MCNPX – New Features Demonstrated

Burnup/Depletion and Delayed Gammas

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13th UK Monte Carlo User Group Meeting (MCNEG 2007),
Teddington, UK March 28-29, 2007

Outline

- **Overview**
- **New 2.6.c Features**
  - **Burnup/depletion**
  - **Delayed Gammas**
- **Future Development**

Overview

- **Monte Carlo radiation transport code**
  - Extends MCNP 4C to virtually all particles and energies
  - 34 particle types (n,p,e, 5 Leptons, 11 Baryons, 11 Mesons, 4 LI)
  - Continuous energy (roughly 0-100 GeV)
  - Data libraries below ~ 150 MeV (n,p,e,h) and models otherwise
- **General 3-D geometry**
  - 1st & 2nd degree surfaces, tori, 10 macrobodies, lattices
- **General sources and tallies**
  - Interdependent source variables, 7 tally types, many modifiers
- **Supported on virtually all computer platforms**
  - Unix, Linux, Windows, OS X (parallel with PVM or MPI)

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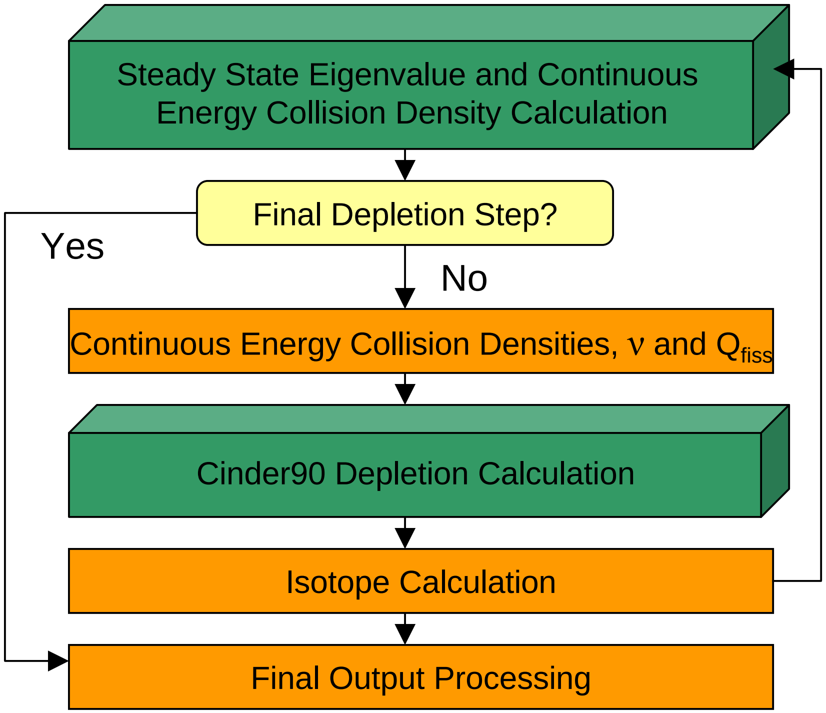
Existing Burnup Capabilities

- **Numerous "scripts" written to link MC codes to depletion codes**
  - MOCUP (MCNP/ORIGEN2, INEL, 1995)
  - MC-REBUS (MCNP/REBUS, ANL, 1998)
  - OCTOPUS (MCNP/FISPACT, ECN NRG Netherlands, 1998)
  - MCB (MCNP/Custom, RIT Sweden, 1999)
  - MonteBurns2 (MCNP/ORIGEN2 or CINDER90, LANL, 1999)
  - MCWO (MCNP/ORIGEN2, INEEL, 2000)
  - BURNCAL (MCNP/Custom, SNL, 2002)
  - MCODE (MCNP/ORIGEN2, MIT, 2002)
- **Disadvantages of a "link" approach**
  - Several input files to create and understand
  - Numerous input/output files to manage
  - Approximations to convert data from one format/code to another

Monte Carlo Linked Depletion Process



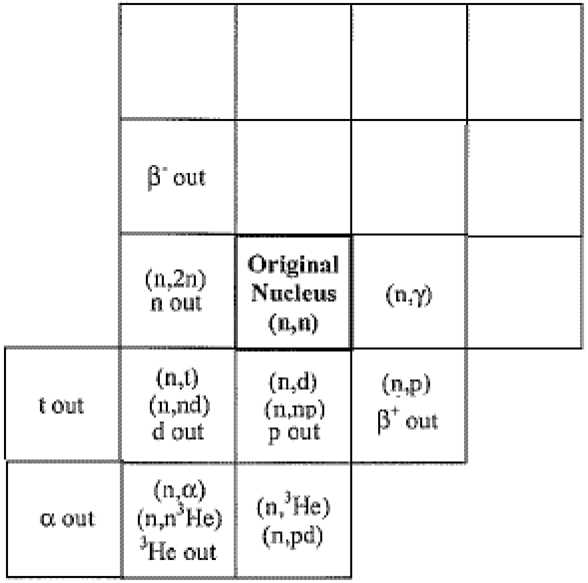
- Steady state Monte Carlo using MCNPX, depletion utilizing CINDER90

CINDER90

- CINDER90 is a FORTRAN program or "code" with a data library used to calculate the inventory of nuclides in an irradiated material
  - Nuclide Inventory Code
    - Follows the conversion of a nuclide to a different nuclide by a particle absorption and/or radioactive decay
- 1960 at Bettis Atomic Power Laboratory (BABL) in support of thermal reactor simulation calculations
- All Cinder version use solve for independent contributions to atom densities in each of a number of linear chains (Markovian Chains)
- Reactors and Accelerators (LANL– APT program)
- Rather than using a preexisting chain structure, each path for each nuclide defined by available data is followed until test of significance are failed.

