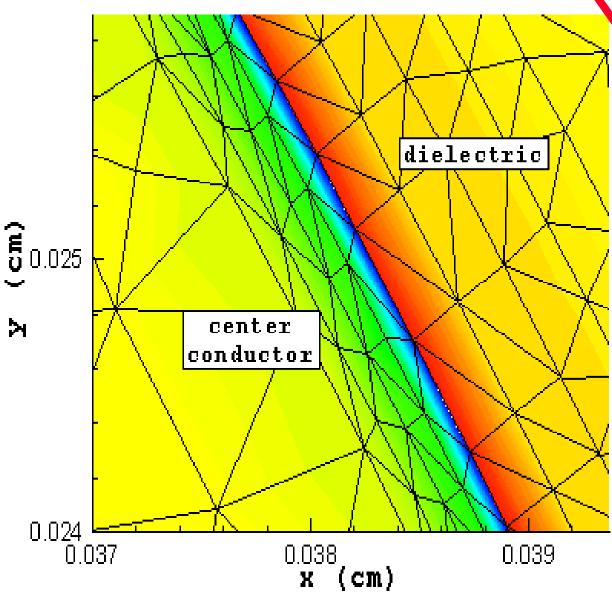
## Table 1: Polynomials Represented Exactly by Basis Functions

| | tri3 | quad4 | tri6 | quad8 | tet4 | hex8 | tet10 | hex20 |
|---|---|---|---|---|---|---|---|---|
| 1 | * | * | * | * | * | * | * | * |
| x | * | * | * | * | * | * | * | * |
| y | * | * | * | * | * | * | * | * |
| z | | | | | * | * | * | * |
| xy | | * | * | * | | * | * | * |
| xz | | | | | | * | * | * |
| yz | | | | | | * | * | * |
| xyz | | | | | | * | | * |
| $x^2$ | | | * | * | | | * | * |
| $y^2$ | | | * | * | | | * | * |
| $z^2$ | | | | | | | * | * |
| $x^2y$ | | | | * | | | | * |
| $x^2z$ | | | | | | | | * |
| $y^2x$ | | | | * | | | | * |
| $y^2z$ | | | | | | | | * |
| $z^2x$ | | | | | | | | * |
| $z^2y$ | | | | | | | | * |
| $x^2yz$ | | | | | | | | * |
| $y^2xz$ | | | | | | | | * |
| $z^2xy$ | | | | | | | | * |

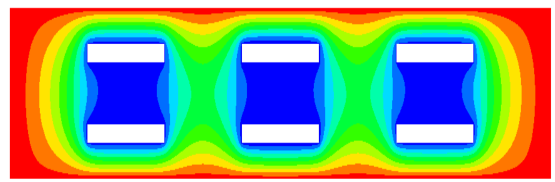
# CEPTRE and EMPHASIS (CABANA) EM Pulse in Cables

*Deterministic (CEPTRE)*

Charge density, currents, & energy deposition at given time




**Electric field intensity**



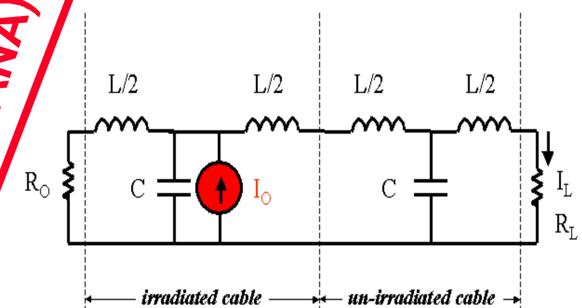
***Electrostatics solved simultaneous with lumped circuit model of cable***

Drive current as a function of time

(CABANA)

