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Deterministic Neutron Transport at LANL: The PARTISN Code

Seminar for UNM

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Neutron Transport

- The Linearized Boltzmann transport equation describes the bulk motion of neutrons in a material

$$\left(\frac{1}{v} \frac{\partial}{\partial t} + \hat{\Omega} \cdot \vec{\nabla}_r + \Sigma_t\right) \psi(\vec{r}, \hat{\Omega}, E, t) = \dot{Q}(\vec{r}, \hat{\Omega}, E, t) +$$
$$\int_{4\pi} d\hat{\Omega}' \int_{E_{min}}^{E_{max}} dE' \Sigma_s(\hat{\Omega}' \cdot \hat{\Omega}, E' \rightarrow E) \psi(\vec{r}, \hat{\Omega}', E', t) + \int_{E_{min}}^{E_{max}} dE' \bar{v} \Sigma_f(E' \rightarrow E) \phi(\vec{r}, E', t)$$

Initial condition: $\psi(\vec{r}, \hat{\Omega}, E, t_0) = 0$
Boundary condition: $\psi(\vec{r}_B, \hat{\Omega}, E, t) = 0, \hat{\Omega} \cdot \vec{n}_B > 0$

- This equation is a time-dependent integro-differential equation with seven degrees of freedom for 3-D (six for 2-D, four for 1-D sphere/slab)
- Describes the *mean* neutron behavior (we'll get back to this!)
- All of the information about how the neutrons interact with the material is incorporated via the cross sections, Σ_x

Neutron Diffusion

- Integrating over angle gives:

$$\left(\frac{1}{v} \frac{\partial}{\partial t} + \Sigma_t\right) \phi(\vec{r}, E, t) + \vec{\nabla}_r \cdot \int_{4\pi} d\Omega \hat{\Omega} \psi(\vec{r}, \hat{\Omega}, E, t) = \int_{4\pi} d\Omega \dot{Q}(\vec{r}, \hat{\Omega}, E, t) + \int_{E_{min}}^{E_{max}} dE' \Sigma_s(E' \rightarrow E) \phi(\vec{r}, E', t) + \int_{E_{min}}^{E_{max}} dE' \bar{v} \Sigma_f(E' \rightarrow E) \phi(\vec{r}, E', t)$$

- Apply Fick's Law: $\vec{J} = \int_{4\pi} d\Omega \hat{\Omega} \psi(\vec{r}, \hat{\Omega}, E, t) \approx -D(\vec{r}, E) \vec{\nabla}_r \phi(\vec{r}, E, t)$

$$\left(\frac{1}{v} \frac{\partial}{\partial t} + \Sigma_t\right) \phi(\vec{r}, E, t) - \vec{\nabla}_r \cdot D(\vec{r}, E) \vec{\nabla}_r \phi(\vec{r}, E, t) = \dot{Q}(\vec{r}, E, t) + \int_{E_{min}}^{E_{max}} dE' \Sigma_s(E' \rightarrow E) \phi(\vec{r}, E', t) + \int_{E_{min}}^{E_{max}} dE' \bar{v} \Sigma_f(E' \rightarrow E) \phi(\vec{r}, E', t)$$

- Smaller phase space, but only accurate for isotropic/weakly-anisotropic fluxes

Neutron Transport: Solution Methods

Monte Carlo (Stochastic)

- Models the 'random walk' taken by particles through the system—the energy, angle and location of a particle are discrete quantities
- Discrete events are sampled from probability density functions (cross sections)
- If we are interested in the mean, then we must run enough histories to get good statistics (reasonably smooth distribution function)

SN/Discrete Ordinates (Deterministic)

- Numerically solve a PDE
- Trace the distribution function through space along discrete velocities (angle + energy)
- Derivatives in time and space move particles between time steps and spatial cells
- Changes in energy and direction due to scattering and fission (absorption and re-emission) events lead to coupling in the equations for the energy groups and angles
- Derivatives in direction for curvilinear geometries

Neutron Transport: Solution Methods

Monte Carlo (Stochastic)

1. To improve accuracy, must reduce the variance → More particle histories
2. Variance reduction via source biasing, weight windows, Russian Roulette etc.
3. Can struggle with obtaining a smooth solution due to noise
4. Can use continuous energy or multigroup cross sections

