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Update on the Integration of Neutron Multiplicity Analysis into GADRAS

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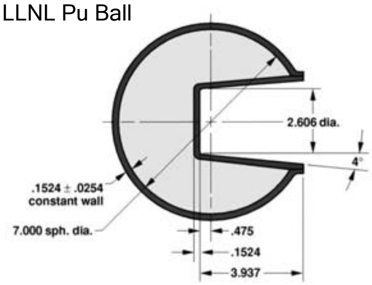
Introduction

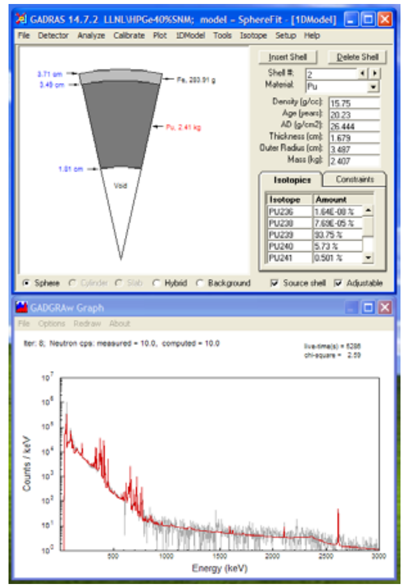
- GADRAS uses deterministic transport methods to synthesize gamma spectrum and neutron count rate from 1D transport models
- Transport modeling embedded in nonlinear optimization to find model parameters that match measured gamma spectrum & neutron count rate
- Simultaneous analysis of gamma spectrum & neutron count rate usually produces a better constrained solution
- Neutron count rate not a very rich metric of neutron field
- Developed method to synthesize Feynman-Y from time-dependent deterministic transport calculations

GADRAS Transport Model Optimizer

- Example: estimate mass and inner void radius of LLNL Pu sphere
- GADRAS uses Levenberg-Marquardt nonlinear optimization to search for model dimensions that minimize error between calculation and measurement
- Converged solution represents best (in least-squared-error sense) estimate of source configuration

LLNL Pu Ball





•Example based on LLNL measurement of unclassified plutonium sphere

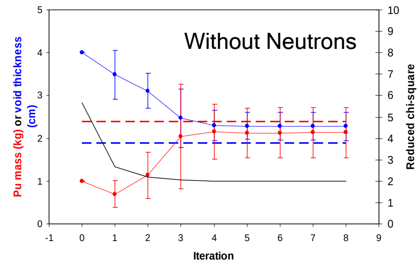
•2.4 kg weapons-grade plutonium metal sphere with frustum removed

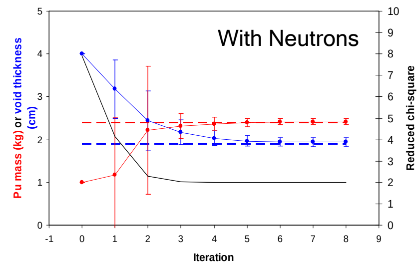
•Model at top-right shows best 1D estimate of source configuration

•Actual convergence time is less than 2 minutes on standard desktop computer

Simultaneous Analysis of Gamma & Neutron Signatures

- Example: estimate mass and inner void radius of LLNL Pu sphere
- Chart at top-right shows convergence on model parameters when only gamma spectrum is analyzed
- Solution tends to underestimate Pu mass because innermost Pu has weak effect on gamma spectrum
- Chart at bottom-right shows convergence when gamma spectrum and neutron count rate are analyzed simultaneously
- Solution converges on correct Pu mass
- Uncertainties are smaller





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Technical Approach

- Compute neutron multiplicity metrics using deterministic transport
  - Use transport models (instead of point models) to accurately model system dynamics
  - Use deterministic transport to keep calculations fast
  - Try to adapt existing transport solver(s) to this application

- Possible to compute moments of multiplicity distribution using standard Boltzmann transport solver
  - Moments require solution to forward and adjoint neutron transport problem
  - Moments vs. coincidence gate width require solution of forward time-dependent neutron transport problem