*2D quasi-electrostatic solver with radiation-induced conductivity models*

*Circuit analysis module (SPICE)*




$I_O$ is the radiation induced current source

Transmission line effects and circuit termination response



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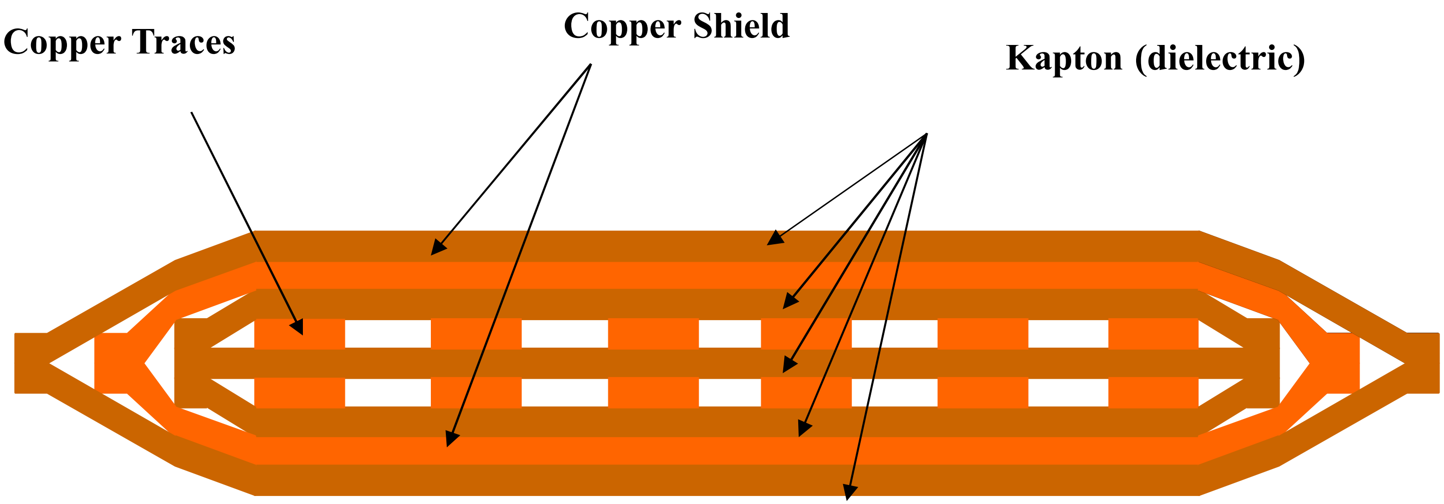
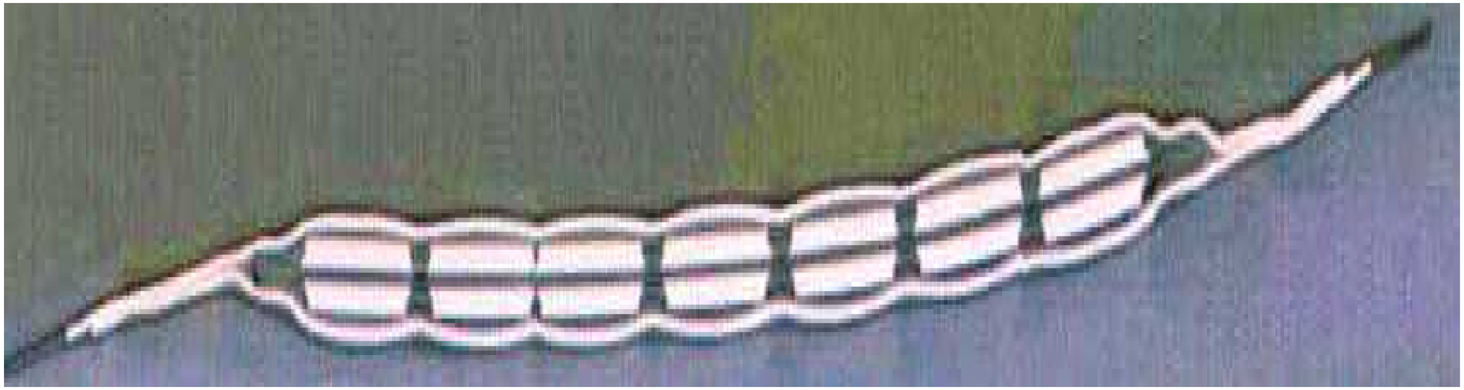
# Design vs. As-built

## Design Geometry (prototype)




## Real Geometry as Manufactured





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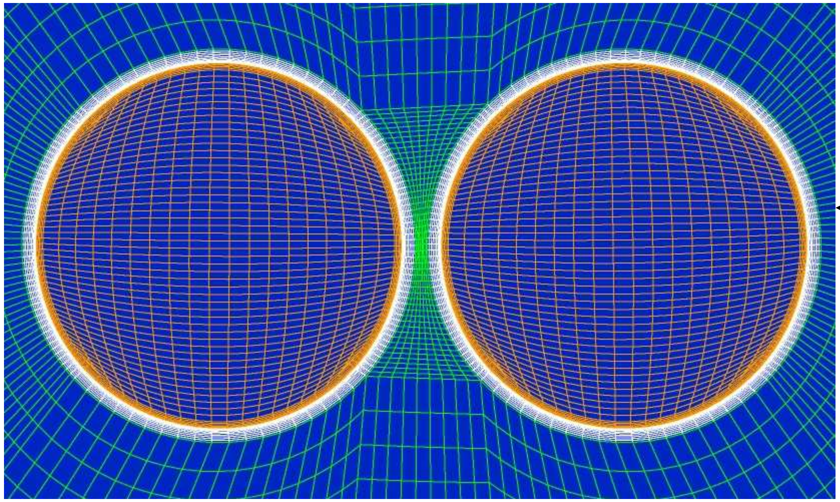
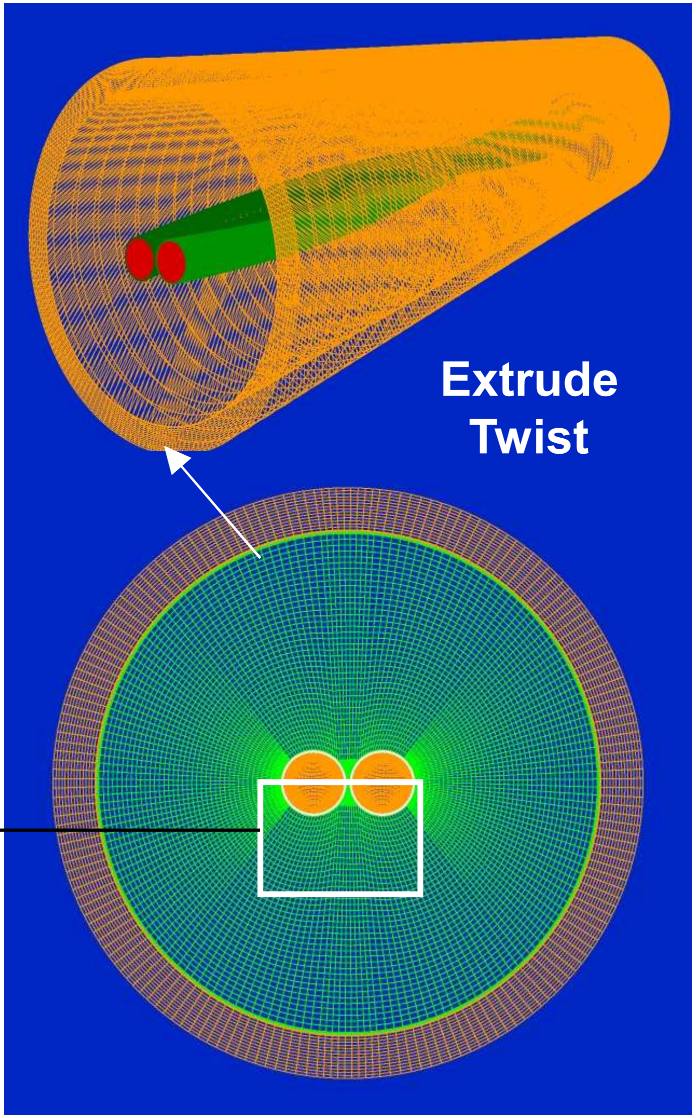
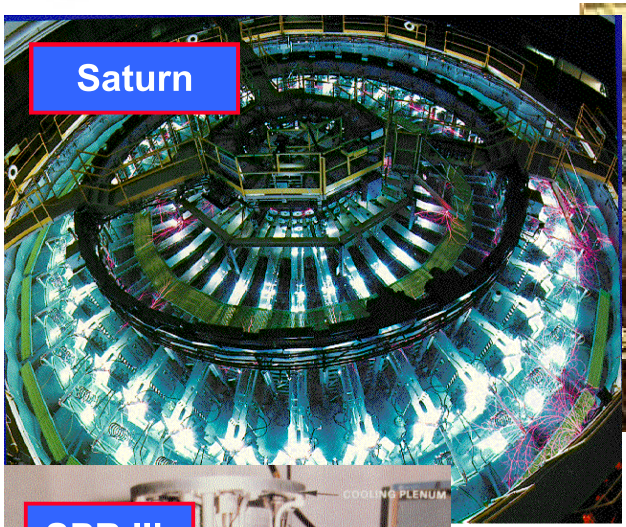
# CEPTRE: 3D Model Geometry and Meshing