SN/Discrete Ordinates (Deterministic)

1. To improve accuracy, add unknowns → more angles and groups (sometimes), smaller spatial cells and time steps
2. This does not have to be done uniformly—refine in 'important' regions of phase space
3. Can obtain a smooth solution, but subject to discretization errors, ray effects, negative fluxes
4. Must use multigroup cross sections

Neutron Cross Sections

- Evaluated through a combination of experimental results, theoretical models and expert judgment
- Resonances due to discrete excitation energies of atomic nuclei
- ‘Continuous energy’ cross sections may contain upwards of 10^4 points!
- The greatest source of uncertainty in almost any transport calculation

Figure: Fission Cross Sections of Various Isotopes

Neutron Cross Sections—Multigroup-in-Energy

- Monte Carlo codes can use continuous energy cross sections
- Deterministic codes must discretize in energy → Multigroup
 - Assume that the energy spectrum of the neutrons is known → ‘weight function’
 - Choose energy group boundaries *carefully*
 - Use the weight function and energy group boundaries to generate ‘multigroup cross sections’
 - Adjust the multigroup cross sections by tuning them to match experimental criticality benchmarks
 - Multigroup cross section sets are tailored to specific applications
 - Can also be used in for Monte Carlo → More efficient sampling of the cross section
 - Resonance self-shielding can be an issue (we’ll come back to this)

Figure: U-235 Total Cross Section
(Thomas Saller)

Angles + Energy = Velocity!

Velocity Mesh

- Solving the transport equation involves taking integrals over angle
- The angular variable, $\hat{\Omega}$, is discretized using numerical quadrature, which also provides a way to do those integrals:

$$\int_{4\pi} d\hat{\Omega} \psi(\hat{\Omega}) \approx \sum_{n=1}^N w_n \psi(\hat{\Omega}_n)$$

- The transport equation is solved for discrete directions of travel, $\hat{\Omega}_n$

PARTISN Code Capabilities

- PARTISN: PARallel, TIme-dependent SN
- Solves both the static and time-dependent forms of the linear Boltzmann transport equation
 - Forward and adjoint mode
 - Static Eigenvalues: k and α
 - Time-dependent stochastic neutron transport equations:
 - Probability of Initiation (static) & Probability of Survival: Probability of obtaining a divergent chain
 - Moments of the (instantaneous) neutron and (total) fission numbers
- Discretization strategies:
 - Discrete ordinates approximation for treating the angular variable
 - Multigroup in energy
 - Diamond difference (standard or adaptive weighted) for the spatial variable
 - Crank-Nicholson in time
 - Set-to-zero fixup to maintain positivity (negative sources, strong gradients, large spatial cells)
- Acceleration via diffusion synthetic acceleration method or the transport synthetic acceleration
- Parallelization is performed via 2-D spatial decomposition (“KBA”) and/or Jacobi iteration for energy decomposition

Radiation Transport Applications in CCS-2

The transport project in CCS-2 develops neutron and x-ray transport codes

- Neutral particle, linear transport
 - Nuclear reactor simulations
 - Criticality (k -effective)
 - Isotope depletion
 - Shielding
 - Medical, e.g., brachytherapy
 - Oil well logging
 - Supernova explosion
- Nonlinear transport of thermal x-rays
 - Inertial confinement fusion
 - National Ignition Facility (Lawrence Livermore)
 - Laboratory for Laser Energetics (Rochester)
 - Astrophysics (Center for Theoretical Astrophysics, Los Alamos)
 - Z Pulsed-Power machine (Sandia)

PARTISN – Neutron/Gamma Deterministic Transport

Our team adds new physics, develops better solution methods, translates these into software and helps our users understand their results

- Our worldwide users perform a wide variety of 1-D/2-D/3-D calculations, so we require robust and efficient methods for reducing transport solution iterations (e.g., “KBA” sweeps, Diffusion Synthetic Acceleration)
- We have long been involved with work and research in nuclear application areas such as criticality safety, reactor engineering/shielding, sensitivity analysis, inverse problems, etc.
- We are also applying our methods and solvers to non-traditional areas such as the r-process in core-collapse in supernovae and neutron-star mergers → material-motion effects

