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Adjoint Weighting Methods Applied to Monte Carlo Simulations of Applications and Experiments in Nuclear Criticality

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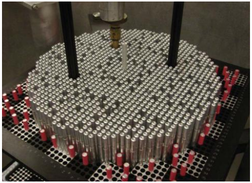
Outline

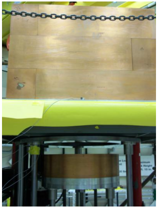
My Goals of Methods Development

- Develop Monte Carlo radiation transport methods and simulation software for engineering analysis that are robust, efficient, and easy to use.
- Provide computational resources to assess and improve the predictive capability of radiation transport methods and nuclear data.

- Focus of my research is on criticality and applications that use fissionable material.

Applications Involving FIssionable Material





Nuclear Criticality – Why it Matters

- When nuclear criticality is achieved, a system is in a configuration such that a runaway nuclear chain reaction will occur.
- Resulting radiation doses are often lethal and cannot be mitigated by time, distance, and shielding.
- Small changes in configuration can be the difference between life and death.
- We have no innate sensing ability to detect how close we are to criticality.
- **Handling fissionable material without criticality controls is like walking near a cliff on a very foggy day.**

How to Predict Criticality

- Experiments
  - Ideal option, and only one in the early days.
  - Difficult and expensive to perform in modern regulatory environment.
  - Few facilities available today, but large databases are available for criticality.
- Simulation
  - Not as good as reality, but with modern computing, this has become the preferred option.
  - Mature software, nuclear data, computational platforms.
  - Often, **but not always**, good quantitative agreement with experiment.
- Experiments and simulation supplement each other.

Assessing Criticality with Simulations

- Solve k-eigenvalue form of the linear radiation transport equation (RTE):

$$\left(\hat{\mathbf{\Omega}} \cdot \nabla + \Sigma_t\right) \psi(\mathbf{r}, \hat{\mathbf{\Omega}}, E) = \iint dE' d\mathbf{\Omega}' \, \Sigma_s(E' \to E, \hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}}) \psi(\mathbf{r}, \hat{\mathbf{\Omega}}', E') + \frac{1}{k_{\text{eff}}} \iint dE' d\mathbf{\Omega}' \, \chi(E' \to E) \nu \Sigma_f(E') \psi(\mathbf{r}, \hat{\mathbf{\Omega}}', E')$$

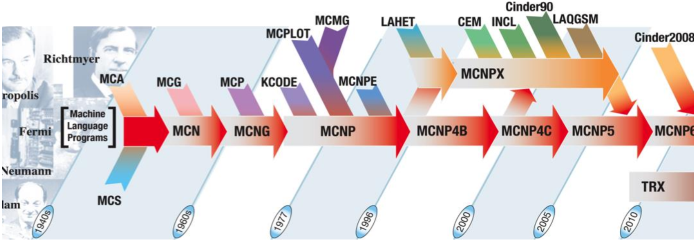
- Find fundamental eigenvalue k_{eff} and corresponding eigenfunction.
- k_{eff} is a mathematical factor that balances gains and losses.
- ψ represents the neutron distribution for this adjusted system.

- Two classes of methods available for solving this equation:
  - Deterministic (diffusion theory, P_n, S_n, MOC, etc.)
  - Monte Carlo

Monte Carlo Basics

- The Monte Carlo method does not solve the RTE in a direct, mathematical sense.
- Rather, it simulates the underlying radiation physics that the equation describes.
  - The neutron transport equation describes mean-value radiation behavior.
  - Monte Carlo simulation makes counts of responses (e.g., reaction rates) from the radiation physics and takes the mean average.
  - Because these correspond, the solution to the transport equation can be inferred from the Monte Carlo simulation.
- The eigenvalue problem is solved iteratively
  - Guess k_{eff} and ψ, transport neutrons one fission generation (an iteration), estimate k_{eff} and store fission neutrons as the new source.
  - After many iterations, the process converges and results may be obtained.

MCNP



- General-purpose, production Monte Carlo radiation transport software developed and maintained by Los Alamos National Laboratory.
- Continuous-energy physics supporting both neutral and charged particle transport.
- Wide range of applications: criticality safety, shielding, research reactors, medical physics, high-energy physics, stockpile stewardship, etc.
- Available from RISCC. Over 10,000 users.