- Conductors twisted along the center line of the cable
- Cross sections of dielectric and shield regions have perfect circular shape and are uniform along the cable
- Periodic structure
- Challenging mesh generation to accommodate
  - µm-size cells near conductor/insulator interface
  - Minimize element counts

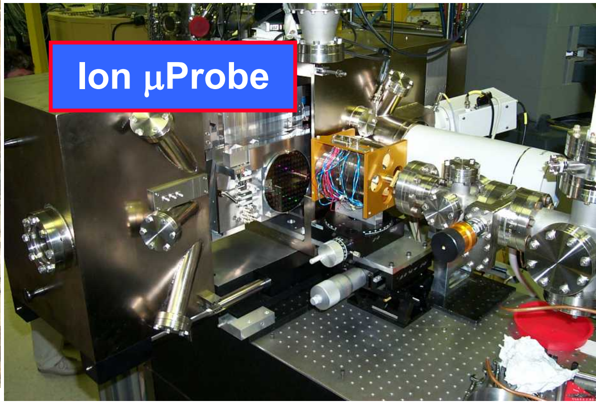


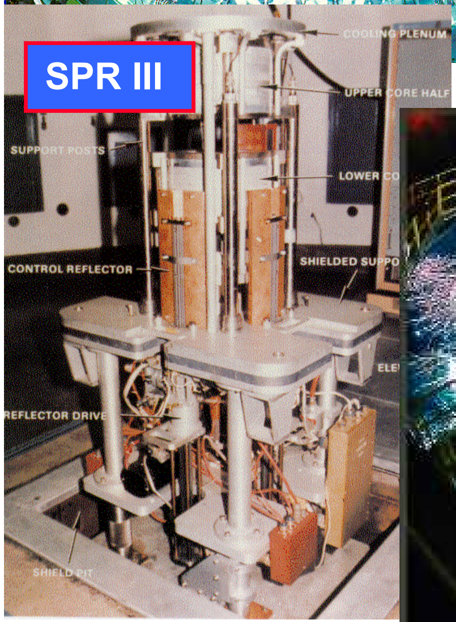


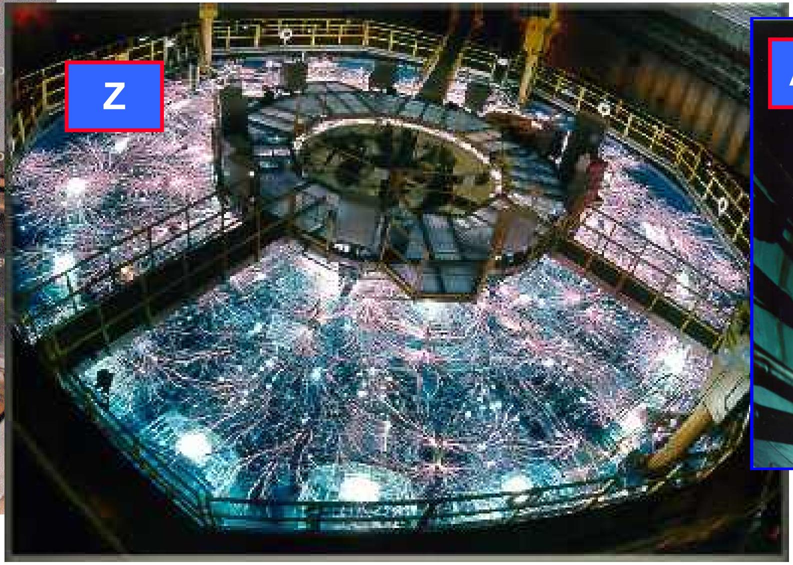
# *Sandia Radiation facilities used for testing, research and code validation*







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# RADIATION

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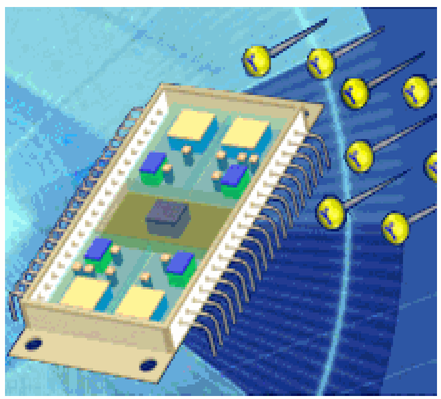


# RESRI

is a collaboration between universities and Sandia to support research in radiation effects. Read more about RESRI here >>

**Objectives**

- Develop a pool of well-trained scientists and engineers to support the Radiation Effects Requirements of the nation's Stockpile Stewardship mission
- Provide opportunities for top students to learn about radiation and its effects on materials and electronics by participating in state-of-art experiments on Sandia's radiation facilities, or by participating in the development of advanced physical and numerical algorithms for codes that model the transport of radiation through matter.