Isotopes Tracked

- Capturing every possible decay chain product from every isotope generated during the depletion process would be extraordinarily memory intensive
- MCNPX utilizes the isotope generator algorithm to determine all the immediate daughter isotopes created from a burn material reaction, and tracks those isotopes during the transport process
- CINDER90 does track isotope concentrations for 3456 isotopes (1325 fission products)
  - Only those isotopes utilized in the steady state transport calculation contain isotope abundance data in the output file



n = neutron
p = proton
d = deuteron
t = triton

α = alpha particle
β^- = beta minus (negative electron)
β^+ = beta plus (positron)
ε = electron capture

Fission Product Tiers

- Certain Monte Carlo linked depletion codes force the user to input every fission product to be tracked during the depletion process
- MCNPX offers the user preset fission product “tier”s
- Eliminates the task of inputting every fission product to be tracked
- MCNPX offers three fission product tiers
  - Tier 1. (default) Zr-93, Mo-95, Tc-99, Ru-101, Xe-131, Cs-133, Cs-137, Ba-138, Pr-141, Nd-143, Nd-145
  - Tier 2. Isotopes contain in the fission product array that are included in the current cross section library file (XSDIR) for MCNPX version 2.6.C. All fission products having ENDF-VII cross sections and yield data in the CINDER library file; 220 fission products.
  - Tier 3. All isotopes contained in the fission product array
- The user then has the option to eliminate certain isotopes from a tier if necessary

Depletion Equation
C+B → A →

$$\frac{dN_A}{dt} = -\lambda_A N_A - \left[\sum_g \sigma_{a_g}^{A} \phi_g\right] N_A + \lambda_B N_B + \left[\sum_g \sigma_{a_g}^{C} \phi_g\right] N_C$$

$-\lambda_A N_A$ = loss due to radioactive decay of A

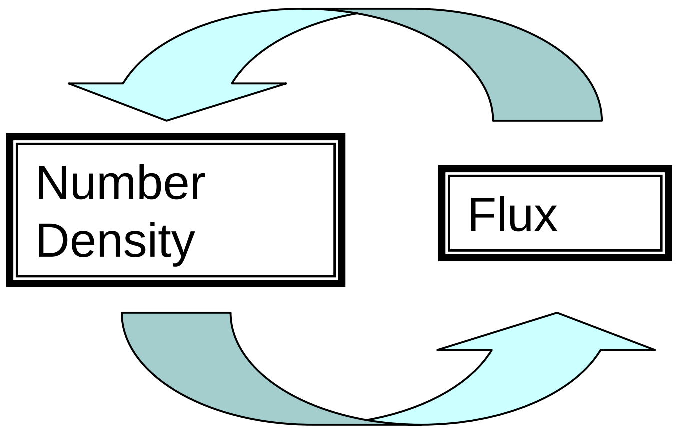
$\left[\sum_g \sigma_{a_g}^{A} \phi_g\right] N_A$ = loss due to neutron capture by A

$\lambda_B N_B$ = gain due to decay of B to A

$\left[\sum_g \sigma_{\gamma_g}^{C} \phi_g\right] N_C$ = gain due to transmutation of C to A via neutron capture

Nonlinear Problem

$$\frac{dN_A}{dt} = -\lambda_A N_A - \left[\sum_g \sigma_{a_g}^A \phi_g\right] N_A + \lambda_B N_B + \left[\sum_g \sigma_{a_g}^C \phi_g\right] N_C$$

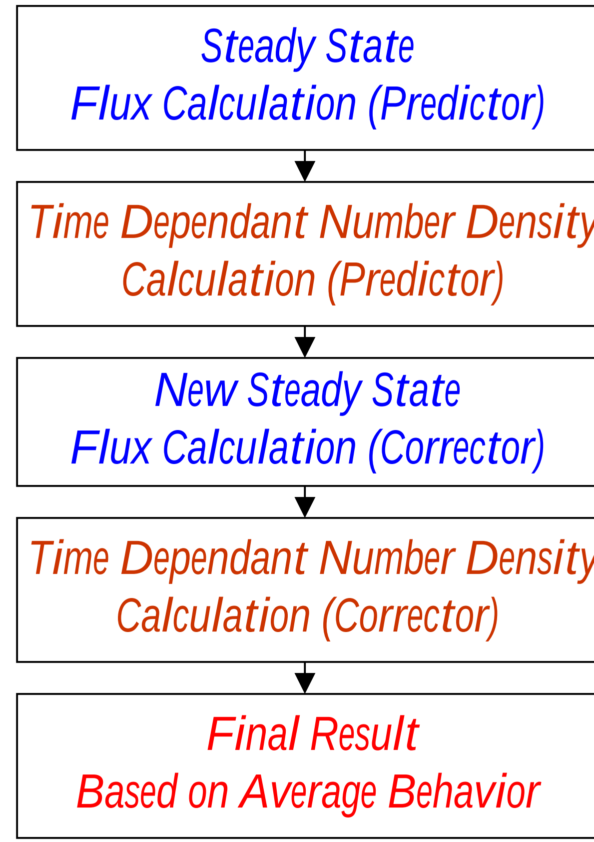


- The depletion equation uses time-dependent fluxes, interaction rates, and nuclide number densities to determine the time-dependent nuclide inventory

- Unfortunately, the time-dependent flux also is dependent on the time-dependent nuclide density, thus making the depletion equation **NONLINEAR**.

