Computational Simulations in Non-proliferation, Nuclear Detection, and Forensics Research at University of Florida

Presented by

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FP&L Endowed Term Professor -- 2007.2010

Florida Institute of Nuclear Detection and Security

Nuclear & Radiological Engineering

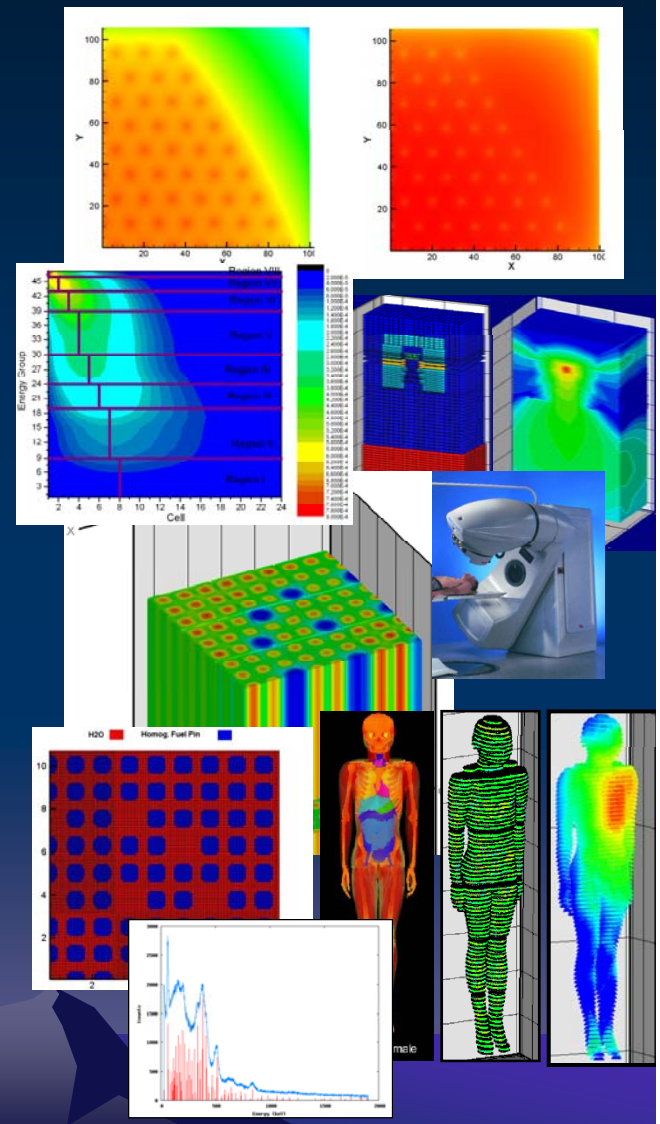
University of Florida

General Theme

- **Non-Proliferation and Reactor Physics.**
  - Computational radiation transport methods should always have an integral role in non-proliferation and power research and engineering
- **Radiation Detection.**
  - It is important to recognize how computational simulation can improve non-proliferation and nuclear forensics detection modalities
- **Advanced Education and Training.**
  - Application of simulation methods in graduate research enables us to produce top quality researchers who are ready to solve problems in industry
  - Maintaining a ***pipeline of qualified people***

Basis for Research at UF

- **Depth & Breadth of Experience in *Nuclear Engineering applications***
- **Broad Mosaic of Capabilities**
  - 3-D Transport Theory, Serial & Parallel Computation, Algorithm Development, Experimental Verification, & Device Development
- Ongoing work in
  - …SNM Detection, Detector Development, Noise Reduction, 3-D Parallel Transport, Reactor Modeling and Fuel Burnup, Whole Body Medical Phantom dosimetry, Heat Transfer, X-ray backscatter…



Overview

- Applications of deterministic and Monte Carlo Methods in understanding radiation transport
  - Codes and Methods
  - Source profiling and simulation of SNM signatures
  - Detector characterization and enhancement
  - Optimization of counting systems in SNM detection
  - Asymmetric approaches in hybrid methods (AA work)
  - Importance of whole core modeling and 3-D depletion
  - Advanced methods (differencing schemes, cross sections) for better accuracy
  - Development of new simulation tools supporting technical nuclear forensics

Radiation Transport Theory

- **Boltzmann transport methods**

$$\left(\mu\frac{\partial}{\partial x}+\eta\frac{\partial}{\partial y}+\xi\frac{\partial}{\partial z}\right)\psi_g(x,y,z,\mu,\varphi)+\sigma_g(x,y,z)\,\psi_g(x,y,z,\mu,\varphi)=$$

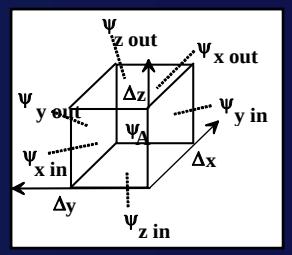
$$\sum_{g'=1}^{G}\sum_{l=0}^{L}(2l+1)\,\sigma_{s,g'\to g,l}(x,y,z)\,\{P_l(\mu)\phi_{g',l}(x,y,z)+2\sum_{k=1}^{l}\frac{(l-k)!}{(l+k)!}P_l^k(\mu)\cdot$$

$$\left[\phi^k_{C\,g',l}(x,y,z)\cos(k\varphi)+\phi^k_{S\,g',l}(x,y,z)\sin(k\varphi)\right]\}+\frac{\chi_g}{k_0}\sum_{g'=1}^{G}\nu\sigma_{f\,g'}(x,y,z)\,\phi_{g',0}(x,y,z)$$

  - **Monte Carlo method**
  - **Discrete Ordinates (S_N) method**
- **Track particles traveling in different directions, energies, 3-D spatial locations**
  - **Each has *Advantages* (+) , *Disadvantages* (-), *Issues***
- ***Both methods* can take advantage of parallel HPC**

Deterministic Discrete Ordinates (S_N)

Solves Discretized Boltzmann Transport Equation:



$$\hat{\Omega}\cdot\nabla\psi_g(\vec{r},\hat{\Omega})+\sigma_g(\vec{r})\psi_g(\vec{r},\hat{\Omega})$$