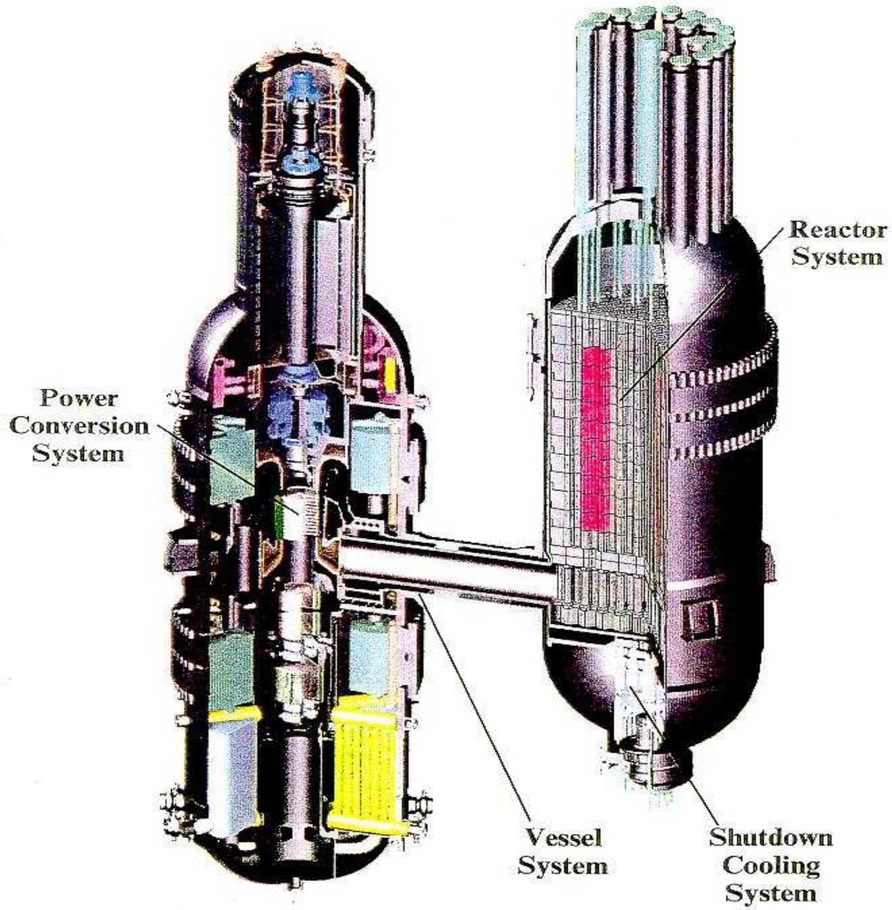
# *Nuclear Energy Activities At Sandia National Labs*

- ***Generation IV Advanced Nuclear Power Systems***
- ***Nuclear Hydrogen Initiative***
- ***Space Nuclear Power and Propulsion Systems***

# Nuclear Energy Research at SNL Advanced Nuclear Power Systems

- Generation IV (Advanced Reactors – DOE NE)
  - Generation IV Program investigating advanced reactor concepts for next generation nuclear power plants
  - Goals – passively safe, reduced waste, proliferation resistant, more efficient and cost effective
- Major SNL Activities
  - Advanced Power Conversion
    - » Develop more efficient / economical electrical power conversion systems for the next generation power plants
    - » Supercritical CO2 Cycles, (500 - 700 C)
    - » High Temperature Helium Brayton Cycles (700 – 1000 C)
  - Hydrogen Production from Nuclear Energy
    - » Theromchemical cycles - Sulfur-Iodine
    - » SNL developing high temperature H2SO4 decomposition technology for Sulfur based cycles

