

LA-UR-13-23172

Approved for public release; distribution is unlimited.

Title: A Millenial's Perspective on the Future of
Monte Carlo Radiation Transport

Author(s): Kiedrowski, Brian C.

Intended for: M&C 2013, SUn Valley ID, May 6, 2013



Disclaimer:

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

A Millennial's Perspective on the Future of Monte Carlo Radiation Transport

Brian C. Kiedrowski
Los Alamos National Laboratory

ANS Mathematics & Computation 2013 Topical
Sun Valley, Idaho
May 6, 2013

***Contributors: Ben Betzler (Michigan), Keith Bledsoe (ORNL), Forrest Brown (LANL),
Tim Burke (Michigan), Sean Carney (Michigan), Josh Danczyk (Caterpillar Inc.),
Jesson Hutchinson (LANL), Bill Martin (Michigan), Chris Perfetti (ORNL),
Brad Rearden (ORNL), Mike Rising (LANL), Paul Romano (KAPL),
Anthony Scopatz (U. Chicago), C.J. Solomon (LANL), Paul Wilson (UW-Madison)***

Abstract

Monte Carlo was once referred to as “the method of last resort” for radiation transport problems. Today, with continuing advances in both methods and computing, the use of Monte Carlo is rapidly becoming routine for applications once thought unthinkable. In the next decade or two, I predict that Monte Carlo transport will be commonly used for multiphysics applications for static and transient analysis, parameter space analysis for design optimization for both forward and inverse problems, and uncertainty and bias quantification. To address these upcoming needs, I see many exciting areas in methods research including: hybrid methods for rapid statistical and eigenvalue source convergence, genetic algorithms for design, methods for efficiently simulating and analyzing correlated signals for radiation detection applications, new data access paradigms for massively parallel calculations, schemes for handling arbitrary numbers of temperatures, and sensitivity analysis to compute response derivatives. Despite our methods research being at the cutting edge, our production radiation transport codes often lag behind modern software engineering practices and will need to become more agile and adaptable to handle future applications or risk becoming extinct. As an example, I will discuss some of the challenges that the MCNP Monte Carlo code faces toward addressing our future needs.

Overview

- **My perspective as a millennial (someone born between 1981-2001) on Monte Carlo radiation transport.**
- **Address my opinions on the following questions:**
 - **What kinds of Monte Carlo radiation transport calculations that are prohibitive today will be routine 10-20 years from now?**
 - **What research efforts today in methods are helping us get there?**
 - **What are the challenges in computing that we as a community will need to address along the way?**

Monte Carlo Basics

- Solve the neutron transport equation:

$$\frac{1}{v} \frac{\partial \psi}{\partial t} + \mathbf{\Omega} \cdot \nabla \psi + \Sigma \psi = \iint \Sigma_s \psi \, dE' d\mathbf{\Omega}' + Q$$

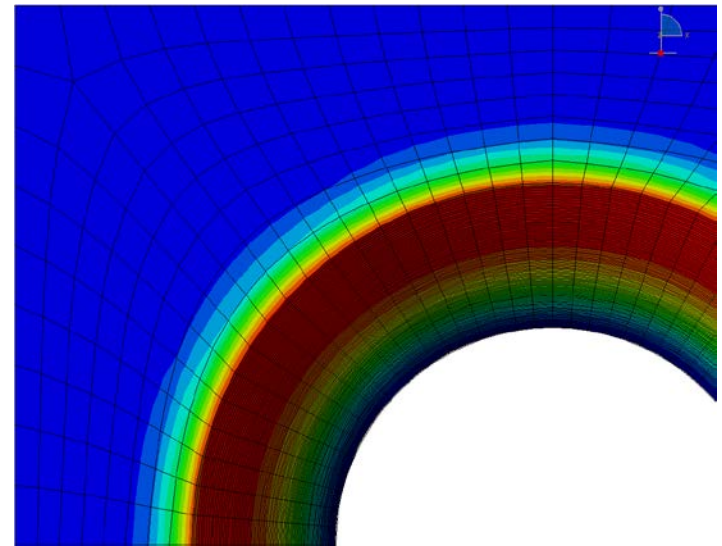
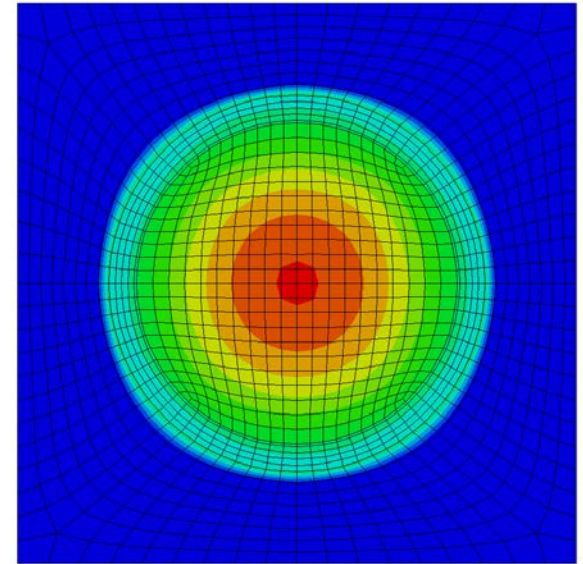
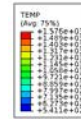
- The function ψ is the mean value of radiation behavior.
- **Method:**
 - Simulate random behavior of particles of radiation
 - Find averages based on that simulation
 - The averages correspond to solutions of the transport equation
- Advantage: Can get very accurate results (with good models, data)
- Disadvantage: Random solution technique = slow convergence

Future Routine Calculations

- **Radiation transport is needed for many applications:**
 - Nuclear reactor design, radiation detection, shielding, criticality safety, medical physics, accelerators, etc.
- **Today, Monte Carlo techniques are used to some degree in all of them.**
- **Cutting across many of these areas, what kinds of Monte Carlo calculations are a decade or two away from being a routine part of engineering analysis?**
 - Multiphysics with feedback
 - Design space analysis and optimization
 - Uncertainty and bias quantification

Multiphysics

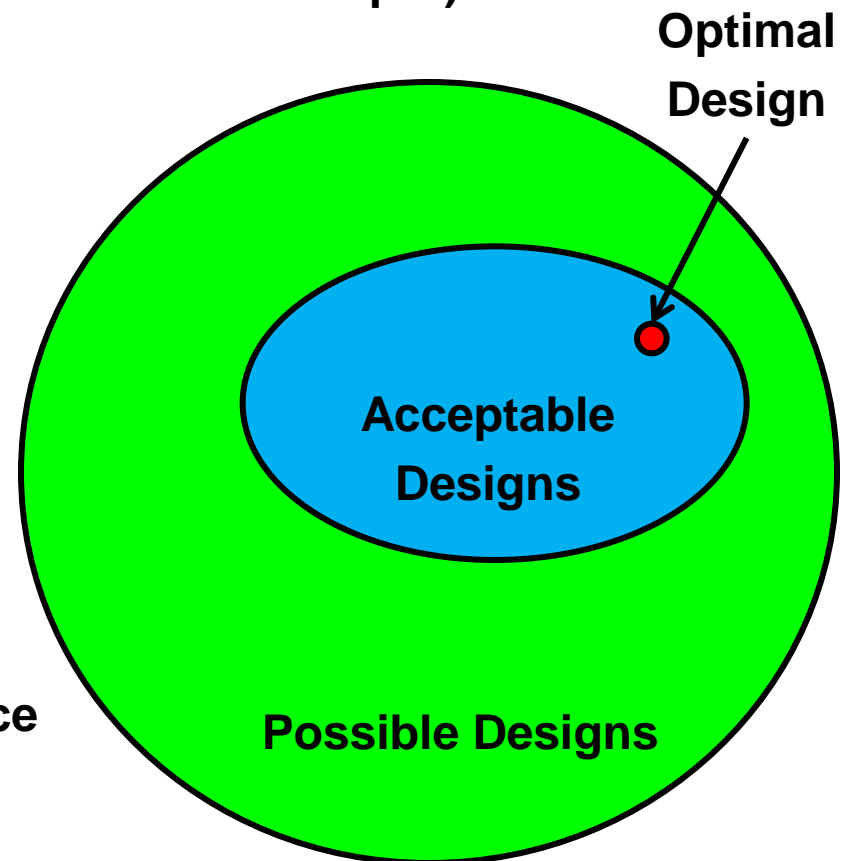
- Monte Carlo will be routinely used for the radiation transport of static and transient multiphysics analysis.
- Challenges:
 - Transport on geometry from CAE tools.
 - Statistical noise tends to break many thermal, fluids, etc. analysis methods.
 - Mapping of meshes from different physics.
 - Feedback methodology and operator splitting (self-consistency), ensuring convergence to correct solution