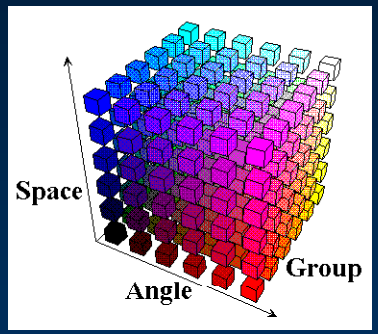
$$=\sum_{g'=1}^{G}\int_{4\pi}d\Omega'\,\sigma_{s\,g'\to g}(\vec{r},\hat{\Omega}'\cdot\hat{\Omega})\,\psi_g(\vec{r},\hat{\Omega}')+q_g(\vec{r},\hat{\Omega})$$

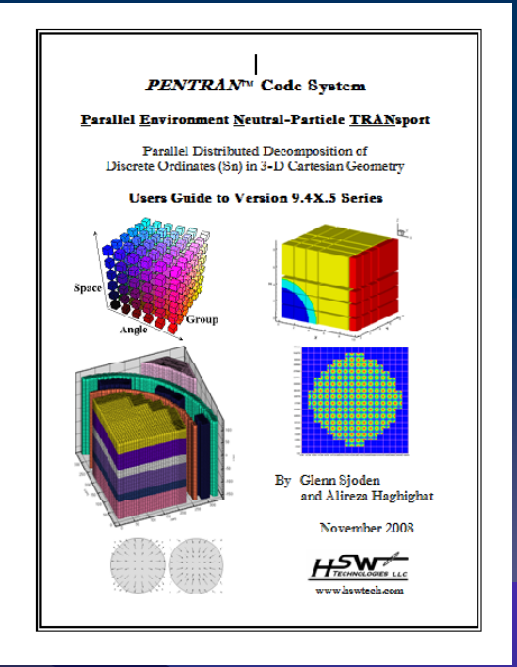
Over specific <u>*directions*</u>, <u>*energies*</u> in different <u>*spatial locations*</u> in 3-D

- **Advantages:**
  - Model entire geometry;
  - Fast and accurate;
  - Global flux distribution;
  - Parallelization in *angle, energy, space, or all*
- **Disadvantages:**
  - Proper multi-group cross sections;
  - Geometry requires effective discretization;
  - Memory, storage, differencing scheme issues.

PENTRAN Code System

- *"P*arallel *E*nvironment *N*eutral-particle *TRAN*sport"
- Over 13 years of continuous development
  - Introduced in 1996 by Sjoden & Haghighat
  - Parallel S_N in *angle*, *energy*, and *space* & *I/O*
  - ANSI FORTRAN over 39k lines
  - Industry standard FIDO input
- Solves 3-D Cartesian Sn Equations
  - Multigroup, anisotropic transport problems
- Forward and adjoint mode
  - Fixed source
    - Criticality eigenvalue problems




PENTRAN™ Code System

Parallel Environment Neutral-Particle TRANsport

Parallel Distributed Decomposition of Discrete Ordinates (Sn) in 3-D Cartesian Geometry

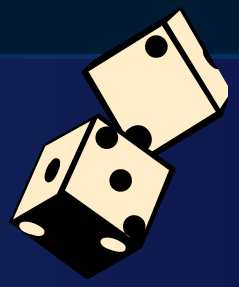
Users Guide to Version 9.4X.5 Series

By Glenn Sjoden and Alireza Haghighat

November 2008

www.hswtech.com

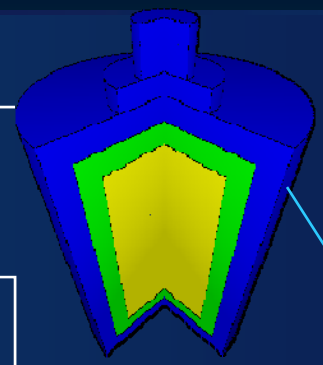
Monte Carlo – MCNP5



- Advantages
  - Traditional, straight forward;
  - Geometrically precise;
  - Robust particle physics--Continuous-Energy xsec;
  - Parallelization obvious: particle histories.
- Disadvantages:
  - Processing time, Non-analog variance reduction;
  - Inherent statistical uncertainties;
  - “Global” solution difficult to obtain.

Define equivalent models (e.g. consistent source &tally definitions) to those used in PENTRAN models.
-- Cross section libraries:
- PENTRAN/BUGLE-96 (47 neutron, 20 photon energy groups);
- MCNP5 – continuous “pointwise” ENDF/B-VI.

SNM Source Characterization



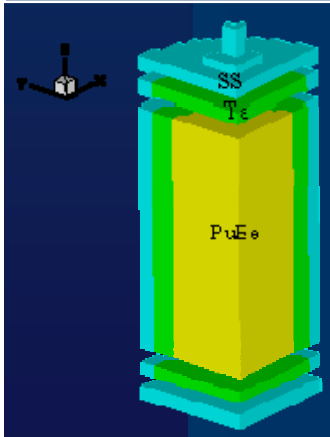
Computational

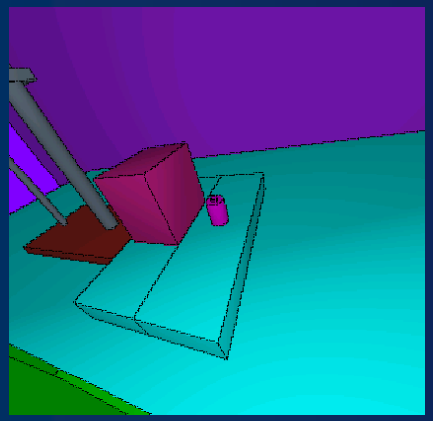
Deterministic S_N
PENTRAN

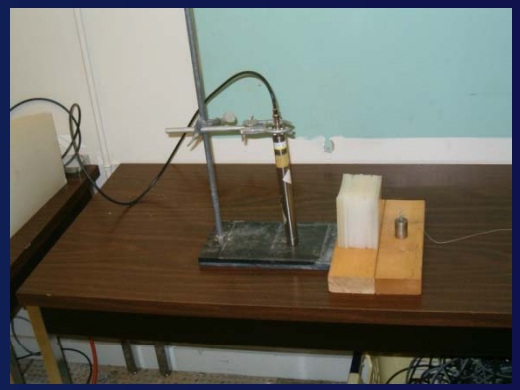
Monte Carlo
MCNP5

Source Description;
Neutron Emission;
Pu Age Estimation;
Effective Dose;
Benchmark Problem
Simulation vs
Experimental

