SAND2021-12764PE

Sandia National Laboratories

Exceptional service in the national interest

Adventures of a Mid-Career Mathematician in Radiation & Electrical Sciences

Heidi K. Thornquist

Org. 1355 (Electrical Models & Simulation)

1400 Postdoc and Early Career Seminar Series

September 14th, 2021

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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Overview

- Let me introduce myself …
- Early career at Sandia
- How did I get to 1300?
- What goes on in 1300 and how could it impact you?
- Questions

Educational background

Humboldt State University

Arcata, CA

B.A. Applied Mathematics (major)

Computer Information Systems (minor)

Rice University

Houston, TX

M.A. / Ph.D. Computational and Applied Mathematics

"*Fixed-Polynomial Approximate Spectral Transformations for Preconditioning the Eigenvalue Problem*"

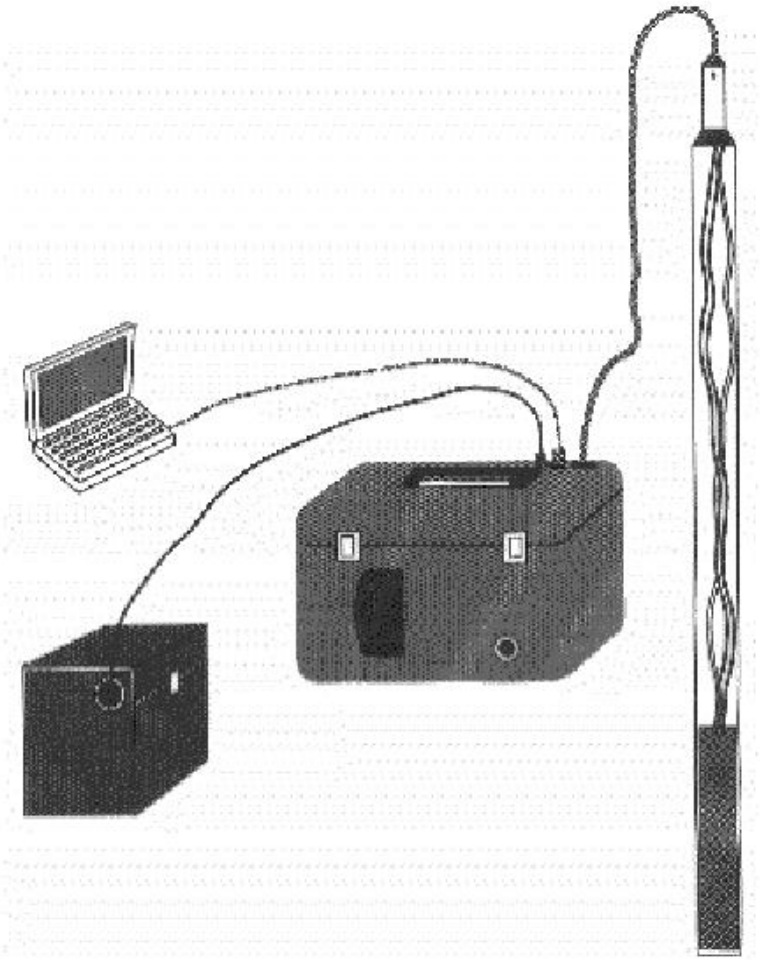
Undergraduate research experience

SERS Internship (LANL, Fall 1996)

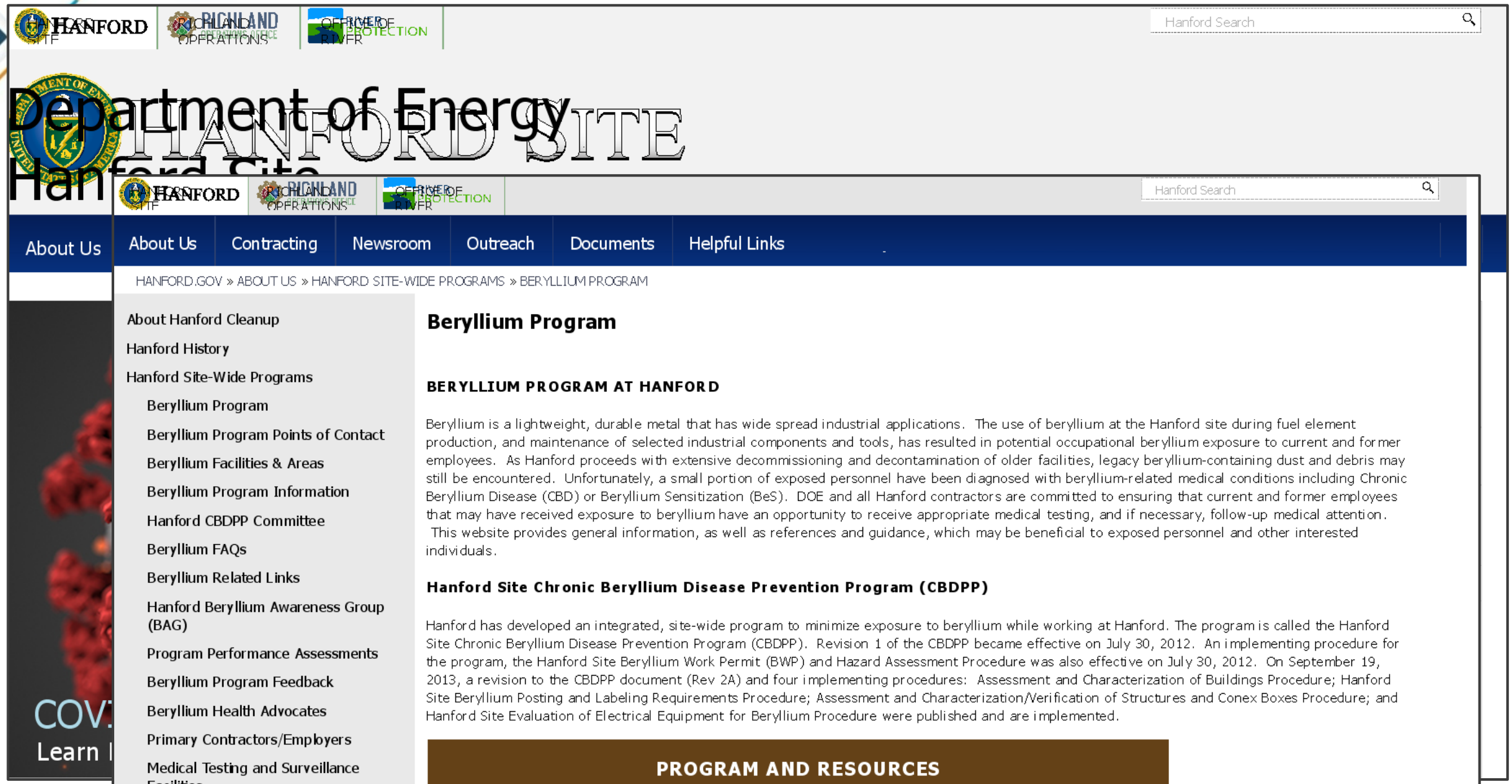
- Developed software in Basic to analyze plasma and electron density from a laser-induced breakdown spectroscopy (LIBS) spectrum.