Outline

Adjoint of the RTE

- Adjoint RTE reverses direction of streaming, scattering, and fission:

$$
\begin{aligned}
&\left(-\hat{\mathbf{\Omega}} \cdot \nabla + \Sigma_t\right) \psi^\dagger(\mathbf{r}, \hat{\mathbf{\Omega}}, E) \\
&- \iint dE' d\mathbf{\Omega}' \, \Sigma_s(E \to E', \hat{\mathbf{\Omega}} \cdot \hat{\mathbf{\Omega}}') \psi^\dagger(\mathbf{r}, \hat{\mathbf{\Omega}}', E') \\
&= \frac{\nu \Sigma_f(E)}{k_{\text{eff}}} \iint dE' d\mathbf{\Omega}' \, \chi(E \to E') \psi^\dagger(\mathbf{r}, \hat{\mathbf{\Omega}}', E')
\end{aligned}
$$

- Adjoint function $\psi^\dagger$ can be thought of as the importance with respect to the right-hand side of the equation, the fission source.

k-Eigenvalue Importance: Thought Experiment

- The importance is the propensity of neutrons at $\mathbf{r}, \hat{\mathbf{\Omega}}, E$ toward driving the self-sustaining chain reaction.

- Consider the following thought experiment:
  - A critical assembly starts with no neutrons.
  - Insert a neutron into the assembly at $\mathbf{r}, \hat{\mathbf{\Omega}}, E$ and wait a "long time".
  - Take a count of the number of neutrons in the assembly and record this number.
  - Flush the neutrons out of the system, and repeat this over and over.
  - The mean of the counts is proportional to the importance at $\mathbf{r}, \hat{\mathbf{\Omega}}, E$.

- What if the system is not critical?
  - System considered is a mathematical model where $1/k_{\text{eff}}$ balances losses and gains.

Why Care About the Adjoint Function in Criticality?

- Practically speaking, the adjoint function has convenient mathematical properties that allow the construction of simple models to estimate:
  - Kinetic behavior of reactors near criticality.
  - Perturbations for small changes in reactor configuration.
  - Sensitivity coefficients for uncertainty quantification.
- These models have terms that are adjoint-weighted integrals over some domain:

$$\left\langle \psi^{\dagger}, A\psi \right\rangle$$

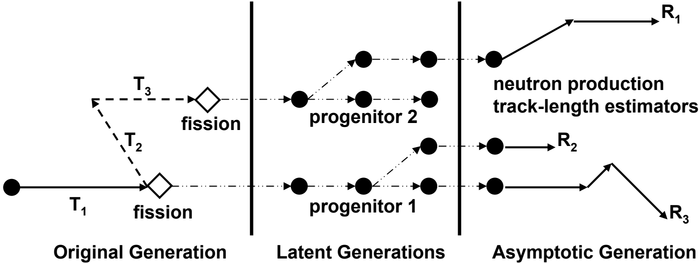
- Goal is to develop a method that can evaluate these integrals in a forward simulation with minimal additional computational cost.

Adjoint Weighting During Forward MC Simulation

- Eigenvalue calculations are an iterative process.
- Any state during a Monte Carlo random walk can be thought of as a point where a neutron is introduced into the system.
- If these states can be tracked and linked to their future behavior after several generations, estimates of the importance of those events can be made.
- User must decide how many generations constitute a "long time".
    - Empirical studies show 5-10 generations sufficient for most problems.
- Otherwise, no mesh or discretization is needed beyond that already in the forward simulation.

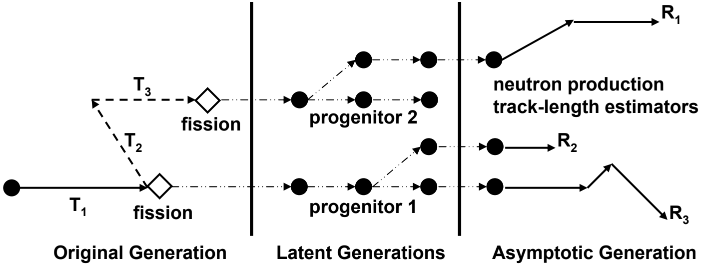
Adjoint Weighting During Forward MC Simulation

- In the first (original) iteration (generation):
  - Record events representing the kernel times the neutron flux (normal Monte Carlo tallies).
  - For each recorded event, tag the neutrons, and associate tags with their events.
  - Events and tags should be combined as possible to limit storage requirements.
  - Progeny of neutrons from fission inherit their tags.



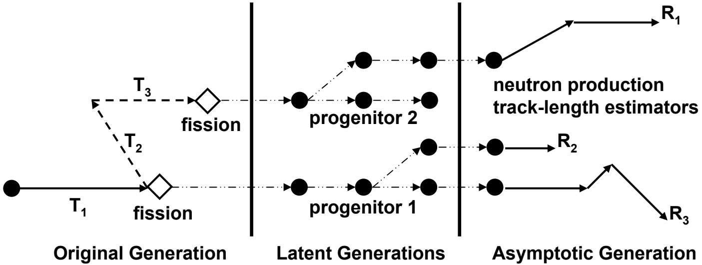
Adjoint Weighting During Forward MC Simulation

- In the subsequent (inner) iterations:
  - Neutron progeny inherit their existing tags, which propagate through the iterations.
  - No additional scores made to the tallies until the final (asymptotic) generation.