Experimental

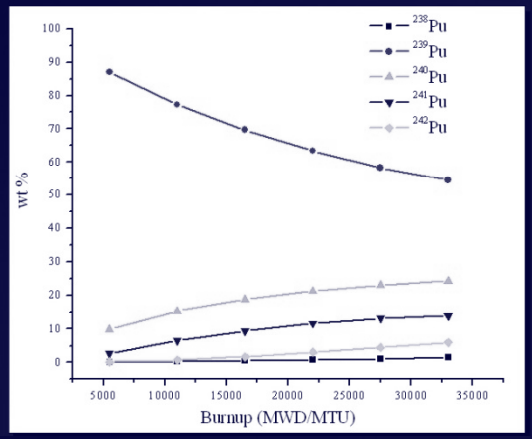




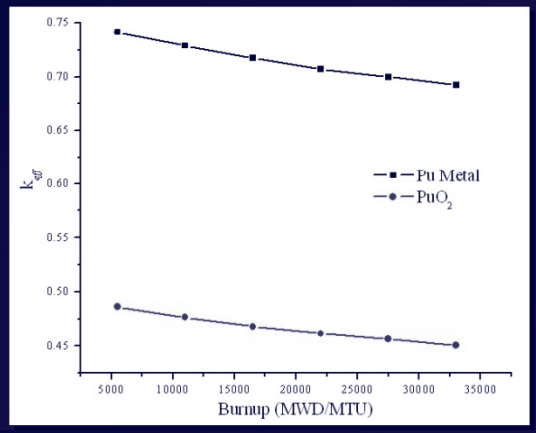


Ghita, Sjoden, & Baciak, "*A Methodology for Experimental & 3-D Computational Radiation Transport Assessment of Pu-Be Neutron Sources,"* *Nuclear Technology,* **159**, 319-331 (2007)

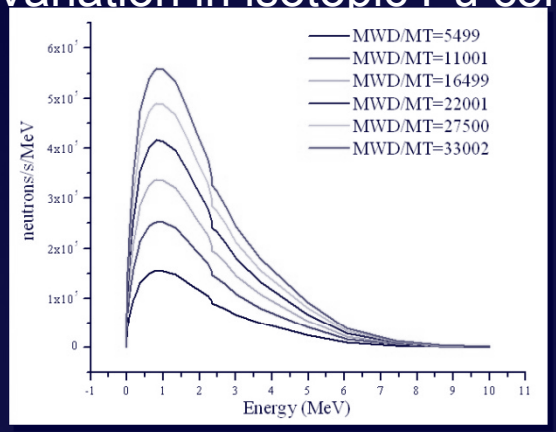
Intrinsic source trends: PWR-Generated Pu