Figure: R-Process Nucleosynthesis
Rapid neutron capture in these types of events is believed to account for the creation of roughly half the abundance of materials heavier than Fe

PARTISN – Neutron/Gamma Deterministic Transport

- Six dedicated team members (5 staff, 1 postdoc) who spend varying amounts of time working on the code and supporting LANL users
 - Currently, about 113k lines of (mostly) modern Fortran
 - Methods development
 - Material-motion advection algorithms
 - Using machine learning to improve multigroup data
 - Self-shielding corrections for multigroup data
 - Solutions to the stochastic neutronics equations
 - Use of Block Adaptive Mesh Refinement (AMR)
 - Efficient and scalable computational transport solution methods for massively parallel architectures using a “MPI+X” paradigm
 - Software maintenance
 - Bug fixes
 - Code modernization
 - User support
 - Help our users run the code *and* understand their results
- We generally have at least one summer student intern
- The code is available through RSICC and it is installed on LANL and LLNL machines

PARTISN Future Research Interests

- Solution methods for the transport equation with neutron-neutron scattering
- Time-dependent multigroup weighting functions
- Relativistic moving material corrections
- Collaborations with NEN-2 (Advanced Nuclear Technology) on FVM, Rossi-alpha, etc.
- Neutron-Diagnosed Sub-critical Experiments (NDSE)
- Pre-initiation experiments (GODIVA-IV)
- Anisotropic fission (once data is available)

Stochastic Neutronics

Stochastic Neutron Behavior

Deterministic Regime

Strong neutron source

Gaussian-like, approaches a delta-function at the mean as the source rate increases

Figure: PDF of y (the ratio of neutron number, n , to mean neutron number, $\langle n \rangle$) for various source rates, S

Stochastic Regime

Weak neutron source, i.e., spontaneous fission
Most likely outcome is zero neutrons, but long tail

- Nuclear fission is a fundamentally stochastic process, so the outcome of any one fission is known only probabilistically
- Deterministic behavior of a fissile system is the result of individual fission chains overlapping to the extent that they become indistinguishable
 - Mean neutron behavior drives the evolution of the neutron population → Predictability!
- Stochastic behavior occurs when the source is weak or the neutron population is very small
 - Overlapping does not occur → Must account for the inherent stochasticity of fission (number of neutrons emitted is probabilistic)
- This occurs in criticality accident scenarios, passive detection of spontaneous fission sources, reactor startup, criticality excursions in spent fuel, burst reactors, etc.

Use of “Point-Models” to Describe Stochastic Behavior

- “Point-Models,” for which time is the only phase-space variable, have long been used in neutron transport to generate simple, analytic representations of fissile systems
- Feynman and Bell pioneered their use at LANL for stochastic systems, deriving an analytic gamma distribution that approximates the PDF of n , the instantaneous neutron number:

$$P(n) = \left(\frac{n}{\langle n \rangle}\right)^{\eta-1} \frac{\eta^\eta}{\langle n \rangle \Gamma(\eta)} e^{-\eta \frac{n}{\langle n \rangle}} \quad \text{for} \quad \eta = \frac{S \cdot POI}{\alpha}$$

- $\langle n \rangle$ is the mean neutron number in the system at some point in time, t_f , given that there were no neutrons at the initial time, t_0
- Even though the model is based on a point-model, information about the geometry and the neutron velocity can be incorporated by computing $S \cdot POI$ and α using a full phase-space transport code
- The model is limited by the fact that it does not allow for *time-varying* geometries
- Bell also derived a system of probabilistic, *full phase-space* transport equations that can be solved using a deterministic transport code → Available in PARTISN

Use of “Point-Models” to Describe Stochastic Behavior

- Work by Prinja showed that a related analytic expression could be derived for the cumulative fission number, f :

$$P(f) = \frac{\sigma_n}{\sigma_f} \left(\frac{\sigma_n}{\sigma_f} \frac{f - \langle f \rangle}{\langle n \rangle} + 1 \right)^{\eta-1} \frac{\eta^\eta}{\langle n \rangle \Gamma(\eta)} e^{\frac{\sigma_n}{\sigma_f} \frac{f - \langle f \rangle}{\langle n \rangle} + 1}$$