Adjoint Weighting During Forward MC Simulation

- In the final (asymptotic) iteration in the block:
  - Neutron populations are assumed to be converged to their asymptotic value (i.e., infinite time).
  - Record the number of neutrons produced by a track-length estimator of fission neutron production.
  - Multiply these by their appropriate scores from recorded events to estimate the importance-weighted integrals by Monte Carlo.
  - Repeat the process until desired statistical precision obtained.



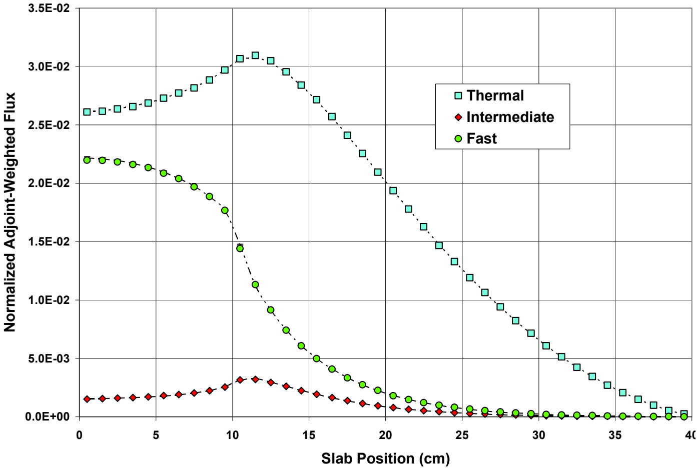
Results: Adjoint-Weighted Flux

- Estimate adjoint-weighted flux averaged over some region R.

$$\overline{\psi^\dagger \psi} = \left\langle \psi^\dagger, \psi \right\rangle_R .$$

- Compare deterministic (S_n in Partisn) and Monte Carlo solutions.
  - Simple 3-group slab problem.
  - Two regions: left is fuel and right is moderator.
  - Reflecting boundary on left, vacuum on right.

Results: Adjoint-Weighted Flux



Outline

Point Kinetics Model

- The point kinetics model is a simple description of neutron behavior in a reactor.
- Assumes flux is time separable and the spatial flux is distributed as the fundamental mode.

$$\frac{dn}{dt} = \left(\frac{\rho - \beta_{\text{eff}}}{\Lambda}\right) n(t) + \sum_i \lambda_i C_i(t) + q$$

$$\frac{dC_i}{dt} = \frac{\beta_i}{\Lambda} n(t) - \lambda_i C_i(t), \quad i = 1 \ldots 6$$

- How are the parameters in this model estimated?

Point Kinetics Parameters

- The point kinetics parameters may be measured or calculated.
- The parameters are ratios of adjoint-weighted integrals:

$$\Lambda = \frac{\left\langle \psi^\dagger, \frac{1}{v}\psi \right\rangle}{\langle \psi^\dagger, F\psi \rangle}$$

$$\beta_{\text{eff}} = \frac{\left\langle \psi^\dagger, B\psi \right\rangle}{\langle \psi^\dagger, F\psi \rangle}$$

- Here v is the neutron speed, F is the fission integral, and B is the fraction of the fission integral producing delayed neutrons.

Point Kinetics Parameter Verification and Validation

- Show that the method is correctly estimating point kinetics parameters by:
  - Verification with analytic solutions.
  - Verification with another method (Partisn).
  - Validation with experimental delayed critical Rossi-α measurements.

$$\alpha_{DC} = -\frac{\beta_{\text{eff}}}{\Lambda}.$$

Analytic Solution

- Two-group, infinite-medium problem with two delayed neutron groups:

$$\Lambda = \frac{\frac{1}{v_1}\frac{\Sigma_{s12}}{\Sigma_{R2}} + \frac{1}{v_2}\frac{\Sigma_{s12}}{\Sigma_{R2}-\xi_2\nu\Sigma_f}}{\left\{\frac{\Sigma_{s12}}{\Sigma_{R1}}\left[(1-\beta)+\xi_1\right]+\xi_2\right\}\frac{\nu\Sigma_f\Sigma_{s12}}{\Sigma_{R2}-\xi_2\nu\Sigma_f}} = 44/3 \ \ \mathrm{ns},$$

$$\beta_{\mathrm{eff}} = \frac{\frac{\Sigma_{s12}}{\Sigma_{R1}}\xi_1 + \xi_2}{\frac{\Sigma_{s12}}{\Sigma_{R1}}\left[(1-\beta)+\xi_1\right]+\xi_2} = 1/2,$$

$$\alpha = -\frac{\left[\frac{\Sigma_{s12}}{\Sigma_{R1}}\xi_1 + \xi_2\right]\frac{\nu\Sigma_f\Sigma_{s12}}{\Sigma_{R2}-\xi_2\nu\Sigma_f}}{\frac{1}{v_1}\frac{\Sigma_{s12}}{\Sigma_{R2}} + \frac{1}{v_2}\frac{\Sigma_{s12}}{\Sigma_{R2}-\xi_2\nu\Sigma_f}} = -3/88 \ \ \mathrm{ns}^{-1}.$$

- ξ_g is defined as the sum, over precursor index i, of all $\chi_{ig}\beta_i$.