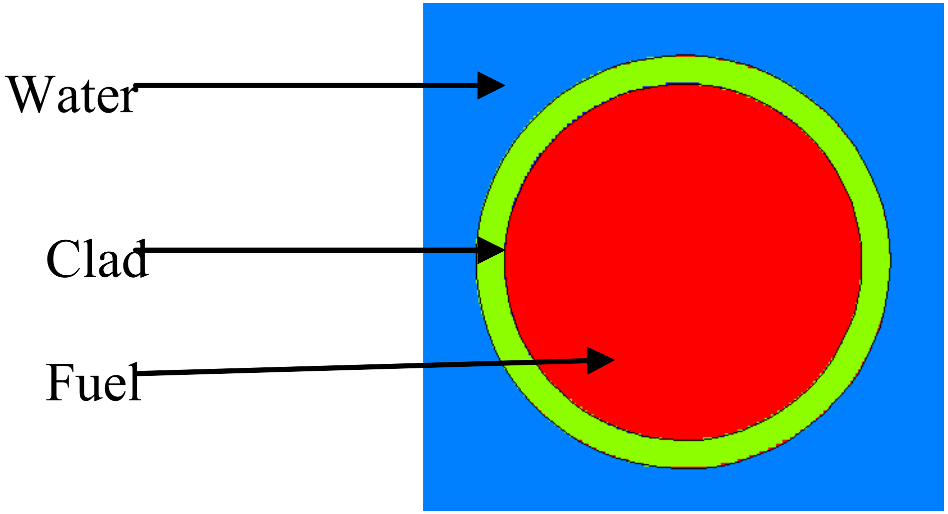
Predictor-Corrector Method

- Time-dependant flux is set to a constant value over the burn step
- A "predicted" value of the number densities, fluxes, and interaction rates is calculated for a time step duration
- Values then are "corrected" by redepleting the system over the time step implementing the newly calculated fluxes and interaction rates
- The hope of implementing such a calculation is to deplete the system using a best representation of the average of the time-dependent parameters
- The two separate predictor-corrector methods tested
  - CELL-2 and MONTEBURNS



Benchmark Calculation

Infinitely reflected "MOX" pin cell geometry with borated water



Fuel Composition

ZAID	Atom Fraction
8016.60c	4.59E-02
92235.60c	1.45E-04
92238.60c	1.99E-02
94238.60c	1.15E-04
94239.60c	1.03E-03
94240.60c	7.97E-04
94241.60c	3.40E-04
94242.60c	5.64E-04

Water Composition

ZAID	Atom Fraction
1001.60c	4.77E-02
8016.60c	2.39E-02
5010.60c	3.63E-06
5011.60c	1.62E-05

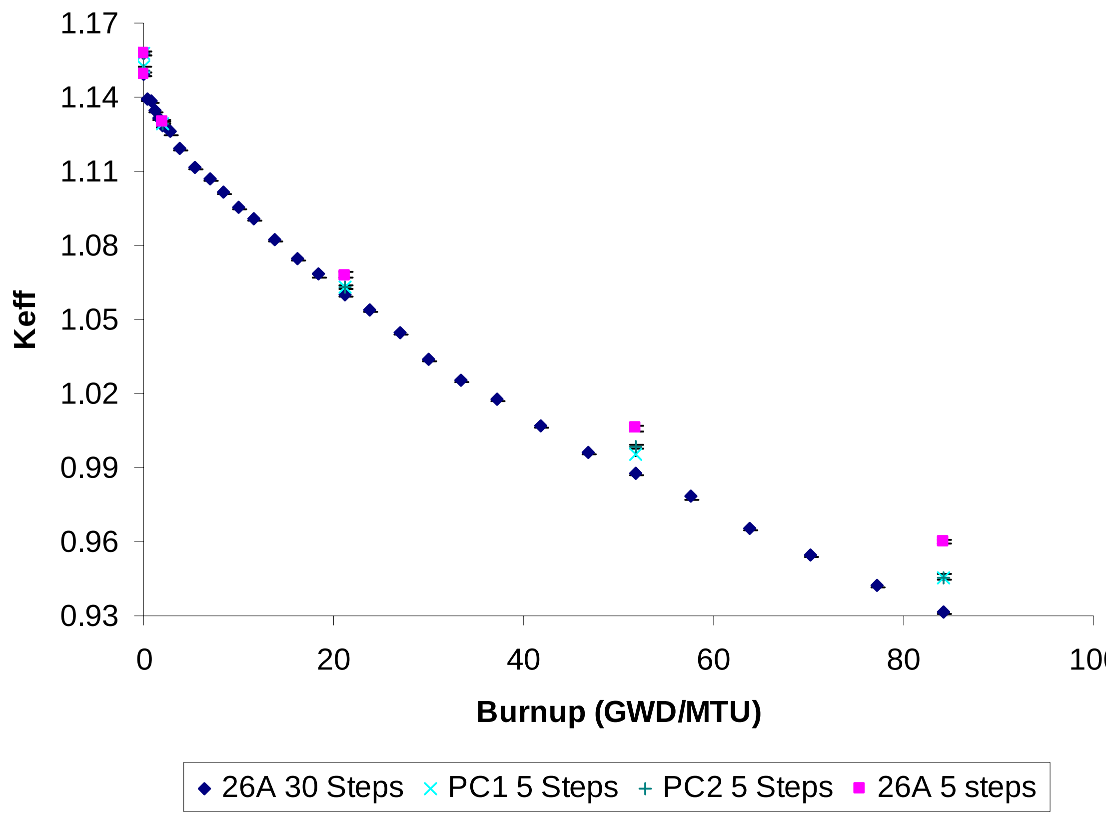
- Entire Cell 1.33 cm X 1.33 cm X 365 cm
- Fuel 0.4095 cm radius
- Clad 0.0655 cm thick