Images from Tim Burke

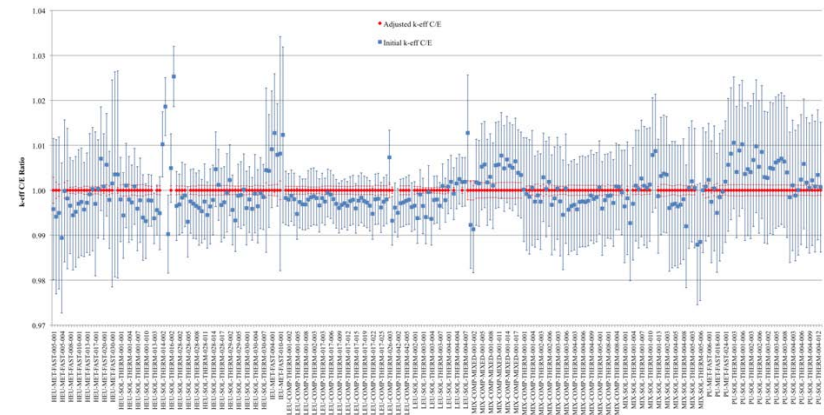
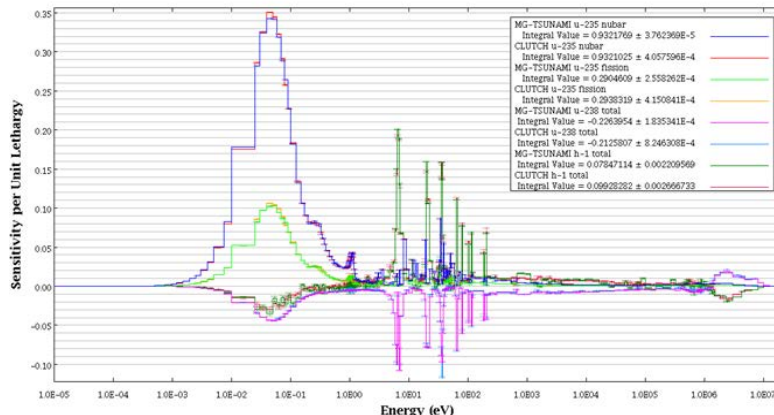
Design Space Analysis and Optimization

- Design involves numerous calculations and searching for optima based on a set of criteria and constraints
 - Forward problem (inputs given, outputs obtained)
 - Inverse problem (outputs given, find best match input)
- Challenges
 - For small enough spaces, brute force Monte Carlo works.
 - Otherwise need more sophisticated search methods:
 - Generalized Least Squares
 - Differential Evolution
 - Genetic Algorithms
 - Data management of design space calculations (big data).



Uncertainty and Bias Quantification

- For safety applications and validation, it is important to be able to provide reliable estimates of uncertainties.
 - Arise from: densities, enrichments, compositions, geometry, temperatures, **nuclear data**, etc.
- Sensitivity analysis is needed to explain the origins of most of the uncertainty and bias in calculations
 - Drives margins and reduces design conservatism (**saves money!**)
 - Predictive capability to remove the need for or to identify focused experiments to improve computer models and data.



Images from Chris Perfetti

Current Research and Development Efforts

- What is being researched today to help us get there?
- Hot topic areas include:
 - Convergence with hybrid and matrix methods
 - Temperature treatments
 - Optimization and genetic algorithms
 - Signal analysis and correlations
 - Sensitivity analysis
 - New parallel and data access paradigms
 - Many more there just is not time to discuss!

Slow Statistical Convergence

- Monte Carlo may get very accurate answers (assuming good models, nuclear data, etc.), but doing so may take a long time.

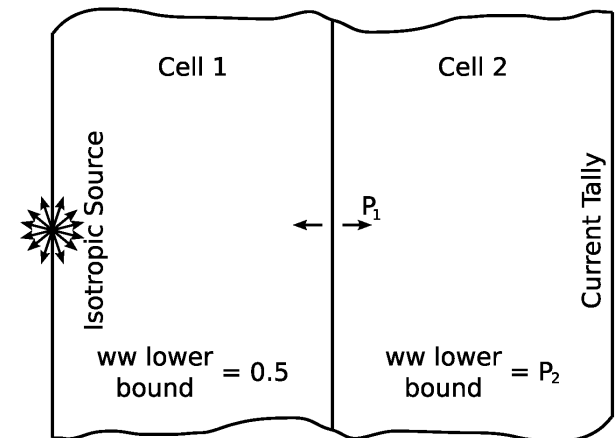
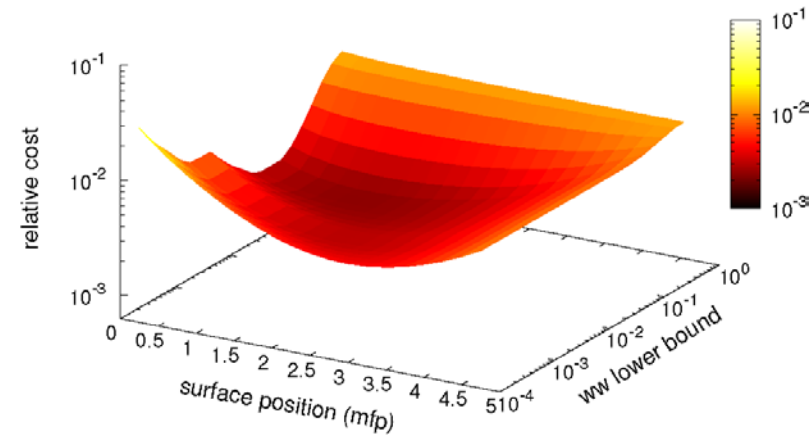


$$\text{Convergence} \sim \frac{\text{Const}}{\sqrt{N}}$$

- As computers get faster, the problems engineers want to solve get harder!
- Need to be clever and apply variance reduction techniques to solve many problems in a reasonable amount of time.
 - How do we pick the parameters to minimize the constant?
 - Is it possible to break the speed limit?