# *Very High Temperature Gas Cooled Reactor (VHTR)*

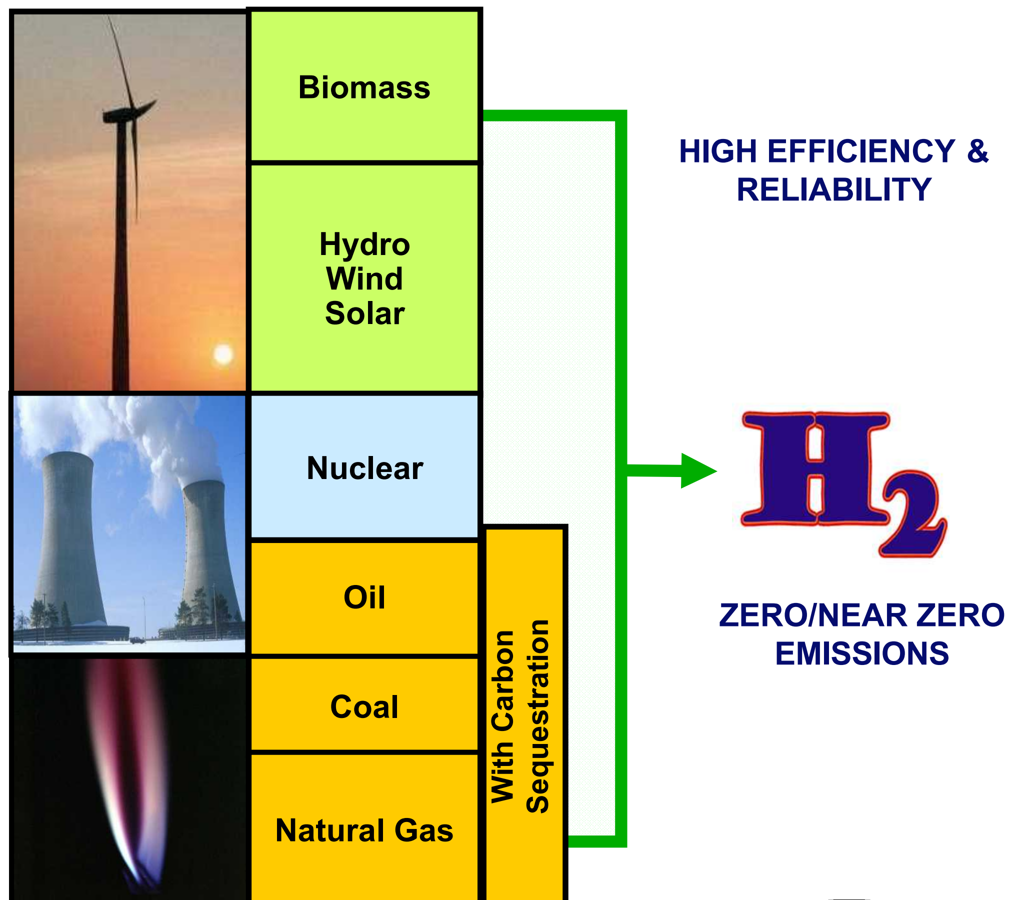



- Thermochemical or High Temperature Electrolysis Hydrogen production
- Robust passive safety capability
- Goals up to 1000 C outlet, 1250 C fuel temperatures
- ~50 % electrical conversion efficiency
- Prismatic or Pebble fuel geometry, direct/indirect cycle He cooled
- R&D focuses on high temperature fuels, coatings, materials, fuel cycle, waste form for graphite/carbide fuels
- Focus of US advanced reactor research effort

# *DOE Hydrogen Program -- Develop Multiple Options for Hydrogen Production*

- **Goal: Demonstrate cost effective Technologies for the production of hydrogen by nuclear energy**

- **Nuclear energy provides option for large scale hydrogen production**
- **Does not produce greenhouse gases or other air-borne pollutants**
- **Not dependent on fossil resources**

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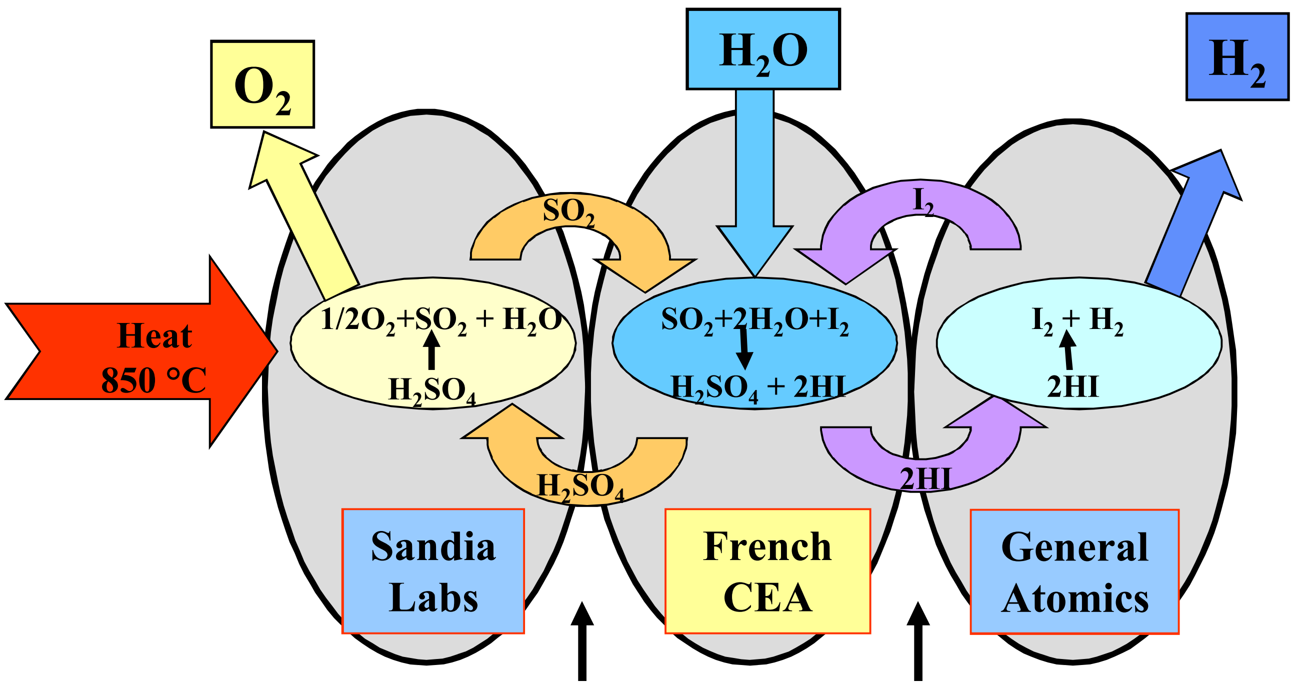
# *Sulfur Iodine Cycle*

- **Sulfur-Iodine cycle (INERI – CEA, GA, SNL)**
  - **Develop component reaction sections for S-I process**
  - **Preliminary design of $H_2SO_4$ and HI decomposition sections**
  - **Assessment of candidate high-temperature materials**




**Interface Issues**

•Species, Concentrations, Recycle Flows, Pressure, Temperature, Control, Configuration



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# *Space Nuclear Power Initiative*