Analytic Solution Results

	Analytic	MCNP	C/E
Λ (ns)	14.66667	14.66548 ± 0.00110	0.99992
β_{eff}	0.50000	0.50003 ± 0.00005	1.00006
α (ns^{-1})	-3.40909 x 10^{-2}	-3.40955 $\pm$ 0.00044 x 10^{-2}	1.00013

Comparison with Partisn (S_n)

#	G	Description
1	4	Bare fast slab
2	4	Metal slab with a moderating reflector
3	2	Metal slab, thermal absorber, and moderating reflector
4	8	Bare intermediate spectrum slab
5	4	Bare fast sphere
6	4	Reflected fast sphere
7	4	Subcritical bare fast slab ($k = 0.78$)
8	4	Supercritical bare fast slab ($k = 1.14$)

Comparison with Partisn (S_n) Results

#	Partisn	MCNP	C/E	I
1	9.79325 ns	9.79675 ± 0.00188 ns	1.00036	0.99021
2	135.19020 us	135.22164 ± 0.03384 µs	1.00023	1.14537
3	49.16822 ns	49.20663 ± 0.01863 ns	1.00078	0.00488
4	112.05232 us	112.29905 ± 0.13692 µs	1.00220	1.11580
5	1.72115 ns	1.72121 ± 0.00032 ns	1.00003	0.86498
6	10.18997 ns	10.18794 ± 0.00233 ns	0.99980	0.56477
7	10.17161 ns	10.17110 ± 0.00230 ns	0.99995	1.05365
8	9.67254 ns	9.67168 ± 0.00166 ns	0.99990	0.96534

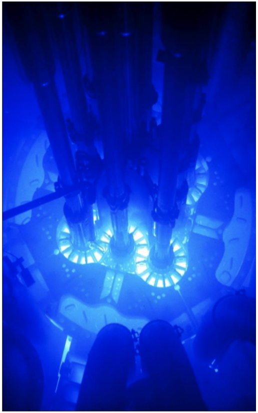
Comparison with Experimental Benchmarks

- Comparisons of Monte Carlo (MCNP) calculations with ENDF/B-VII.0 data and experimental measurements of Rossi-α (in ms^{-1}).

	Experiment	MCNP	C/E
Godiva	-1100 $\pm$ 20	-1139.57 $\pm$ 2.35	1.017
Jezebel-239	-640 $\pm$ 10	-640.238 $\pm$ 2.374	1.000
BIG TEN	-117 $\pm$ 1	-115.518 $\pm$ 0.219	0.987
Jezebel-233	-1000 $\pm$ 10	-1071.18 $\pm$ 3.50	1.071
Flattop-233	-271 $\pm$ 3	-292.401 $\pm$ 0.808	1.079
Stacy-29	-0.122 $\pm$ 0.004	-0.122155 $\pm$ 0.00296	1.001
WINCO	-1.1093 $\pm$ 0.0003	-1.11723 $\pm$ 0.00311	1.007

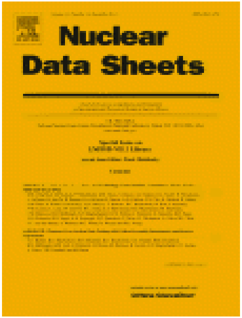
End-User Application: Advanced Test Reactor

- ATR uses point kinetics for safety analysis.
- Former approach involved using deterministic methods to calculate parameters.
- Difficult geometry to model, self shielding is important, and therefore required over a month of work by an engineer.
- Approach in MCNP requires minimal time by the user and (at most) hours of computational time.
- Results from MCNP agree with former approach.



End-User Application: Nuclear Data Validation

- Prediction of experimental measurements inform the development of any nuclear data library.
- The latest US library, ENDF/B-VII.1, used this capability in MCNP to benchmark to β_{eff} and α_{DC} measurements for the first time.
- Error found in the β_i of all actinides in previous library ENDF/B-VII.0; fixed in ENDF/B-VII.1.
- After fix, results show generally good agreement with measurement.