- Developed a method to compute Feynman-Y (variance-to-mean) vs. coincidence gate width that uses PARTISN time-dependent deterministic transport solver

Current Transport Framework

- Current framework solves coupled electron/neutron/photon transport problems
  - Uses ONEDANT for neutron transport
  - Uses ONELD for electron and photon transport
  - Uses ray-tracing to synthesize discrete photon lines

- Neutron solution coupled to photon source term by spontaneous & induced fission and (n, g) reactions
- Electron solution coupled to photon source term by Bremsstrahlung

- Photon and neutron leakage current folded with detector response models to synthesize gamma spectrum & neutron count rate

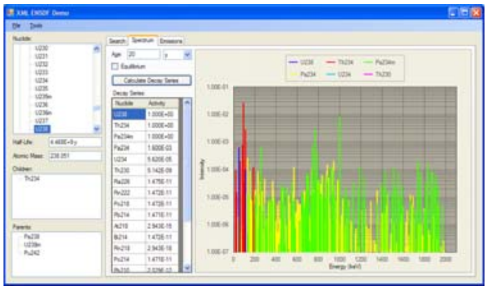
- Extending framework to compute Feynman-Y required a complete overhaul of current transport framework

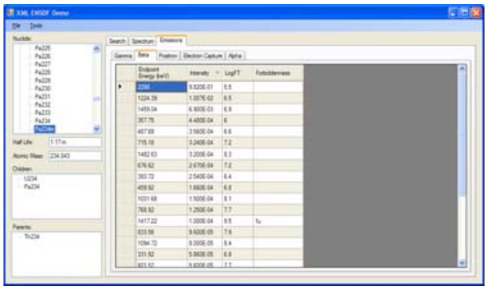
Changes to Transport Framework

- Developed new nuclide/emission database based on Evaluated Nuclear Structure Data Files (ENSDF)
- Integrated SOURCES-4C for neutron source term generation
- Developed new neutron cross-section library that includes neutron upscatter
- Replaced ONEDANT transport engine with PARTISN
- Integrated models of induced fission neutron multiplicity distributions
- Developed new (n, γ) reaction database based on MCNP libraries
- Implemented time-dependent transport calculations of Feynman-Y vs. coincidence gate width

Nuclide Database

- Developed new nuclide database from ENSDF
  - Tabulates branch ratios & emission probabilities for over 3700 nuclides
  - Translated to self-describing XML database
- About 1100 nuclides in new GADRAS database
  - Retained every nuclide with ancestor that has $T_{½} \geq 60$ minutes
  - Tabulates alpha, beta, positron, EC, and gamma emissions
  - U235, U238, Pu239, Pu240, and Am241 gamma spectra corrected to match benchmarks
  - Solves branching Bateman decay equations to generate decay series





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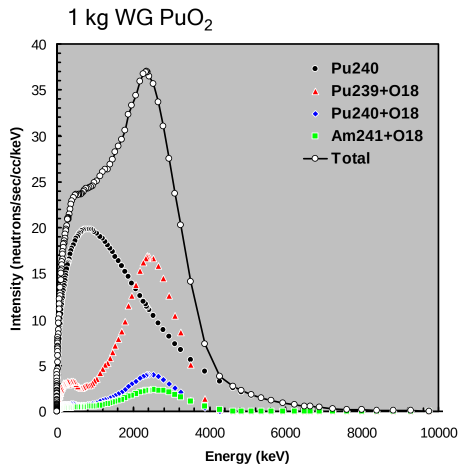
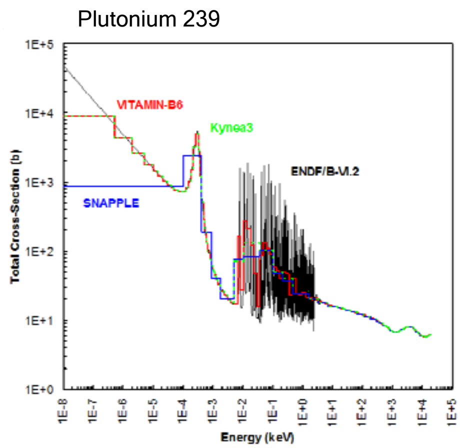
Neutron Source Terms using SOURCES-4C