- **NASA Prometheus Project will develop and deploy a space nuclear power/propulsion system for extended space missions (Prometheus, JIMO mission, NASA, NR, NGST)**
  - **JIMO (Jupiter Icy Moons Orbiter) Project ~2017 launch with few hundred kWe nuclear reactor power source**
  - **SNL supports NGST – Spacecraft developer**
  - **Anticipate support for NR (Safety, Design)**
- **RTG (Radioisotope Thermoelectric Generator) Launch Safety Program (DOE NE-50)**
  - **Launch safety analysis and testing for commercial and defense space applications**



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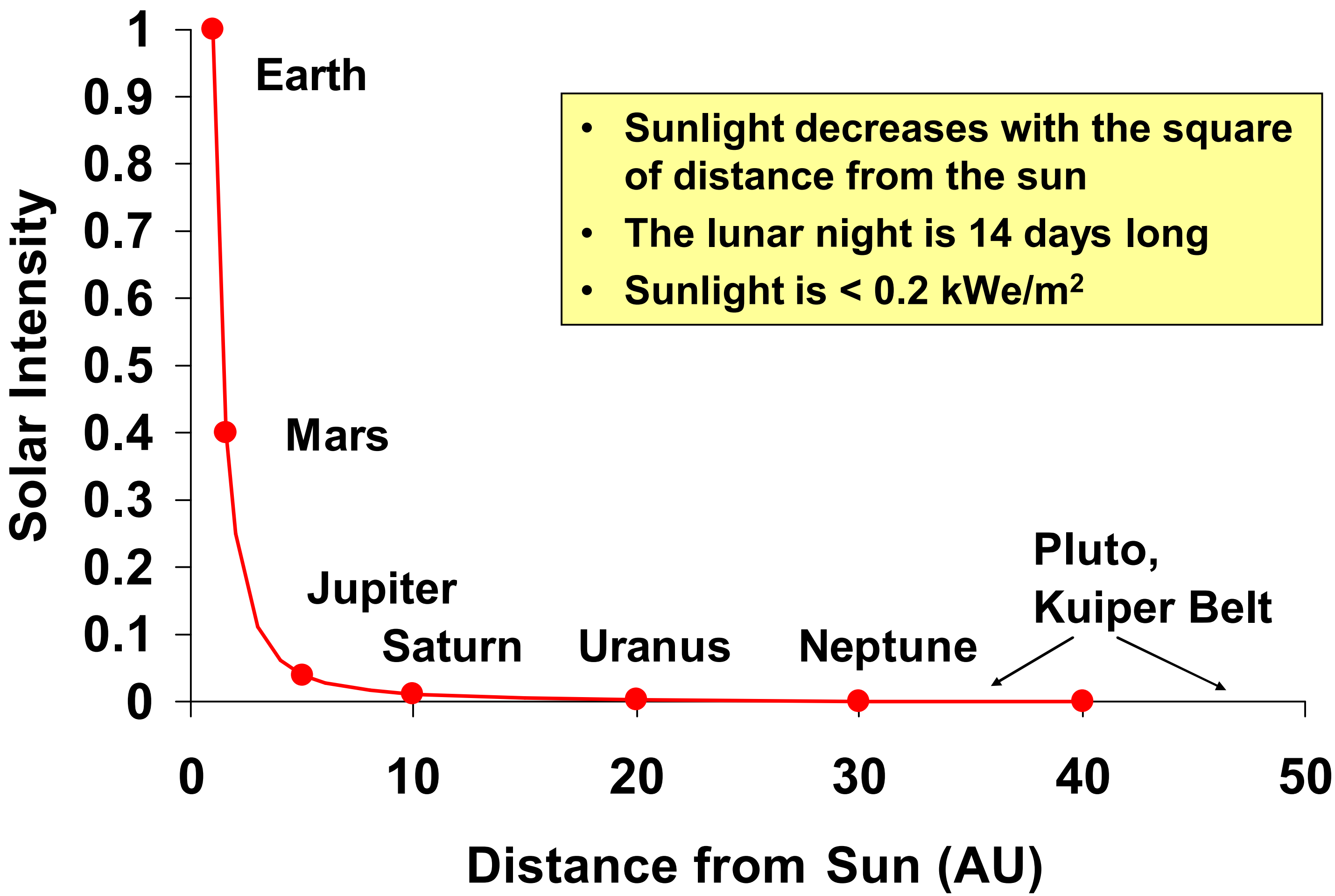
# *Fission systems can provide power where sunlight is faint or obstructed*

- Sunlight decreases with the square of distance from the sun
- The lunar night is 14 days long
- Sunlight is < 0.2 $kWe/m^2$