UGS (LANL, Summer 1997)

- Updated Basic software used in the operation of the field-portable LIBS analyzer.
- Tested the effectiveness of LIBS in detecting beryllium contamination in water-saturated soil samples.



Why is this important? Who does this benefit?


HANFORD SITE
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OFFICE OF RIVER PROTECTION
Hanford Search
Department of Energy
Hanford Site
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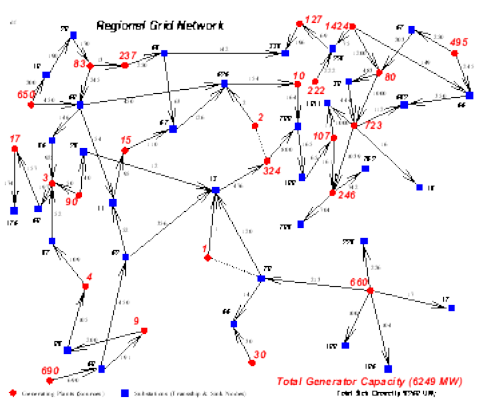
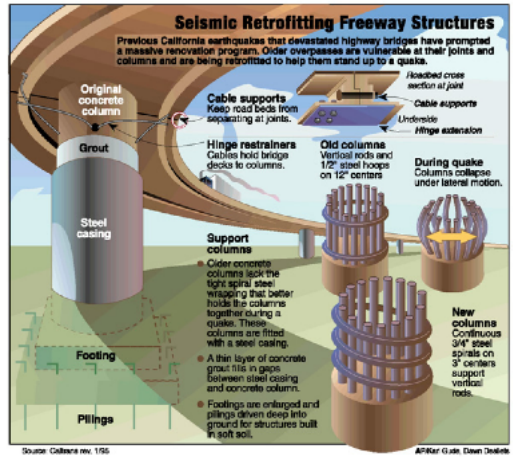
Hanford History
Hanford Site-Wide Programs
Beryllium Program
Beryllium Program Points of Contact
Beryllium Facilities & Areas
Beryllium Program Information
Hanford CBDPP Committee
Beryllium FAQs
Beryllium Related Links
Hanford Beryllium Awareness Group (BAG)
Program Performance Assessments
Beryllium Program Feedback
Beryllium Health Advocates
Primary Contractors/Employers
Medical Testing and Surveillance Facilities
General Resources
Beryllium Program Implementing Procedures
Hanford Workers Compensation
Beryllium Program
BERYLLIUM PROGRAM AT HANFORD
Beryllium is a lightweight, durable metal that has wide spread industrial applications. The use of beryllium at the Hanford site during fuel element production, and maintenance of selected industrial components and tools, has resulted in potential occupational beryllium exposure to current and former employees. As Hanford proceeds with extensive decommissioning and decontamination of older facilities, legacy beryllium-containing dust and debris may still be encountered. Unfortunately, a small portion of exposed personnel have been diagnosed with beryllium-related medical conditions including Chronic Beryllium Disease (CBD) or Beryllium Sensitization (BeS). DOE and all Hanford contractors are committed to ensuring that current and former employees that may have received exposure to beryllium have an opportunity to receive appropriate medical testing, and if necessary, follow-up medical attention. This website provides general information, as well as references and guidance, which may be beneficial to exposed personnel and other interested individuals.
Hanford Site Chronic Beryllium Disease Prevention Program (CBDPP)
Hanford has developed an integrated, site-wide program to minimize exposure to beryllium while working at Hanford. The program is called the Hanford Site Chronic Beryllium Disease Prevention Program (CBDPP). Revision 1 of the CBDPP became effective on July 30, 2012. An implementing procedure for the program, the Hanford Site Beryllium Work Permit (BWP) and Hazard Assessment Procedure was also effective on July 30, 2012. On September 19, 2013, a revision to the CBDPP document (Rev 2A) and four implementing procedures: Assessment and Characterization of Buildings Procedure; Hanford Site Beryllium Posting and Labeling Requirements Procedure; Assessment and Characterization/Verification of Structures and Conex Boxes Procedure; and Hanford Site Evaluation of Electrical Equipment for Beryllium Procedure were published and are implemented.
PROGRAM AND RESOURCES
DOE-0342 Hanford Site Chronic Beryllium Disease Prevention Program
DOE-0342 Implementing Procedures

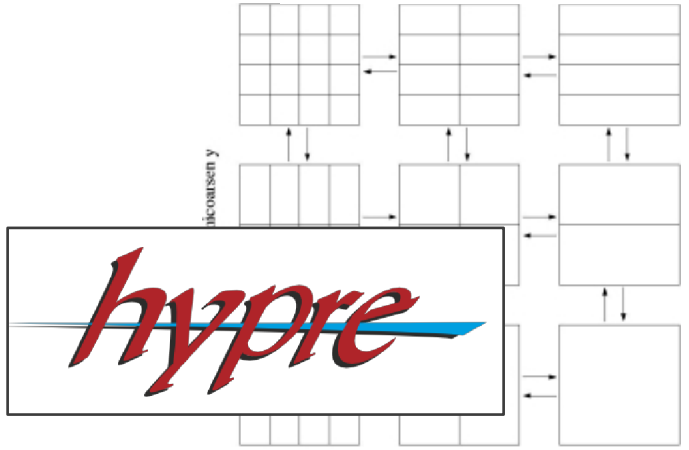
Graduate research experience





- **LANL, Summer 1998**
  - Simulation of deregulated power markets
  - Damage identification project for seismic retrofitting

- **LLNL, Summer 1999**
  - Developed a hybrid multigrid method for preconditioning highly anisotropic problems
    - Sparse grids domain decomposition (Zenger, Griebel)
    - Multiple Semi-coarsened Grid (MSG) technique (Mulder, et al.)