Hybrid Methods for Convergence Acceleration

- **Adjoint-based approaches**
 - Use adjoint function as importance
 - Examples: CADIS and FW-CADIS
- **Cost optimization with second moments**
 - Deterministically calculate MC variance
 - Optimize VR for figure of merit
- **Learning algorithms for geometric convergence**
 - Gain information from random walks
 - Theoretical convergence rate is **geometric**
 - How to prevent false learning?

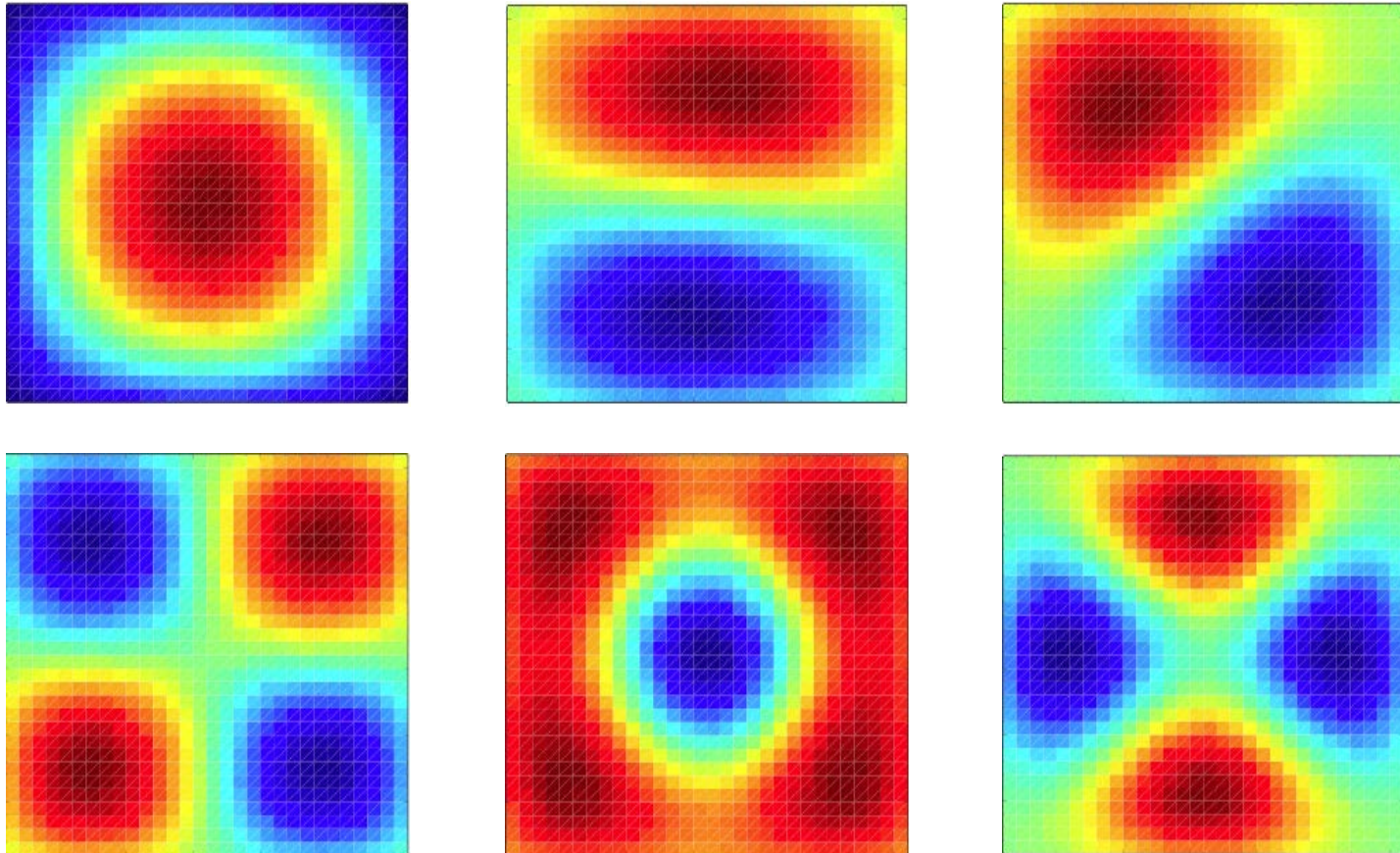


Reactor Analysis Issues

- Reactor applications are typically solved as eigenvalue problems.
- In addition to statistical convergence, the source is unknown and must be converged from an initial guess.
 - Much work to accelerate with higher modes/matrix methods
 - Higher modes may also be used to approximate correlation effects to get better confidence interval estimates
- Reactor transients may also be described with higher modes
 - Examples: Control rod movement, xenon oscillations, temperature feedback
- Thermal analysis with feedback requires appropriate temperature treatments
 - How to efficiently handle 1000's of temperatures?