- $\langle f \rangle$ is the mean number of fissions that occur on $t \in [t_0, t_f]$ and σ_n and σ_f are the standard deviations of the distributions
- Number of fissions is directly related to emitted energy and is therefore more relevant than neutron number for quantifying energy release, e.g., analysis of criticality accident scenarios
- Prinja also derived *full phase-space* equations for the fission number → Available in PARTISN

Full Phase-Space Equations for the Moments of n and f

- The equation for each moment, $\overline{g^k}$, is identical in form to the other moments of the fission number, f , and the neutron number, n
- However, the equations for $\overline{n^k}$ and $\overline{f^k}$ have different sources and initial conditions
- They equations are **standard linear adjoint transport equations** with a source term, S_k , that depends on the lower-order moments

$$\left(-\frac{1}{v} \frac{\partial}{\partial t} - \hat{\Omega} \cdot \vec{\nabla}_r + \Sigma_t\right) \overline{g^k}(\vec{r}, \hat{\Omega}, E, t) = S_k(\vec{r}, \hat{\Omega}, E, t; \overline{g} \dots \overline{g^{k-1}}) + \int_{4\pi} d\hat{\Omega}' \int_{E_{min}}^{E_{max}} dE' \Sigma_s(\hat{\Omega} \cdot \hat{\Omega}', E \rightarrow E') \overline{g^k}(\vec{r}, \hat{\Omega}', E', t) + \bar{v} \Sigma_f(E) \int_{E_{min}}^{E_{max}} dE' \chi(E \rightarrow E') \overline{g^k}(\vec{r}, E', t)$$

Initial condition: $\overline{n^k}(\vec{r}, \hat{\Omega}, E, t_{final}) = 1$ & $\overline{f^k}(\vec{r}, \hat{\Omega}, E, t_{final}) = 0$

Boundary condition: $\overline{g^k}(\vec{r}_B, \hat{\Omega}, E, t) = 0, \hat{\Omega} \cdot \vec{n}_B < 0$

- Accounts for variation in the solution due to the fission multiplicity distribution

DISTRIBUTIONS OF FISSION NEUTRON NUMBERS

FIG. 4. Experimental noncumulative neutron emission probabilities. The continuous curves are for a "Gaussian" distribution. Experimental data are from references 14-16; standard deviations are shown.

Table: Source terms

$$\Lambda_k(E) = \frac{\Sigma_f(E)}{i!} \sum_{j=i}^I \frac{i!}{(j-i)!} p_j$$

$$\langle \overline{g^k} \rangle = \int_{E_{min}}^{E_{max}} dE' \chi(E \rightarrow E') \overline{g^k}(\vec{r}, E', t)$$

$\overline{g^k}$	S_k
$\overline{n}$	0
$\overline{n^2}$	$2\Lambda_2 \langle \overline{n} \rangle$
$\overline{f}$	Λ_0
$\overline{f^2}$	$\Lambda_0 + 2\langle \overline{f} \rangle (\Lambda_1 + \Lambda_2 \langle \overline{f} \rangle)$

Full Phase-Space Descriptions of Stochastic Behavior

- Our codes can perform full phase-space computations as well as incorporate changing geometries
 - MCATK**: Analog Monte Carlo tracks individual fission chains to compute n and $f \rightarrow$ The outcomes are tallied to form the distributions and compute their moments (*Travis Trahan*)
 - PARTISN**: Equations for the moments of n and f are solved directly
- The moments can be used to compute the analytic PDF parameter, η

Table: System parameters computed using MCATK and PARTISN (21 energy groups) for a 6.5 cm sphere of Pu

	α (μs^{-1})	$\eta = \frac{S \cdot POI}{\alpha}$	$\eta = \left(\frac{\langle n \rangle}{\sigma_n} \right)^2$	$\langle n \rangle$	$\langle f \rangle$
PARTISN	7.7184	1.5024e-3	1.3951e-3	5.8661	60.625
MCATK	7.7253	--	1.3641e-3	5.8659	61.438

Figure: PDFs of f and n at $t_f = 0.5 \mu s$

- Direct tally from MCATK (target solution)
 - Analytic gamma PDF with MCATK η from table
 - Analytic gamma PDF with PARTISN η from table
- Agreement is good for n and large f .
(The discrepancy for small f is due to fission chains that die before t_f .)