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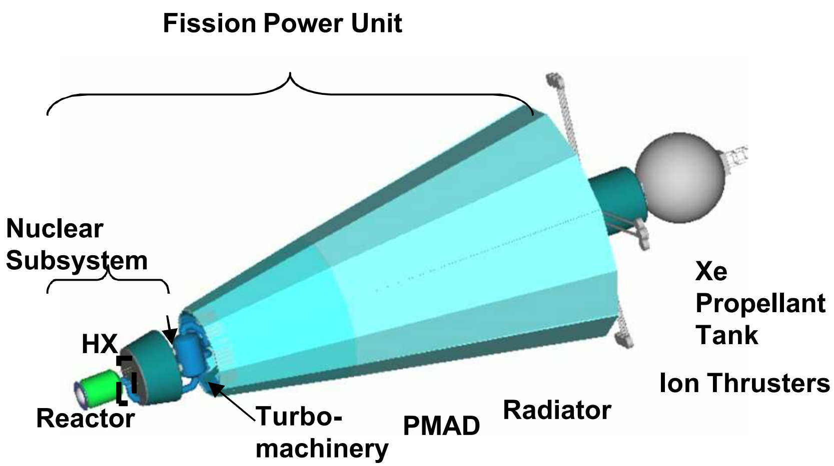
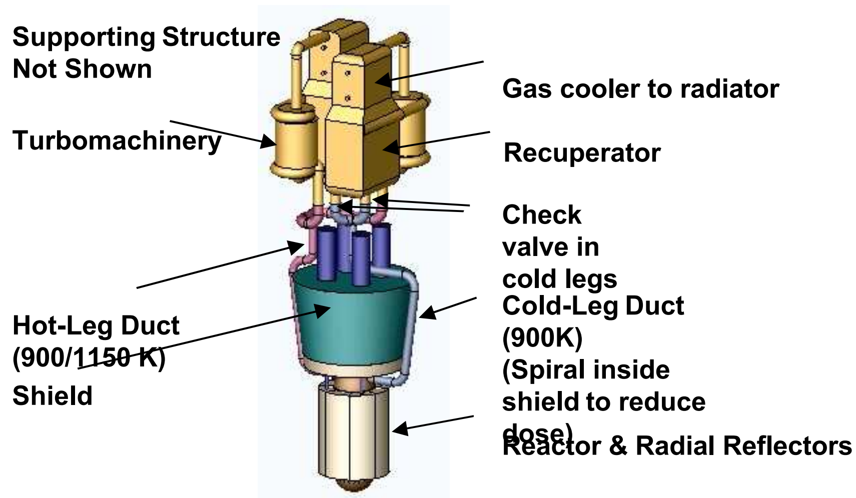
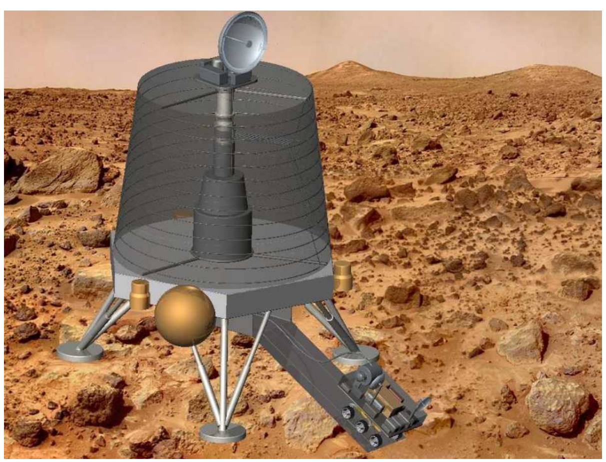
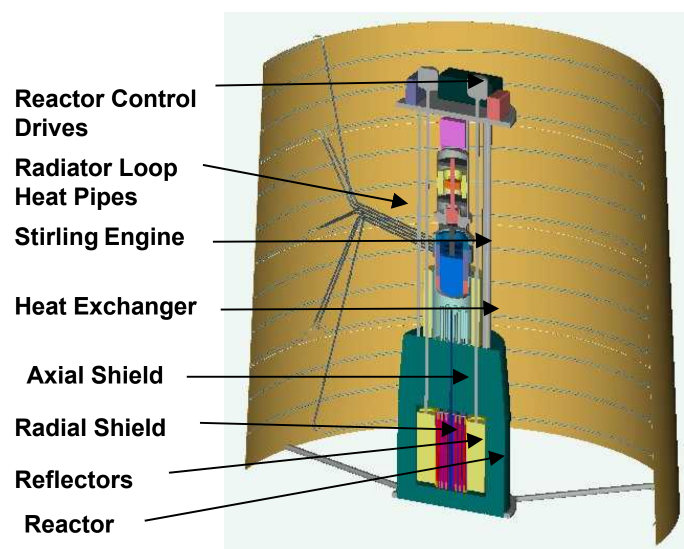
# *SNL participated on DOE/NASA studies that were precursor to the JIMO Project*



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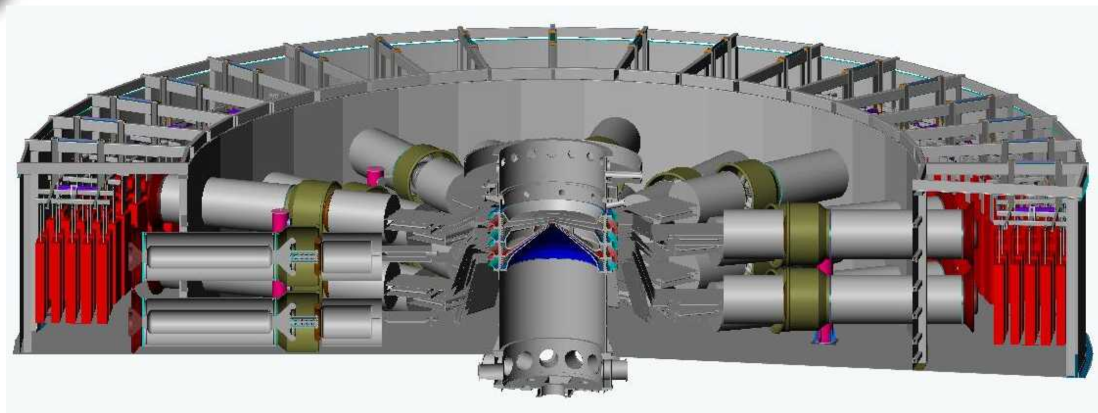
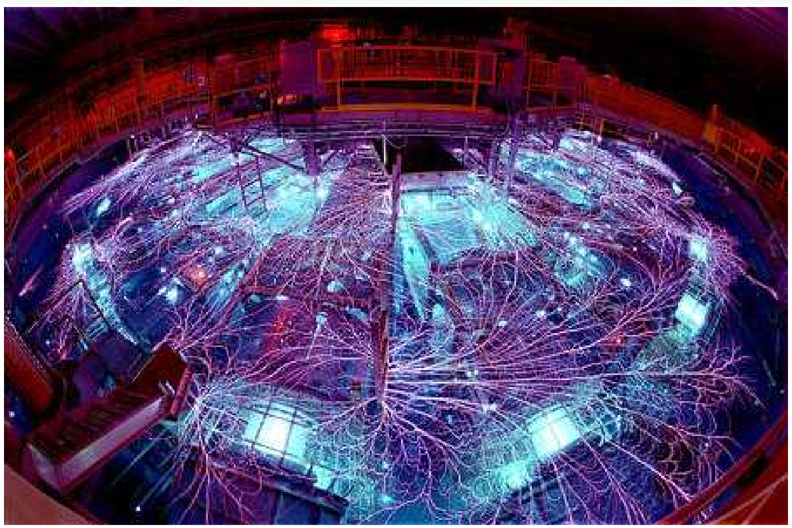
# *Inertial Fusion Energy (IFE) Research at Sandia National Laboratories*