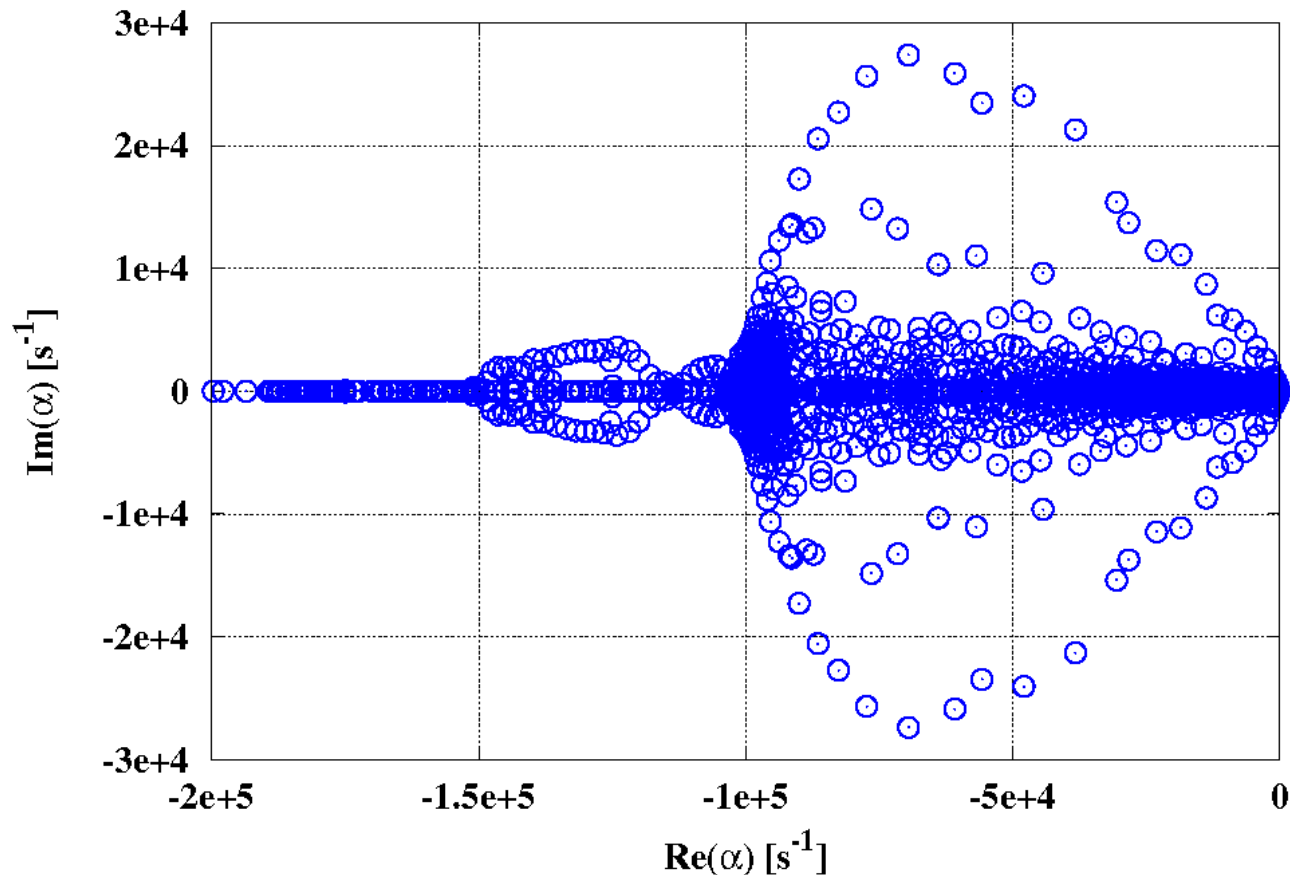
Matrix Methods and Higher Eigenmodes

- Matrix methods allow for 100+ eigenmodes to be obtained routinely today for the k-eigenvalue problem
 - First six modes for 2-D Pressurized Water Reactor



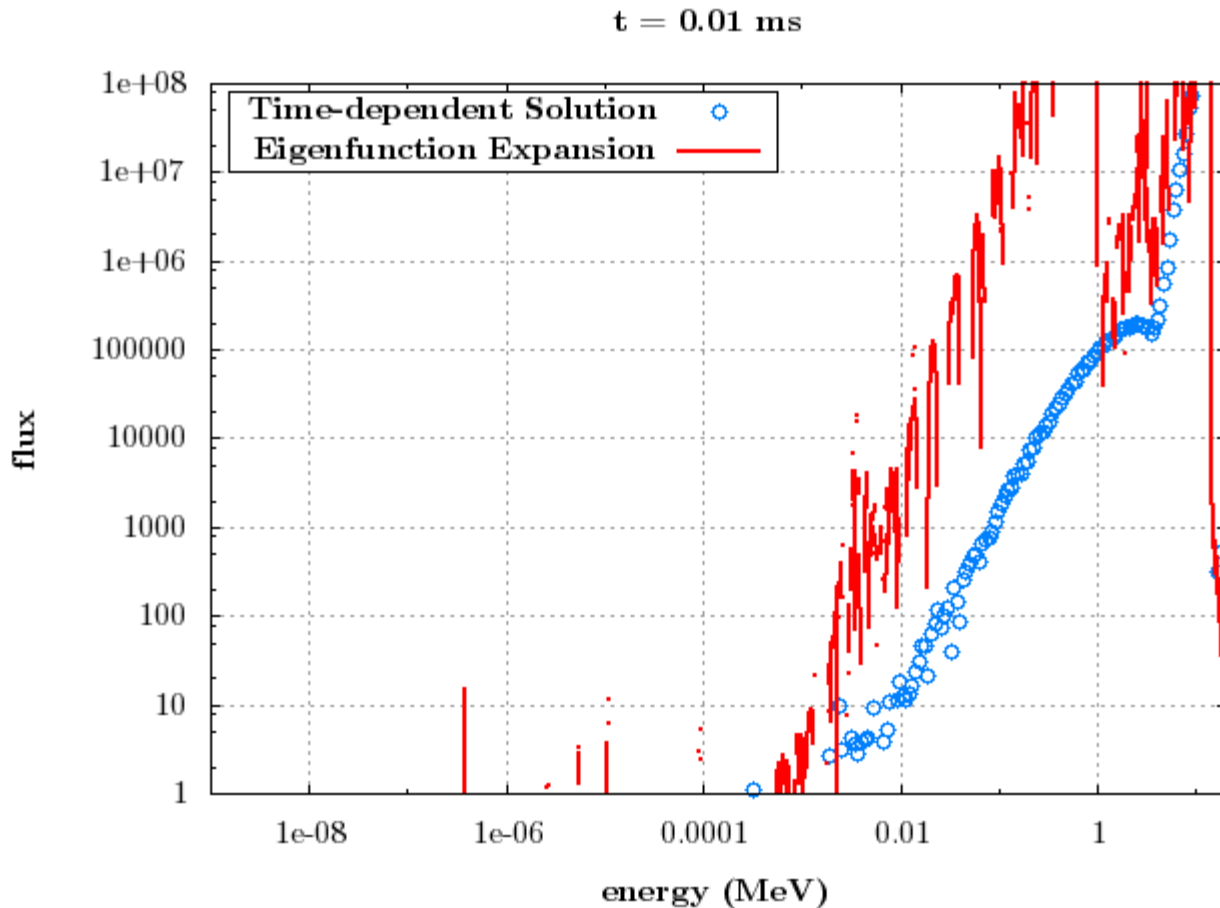
Matrix Methods and Higher Eigenmodes

- Dynamic (alpha) modes for transient analysis may make modal methods attractive.
 - First 3,000 eigenvalues for neutrons in subcritical graphite-UO₂ Mix



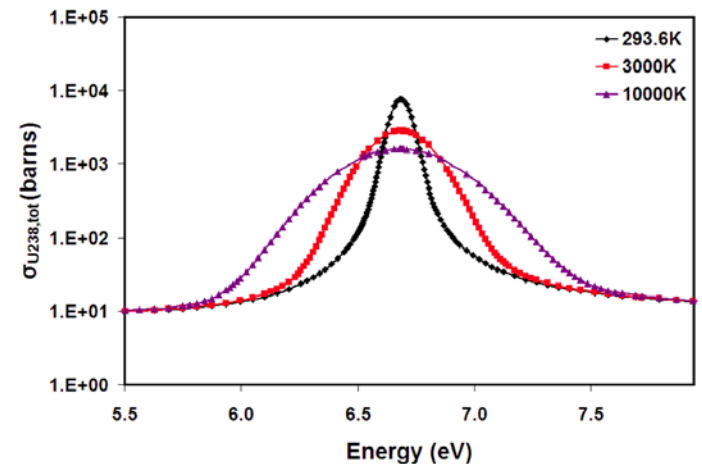
Matrix Methods and Higher Eigenmodes

- Dynamic (alpha) modes for transient analysis may make modal methods attractive.



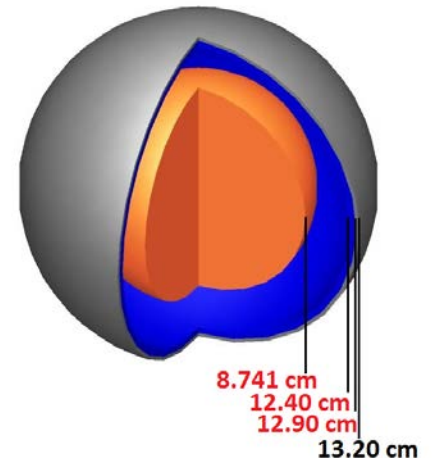
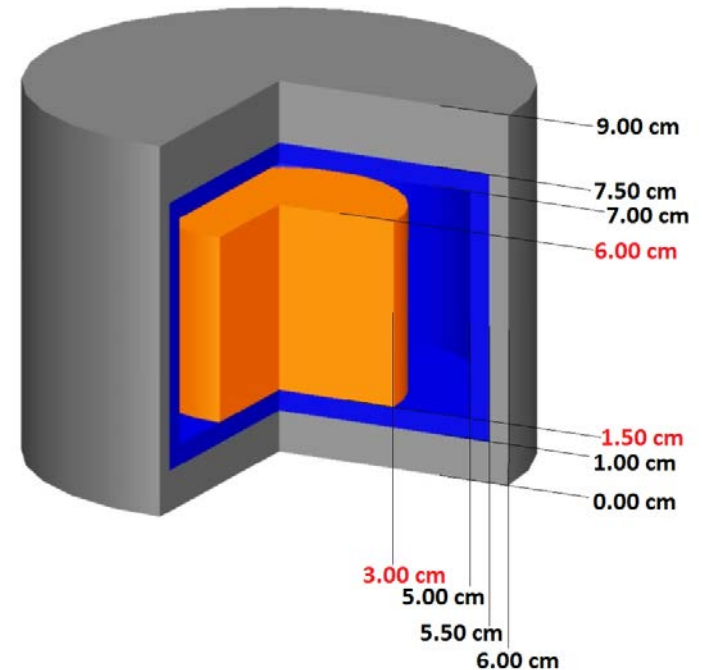
Temperature Treatments