- **LANL, Summer 2002**
  - Developed a physics-based preconditioner for Newton-Krylov methods used in ocean circulation modeling
  - Performed bifurcation / stability analysis using fixed-polynomial approximate spectral transformations

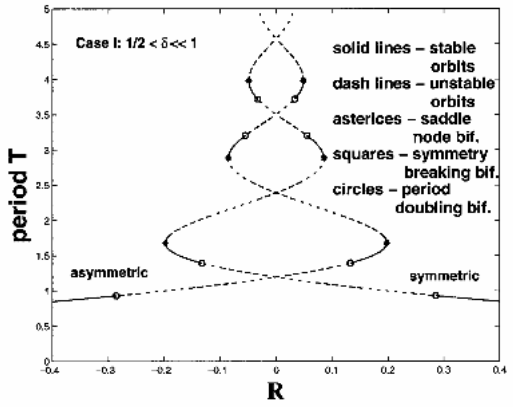


FIG. 5. Bifurcation diagram for a case I Shilnikov phenomenon (1/2 , d K 1), indicating the *half* period of the symmetric principal orbit and the full period of the asymmetric principal orbit. The principal orbits are asymptotic to a pair of homoclinic orbits at R 5 0.

Cort Kreer and Sarah Harman, DOE

DOE Laboratories

There are 17 DOE laboratories that …

- Execute long-term government scientific and technological missions, often with complex security, safety, project management, or other operational challenges
- Develop unique, often multidisciplinary, scientific capabilities beyond the scope of academic and industrial institutions, to benefit the Nation's researchers and national strategic priorities
- Develop and sustain critical scientific and technical capabilities to which the government requires assured access

National Nuclear Security Agency (NNSA) and its labs *"work to enhance national security through the military application of nuclear energy"*

- Los Alamos National Laboratory
- Lawrence Livermore National Laboratory
- Sandia National Laboratories

Sandia National Laboratories is responsible for the development, testing, and production of specialized nonnuclear components and quality assurance and systems engineering for all U.S. nuclear weapons.
[https://www.energy.gov/nnsa/locations]

Early career @ Sandia

In 2003, joined Sandia (in what is currently 1400) to become a Trilinos developer

- Anasazi: Generic templated framework for developing iterative algorithms for solving large-scale eigenproblems
- Belos: Generic templated framework for developing iterative algorithms for solving large-scale linear systems
- Teuchos: Collection of common utilities and tools that can be used by Trilinos packages

Observed (what seemed like) the exponential growth of capabilities provided by Trilinos, targeting the diverse needs of application codes at Sandia

Trilinos

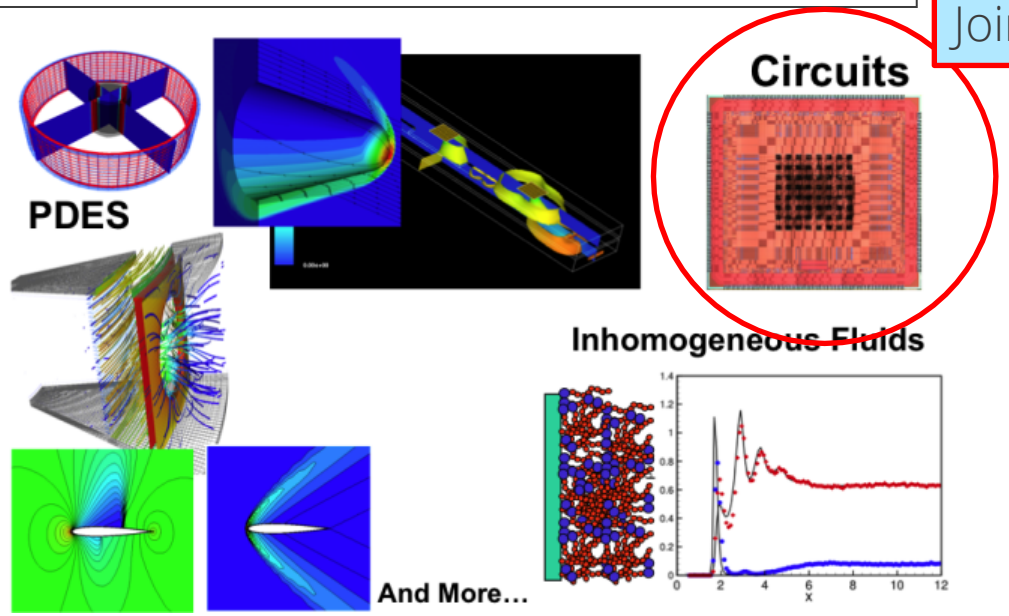
- R&D 100 Winner
- Open Source
  - Accessible via GitHub

Laptops to Leadership systems

- Geometry, Meshing
- Discretizations, Load Balancing
- Scalable Linear, Nonlinear, Eigen, Transient, Optimization, UQ solvers
- Scalable I/O, GPU, Manycore

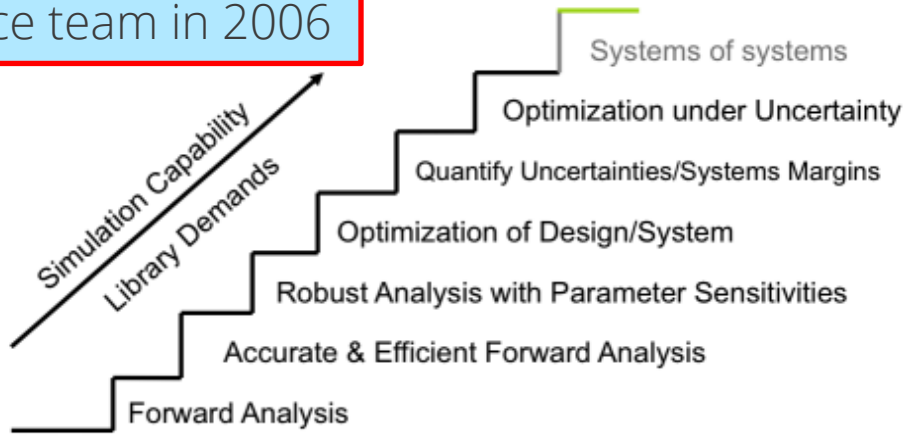
- 60 Packages
- Binary distributions

"An Introduction to Trilinos"
Presented by: Jennifer Loe
August 31, 2021



Joined the Xyce team in 2006

Transforming Computational Analysis To Support High Consequence Decisions



Each stage requires *greater performance* and *error control* of prior stages:
Always will need: more accurate and scalable methods.
more sophisticated tools.