- Integrated SOURCES-4C neutron spectrum code into GADRAS
- Uses Watt fission neutron spectra for 30 nuclides
- Computes (α, n) spectra from α-transport
  - Homogeneous material regions
  - Interfaces between materials
  - 48 alpha emitters
  - 16 target nuclides
  - Over 750 (α, n) spectra
- Example at right shows prominent source terms for 1 kg of weapons-grade plutonium oxide



Neutron Cross-Sections

- Current transport engine uses 47-group neutron cross-sections without upscatter (SNAPPLE)
- Found that k-effective and Feynman-Y calculations were inaccurate for highly thermalized problems
- Developed new cross-section library (Kynea3)
  - Merges fine-group VITAMIN-B6 library with coarse-group SNAPPLE library
  - Retains upscatter and group structure of VITAMIN-B6 at low energy, group structure of SNAPPLE at high energy



Effect of Upscatter on Multiplication Calculations

- Neutron upscatter: at very low energies, a neutron can emerge from a scatter interaction with more kinetic energy than it had when it entered the interaction
- In thermally fissioning materials slower neutrons are more likely to sustain fission chain-reactions
- Downscatter tends to increase multiplication
- Upscatter tends to decrease multiplication
- Without upscatter, can't accurately estimate multiplication for highly moderated systems

BeRP Ball Multiplication

Poly Thickness (in)	Subcrit Benchmark	MCNP		PARTISN		
		Spherical	Actual	SNAPPLE	Kynea3	VITAMIN-B6
0	4.6	4.4	4.4	4.0	4.0	4.0
0.5	5.7	5.7	5.6	5.4	5.4	5.4
1	7.4	7.7	7.3	7.3	7.4	7.4
1.5	9.8	10.3	9.6	10.3	10.1	10.1
3	15.5	16.5	15.1	24.0	16.5	16.5
6	N/A	17.5	15.7	36.6	18.3	18.2

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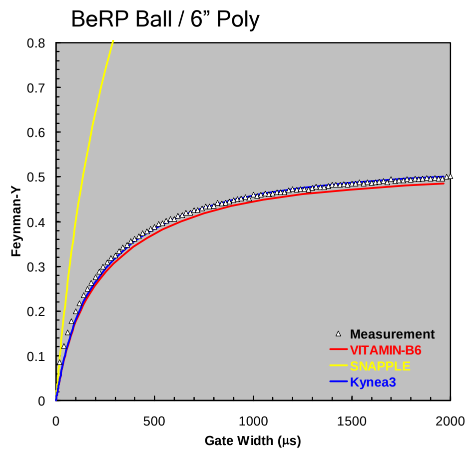
•Multiplication estimates for LANL BeRP ball

•Unclassified 4.5 kg solid sphere of alpha-phase weapons-grade plutonium metal

•Reflected by spherical shells of high-density polyethylene between 0” (no reflector) and 6” thick

Effect of Upscatter on Feynman-Y Calculations

- Downscatter shifts neutron population toward lower energies
  - Increases multiplication → increases Feynman-Y amplitude
  - Increases neutron lifetime → slows Feynman-Y rise-time
- Upscatter shifts neutron population back toward higher energies
  - Decreases multiplication → decreases Feynman-Y amplitude
  - Decreases neutron lifetime → speeds Feynman-Y rise-time
- Can't accurately calculate Feynman-Y for highly moderated systems without upscatter



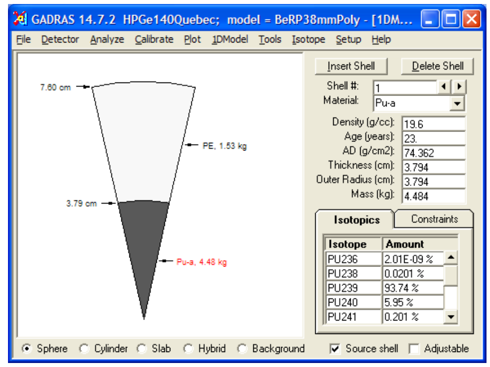
PARTISN Transport Solver

- Replaced ONEDANT solver with its successor PARTISN (Parallel Time-Dependent S_N)