- **Appropriate elastic scattering near resonances**
 - Removal of constant cross section approximation employed in most production Monte Carlo codes
- **Doppler broadening that is automatic and efficient in both speed and memory:**
 - “On-the-Fly” Method (MCNP)
 - “Explicit Target Thermal Motion” Method (Serpent)
- **Almost a solved problem, but what about...**
 - $S(\alpha, \beta)$ and unresolved resonances?
 - Application to temperature coefficients, feedback?



Optimization and Genetic Algorithms

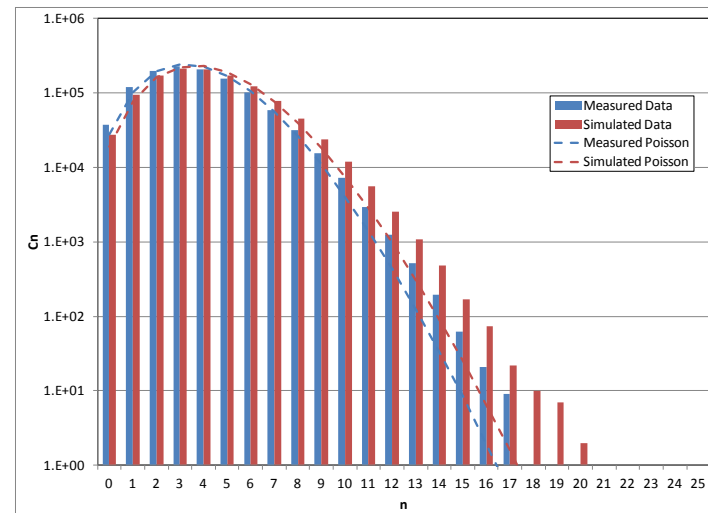
- **Determine optimal design**
 - Forward problem based upon a set of design criteria
 - Inverse problem based upon best match of measurable
- **Approaches**
 - Perturbation based
 - Gradient based optimization
 - Stochastic optimization
- **Challenges**
 - Dimensionality of spaces
 - Local optima, degeneracy
 - Searching results “big data”



Images from Keith Bledsoe

Signal Analysis and Correlations

- Many applications involving radiation detection and safeguards cannot be handled with the classic mean-value treatment.
 - Requires strict energy and momentum conservation, which many Monte Carlo codes and nuclear data do not yet support.
 - Often measures the correlations between detector signals (e.g., Rossi Alpha) or moments of counts (e.g., Feynman Variance).
- Having correlated responses may help resolve degeneracy issues faced in many inverse problems.



Images from Jesson Hutchinson

Sensitivity/Uncertainty Analysis

- Providing uncertainty estimates determines design margins.
- Methods:
 - Perturbation theory (MG + CE)
 - Polynomial chaos
 - Brute force Monte Carlo
- Sensitivity analysis can determine sources of uncertainty and bias
 - Smaller design margins = lower cost
- Challenges
 - More and better covariance data
 - Temperature correlations
 - Data adjustment, experiment design
 - Non-linear problems, multiphysics

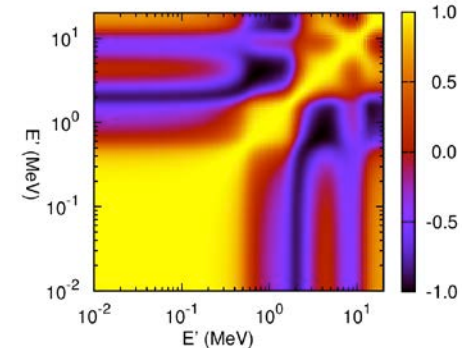
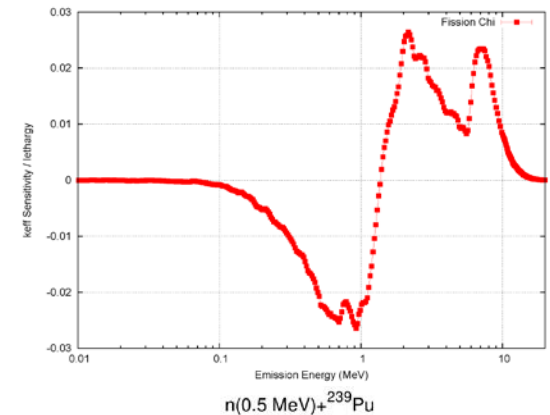
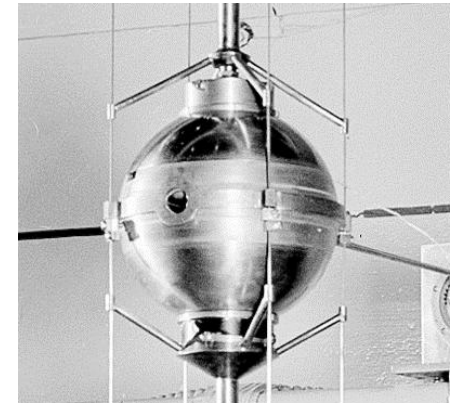
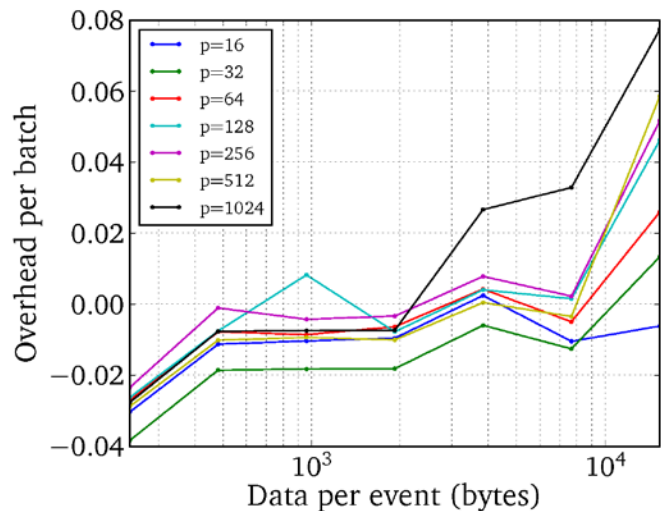


Image from Mike Rising

Parallel Methods

- **Must utilize computational resources on current and future architectures to take advantage of Moore's Law.**
 - **Parallel execution: MPI + Threads (OpenMP) + ???**
 - **Heterogeneous architectures: CPUs + GPUs + MICs + ???**
- **Challenge of handling data transfer across network for parallel scaling**
 - **More overall memory on cluster, but probably less per core**
 - **Domain decomposition, data decomposition, tally servers, ???**