Why is Xyce/Trilinos important? Who does this benefit?

- Comprehensive Test Ban Treaty (CTBT), signed in 1996, is a multilateral treaty that bans all nuclear tests, for both civilian and military purposes, in all environments
  - Limited environments in which "build and test" engineering could be used; increased need for modeling and simulation (mod-sim)
  - Advanced Simulation & Computing Initiative (ASCI), 1995
  - Qualification Alternatives to the Sandia Pulsed Reactor (QASPR), 2005

- Sandia ensures electrical systems survivability in hostile environments
  - Survivability: System and all components must retain mechanical/structural integrity and electrical components must continue to operate as designed
  - Hostile: Radiation (neutron, gamma, x-ray, and electromagnetic) environments

Sandia National Laboratories is responsible for the development, testing, and production of specialized nonnuclear components and quality assurance and systems engineering for all U.S. nuclear weapons.
[https://www.energy.gov/nnsa/locations]

How can analog simulation ensure electrical systems survivability?

Provides tradeoff between fidelity and speed/problem size

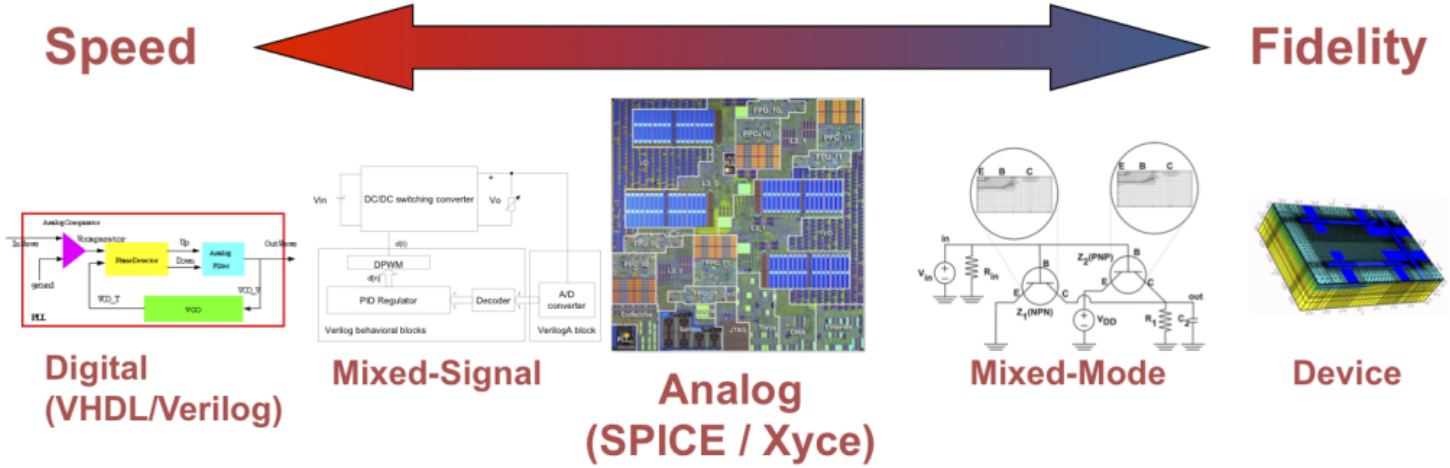
- Models network(s) of devices coupled via Kirchoff's current and voltage laws

$$\boxed{f(x(t)) + \frac{dq(x(t))}{dt} = b(t)}$$

- Xyce enables full system parallel simulation for large integrated circuits

Essential simulation approach used to verify electrical designs

- SPICE is the defacto industry standard (PSpice, HSPICE, etc.)
- Xyce supports NW-specific device development

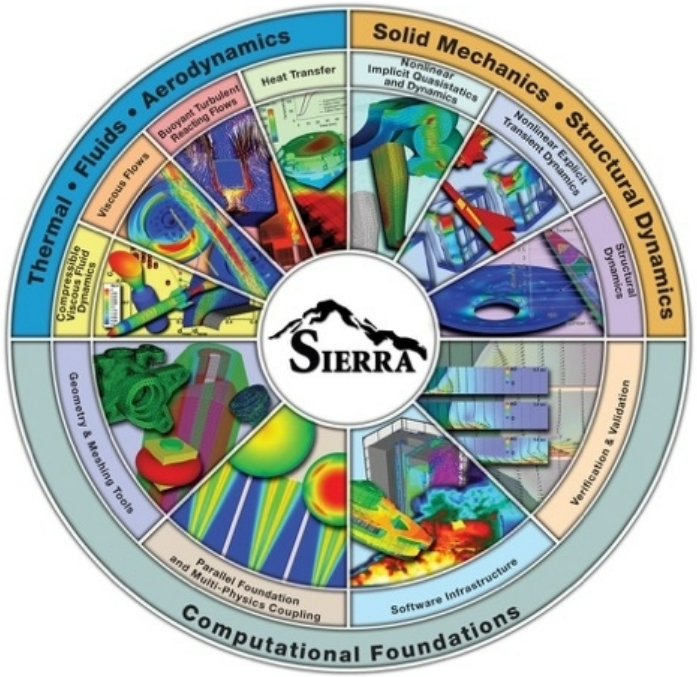


Sandia's Advanced Simulation & Computing (ASC) Code Suites

RAMSES

ITS SCEPTRE NuGET EIGER EMPHASIS Xyce Charon
CHEETAH Gemma EMPIRE

Electromagnetics, Radiation and Electrical Code Suite



Engineering Mechanics Code Suite

RAMSES
ITS SCEPTRE NuGET EIGER EMPHASIS Xyce Charon
CHEETAH Gemma EMPIRE

RAMSES

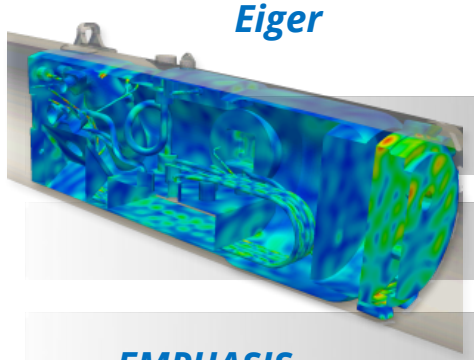
Radiation Analysis, Modeling and Simulation for Electrical Systems