- PARTISN is used to solve:
  - Static forward and adjoint neutron transport problem: used to compute neutron count rate and Feynman-Y asymptote
  - Dynamic forward neutron transport problem: used to compute Feynman-Y dependence on coincidence gate width

- Users won't notice a difference most of the time
  - Runtime for Feynman-Y calculations are longer
  - Can model spherical, cylindrical, and slab geometries

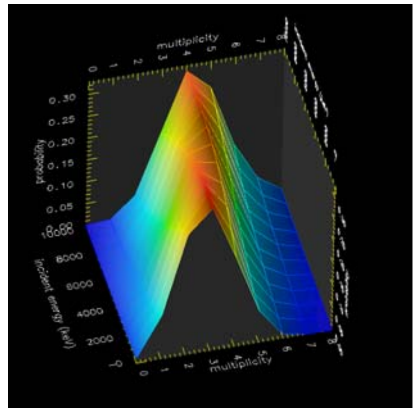
BeRP Ball / 1.5" Poly



Induced Fission Neutron Multiplicity Distributions

- Integrated Zucker & Hölden models for induced fission neutron multiplicity distribution
- Based on measurements of U235, U238, and Pu239
- Valentine (ORNL) developed prescription for adapting Z&H distributions to other nuclides
  - U235 → U233
  - U238 → U232, U234, U236
  - Pu239 → Pu241

Pu239 Induced Fission



(n, γ) Reaction Cross-Sections

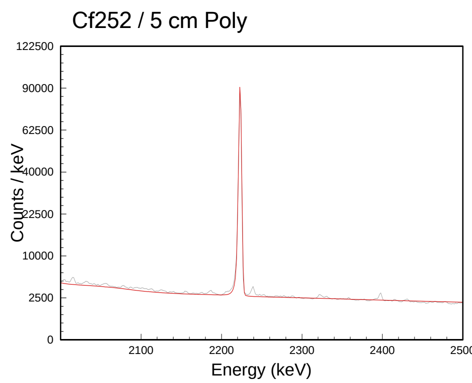
- Extracted (n, γ) reaction cross-sections from MCNP ENDF66 and ACTI libraries

- New GADRAS (n, γ) database contains:
  - 76 nuclides and elements
  - Over 10,000 gamma lines

- New (n, γ) calculations also correctly distribute energy of primary photons

$$E_\gamma = E_\gamma^0 + \frac{A}{A+m} E_n$$

- New database generally improves accuracy of (n, γ) calculations, still needs a lot of testing



Computation of Feynman-Y from Deterministic Transport

- Feynman-Y exhibits two notional features
  - Asymptotic value
  - Shape dependent on coincidence gate width
- Asymptote
  - Computed from static forward and adjoint transport solution
  - Accounts for relative contribution of source and induced fission neutrons
  - Source term for adjoint problem is detection efficiency – adjoint flux "weighting function" represents importance to detection
- Shape
  - Computed from solution to dynamic step response problem
  - Forward source term is instantaneously stepped
  - Leakage current is folded with detector cross-section & impulse response
  - Detector response is integrated over gate width

Computation of Feynman-Y Asymptote

- Excess variance comes from source and induced fission

$$\frac{\sigma^2}{\mu} = 1 + Y \qquad \sigma^2 = \mu + {}_2S_0 + {}_2S$$

- Variance of source neutron production Q

$${}_2S_0 = \int d^3r \int dE \, \frac{\overline{\nu_0(\nu_0 - 1)}}{\overline{\nu_0}} \, Q(\vec{r}, E) \, I_0^2(\vec{r}) \qquad I_0(\vec{r}) = \int dE' \, \frac{\chi_0(\vec{r}, E')}{4\pi} \, \varphi^\dagger(\vec{r}, E')$$