Full Phase-Space Descriptions of Stochastic Behavior

- Dynamic Uranium Test Problem
 - 17.25 cm sphere with a time-varying mixture of U-235 and U-238 where
$$\rho_{235} = 14 - 6C \frac{g}{cm^3},$$
$$\rho_{238} = 1 + 6C \frac{g}{cm^3}$$
and C varies linearly between time points
 - Uniformly distributed volume source in group 7 (14-14.25 MeV) emitting 0.1 n/s

Figure: Moment comparison PARTISN vs. MCATK
MCATK results were generated using ENDF-VII.1 data, time biasing and 50 independent runs with 554400 fission chains each (Travis Trahan)
PARTISN results generated using MENDF71x data library, 133 groups, 120 spatial cells, S-20 and P-3 scattering/flux moments

Self-Shielding Corrections

Thomas Saller

The Multigroup Approximation

- Cross sections are continuous in energy but generally cannot be defined by an analytic function
- In the multigroup approximation, the energy range is broken up into a series of ‘groups,’ and the cross section for reaction x is averaged over these ranges by some weight function $f(E)$:

$$\sigma_{x,g}^i = \frac{\int_{E_{g+\frac{1}{2}}}^{E_{g-\frac{1}{2}}} \sigma_x^i(E) f(E) dE}{\int_{E_{g+\frac{1}{2}}}^{E_{g-\frac{1}{2}}} f(E) dE}$$

- Obtaining accurate multigroup cross sections requires an accurate $f(E)$
- The ideal weight function would be the flux of the problem of interest, which is not known a priori → use a “best guess”
- At LANL, we use the TD weight function, which consists of a Maxwellian at low energies, a $1/E$ slowing down range, a fission spectrum at high energies, and a 14.1 MeV fusion peak

Figure: LANL group structures and weight function

Self-Shielding Corrections in PARTISN

- Spectrum changes due to the mixing of isotopes (particularly resonant isotopes) is referred to as “self-shielding”
- PARTISN uses the Bondarenko method to account for self-shielding effects
- In the Bondarenko method, the macroscopic total cross section of a material is broken up into two parts:

1. $\sigma_t^i(E)$: Microscopic cross section of isotope i
2. $\sigma_0^i(E)$: Background cross section, which depends on all of the other isotopes in a material m

$$\Sigma_t^m(E) = N^i \left(\sigma_t^i(E) + \sigma_0^i(E) \right)$$

- To account for spatial effects, we include an “escape cross section,” Σ_e , in the background cross section:

$$\sigma_0^i = \frac{1}{N^i} \left(\Sigma_e + \sum_{(j \neq i) \in m} N^j \sigma_t^j \right) .$$

- The escape cross section relates the outgoing current from a region to the scalar flux:

$$\Sigma_e(E) = \frac{J^+(E)}{\phi(E)}$$

Self-Shielding Corrections in PARTISN

- The background cross section is used in a cross section processing code (e.g., NJOY) to generate multigroup cross sections as a function of σ_0^i
- In general, multigroup cross sections are “infinitely dilute,” where $\sigma_0 = 10^{10}$ (no self-shielding correction)

Figure: Pu-239 total cross section as a function of σ_0^i

Figure: Uranium sphere with 5 atom-percent U-235
Over time, U-235 is replaced by U-238.
The value of α compares better to MCATK (Monte Carlo) when self-shielding is used.

Self-Shielding Corrections in PARTISN

Figure: Lower energy neutrons experience the epithermal resonances of uranium and plutonium → self-shielding corrections make a big difference!