# *Area IV X-ray Facilities: The Z Accelerator*

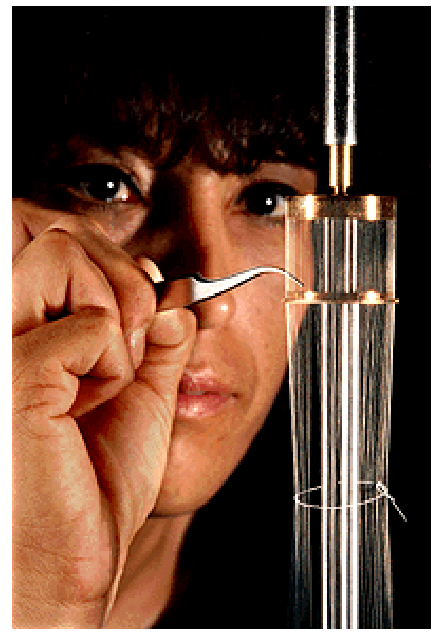


**Z-pinch generation of x-rays**

- **1.8 MJ**
- **230 TW**



**Time exposure photograph of electrical flashover arc produced over the surface of the water in the accelerator tank as a byproduct of Z operation. These flashovers are much like lightning strokes**



**Wires 1/10th width of human hair**

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The *long-term* goal of Z-Pinch IFE is to produce an economically attractive power plant using high-yield z-pinch-driven targets (~3 GJ) at low rep-rate per chamber (~0.1 Hz)

Z-Pinch IFE DEMO (ZP-3, the first study) used 12 chambers, each with 3 GJ at 0.1 Hz, to produce 1000 MWe

The *near-term* goal of Z-Pinch IFE is to address the science issues of repetitive pulsed power drivers, recyclable transmission lines, high-yield targets, and thick-liquid wall chamber power plants



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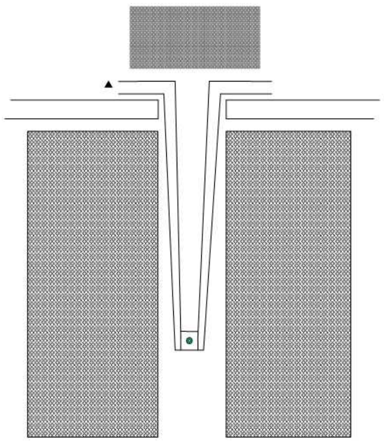
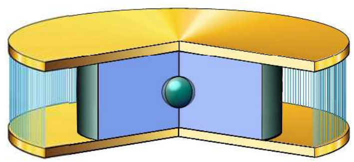
# *Z-Pinch IFE Research*



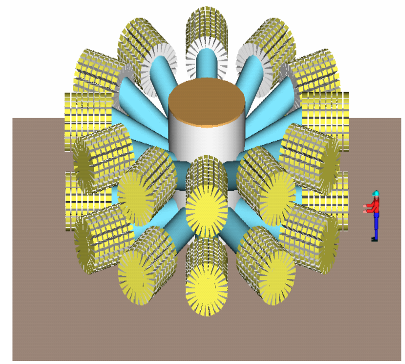
**RTL**

Recyclable transmission line



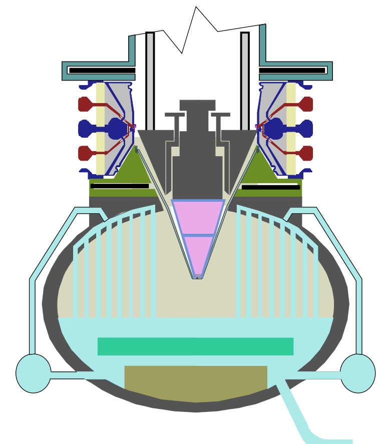
**DH target**

Dynamic Hohlraum



**LTD driver**

Linear Transfomer Driver
(Rep-rateable)



**Chamber**

- **Substantial progress has been made in all areas of Z-Pinch IFE**
- **A growing Z-Pinch IFE program is envisioned**



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# *www.sandia.gov/pulsedpower/ncppri*

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## National Collegiate Pulsed Power Research Institute (NCPPRI)

PPT Main | Programs & Capabilities | **NCPPRI** | Facilities | News and Reviews | Related Resources

The NCPPRI is a laboratory critical skill development program funded by the National Nuclear Security Administration (**NNSA**) to funnel U.S. undergraduate and graduate students into pulsed power research areas. NCPPRI also works with community colleges to develop programs to train pulsed-power technicians.

Time-exposure photograph of electrical flashover arcs produced over the surface of the water in the accelerator tank as a byproduct of Z operation. These flashovers are much like strokes of lightning

**Objectives**

- Develop pool of well-trained scientists and engineers to support pulsed power requirements of the nation's stockpile stewardship mission
- Lay foundation for the next generation of scientists to achieve high-yield, high-gain fusion

**Elements**

- Undergraduate and graduate opportunities
- Competitive selection process
- 13-week summer institute
- Short courses, lectures, tours
- Weekly speaker series
- On-campus research option during academic year
- Technical research paper



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