- Variance of fission neutron production $\nu\Sigma_f\varphi$

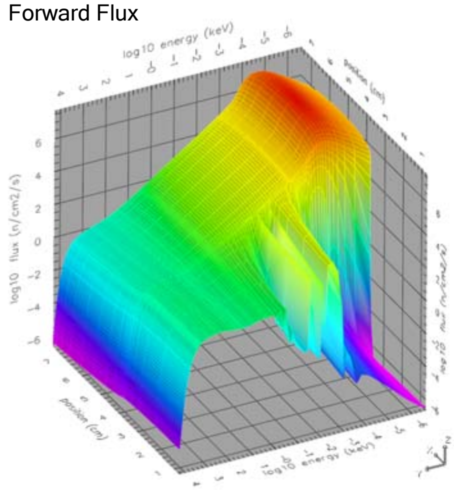
$${}_2S = \int d^3r \int dE \, \overline{\nu(\nu - 1)} \, \Sigma_f(\vec{r}, E) \, \varphi(\vec{r}, E) \, I^2(\vec{r}) \qquad I(\vec{r}) = \int dE' \, \frac{\chi(\vec{r}, E')}{4\pi} \, \varphi^\dagger(\vec{r}, E)$$

- Importances I_0 and I weighted by adjoint flux $\varphi^\dagger$

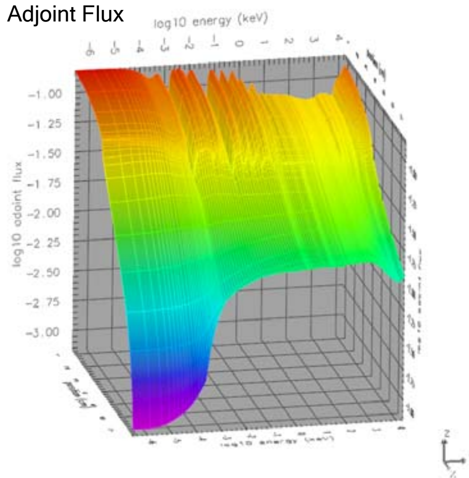
Static Forward and Adjoint Solutions

LANL BeRP Ball / 1.5" Poly Reflector

Forward Flux



Adjoint Flux



Computation of Feynman-Y Shape

- Feynman-Y shape computed from solution to forward dynamic step response problem

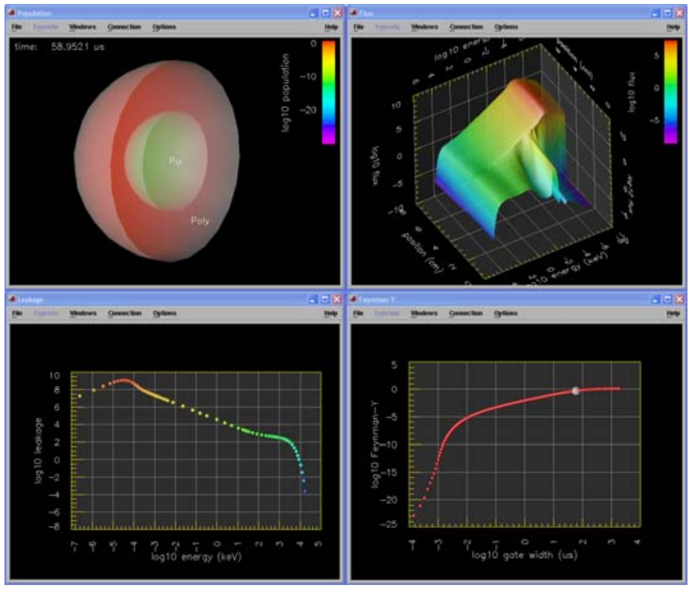
$$Y(T) \propto \frac{1}{T}\int_0^T dt \int_0^t dt'\, h(t-t')\Sigma_d(\vec{r},E)\,\varphi(\vec{r},E,t')$$

- Uses LANL transport solver PARTISN to compute flux φ in response to instantaneous step in forward source term Q

- Time-dependent flux folded with detector cross-section Σ_d and impulse response h