RAMSES/EM
Electromagnetic and Plasma Applications

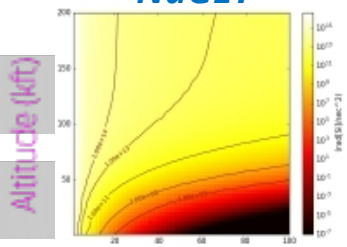
RAMSES/RAD
Radiation Transport Applications

RAMSES/CD
Circuit & Device Response Applications

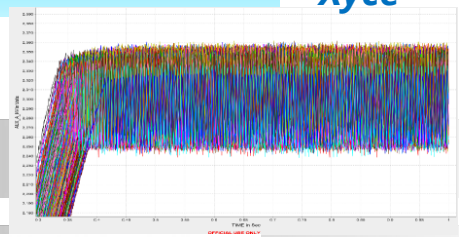
Eiger



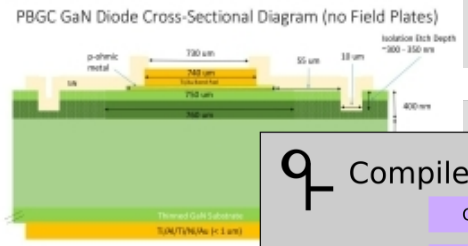
NuGET



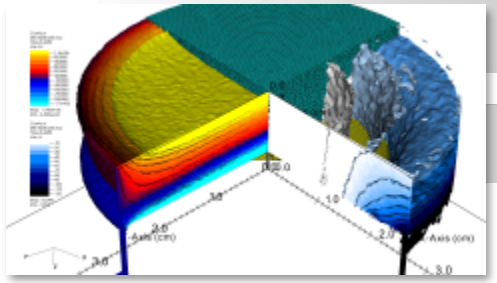
Xyce



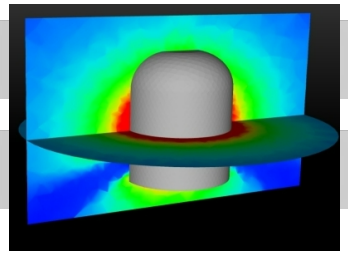
Charon



EMPHASIS



ITS/SCEPTRE



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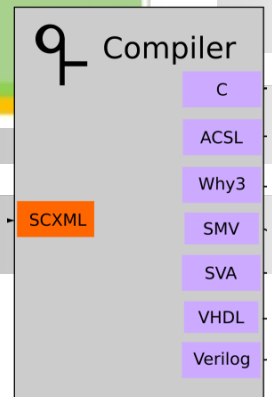


IC
P&EM
V&V
ATDM
CSSE/FOUS

RAMSES capabilities support NW design and qualification

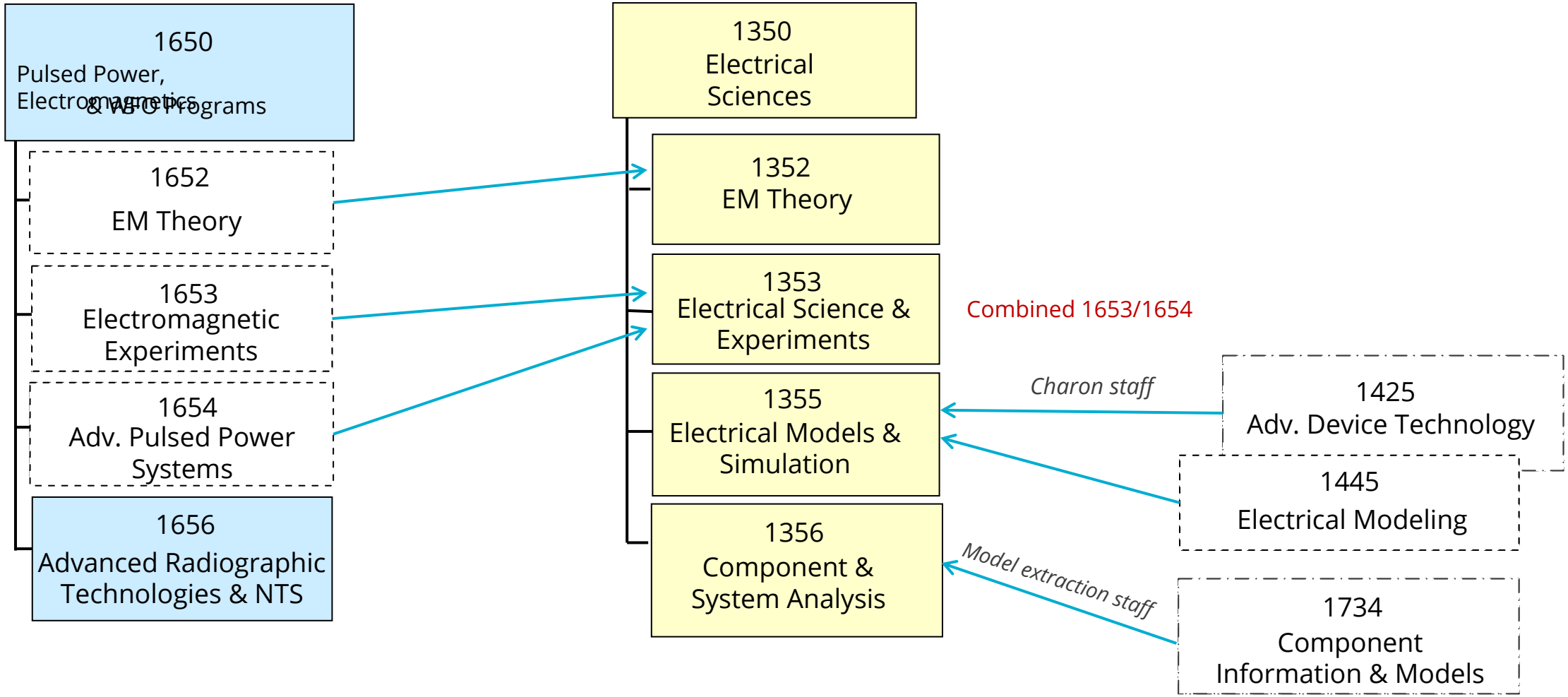
	Code	Physics	Numerics	NW Use Cases
Radiation transport 1300	ITS/Cheetah	γ - e^- transport	Monte Carlo (MC)	Environment Specification, INRAD, Cavity SGEMP, TREE, Impulse, TMS, TSR
	SCEPTRE	γ - e^- transport	Deterministic (DO)	Box & Cable SGEMP
	NuGET	N - γ environment, fireball	Builder/follower trajectory models, MC & DO transport	Environment Specification, QASPR, TREE, Heating, TMS, TSR, Dielectric breakdown
Electromagnetics & Plasma 1600	EMPHASIS/ EMPIRE	EM-Plasma	Time Domain EM with PIC, finite element	Qualification & design: Cable & Cavity SGEMP, Box IEMP, SREMP, Abnormal (Nearby Lightning), development of Environ. Specs
	EIGER/Gemma	Full wave electromagnetic	Frequency domain EM Integral Equation, Method-of-Moments	Qualification & design: Normal and Hostile EMR/EMP, development of Environ. Specs
Circuits & Devices 1400 / 8700	Charon	Transistor carrier transport & recombination	PDE solver Time domain and Frequency domain (in development)	Qualification & design, Neutron Effects, SGEMP
	Xyce	Analog circuit simulation	Non-linear DAE solver Time domain and Frequency domain	Qualification & design: Neutron Effects, SGEMP, Abnormal (Thermal), Normal (Aging, RF), development of Environ. Specs
	Q	Digital Formal Verification	Formal Mathematics	Digital Assurance, Design Verification, Off-Nominal Performance