Tally Server Concept

- **Portions of cluster are dedicated nodes or servers for storing and accruing tallies.**
- **Servers listen for and receive tally scores from compute nodes.**
- **Shows minimal overhead, good scaling.**

Courtesy of Paul Romano

- **Methods and software will need to be adaptable.**

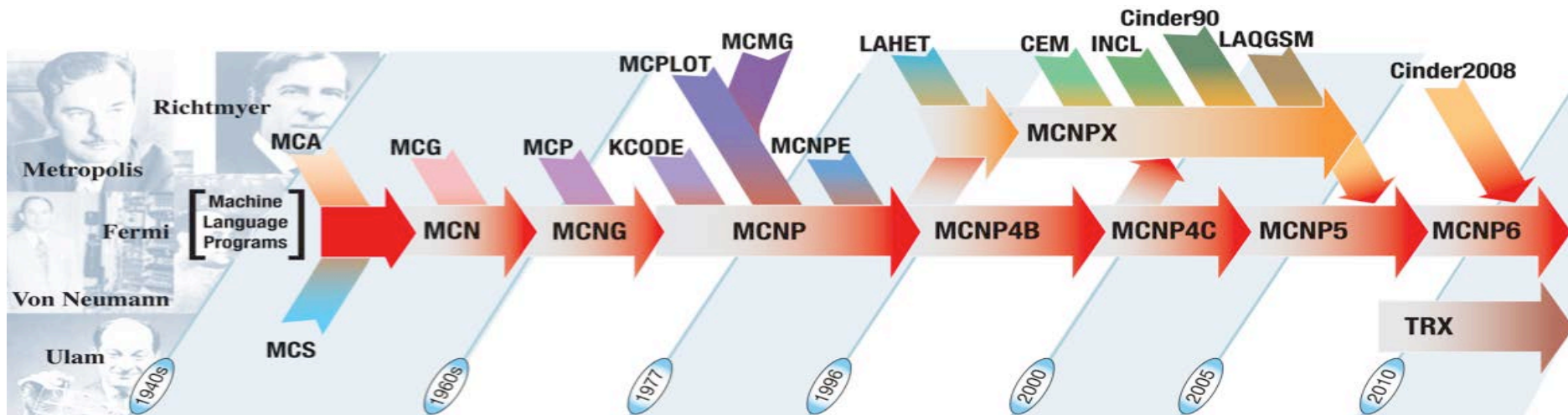
Challenges in Software Engineering

- This was only a small sampling of the exciting methods work going on today.
- We as a community are on the cutting edge for methods research and development.
- But...
 - Will the future engineers be able to take full advantage?
 - Can our aging production-level software infrastructure (the codes) incorporate these new capabilities while supporting advances in computer hardware? Will they even be able to solve current problems on new architectures?
 - Are the design paradigms of today sustainable for the future?

Our Aging Software Infrastructure

- Nuclear engineering software development was pioneering in the field of scientific computing
 - We have a very proud **legacy** of innovation going back to the 1940's.
 - Much of our software was built to support the burgeoning nuclear enterprise during the Cold War Era.
- Times have changed...
 - The explosion of personal computing has changed the focus of computer vendors.
 - Software engineering has evolved as its own discipline and largely left us behind.
 - **Our legacy often makes future development and innovation more difficult!**
- Case study: the MCNP Monte Carlo code

MCNP History



- In the 1950s-1970s, MCNP emerged as pieces of smaller special-purpose codes and evolved since then.
 - MCNP5 focused on modernization and parallelism of the 2000s with focused enhancements for key NNSA initiatives.
 - MCNPX created as a spinoff project for accelerator work and efforts were solely toward capability enhancements for numerous sponsors.
- MCNP6 is a merger of MCNP5 and MCNPX and more
 - MCNP5 has ~100K lines of code
 - MCNP6 has ~400K lines of code

MCNP Software Practices

- Core transport routines of MCNP largely retain the same fundamental coding structure of the past.
 - Modularity not part of the design, efficiency on now long extinct machines was, leading to tangled “spaghetti code”.
 - Different and outdated coding and software development philosophies. Best practices of a very different time.
 - Structural improvements have occurred, but are incremental and do not keep up with addition of new capability.
- Growth in the codebase has made it **very difficult to manage**.
- Poor design practices incur a **technical debt** and when doing future development, **interest is paid** on the debt in the form of extra, non-productive effort.
 - New methods increasingly difficult to implement.
 - Current release is very painful, and subsequent releases will be even worse unless changes are made.

Three Possible Options for MCNP's Survival



Business as Usual

(Continue taking on debt)

As more gets added, costs continue to rise and it becomes increasingly difficult to ensure reliability, becomes unsustainable, and stymies the ability to implement new capability.



Complete Rewrite

(Declare bankruptcy, cut losses)

Requires an unusually large commitment, a focused application, few users, or institutional investments. Not practical for MCNP, but may be for other efforts, e.g., MCATK, MC21, OpenMC, Serpent.



Modernization

(Refinance, pay principal)

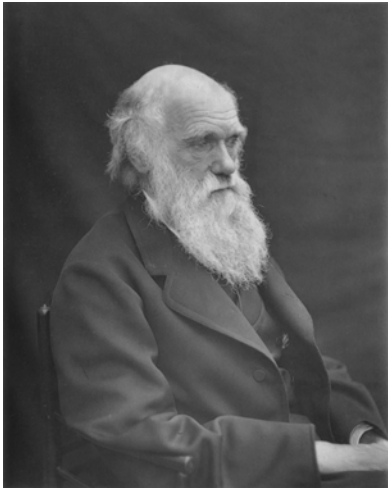
Redesign for modularity, ease of understanding, and adopt modern software design and QA practices. Make adding (and removing) functionality easy and unit testable.

Aggressive Modernization

- For MCNP to exist as an ongoing development project 10-20 years from now, we need to perform **aggressive modernization**.
 - Old development models and paradigms unsustainable with a significantly larger codebase, changing hardware, skills of prospective employees, etc.
- Core routines of MCNP in serious need of restructuring.
 - Make capability development, testing, and maintenance easier.
- As developers, we must change our practices.
 - Adopt best practices and peer review at all phases of design.
 - The single integrator (hero) model cannot work with large software packages (too big with too many different capabilities), need teams of experts managing core capabilities.
- This applies to any large legacy code if it hopes to move into the next few decades as a viable development platform.

A Guiding Principle for Software Design

- A misquote, often mistakenly attributed to Charles Darwin, but applicable to software design in general:



“It is not the strongest of the species that survives, nor the most intelligent that survives. It is the one that is most adaptable to change.”

- **NOT** Charles Darwin

- Adaptability needs to be a conscious design goal for production radiation transport software.
 - Software developers of new codes following today’s modern best practices need to continue to adapt to new paradigms and be vigilant or they too will eventually reach a similar situation.