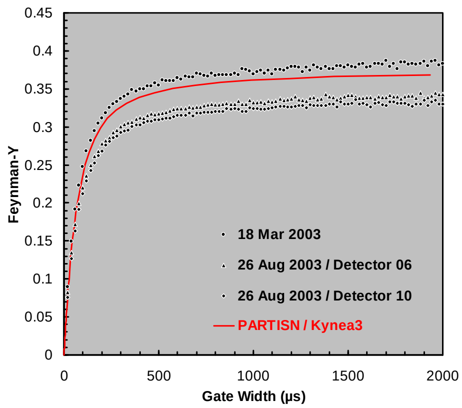
- Integrated over coincidence gate width T

Computation of Dynamic Response



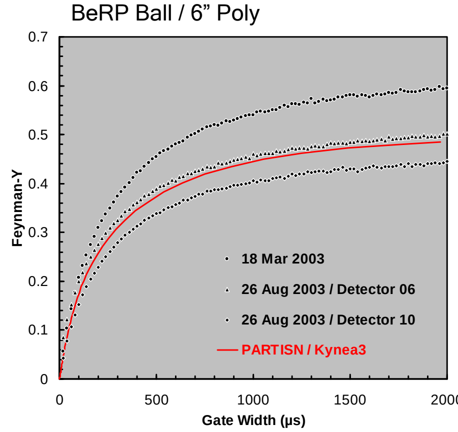
Initial Test Results

Bare BeRP Ball



Comp. Time: 2.5 sec

BeRP Ball / 6" Poly



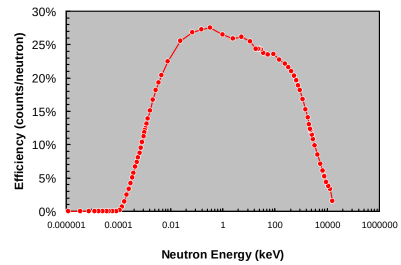
Comp. Time: 13.0 sec

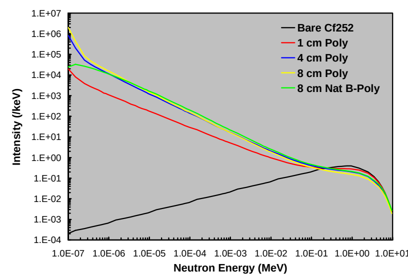
Neutron Detector Calibration

- Neutron detector efficiency vs. energy unfolded from of measurements
  - Measure neutron count rate:
    - Bare Cf252
    - Cf252 in polyethylene spherical shells up to 4 cm thick
  - Count rates used to index into lookup table containing efficiency vs. energy pre-calculated by Monte Carlo

- We've observed some problems modeling very highly moderated sources

- Extending calibration set to use thicker moderators





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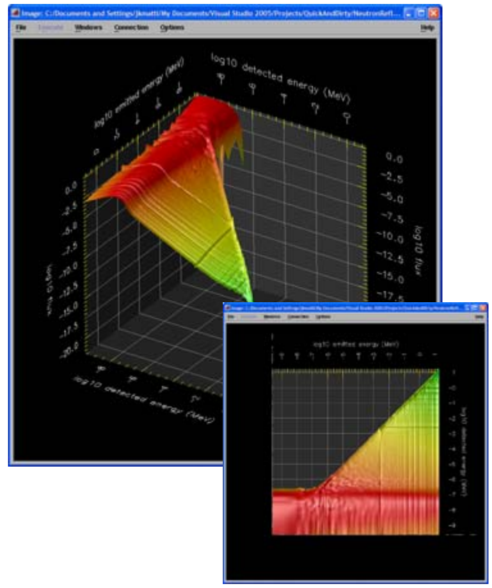
Neutron Environmental Scattering

- Neutron scattering off reflecting surfaces (floor, walls) creates an albedo source of neutrons in addition to direct source
- Augments neutron detector response

- Using MCNP to compute reflection "transform matrix"
- Matrix tabulates probability of detection versus:
  - Neutron energy emergent from source
  - Neutron energy incident on detector
- Matrix calculated for several source-detector and source-reflector distances

- Can fold neutron leakage spectrum with transform matrix and detection efficiency to estimate response to reflected neutrons