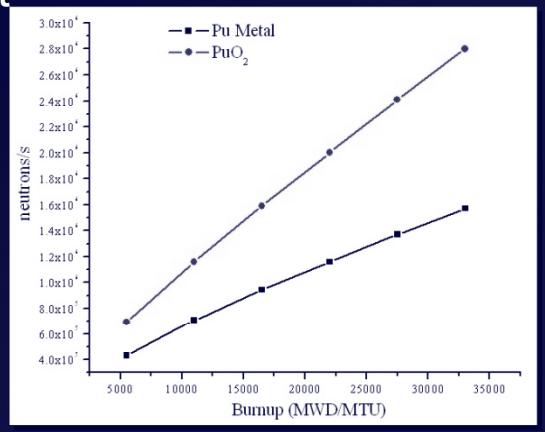


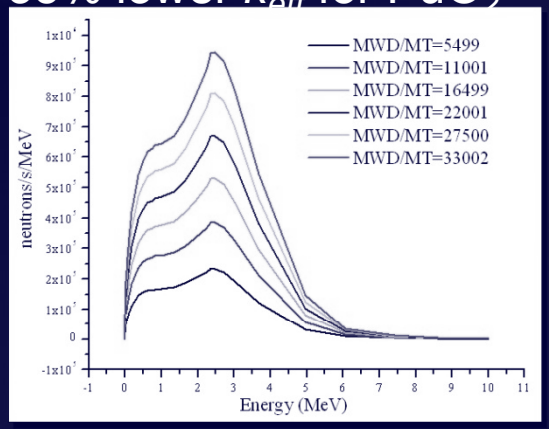
Variation in isotopic Pu content



35% lower k_{eff} for PuO_2

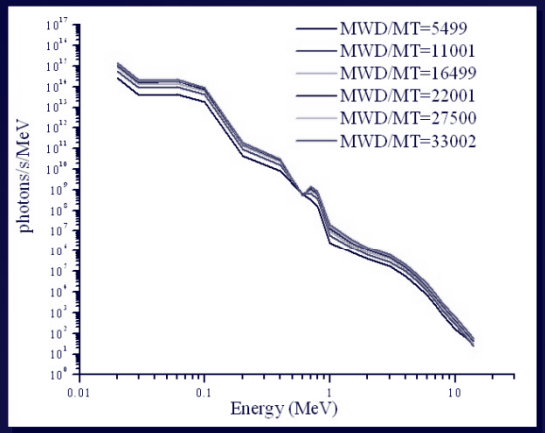


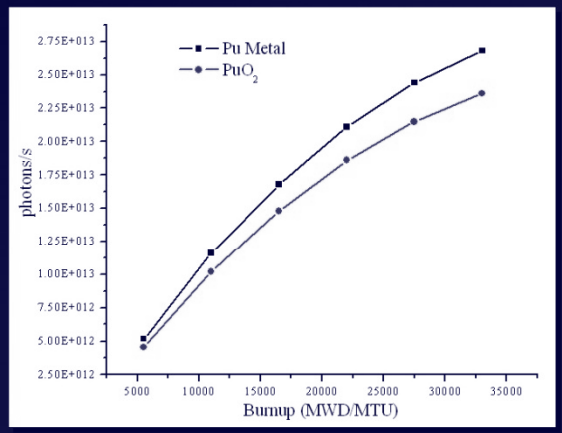


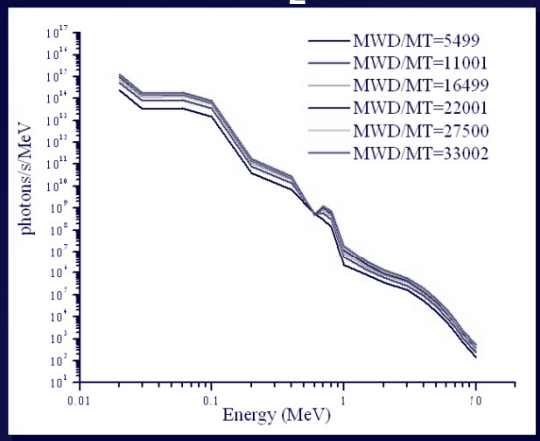


Pu metal

PuO_2



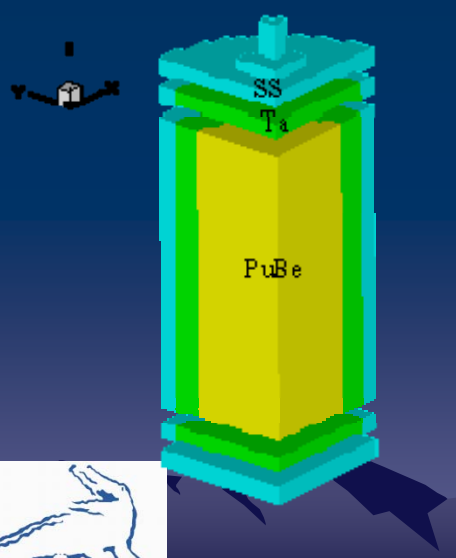


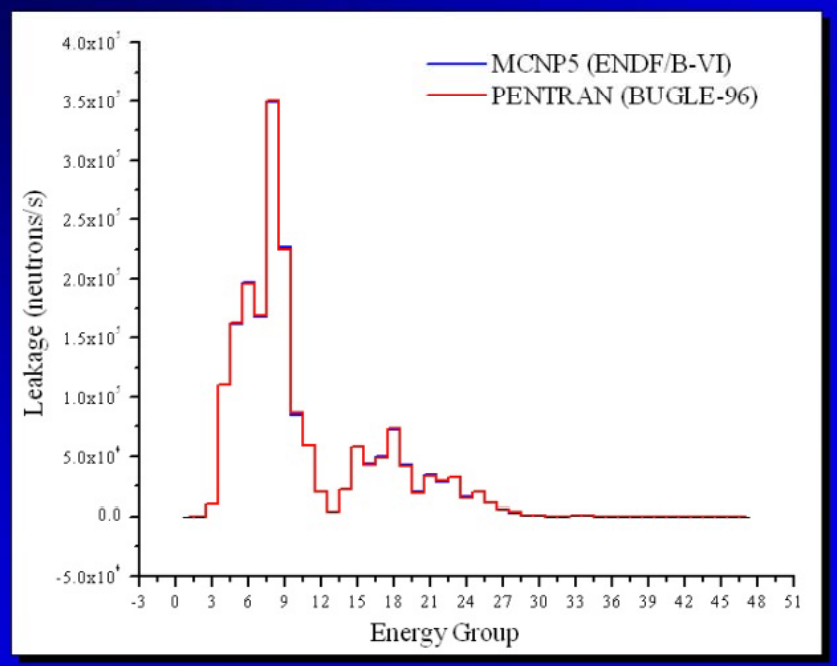


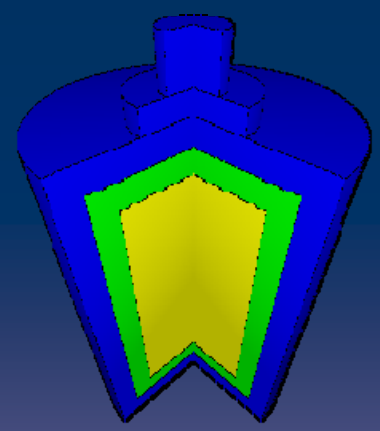
Pu-Be Neutron Leakage

PENTRAN - using BUGLE-96
- 6,452 3-D mesh cells
- 1/4 symmetry
- S_{24} angular quadrature
- P_3 scattering anisotropy
- ➢ 1.8527E+06 n/s
- ➢ k_{eff}=0.03567

MCNP5 (1σ) - using ENDF-BVI point wise "continuous" energy library
- nonu card (no multiplication)
- ➢ 1.8528E+06 (0.01%) n/s
- ➢ k_{eff} = 0.03576 ± 0.00001







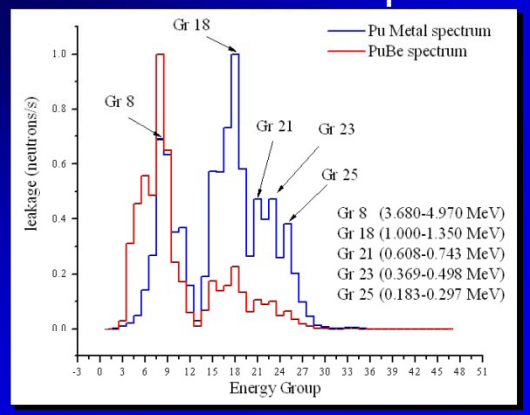
SNM Signature Simulation: Pu-Be n-Source Capsule Shielded to Emulate a WGPu Neutron Spectrum