User Data Handling

- **Transport codes require engineers to prepare inputs and to post process output data**
 - Many scripts exist for this purpose, either homegrown or prepackaged with software
 - For the former case, engineers are constantly reinventing the wheel
- **Computer time has largely become relatively cheap, whereas the time spent by the engineer is expensive.**
- **How can we as developers make work easier (and less costly) for the engineer?**
 - Standardized formats and libraries
 - Publicly available, open source data processing utilities
 - Robust data and file management needed to handle massive data from different designs or parameters of same design

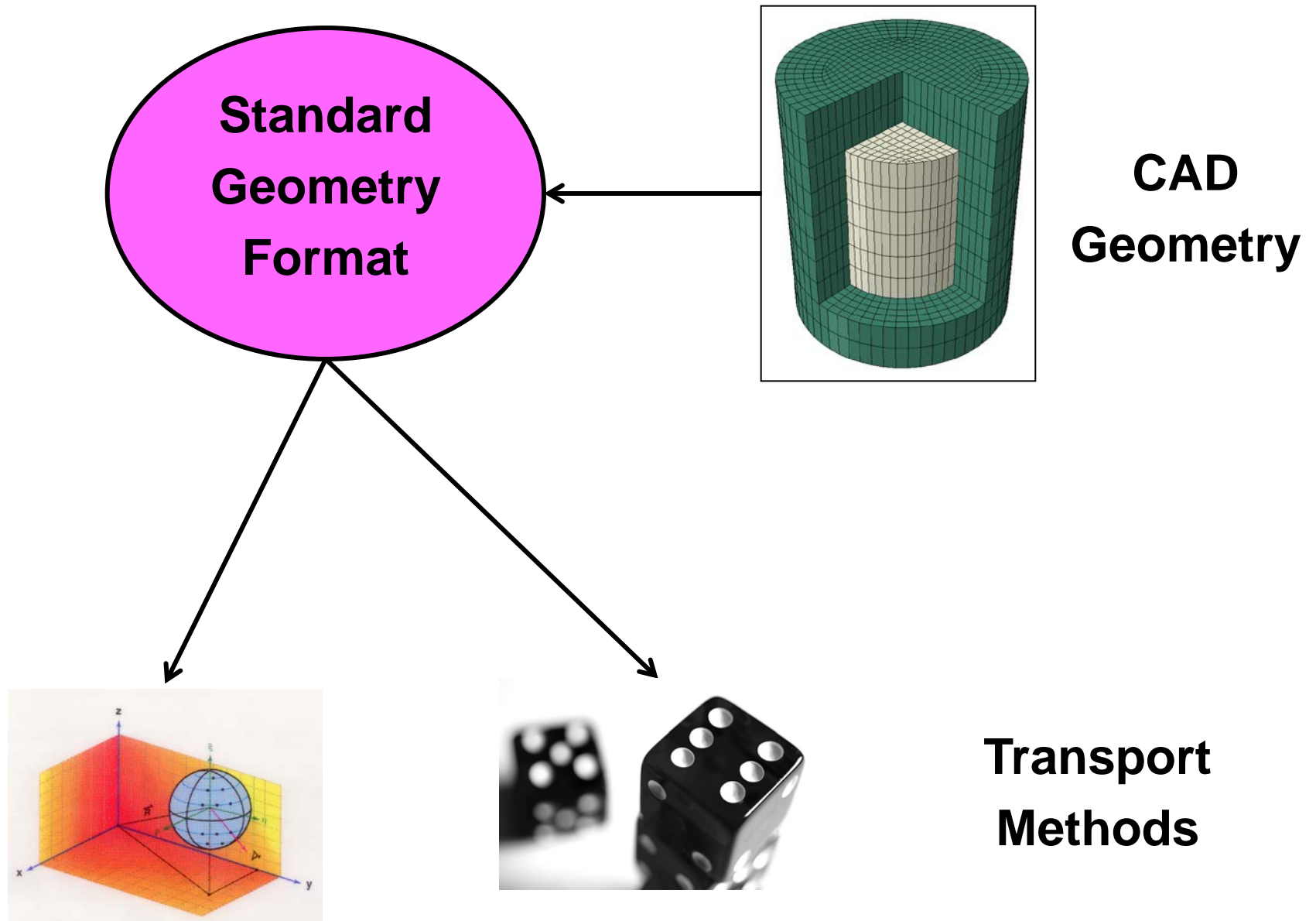
Standardized Formats for Radiation Transport

- **Proposal: Revisit the idea of developing a set of **standardized formats for radiation transport applications**.**
 - Would cover as many possible things transport codes need as part of their workflow.
 - Needs commitment from radiation transport code developers and applications professionals with international support.
 - Develop and publish standards that code developers may implement as part of their I/O processes.
- **This was tried in the 1970s (CCCC) in the “punch card era”.**
 - Formats are today “old fashioned” and predate advances in data representation and storage (e.g., XML was not codified until the mid 1990s!)
 - New capabilities in this area mean we should perhaps give this another look.
 - File formats need to be **general, self-describing, and extensible**!