Burnup Criteria

- 5000 particles per cycle, skipping the first 5 cycles, for 300 cycles
- The fuel pin was depleted at a power of 66.956 kWt for 2191 days
- Examined cases:
  - No predictor Method
    - 30, 20, 10 and 5 time steps
  - MONTEBURNS method
    - 15, 10 and 5 time steps
  - Cell 2 Method
    - 15, 10 and 5 time steps

Burnup Steps (GWD/MTU)				
30	**20**	**15**	**10**	**5**
0.00E+00	**0.00E+00**	**0.00E+00**	**0.00E+00**	**0.00E+00**
2.48E-02	**2.48E-02**	**2.48E-02**	**2.48E-02**	**2.48E-02**
4.09E-01	4.09E-01	4.09E-01	**1.94E+00**	**1.94E+00**
7.93E-01	7.93E-01	1.18E+00	1.15E+01	**2.11E+01**
1.18E+00	1.18E+00	**1.94E+00**	**2.11E+01**	**5.19E+01**
1.56E+00	1.56E+00	6.74E+00	3.07E+01	**8.41E+01**
1.94E+00	**1.94E+00**	1.35E+01	4.13E+01	
2.71E+00	4.82E+00	**2.11E+01**	**5.19E+01**	
3.86E+00	7.70E+00	2.88E+01	6.24E+01	
5.40E+00	1.15E+01	3.65E+01	7.30E+01	
6.94E+00	1.54E+01	4.42E+01	**8.41E+01**	
8.47E+00	**2.11E+01**	**5.19E+01**		
1.00E+01	2.73E+01	5.95E+01		
1.15E+01	3.34E+01	6.72E+01		
1.39E+01	3.96E+01	7.49E+01		
1.62E+01	4.57E+01	**8.41E+01**		
1.85E+01	**5.19E+01**			
2.11E+01	5.95E+01			
2.38E+01	6.72E+01			
2.69E+01	7.49E+01			
3.00E+01	**8.41E+01**			
3.34E+01				
3.73E+01				
4.19E+01				
4.69E+01				
5.19E+01				
5.76E+01				
6.38E+01				
7.03E+01				
7.72E+01				
8.41E+01				

Results



- Implementing a predictor-corrector method leads to a better approximation of EOL k_{eff}

Future Work – Burnup/Depletion

- Benchmarking!!!
- Increased fission product list
  - Tier 3 may automatically pick up all fission products on xsdir
- Power partitioning for cells using a common burn material
- Adding new materials and making geometry perturbations during the burnup calculation
  - MCNPX currently only transports materials that are specified at BOL
- Calculating number density error and error propagation during the depletion process
  - Toshikazu Taked, Naoki Hirokawa and Tomohiro Noda "*Estimation of Error Propagation in Monte-Carlo Burnup Calculations*" Journal of Nuclear Science and Technology, Vol 36, No. 9, September 1999.
- Automatic burn step generation
  - Determine the placement of the minimal amount of burn steps in order to achieve a reliable answer

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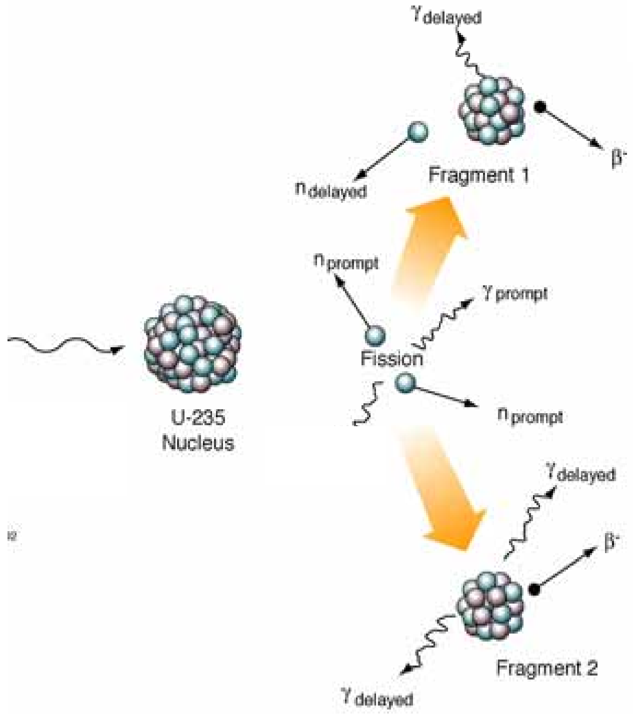
Delayed-Gamma Signatures