Summary

- GADRAS transport framework has received a complete overhaul
- Changes to source term generation, cross-section libraries, transport solver, and reaction libraries improve accuracy of assessments

- Implemented method to compute Feynman-Y vs. gate width using deterministic transport
- Synthesized Feynman-Y without using point model approximation
- Calculations require 1 - 20 seconds

- Integrating analysis of Feynman-Y into GADRAS
- Source models will use simultaneous analysis of gamma spectrum and Feynman-Y
- Expect that simultaneous analysis will better constrain solution to some problems

Upcoming Developments

- Working to integrate Feynman-Y into GADRAS interface and analysis procedures

- KEEP TESTING CHANGES! - working to acquire more and better measurements to test simultaneous gamma spectral / neutron multiplicity analysis

- Trying to identify transport solution options to decrease computational time further

- Interested in modeling neutron reflection feedback into fissile system

Acknowledgments

- Work sponsored by NNSA Offices of Nonproliferation Research & Development (NA-22) and Nuclear Counterterrorism (NA-47)
- Erik Shores of LANL assisted with integration of SOURCES-4C
- Jeff Favorite and Randy Baker of LANL assisted with integration of PARTISN
- Ken Butterfield, Doug Mayo, John Bounds, and Mark Smith-Nelson of LANL provided measurements of BeRP ball

Supplemental Information

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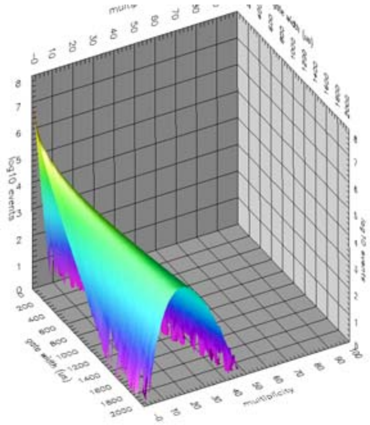
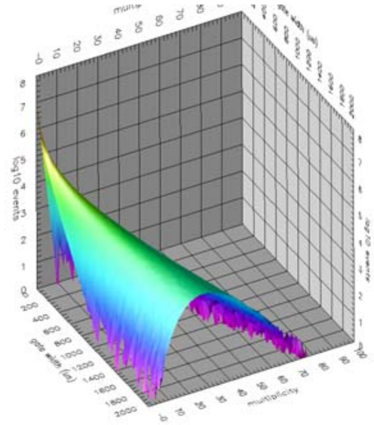
Neutron Multiplicity Distribution

Multiplication ~ 4.5
Generation Time ~ 3 ns



LANL BeRP Ball / Bare

Multiplication ~ 15.5
Generation Time ~ 9 μs



LANL BeRP Ball / 3” Poly Reflector

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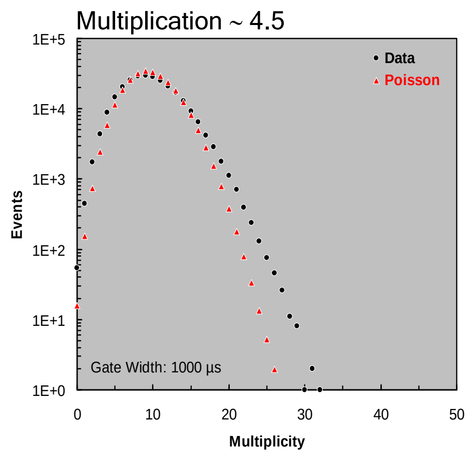
•Los Alamos BeRP ball is an unclassified 4.5 kg sphere of alpha-phase weapons-grade plutonium metal

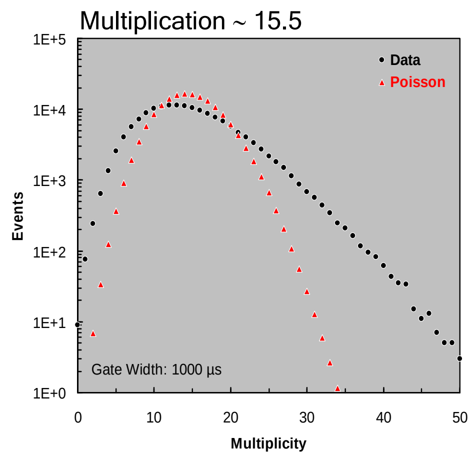
•Constructed for critical and subcritical experiments using various reflecting materials