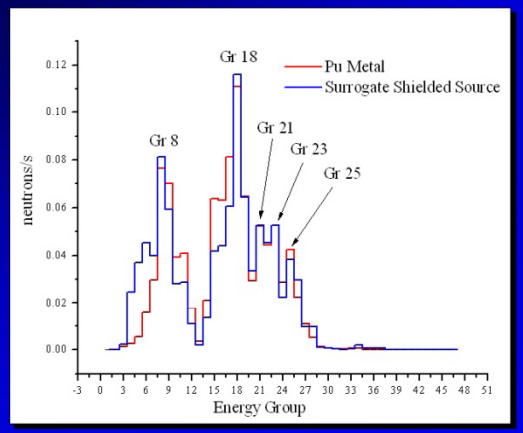
G. Ghita et al., "*WGPu-X Surrogate Shielded Source Design for PuBe*",
UF Invention Disclosure #12609, US Provisional Patent # 61/027988

Designed, constructed, and *laboratory-tested* a ***unique shield design*** that transforms the neutron leakage spectrum of a small 1 Ci PuBe capsule into a softer fission neutron spectrum signature from a large WGPu mass.

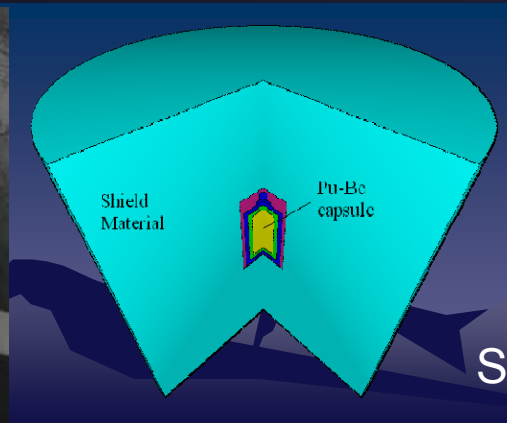
This will enable testing for detection of a significant quantity of weapons plutonium without the expense or risk of testing detector components with real materials.

PuBe vs. Pu metal Spectra



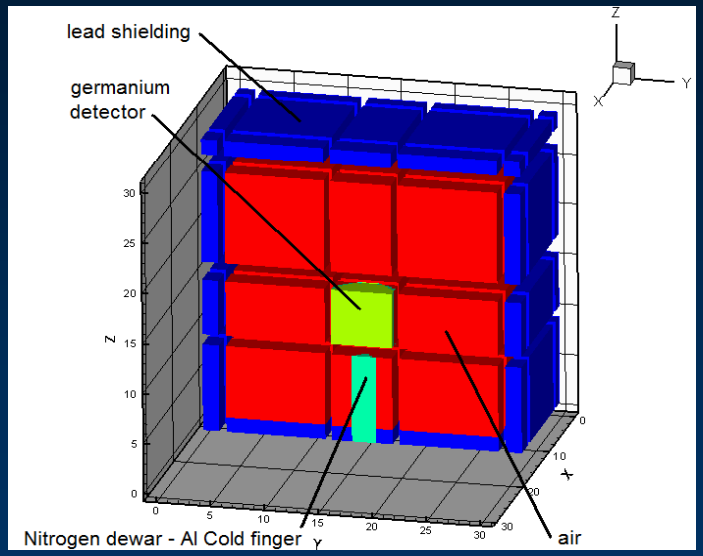


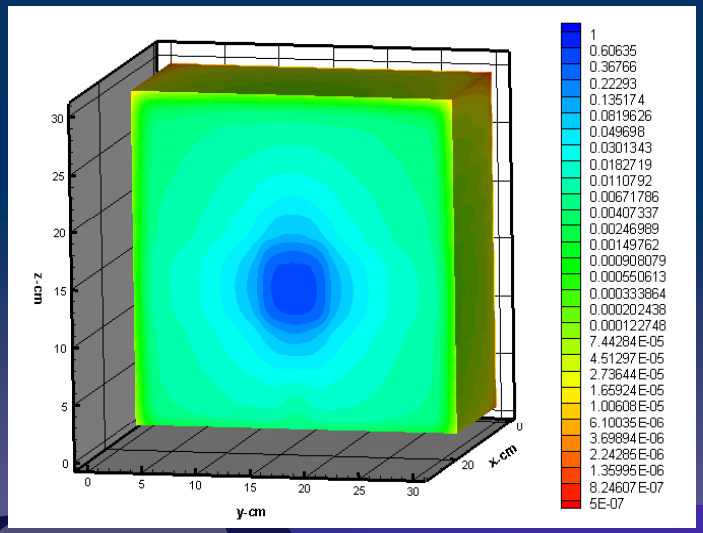
Shielded PuBe vs. Pu metal Spectra



Detector Characterization

- 3-D Adjoint Sn Yields accurate assessment of detector response, efficiency over phase space
- Also
  - (i) Relative and absolute detector efficiency, any sample location
  - (ii) Overall detector performance
  - (iii) Potential detector drift
  - (iv) Probable sample placement / proximity of amorphous source to detector
  - (v) Precise burden of cosmogenic or other nearby background, as applicable.