- Objective

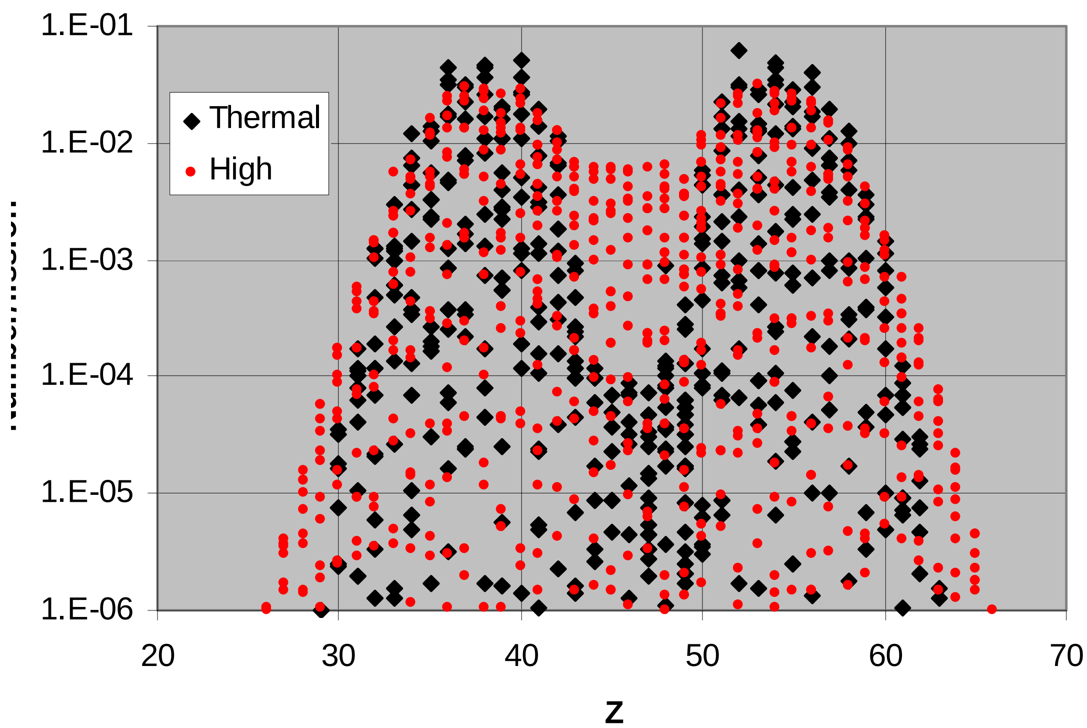
  Develop capability for MCNPX to automate the creation of delayed signatures emitted due to the decay of radioactive:
  - Fission products created by neutron fission or photofission.
  - Residual nuclides created by non-fission transmutation.
- Significance
  - The radioactive decay of fission products, or residual nuclides excited by neutron or photonuclear interaction, frequently results in the emission of gamma/x-rays at times appreciably later than the initiating event: "delayed gammas."
  - The relative amounts of fission products vary with the fissioning isotope and the particle (i.e., neutron, photon, etc.) inducing the fission.
  - The delayed-gamma emissions occur with intensities and at energies that are unique to each radionuclide.
  - These factors permit the identification of the target nuclide and its fission or residual-nuclide products via the delay-gamma spectral signatures.