Remarks

- Verification and validation demonstrates that the method (implemented in MCNP) can calculate point kinetics parameters accurately.
- Calculation requires minimal user interaction: one user parameter and one additional line of input.
- Only small cost in computational time and memory usage.
- Variant of this method being implemented in Serpent.
- Allows for additional benchmarking of kinetic measurements with current experiments.

Outline

Sensitivity Coefficient

- The sensitivity coefficient is the ratio of the relative change in a response R caused by some relative change in some system parameter x:

$$S_{R,x} = \frac{\Delta R/R}{\Delta x/x} = \frac{x}{R}\frac{\Delta R}{\Delta x}$$

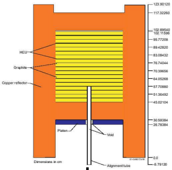
- For this talk, R will be taken to be k_{eff} and x is some segment of nuclear data (e.g., a reaction cross section for a particular isotope in some energy range).

Why Sensitivity Coefficients Matter in Criticality

- The sensitivity coefficient shows what nuclear data most impact k_{eff}.
- Empirically, most of the computational bias (inability of software to predict measurements) in k_{eff} is because of uncertainty in the nuclear data.
- Sensitivity coefficients offer a relatively simple way of showing if two systems are neutronically similar.
- The sensitivity coefficients can therefore be used to assess the predictive capability of software for a particular system based on how well it predicts neutronically similar experimental benchmarks.
- When convolved with cross section covariance data, can get estimates of uncertainties in k_{eff}.

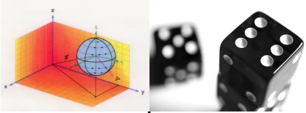
Schematic of a Calculation

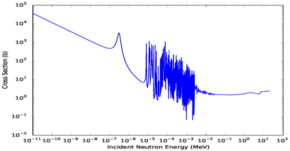
Computational Model



Experiment

Nuclear Data





Results: keff, doses, reaction rates, etc.

History of Sensitivity Analysis in Criticality

- Sensitivity analysis is a well established technique.
  - Has been used for decades with deterministic methods at Argonne National Laboratory, mostly for fast reactor uncertainty quantification.
  - Multigroup Monte Carlo sensitivity/uncertainty analysis has been in SCALE out of Oak Ridge National Laboratory for about a decade.
- Multigroup methods require two Monte Carlo calculations, one forward and one adjoint, and must consider the effect of multigroup collapse (not always easy).
- The adjoint weighting method for kinetics can be applied to sensitivity analysis as well, requiring minimal user input.
- This method has been implemented in MCNP and will be in the next version of SCALE.

Sensitivity Coefficients with Adjoint Weighting

- Perturbation theory can be used to derive an expression for the sensitivity coefficient:

$$S_{k,x} = -\frac{\left\langle \psi^\dagger, \left(\Sigma_x - C_x - \frac{1}{k} F_x\right) \psi \right\rangle}{\langle \psi^\dagger, F\psi \rangle}.$$

- Σ_x is the macroscopic cross section of interest (zero if not a cross section).
- C_x is the scattering integral for nuclear data x (zero if not scattering).
- F_x is the fission integral for nuclear data x (zero if not fission).

Sensitivity Coefficients for Distributions

- Fission χ and scattering distributions have an additional constraint that the area under the curve must be unity.
- The sensitivity coefficient may be adjusted accordingly:

$$\hat{S}_{k,f}(E', E, \mu) = S_{k,f}(E', E, \mu) - f(E' \to E, \mu) \iint dE d\mu \, S_{k,f}(E', E, \mu)$$

- The quantity $\hat{S}_{k,f}$ is often referred to as the constrained or renormalized sensitivity coefficient.

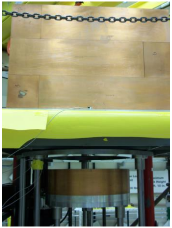
Sensitivity Coefficients for Scattering Moments

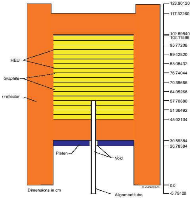
- Often the scattering distributions and uncertainties are given as Legendre moments.
- Can express renormalized sensitivity coefficient $\hat{S}_{k,f}(\mu)$ as Legendre moment sensitivity $\hat{S}_{k,f,\ell}$.
- Given a defined cosine grid with N bins with index i, the ℓth Legendre moment sensitivity is