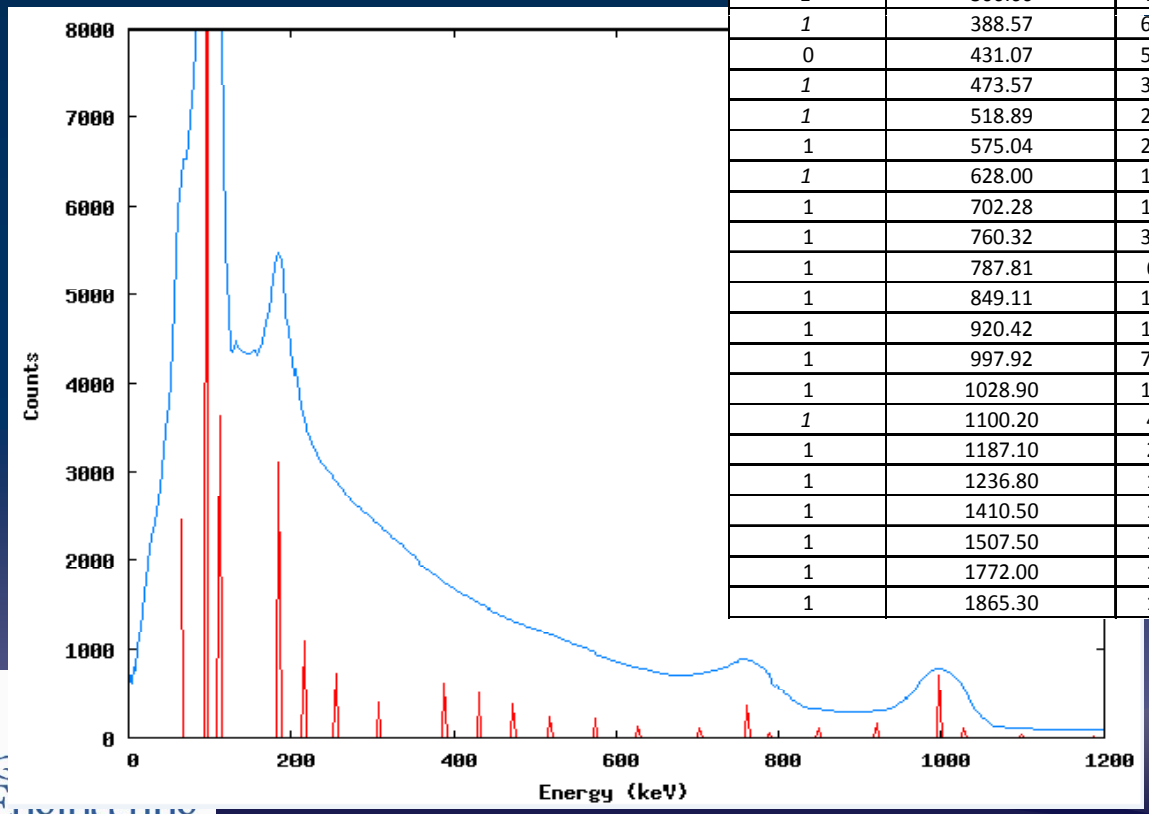




400-410 keV Gamma Importance (ε)

ASEDRA: Deconvolution NatU Results

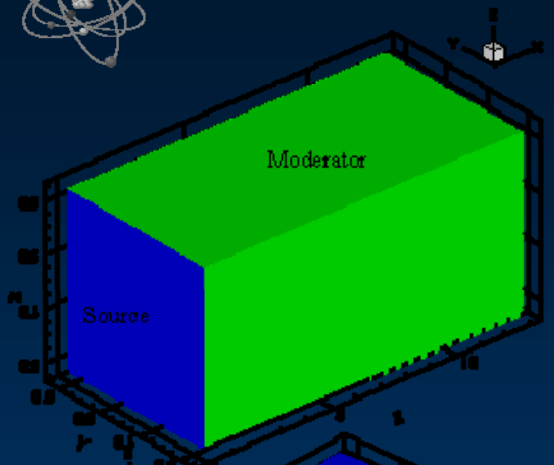
- Extract gamma lines using Detector Response Functions in NaI(Tl)
- Ra-226, Pa-234, others correctly detected…
- Peaks correctly correlated with HPGe, ~<1% in E

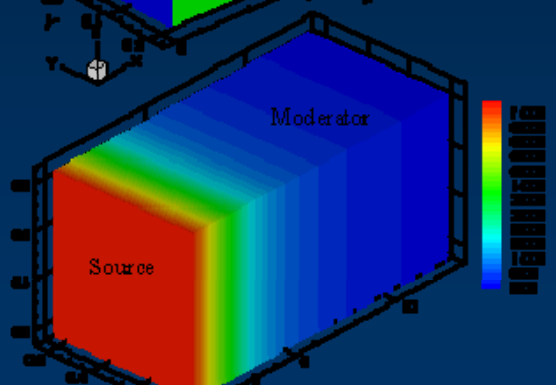


10 min, unshielded 8 kg Natural Uranium , NucSafe 2x2" NaI(Tl) Detector					
HPGe Indicated (1=yes)	E (keV)	Counts	ID	ID keV	Comment
1	64.97	2450.70	Th-234	63.3	in Ge
1	96.05	12715.00	U-238	U	K-L Transition
1	112.18	3640.10	U-238	115.6	U K-edge
1	185.51	3101.90	Ra-226/U-235?	186.2	U-238 daughter
1	215.25	1081.40	Pa-234,m?	227	in 1 hour Ge
1	254.32	722.78	Pa-234?	258.13	in Ge
1	306.66	406.99	Pa-231?	302.7	*U-235 Daughter, possibly in Ge*
1	388.57	625.70	Pu-239?	383	*possibly in Ge*
0	431.07	508.35	Pu-239?	430	Unknown
1	473.57	384.56	Pu-239?	475	*possibly in Ge*
1	518.89	251.55	Ho-166m	529.8	*possibly in Ge*
1	575.04	228.43	Pa-234	569	U-238 daughter
1	628.00	127.33	Bi-214?	609	*out of energy window*
1	702.28	110.04	Pa-234,m	699, 702	in 1 hour Ge
1	760.32	379.53	Pa-234,m	742.8, 755.6	in 1 hour Ge
1	787.81	62.69	Pa-234m	786	U-238 daughter
1	849.11	118.52	Pa-234m	851	in 1 hour Ge
1	920.42	164.87	Pa-234,m	921.7, 926	U-238 daughter
1	997.92	718.74	U-238/Pa-234m	1001	principal gamma
1	1028.90	106.40	Pa-234	1028.7	U-238 daughter
1	1100.20	42.20	Pa-234m	1061.9, 1125	*possibly in Ge*
1	1187.10	25.82	Pa-234m	1193.8	U-238 daughter
1	1236.80	12.98	Pa-234m, Bi-214	1237.2,1238.1	U-238 daughter
1	1410.50	16.76	Pa-234m	1414	in 1 hour Ge
1	1507.50	12.41	Pa-234m	1510.2	U-238 daughter
1	1772.00	16.93	Pa-234m, Bi-214	1765.4, 1764.5	U-238 daughter
1	1865.30	13.77	Pa-234m, Bi-214	1867.7,1847.4	U-238 daughter