The Products of Fission: Radiation & Residuals

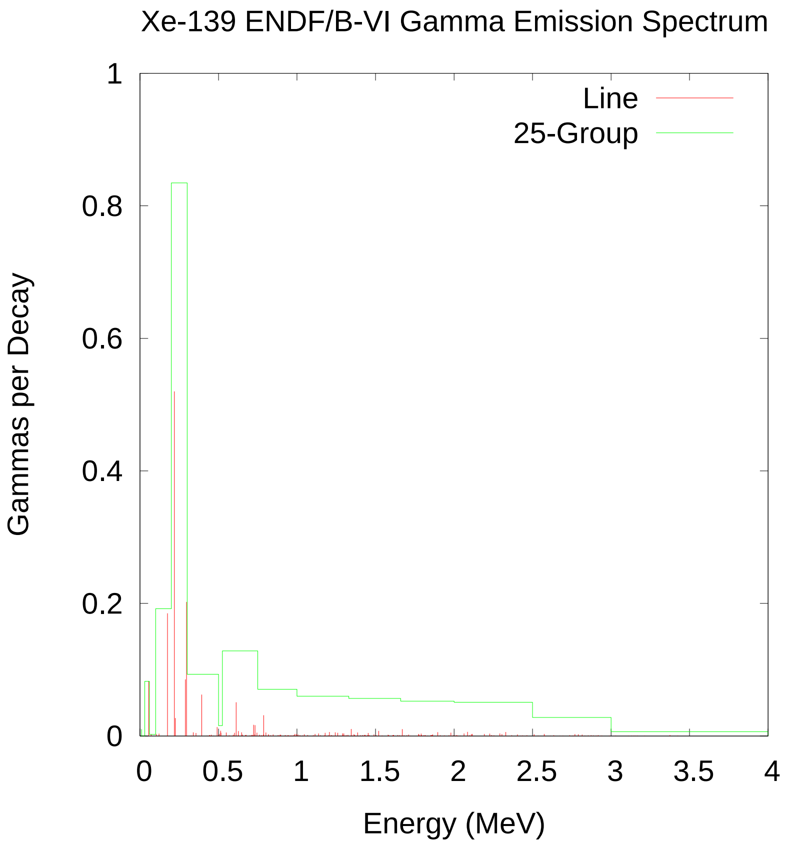
Prompt and Delayed Gammas From Fission

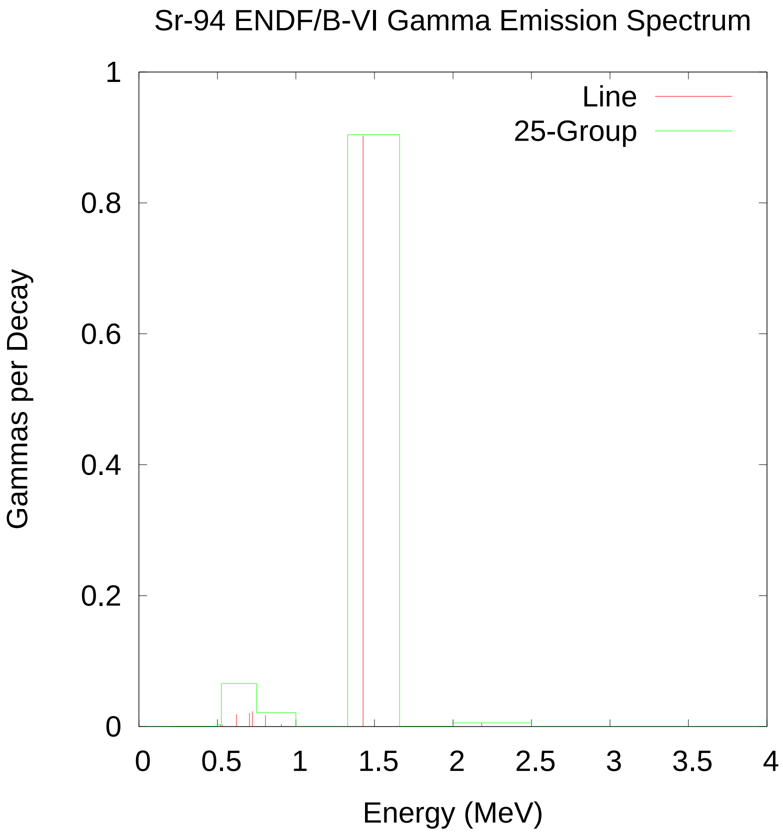


CINDER90 ^{235}U fission-yield curves for thermal and high-energy neutron-induced fission.



^{139}Xe & ^{94}Sr ENDF/B-VI Gamma Emission Spectra

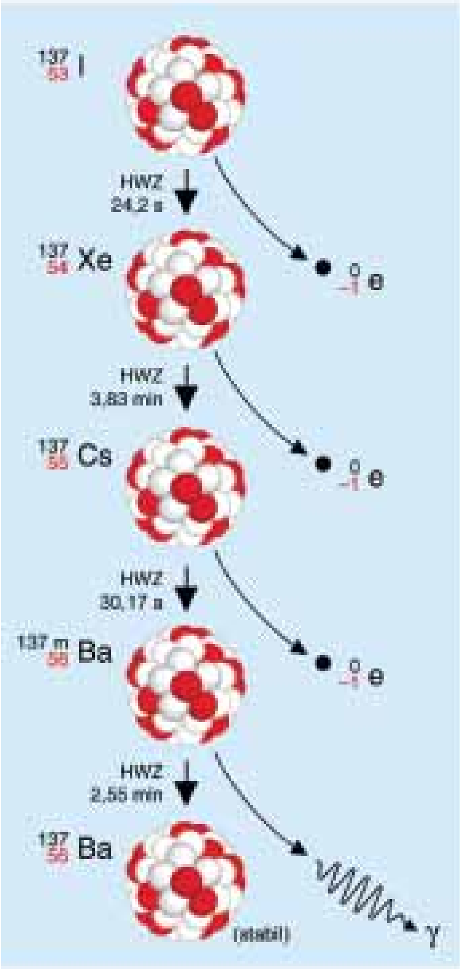




Decay Chains and Emission Sampling

Not only are the fission-products and residual nuclides radioactive sources, but so too are their decay products. Each contributes to the delayed signature. Thus, a fission event may have hundreds or thousands of lines contributing to its signature.