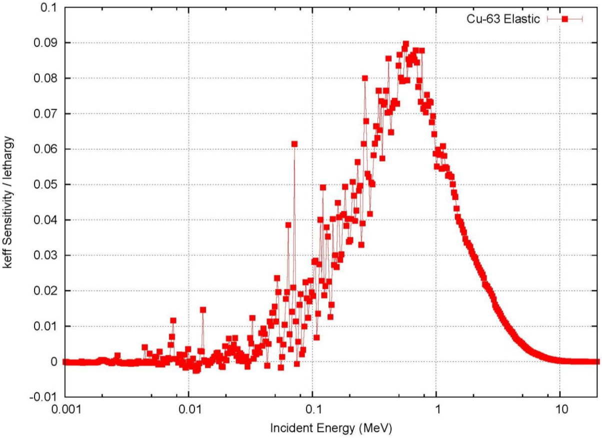
$$\hat{S}_{k,f,\ell} = \frac{2\ell+1}{2} f_\ell \sum_{i=0}^{N-1} (\mu_{i+1} - \mu_i) \frac{P_\ell(\mu_{i+1/2})}{F_{i+1/2}} \hat{S}_{k,f,i+1/2}$$

- $P_\ell(\mu_{i+1/2})$ is the ℓth Legendre polynomial at the cosine bin center.
- f_ℓ is the ℓth Legendre moment of f.
- $F_{i+1/2}$ is the cumulative density function of f integrated over the cosine bin.

Sensitivity Result







Sensitivity Coefficient Verification

- Show that the method is correctly estimating sensitivity coefficients by:
  - Verification with analytic solutions.
  - Verification with another method (multigroup Monte Carlo in SCALE/TSUNAMI).
  - Verification with direct perturbations.

Sensitivity Coefficient Verification: Analytic Solution

- Infinite medium problem with three energy groups:

g	σ_t	σ_c	σ_f	ν	χ	σ_{sg1}	σ_{sg2}	σ_{sg3}
1	2	1/2	0	–	5/8	1	1/2	0
2	4	1	0	–	1/4	0	1	2
3	4	1/2	3/2	8/3	1/8	0	0	2

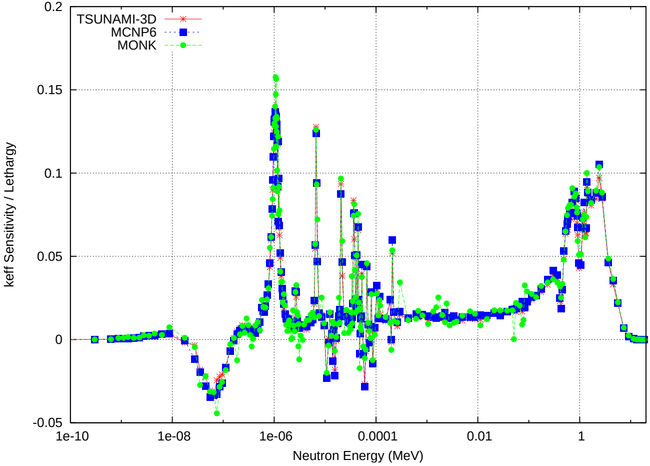
Sensitivity Coefficient Verification: Analytic Solution

x	Exact $S_{k,x}$	MCNP6 $S_{k,x}$	C/E
σ_{c1}	$-5/24$	$-0.20868 \pm 0.10\%$	1.002
σ_{c2}	$-1/4$	$-0.24993 \pm 0.07\%$	0.999
σ_{c3}	$-1/4$	$-0.24985 \pm 0.05\%$	0.999
σ_{f3}	$+1/4$	$+0.25045 \pm 0.16\%$	1.002
ν_3	$+1$	$+1.00000 \pm 0.00\%$	1.000
σ_{s12}	$+5/24$	$+0.20810 \pm 0.16\%$	0.999
σ_{s23}	$+1/4$	$+0.25083 \pm 0.15\%$	1.003

g	Exact $\hat{S}_{k,\chi_g}$	MCNP6 $\hat{S}_{k,\chi_g}$	C/E
1	$-5/24$	$-0.20805 \pm 0.12\%$	0.999
2	$+1/12$	$+0.08339 \pm 0.28\%$	1.001
3	$+1/8$	$+0.12465 \pm 0.17\%$	0.997

Sensitivity Coefficient Verification: TSUNAMI Comparison

- 3-D MOX lattice in water. H-1 elastic cross section sensitivity:



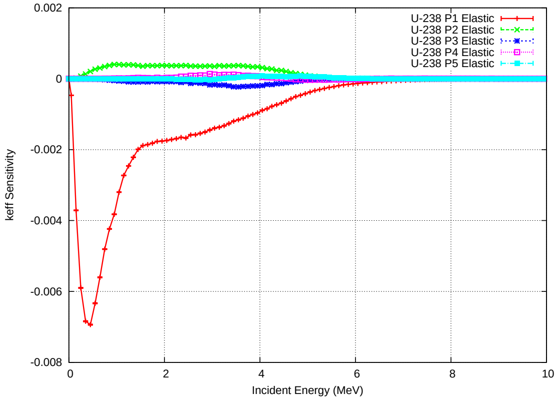
Sensitivity Coefficient Verification: Direct Perturbation

- Spherical core, cylindrical (non-fissionable) reflector.
- Two energy groups, reflector has P_1 anisotropy.
- Perturb reflector P_1 scattering cross section by 10% find Δk and compare with that from adjoint method.