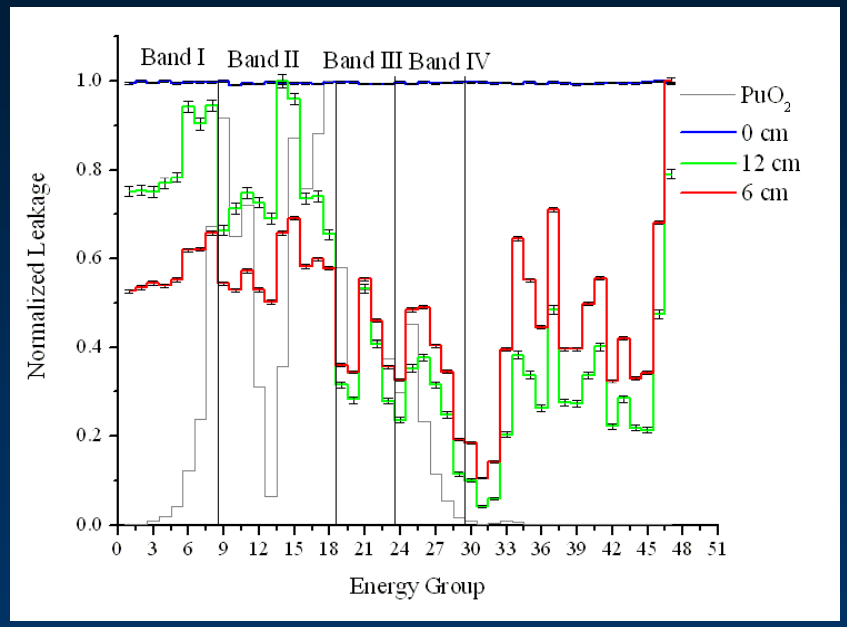
- Development ongoing

Optimization of Gas-Proportional Counters

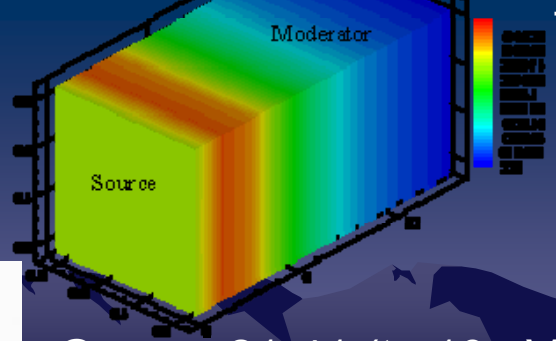




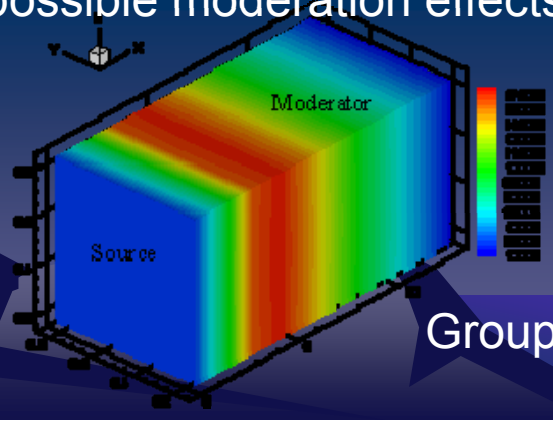
Groups 1-20 (to 0.7 MeV)



- (*n*,*p*) response in ^{3}He assuming that 4-atm ^{3}He is uniformly diluted throughout the block material;
- best possible moderation effects in each material.

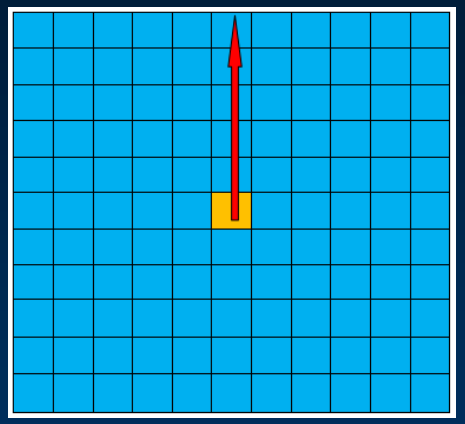


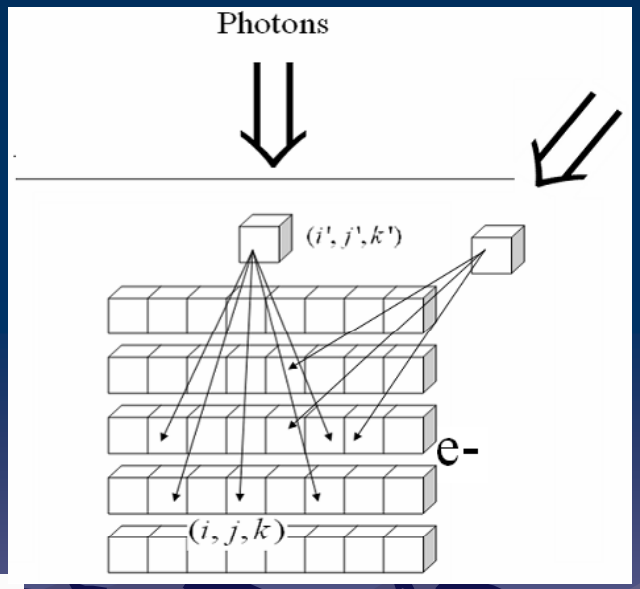
Groups 21-41 (to 10 eV)



Groups 42-47 (thermal)