•All measurements shown in this presentation use polyethylene reflectors varying in thickness from 0 (bare) to 6”

Multiplication Induces Excess Variance



LANL BeRP Ball / Bare



LANL BeRP Ball / 3” Poly Reflector

Feynman-Y: Excess Relative Variance

- Feynman-Y measures excess variance relative to Poisson process

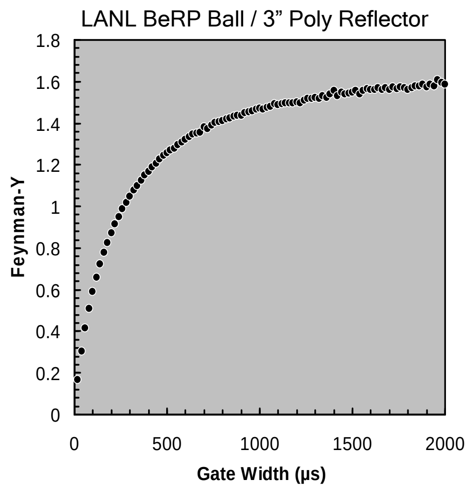
$$\frac{\sigma^2}{\mu} = 1 + Y$$

$$\sigma^2 : variance$$

$$\mu : mean$$

- Y vanishes if counting distribution is purely Poisson
- Y tends to increase with neutron multiplication

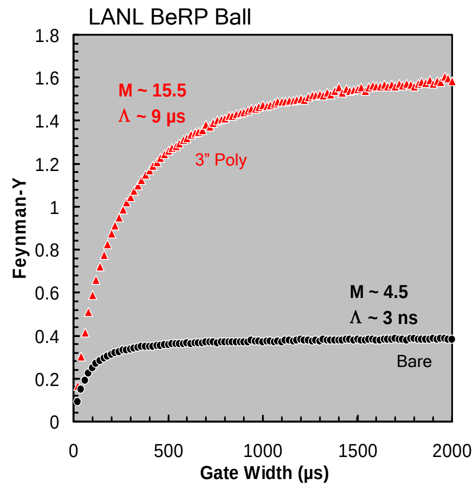
- Usually measured vs. coincidence gate width (counting time)



Effect of Multiplication and Generation Time

- Y is a measure of the second moment of the counting distribution
- Asymptotic value tends to increase with square of neutron multiplication

- Y is a measure of the system's dynamic response
- Shape vs. gate width tends to evolve more slowly with increasing neutron generation time

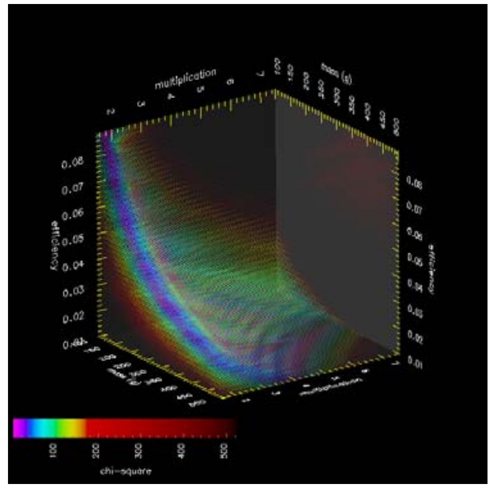


Degeneracy in Neutron Multiplicity

- Neutron multiplicity distribution is a complicated function of source strength (mass), multiplication, leakage and detection probability (efficiency)
- Systems w/ similar products of mass, multiplication, and efficiency exhibit similar multiplicity distributions

- Problem has more degrees of freedom than model
- Many possible models tend to fit measurement equally well
- Can't rely on neutron multiplicity alone to estimate system parameters

LLNL Pu Ball



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