- Direct $\Delta k = -0.00344(4)$.
- Adjoint $\Delta k = -0.00341(1)$.
- Agrees within 1-σ.

Legendre Moment Sensitivity

- Flattop (HEU sphere with spherical natural uranium reflector).
- U-238 Elastic scattering sensitivities as function of incident neutron energy.



Sensitivity Coefficient Applications

- Implemented in MCNP. Currently funded $250k/year to support uncertainty quantification work.
- May be used in support of critical experiment design (required by the NNSA Nuclear Criticality Safety Program).
- Legendre moment sensitivities for scattering distribution has typically been neglected in nuclear data adjustments; it is now possible to include this.

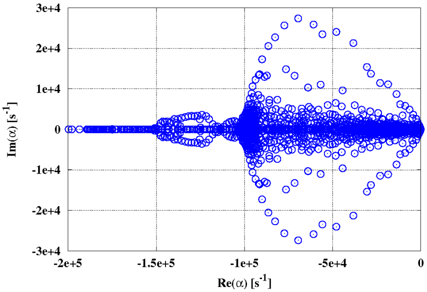
Sensitivity Coefficient Applications

- Support criticality safety validation project for restart of plutonium production at Los Alamos National Laboratory:
  - Develop computational software that automatically finds neutronically similar benchmark experiments.
  - Uses information to compute computational bias and subcritical margins with cross section uncertainties.
  - Technically-based validation required for safe operations with fissionable material.

Outline

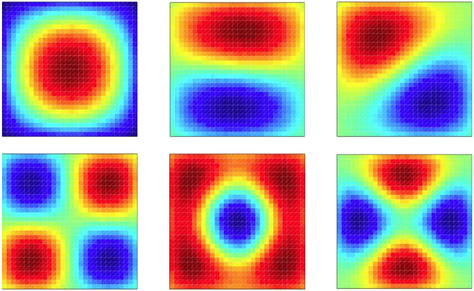
α-Eigenvalue Spectra (Betzler, Michigan)

- Develop continuous-time adjoint Markov transition rate in forward calculation.
- Use linear algebra to solve for discrete approximations of forward and adjoint α-eigenvalue spectra.
- Employ eigenfunction expansion to match time-dependent response measurements.
- Possible validation with new measurements on critical assemblies.



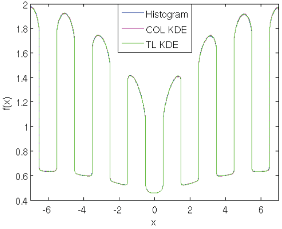
Fission Matrix (Carney, Michigan)

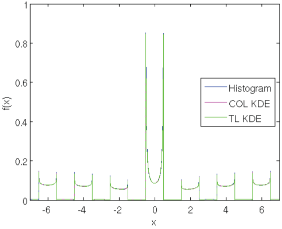
- Use fission matrix to solve for k-eigenvalue modes.
- Applications:
  - Monte Carlo eigenvalue convergence acceleration and detection.
  - Correction of statistical uncertainties in eigenvalue calculations.
  - Higher-order perturbation theory and sensitivity analysis.



Applied Kernel Density Estimators (KDEs) (Burke, Michigan)

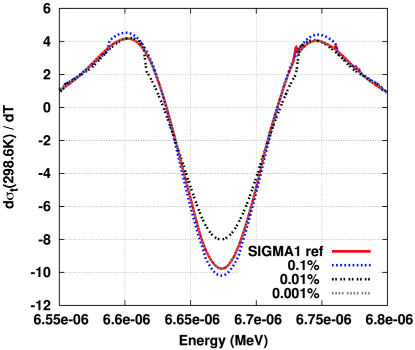
- KDEs offer an alternative approach to tally responses at points.
- Extended to reaction rates in 1-D using mean-free-path based bandwidth.
- Implementation in OpenMC; current work on 2-D and 3-D.
- Possible future efforts:
    - Multiphysics with meshfree methods.
    - Depletion with node-based isotopics, temperatures.





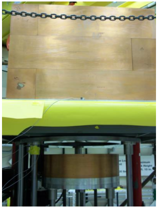
Doppler Reactivity Coefficients (Gonzales, UNM)

- Use sensitivity methodologies for Doppler reactivity coefficients.
- Use temperature series expansion by Yesilyurt to compute cross-section derivatives.
- Effective cross section shows reasonable agreement with direct perturbations.
- Current work is on scattering kernel derivative.