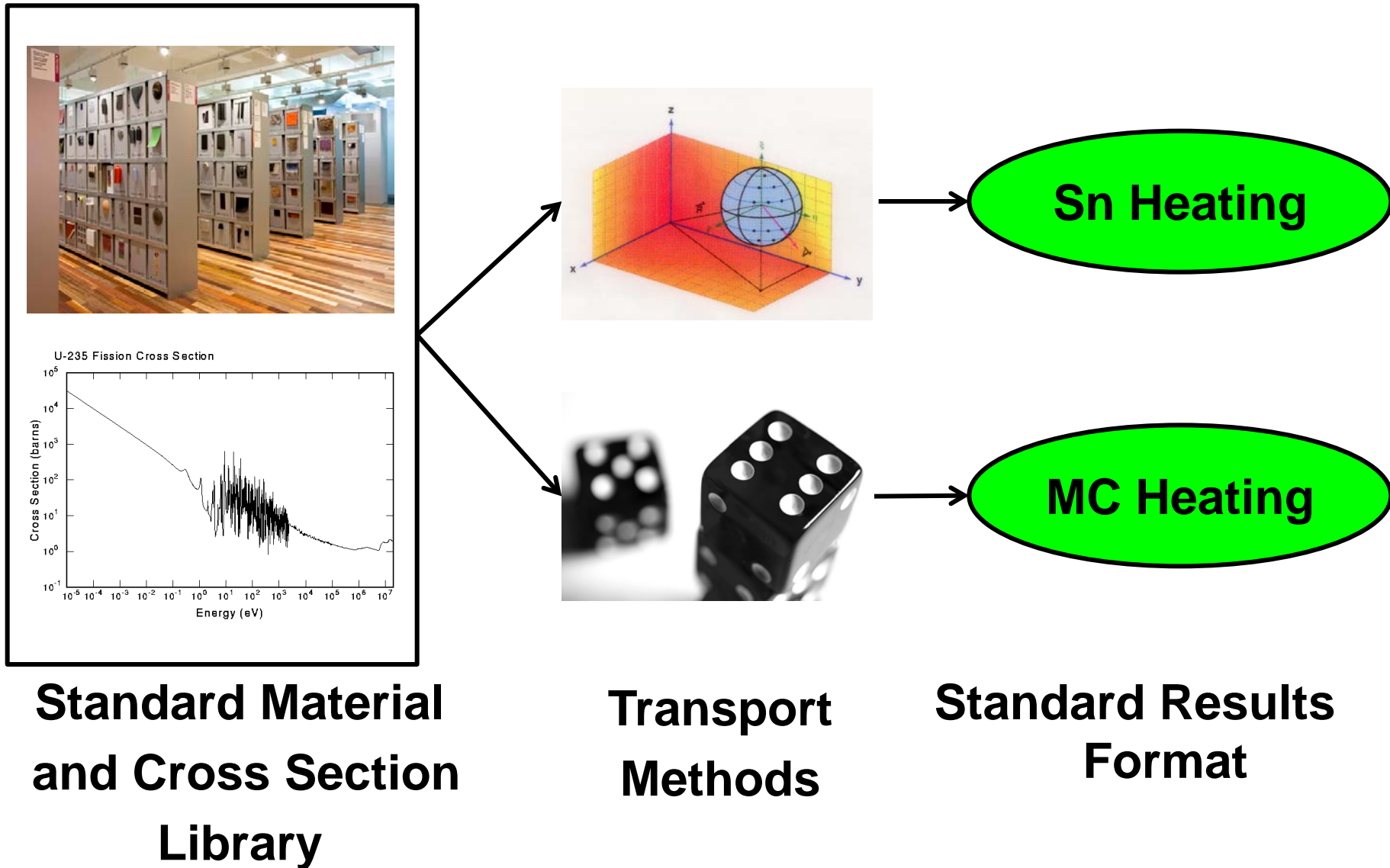
An Issue and a Proposal

- **Common needs:**
 - **Geometry**
 - **Material properties (isotopics, densities, temperatures, etc.)**
 - **Nuclear data (cross sections, decay data, etc.)**
 - **Response functions**
 - **Results (Fluxes, doses, reaction rates, heating, etc.)**
 - **Sensitivities/Uncertainties**
 - **Design parameter descriptions**
 - **Etc.**
- **Each Design Tool within the process (geometry package, transport code, TH solver, etc.) reads/writes data in standardized formats.**
- **Design Tools should be interchangeable and be able to read/write the standardized formats.**

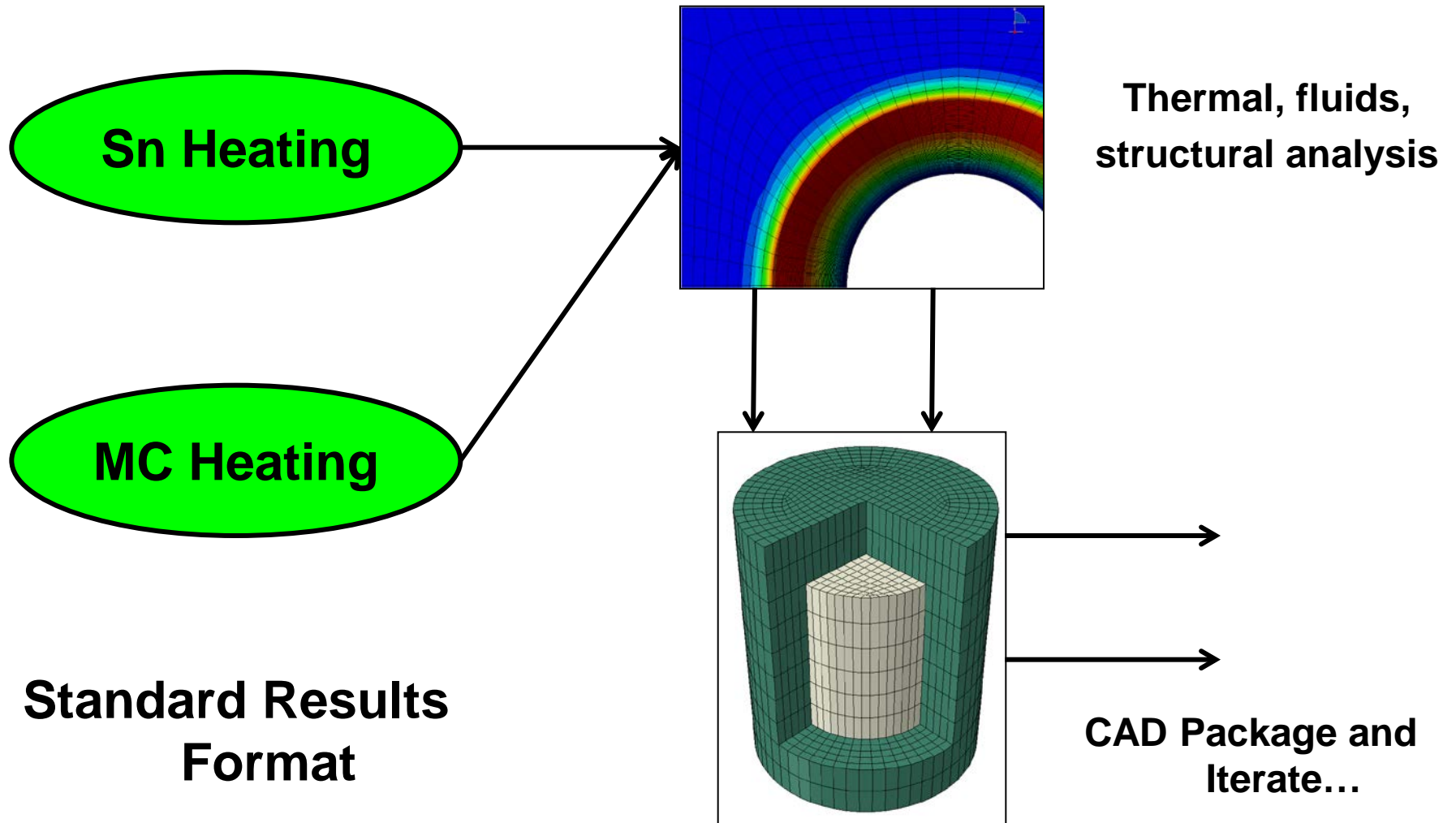
Multiphysics Example: Effect of Transport Method



Multiphysics Example: Effect of Transport Method



Multiphysics Example: Effect of Transport Method



PyNE: Standardized Utilities and Tools

- Open source effort called **Py**thon for **N**uclear **E**ngineering.
- **Goal:** Create an open source set of tools for nuclear engineering applications.
 - Examples: Material/isotopic mixer, ENDF file reader, transport output parser, etc.
 - Website <http://pyne.github.com>
- Having a common library of tools can help reduce the amount of time an engineer needs to perform analysis.
 - PyNE still has separate scripts for each analysis package (e.g., MCNP, Serpent, etc.)
- A good start, but we need many more efforts like this.
 - OpenMC good R&D tool and may provide templates for codes
 - Need a general repository (NEhub) for useful information
 - Will export control in the US hamper our best efforts here?

Summary

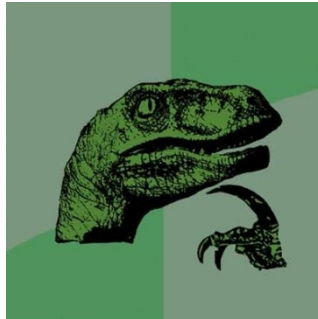
- Monte Carlo radiation transport methods will be used with increasing frequency for a greater number of applications.
- Our community is doing particularly well with methods research and should be able to address future needs.
- Our software engineering and infrastructure requires significantly more attention and/or redesign to adequately meet upcoming challenges.

Questions?

- MCNP, the made-up history...



In the Beginning, the Flying Spaghetti Monster decreed, "Let there be Monte Carlo! And its codes shall be created in my image."



Philosoraptors ponder the first Monte Carlo methods in the mid-cretaceous period.



2500 B.C. First recorded MCNP code in ancient Egypt.



In 1577 A.D. Queen Elizabeth I has MCNP rewritten in the just released Ye Olde FORTRAN77 standard.

- And thanks again to all who contributed to this talk, and thank you all for listening!