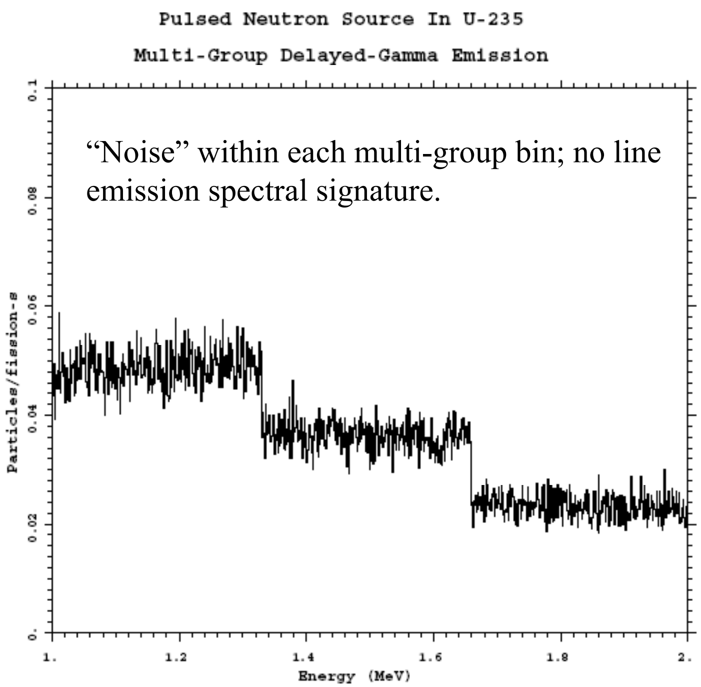
CINDER90 has been integrated into MCNPX to calculate the radioactive decay-chain nuclide densities as a function of time. The nuclide densities, decay constants, and particle (neutron, gamma) emission probabilities are used to calculate distributions that are sampled for particle emission energy and delay time (direction is sampled isotropically).

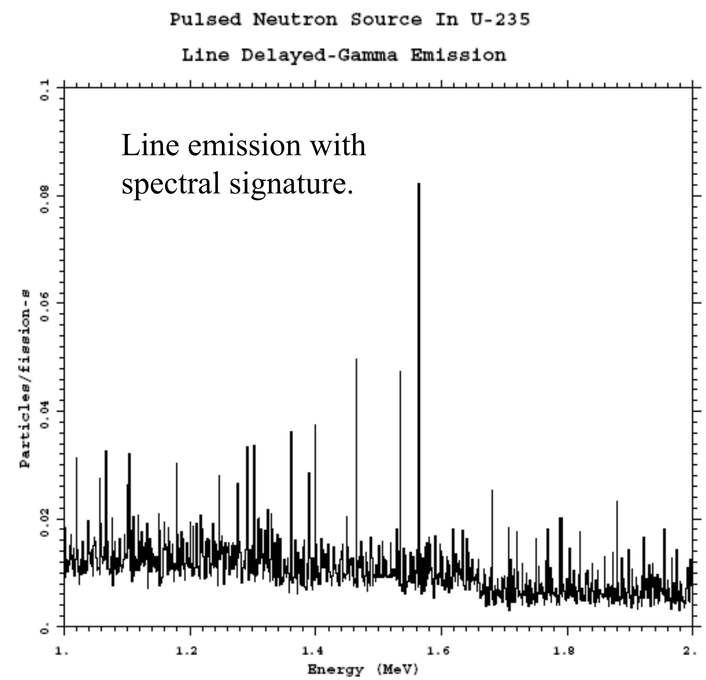


Results: Delayed-Gamma Lines for Neutron-Induced Fission of HEU

- **Sample Model "u5edelay": HEU Uranium Sphere.**
  - 0.01975-cm radius to minimize self-absorption effects.
  - 99.9 at% U-235, 0.1 at% U-238.
  - Pulsed neutron source at t=0, spatially uniform surrounding sphere, fission spectrum.

25-Group and Line Emission Spectra. Surface Current Integrated t=[10^{-4} to 10^{2} s].





Delayed-Gamma Sampling

Integrate over all energy and time

$$S^{L}_{\tilde{i}:\tilde{n}} = \int_0^\infty \int_0^\infty s^{L}_{\tilde{i}:\tilde{n}}(E,t)\,dE\,dt$$

And sum over all $\tilde{i}$, $\tilde{n}$ for the total source:

$$S^{L} = \sum_{\tilde{i}}^{\tilde{I}} \sum_{\tilde{n}}^{N\tilde{i}} \int_0^\infty \int_0^\infty s^{L}_{\tilde{i}:\tilde{n}}(E,t)\,dE\,dt$$