Multi-point Kinetics (Clark, UNLV)

- Historically, there has been poor predictive capability of kinetics measurements of reflected metal systems.
- Spatially resolved, multi-point kinetics models exist that should give better agreement.
- Plan is to apply point kinetics methodologies in MCNP to implement multi-point kinetics in CE Monte Carlo.
- Since reflectors are often non-fissionable, need a collisional eigenvalue kinetics model.
- Goal is to predict and compare with kinetics measurements of a critical system with two coupled assemblies.

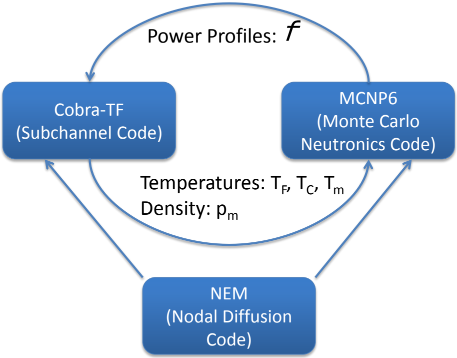


CE Neutron Adjoint and FACEMC (Robinson, Wisconsin)

- Forward-Adjoint Continuous Energy Monte Carlo (FACEMC) software developed by Wisconsin.
- Software designed in a modular fashion to accomodate future development.
- Software is being developed with agile programming practices.
- Seeking permission to release as open source software to serve as a research development platform for radiation transport methods.

MC Coupled Neutronics-Thermal Hydraulics (Bennett, PSU)

- Current effort at PSU is to couple MCNP6 with COBRA-TF (thermal hydraulics code) and NEM (nodal diffusion code) for forward/adjoint solutions for acceleration.
- Possible research area is to study issues with MC calculations (bias, correlation, stability) with TH and depletion.



Reactor Transients (Aures, GRS)

- New collaboration with GRS in Germany to investigate efficient approaches to Monte Carlo reactor transients with feedback.
- Possible research topics:
  - Application of higher-α modes.
  - Perturbation theory with α eigenvalue.
  - Jacobian-Free Newton Krylov with Monte Carlo for neutronics solve.

Outline

Critical Experiment Design with Automated Optimization

- Critical experiments are often performed to assess a weakness in software predictive capability, which are driven by uncertainties in nuclear data.
- Sensitivity analysis provides a means to ensure that the critical experiment addresses that need.
- Sensitivity profiles can be combined with optimization methods to maximize value of the experiment (more information for less money).
- Possible approaches:
  - Derivative-based methods with higher-order perturbation theory.
  - Derivative-free methods with Mesh Adaptive Direct Search method.

Sensitivity/Uncertainty of Transients

- Develop sensitivity methods for the fundamental α eigenvalue.
- The time-dependent nature makes it sensitive to different nuclear data (downscattering, delayed emission fractions, etc.).
- More data from existing or new kinetic measurements of α.
- Is it possible to reformulate eigenvalue equations like we are with the multi-point kinetics work to gain additional insights?

Uncertainty Quantification with Temperature Dependence

- Nuclear data covariances are generated at discrete temperatures.
- Correlations exist between temperatures because of resonance parameter uncertainties.
- How would one handle correlations between temperatures?
- MC software Serpent can handle continuous temperature fields (uses Woodcock or delta tracking).
- How would one perform sensitivity/uncertainty analysis in the presence of continuous temperature fields.

Time-Dependent KDE

- Transients and inertial confinement fusion (ICF) simulations need accurate time-dependent reaction or absorption/reemission rates.
- Discretization in time can lead to causality violations (radiation gets ahead of itself on the subsequent time step).
- Time-dependent KDEs at points with appropriate interpolation may offer a way to minimize this error.
- Possible approach is to have a causality-preserving boundary for KDE.

Automated Variance Reduction

- In the last decade, significant progress has been made on automating variance reduction (VR) with weight windows and source biasing using deterministic methods.
- Optimized weight windows provide significant speedups for some problems (factors of 10-1000+).
- There are other VR techniques (exponential transforms, forced collisions, deterministic transport surfaces, etc.) available.
- Can deterministic methods be used to solve for optimal VR parameters of these other techniques as well?
- Can they be combined to make an even more efficient solution? Perhaps with adaptive learning?

Summary

- My research has focused on developing applications to adjoint weighting in criticality simulations.
- These have been implemented in production Monte Carlo codes like MCNP, Serpent, SCALE, etc. and are robust and simple for an engineer to use.
- Point kinetics and sensitivity analysis have a close coupling with experimental measurements and the development of nuclear data.
- Graduate students who have worked with me have a diverse set of research interests in the area of criticality, reactor physics, and radiation transport simulation.