The Electrical Sciences Consolidation (2013)

Working group recommendations:

- Provide a clearer and more responsive interface to mission partners for challenging electrical problems requiring a more fundamental understanding
- Better integrate and steward our ability to perform predictive electrical simulation (both physical and computational) across our mission needs
- Address specific identified gaps in capability and services
  - Improve ability to assess and respond to electrical issues in support of the Annual Assessment Review
  - Create the ability to perform -- at the level of fidelity required -- a *full system* analysis of ND electrical systems
  - Create substantial capability to assess electromagnetic effects on circuits (combined environments)

Moving from 1400 to 1300 through reorganization



Center 1300 - Radiation & Electrical Sciences

The Radiation & Electrical Sciences Center 1300:

- Develops technologies and operates facilities needed to assess and qualify the performance of nuclear weapons in electromagnetic and severe radiation environments.
- Develops theory, analytical techniques and computer codes to model the effects of radiation, electromagnetics and lightning on nuclear weapons components and systems.
- Conducts experiments to develop and validate these models and applies a broad range of experimental and computational tools to assess the performance of weapons in normal, abnormal and hostile environments.
- Special technologies that are resistant to radiation environments are also developed.

Center 1350 - Electrical Sciences

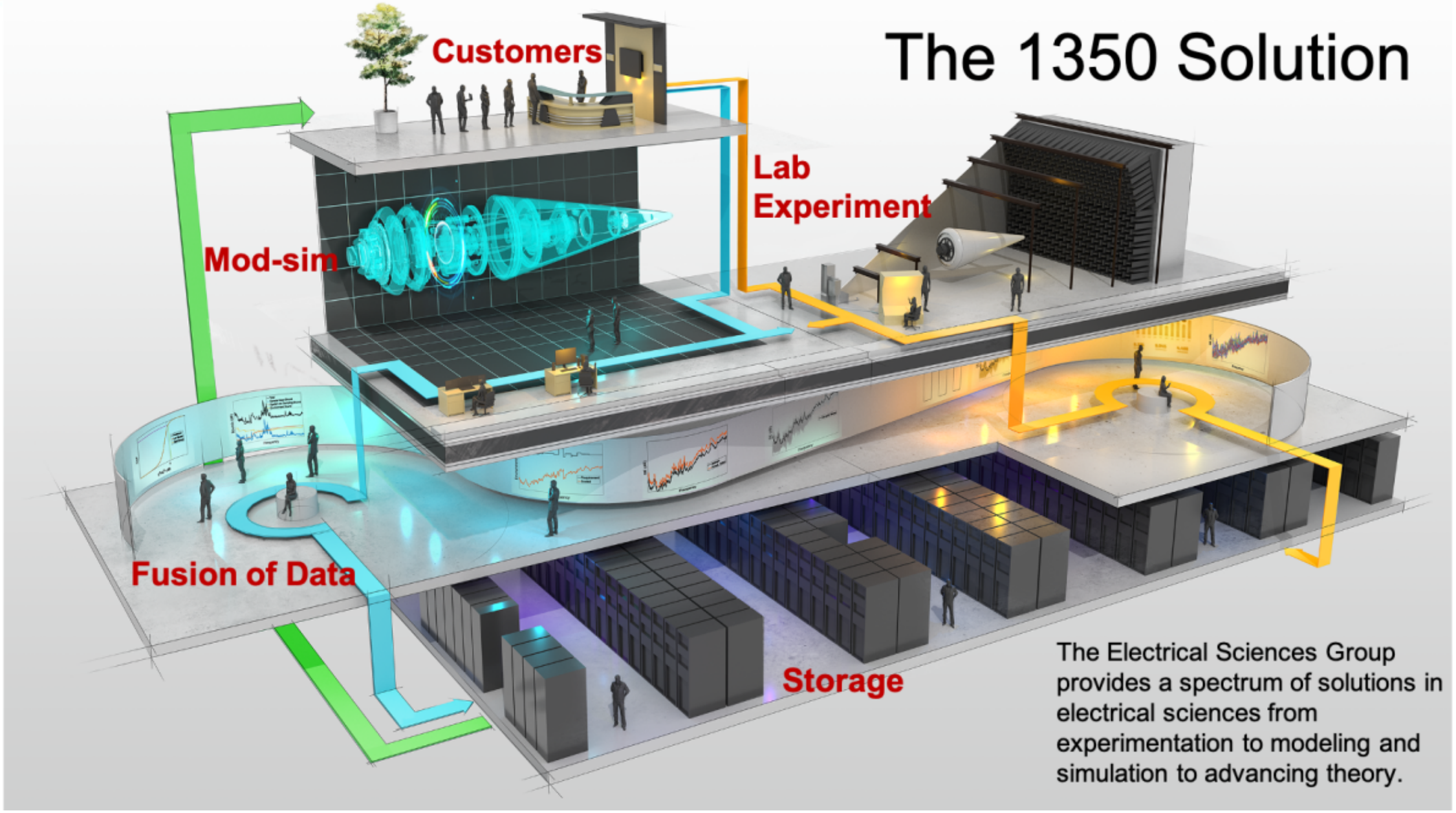
The Electrical Sciences Group provides a spectrum of solutions in electromagnetics environments effects and electrical sciences from experimentation to modeling and simulation to advancing theory.