More moderation →
Slower energy
spectrum

Figure: Self-shielding improves the accuracy of PARTISN in the presence of resonant isotopes

Iron and copper
have high energy
resonances

Moving Material Corrections

Transport in Moving Materials

- The neutron transport equation is generally applied to systems in which the material is assumed to be at rest
- There are instances where material motion can affect the resulting solution
 - Coolant flowing through a nuclear reactor
 - Collapsing stellar cores
- When the material is moving, there is a discrepancy between neutron velocities in the co-moving & lab frames → neutron cross sections are measured in the lab frame
- Using the wrong cross section results in errors in reaction rates & the transport solution
- Even though nuclear cross sections are evaluated with respect to a material at rest, it is the relative velocity between the material & neutrons (i.e., the velocity in the co-moving frame) that is important
 - It is possible to do the transport in the lab frame
 - Use cross sections for the neutron velocity in the co-moving frame
 - The 'effective' total & fission cross sections are not isotropic → complicates the algorithm & may cause instabilities in the solution
- Alternatively, it is possible to transform the transport equation itself into the co-moving frame in which the material is stationary → “Moving Material Corrections”

Transport in Moving Materials

- Transforming to the co-moving frame introduces **spatial** and **momentum** advection terms

$$\frac{\partial N}{\partial t} + \vec{q} \cdot \vec{\nabla}_r N + \vec{\nabla}_r \cdot \vec{u} N + \Sigma_t q N(\vec{r}, \vec{q}, t) = \dot{q}(\vec{r}, \vec{q}, t) + \vec{\nabla}_q \cdot \vec{H} N(\vec{r}, \vec{q}, t)$$

$$\vec{\nabla}_q = \frac{\vec{q}}{q} \left(\frac{\partial}{\partial q} - \frac{\mu}{q} \frac{\partial}{\partial \mu} \right) + \frac{\vec{r}}{r} \frac{1}{q} \frac{\partial}{\partial \mu}$$

$$\vec{H} = \left(\vec{q} \cdot \vec{\nabla}_r + \vec{u} \cdot \vec{\nabla}_r + \frac{\partial}{\partial t} \right) \vec{u}$$

- $\vec{q} = \vec{v} - \vec{u}$ is the neutron velocity in the co-moving frame (material at rest)
- $\vec{u}$ is the material velocity in the lab frame
- $N = \frac{\psi}{q}$ is the neutron density in the co-moving frame
- $\dot{q}$ is a source rate term (scattering, fission, volumetric sources)
- Solve using a three-step operator split procedure:
 - Standard Transport step
 - Spatial Advection step
 - Momentum Advection step

Velocity Mesh

Modeling R-Process Nucleosynthesis in Proto-Neutron Stars

- Core-collapse supernovae are powered by the collapse of a stellar core into either a neutron star or a black hole
- Energy released powers an explosion that disrupts the star & some material falls back onto the newly formed neutron star, creating secondary outbursts
- Fryer et al. argued that these outbursts could be the site of r-process nucleosynthesis, i.e., the formation of elements through the rapid capture of neutrons onto heavy seed nuclei
- This rapid neutron capture process is believed to be responsible for the creation of approximately one half of the atomic nuclei in the universe that are heavier than iron
- In this scenario, heavy 'seed' nuclei (e.g., iron) undergo a series of rapid neutron captures as they fall back toward the neutron star & are then swept up in the outflow

Figure: 1-D model of heavy seed nuclei (nickel) falling into the star (helium)

Modeling R-Process Nucleosynthesis in Proto-Neutron Stars

Figure: Neutron Spectrum at the Ni/He interface
Accounting for material motion changes the energy spectrum of the neutrons, which affects reaction rates

Sensitivity Analysis with SENSMSG

Jeffrey Favorite

SENSMG

- SENSMSG is a tool developed at LANL for calculating **first-order sensitivities** to multigroup cross sections, isotope densities, material mass densities, and interface locations using **PARTISN** and **Generalized Perturbation Theory**
 - Reaction-rate ratios, k_{eff} , and α in critical problems
 - Reaction-rate ratios, reaction rates, and leakage in fixed-source problems

Jeffrey A. Favorite (2018) SENSMSG: First-Order Sensitivities of Neutron Reaction Rates, Reaction-Rate Ratios, Leakage, k_{eff} , and α Using PARTISN, Nuclear Science and Engineering, 192:1, 80-114, DOI: 10.1080/00295639.2018.1471296

Figure: SENSMSG vs. TSUNAMI-1D for Flattop-Pu
Sensitivity of the ratio of ^{237}Np fission to ^{235}U fission to the ^{239}Pu density and fission cross section as a function of energy

Thank you for the opportunity to talk about PARTISN!

Questions?