Delayed-Gamma Sampling

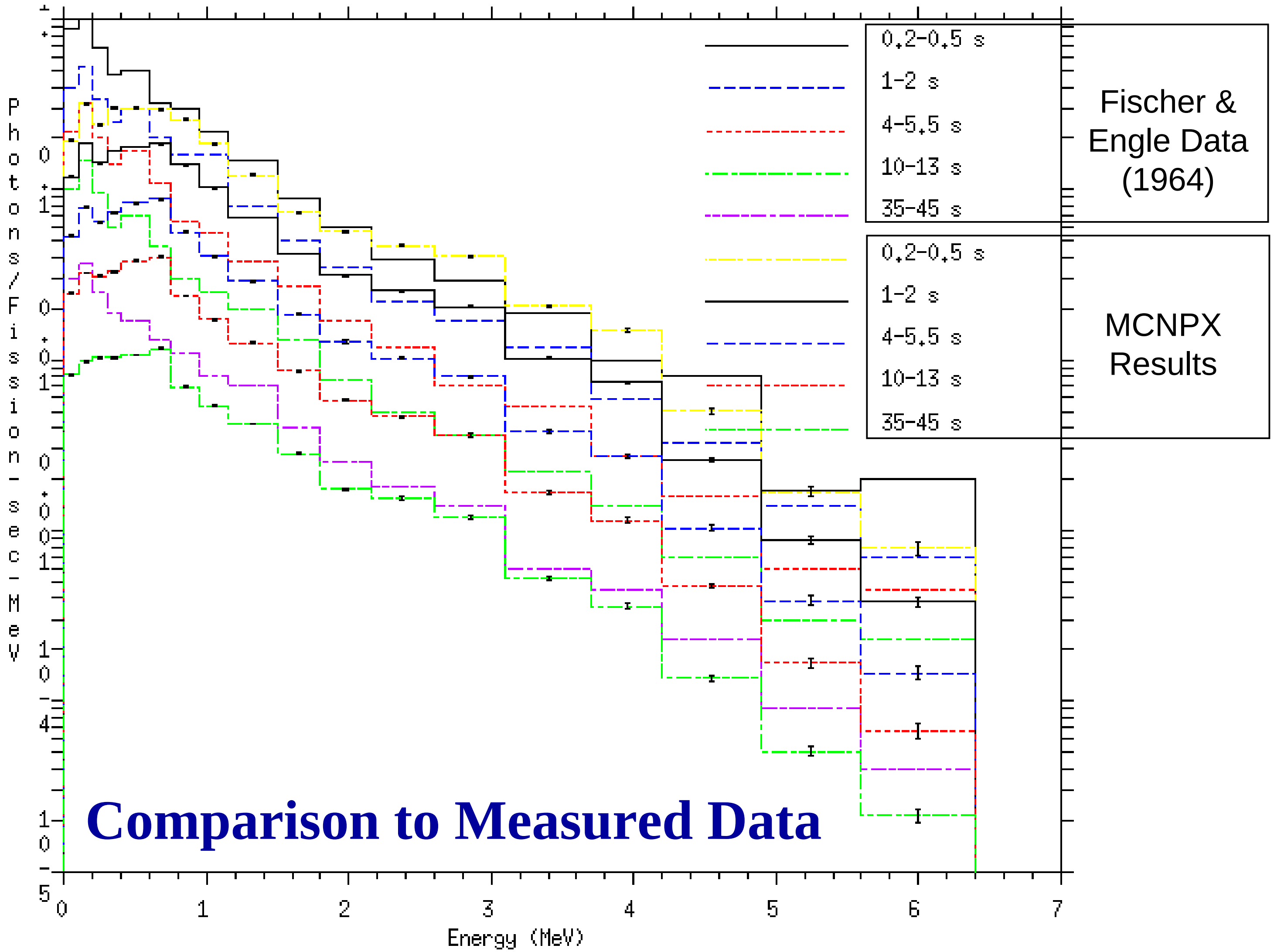
Delayed-gamma cumulative distribution function (energy cdf) that is used to sample delayed-gamma <u>line</u> emission as a function of energy for line emission, $\tilde{K}S$ <u>lines</u>:

$$\Xi^{L}_{J,\tilde{K}S} = \frac{1}{S^{L}} \sum_{\tilde{k}=1}^{\tilde{K}S} \sum_{\tilde{i}=1}^{\tilde{I}} \sum_{j=1}^{J} \frac{\Delta t_j}{2} \sum_{n=1}^{\tilde{N}\tilde{i}} (N_{\tilde{i}:j-1,\tilde{n}} + N_{\tilde{i}:j,\tilde{n}}) \lambda_{\tilde{i}:\tilde{n}} p^{L}_{\tilde{i}:\tilde{k},\tilde{n}} = \frac{S^{L}_{J,\tilde{K}S}}{S^{L}}$$

Energy cdf for <u>multi-group</u> emission, KS energy <u>bins</u>:

$$\Xi^{M}_{J,KS} = \frac{1}{S^{M}} \sum_{k=1}^{KS} \sum_{i=1}^{I} \sum_{j=1}^{J} \frac{\Delta t_j}{2} \sum_{n=1}^{N_i} (N_{i:j-1,n} + N_{i:j,n}) \lambda_{i:n} \overline{P}^{M}_{i:k,n} = \frac{S^{M}_{J,KS}}{S^{M}}$$

Delayed Neutrons and Gammas



Comparison to Measured Data

Summary – Delayed Gamma

- This methods & code-development effort is yielding the capability to calculate high-fidelity time-dependent delayed-gamma signatures.
- The effort has been complicated by:
  - Data complexity (discrete lines, continuum, multi-group) driving algorithm development, storage, execution, and testing.
  - Identifying suitable experimental measured data.
- Accomplishments include equation derivation to verify the m-g coding & extend to lines, the creation of over 10000 lines of coding & 979-nuclide line dataset, PC and cluster executables, initial benchmarking, 300+ pages of documentation, initial journal article manuscript.
- Remaining issues include data adequacy (T-16 vs NNDC), cdf algorithms/fidelity, storage & execution enhancements, non-fission emission, photon-induced emission, line/nuclide identification tallies, extensive validation & verification.

Future Development - MCNPX

- **Heavy-ion tracking and LAQGSM physics model (2.6.?)**
- **Magnetic fields**
- **CAD interface (with spline-surface tracking)**
- **Variance reduction techniques extended to models**
- **Improve point detectors/DXTRAN for models**
- **Extend electron data to 100 GeV**

Future of MCNPX

- **Possible public release of 2.6.0 (Summer 2007)**
- **Version 2.6.D/2.7.A (April 2007)**
  - **Transmutation improvements**
  - **Energy and time weight windows**
  - **Radioactive source option**
  - **Photofission and delayed neutron improvements**
- **MCNPX and MCNP merger**
  - **Hope to preserve all features of both codes**
  - **Preliminary version by Summer 2007**
  - **Public release perhaps by 2008**