	Code	Physics	Numerics	NW Use Cases
Electromagnetics & Plasma	EMPHASIS/ EMPIRE	EM-Plasma	Time Domain EM with PIC, finite element	Qualification & design: Cable & Cavity SGEMP, Box IEMP, SREMP, Abnormal (Nearby Lightning), development of Environ. Specs
	EIGER/Gemma	Full wave electromagnetic	Frequency domain EM Integral Equation, Method-of-Moments	Qualification & design: Normal and Hostile EMR/EMP, development of Environ. Specs
Circuits & Devices	Charon	Transistor carrier transport & recombination	PDE solver Time domain and Frequency domain (in development)	Qualification & design, Neutron Effects, SGEMP
	Xyce	Analog circuit simulation	Non-linear DAE solver Time domain and Frequency domain	Qualification & design: Neutron Effects, SGEMP, Abnormal (Thermal), Normal (Aging, RF), development of Environ. Specs

Facilities

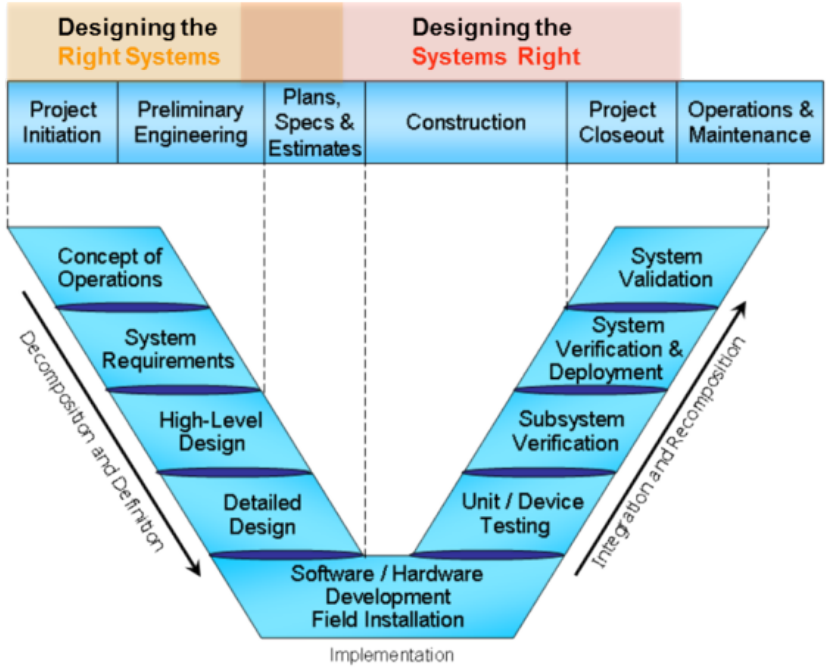
Electromagnetic Environments Simulator (EMES)
Lightning Simulator (SLS)
Reverberation Chamber (RC)
Large Gigahertz Transverse Electromagnetic (GTEM) Cell
Nearby Lightning Facility (NBL)
Sandia Anechoic Chamber (SAC)
Secure Scalable Microgrid Testbed

The 1350 Solution



The Electrical Sciences Group provides a spectrum of solutions in electrical sciences from experimentation to modeling and simulation to advancing theory.

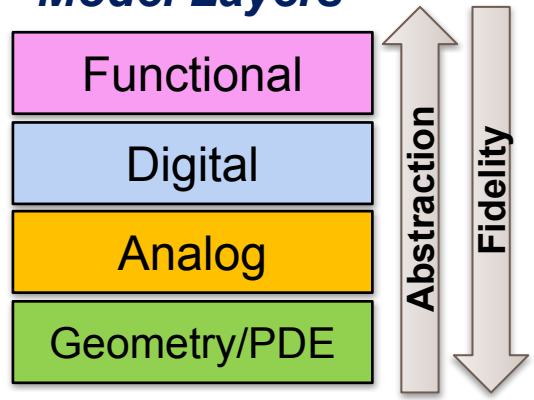
Moving Electrical System Mod-Sim from Qualification to Design

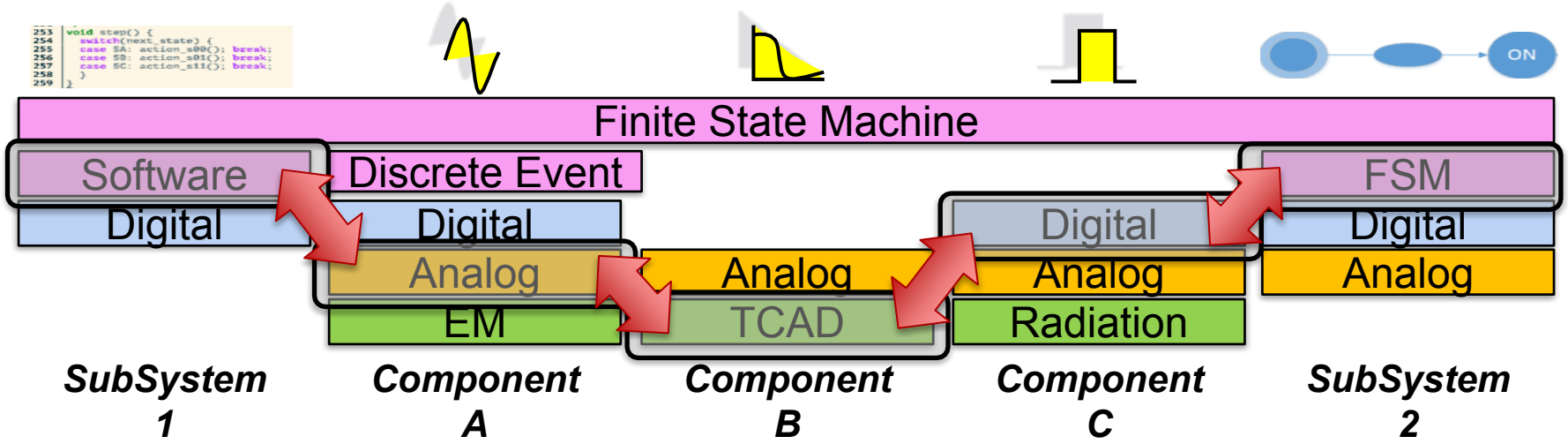


Key Challenges (enable Future Vision & Mod-Sim Integration)

- Interfaces between distinct models and tools
- UQ and V&V for multi-scale, e.g., mixed analog-digital
- Model consistency, selection, and abstraction
- Leverage and integrate with design activities

Model Layers

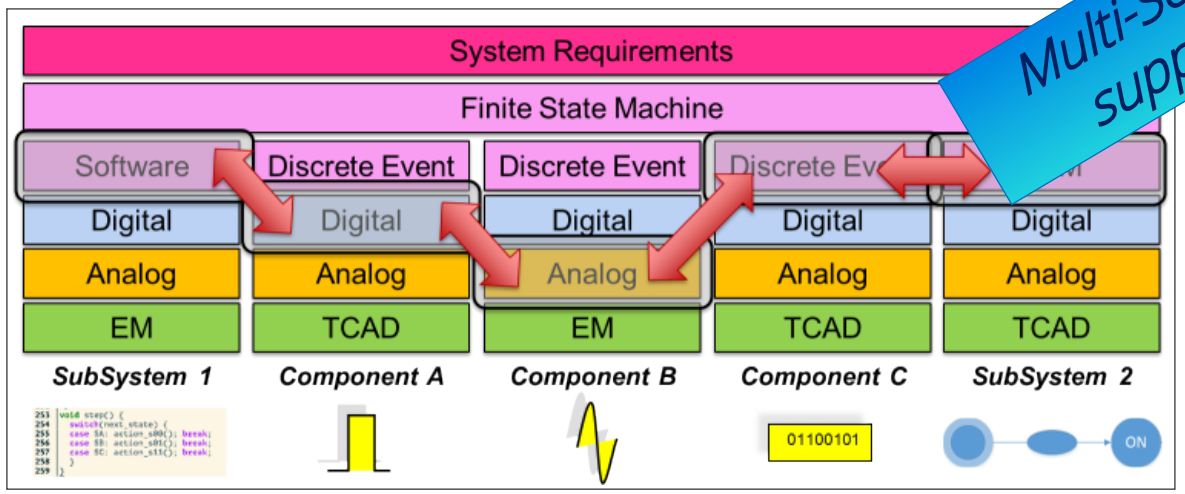


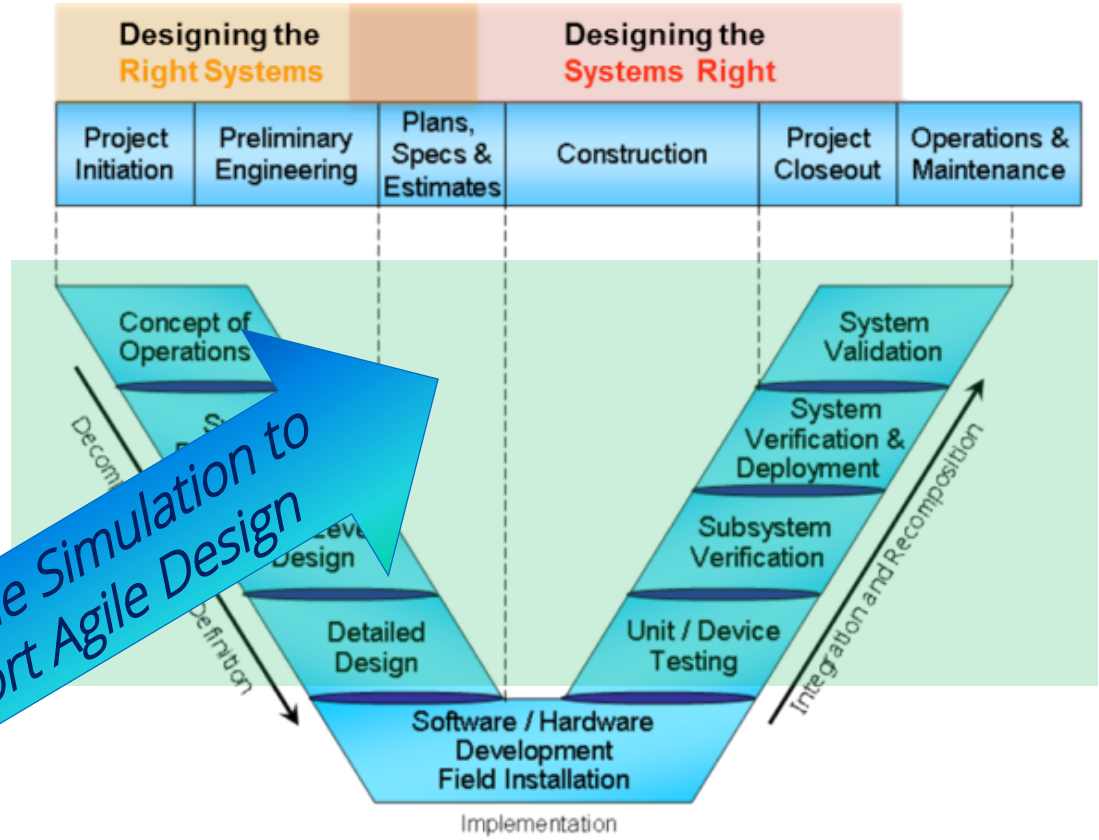


Enable Electrical Model-Based Design Engineering

Agile and Responsive Design aided by
Robust Integrated Mod/Sim Capability

- Credible, uncertainty-informed models available at outset
- Enable early phase design decisions and trade-offs (e.g., requirements, margins)
- Early integration with design teams → Enable rapid design iterations and improved qualification
- Distinct conceptual boundaries in electrical design (model) hierarchy (Ex.: Analog vs. Digital)





Multi-Scale Simulation to support Agile Design

Challenge:
Develop & integrate capabilities to support design engineering

Suggestions

- Disclaimer: Lots of fundamental science and applications to choose from at Sandia
- Ask about why your work is important and who is impacted?
  - LDRD, PMF
- Take advantage of ”open door” policy
  - Attend seminars, even if they are not in your area of expertise
- The opportunities are endless

Questions?