Monte-Carlo Based EDK-S_N





- Charged Particle Transport > 1 Mev
  - Lack of Charged Particle Equilibrium over mesh
  - Not easily handled in 3-D deterministic approaches
- EDK-S_N kernel s from Monte Carlo
  - 11x11x11 cm^3 water box, forward-peaked X-ray source cell at center
  - ~All electrons are absorbed
  - 16 energy groups in 0.5 MeV steps
  - MC: low variances (<1% on average)
  - Full Physics Monte Carlo MCNP5 *F8
  - Projected via Euler Angles on Dose Driving Voxel
  - Scaled by Sn computed photon fluxes
- With PENTRAN+EDK, whole Body doses everywhere in ~1 hour

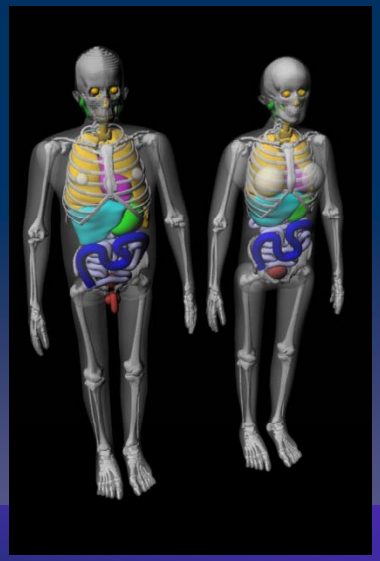
EDK-S_N Organ Dose Computation

Absorbed dose rate (MeV/g.Sec) calculated for the test Phantom 8 MV Uniform beam using EDK-S_N and MCNP5 using *F8(p, e^- mode)

Organ	MC(*F8) (MeV/g.Sec)	(2-sigma) MC Uncertainty	Sn-EDK (MeV/g.Sec)	(MC-EDK)/EDK
Right+ Left Lung	1.35E-01	6.80%	1.41E-01	4.56%
Pancreas	9.47E-05	4.14%	9.85E-05	4.02%
SI W	3.56E-05	4.00%	3.75E-05	5.43%
Spleen	1.11E-04	3.00%	1.18E-04	6.58%
Stomach W	1.86E-04	4.60%	1.94E-04	4.09%
Thyroid	1.41E-05	6.82%	1.38E-05	2.08%
Prostate	2.21E-08	44.00%	2.29E-08	3.62%

Dose rate (MeV/g.Sec) calculated for the test problem using MCNP5 using *F8(p, e^- mode) and MCNP5 F6 tallies

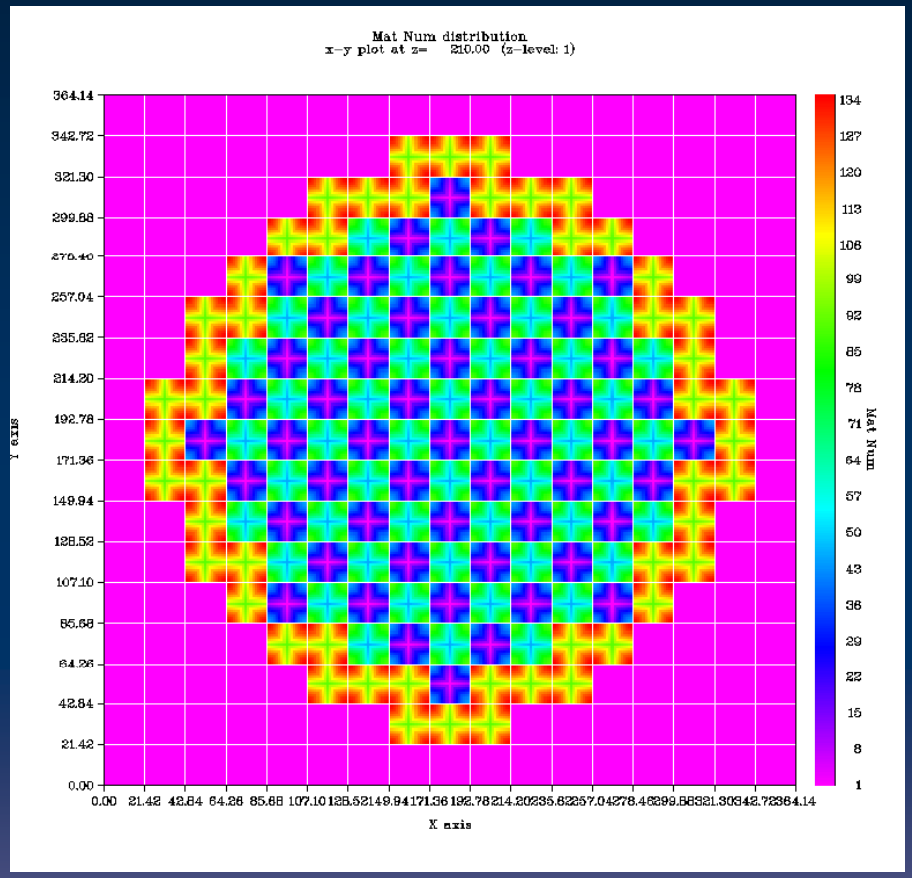
	Dose (Mev/gm.Sec)	2-Sigma-MC	(EDK-MC)/EDK	Running Time
Sn-EDK	2.29E-08	-----	-----	2hr
MC1	2.21E-08	44.00%	3.62%	3.9hr
MC2	2.34E-08	39.20%	2.14%	4.7hr
MC3	2.18E-08	34.40%	5.05%	6.1hr
MC4	2.23E-08	22.20%	2.69%	14.5hr
MC5	2.46E-08	16.86%	6.91%	28.15hr
MC6	2.406E-08	14.14%	4.58%	38.85hr



ALRADS Morphable UF Phantoms (W. Bolch)

Nuclear Power Full Core Transport

- PENTRAN Sn Full 3-D Core (PWR900)
  on IBM BlueGene/P
- Collaborative effort between EDF (T. Courau), IBM,
  HSW Technologies,
  University of Florida
- Goal: Use PENTRAN to simulate high fidelity whole core 3-D models
- Test Parallel Scalability, Performance on 100's to 1000's of BG/P processors,
  10-100M cells,
  2-8 energy groups



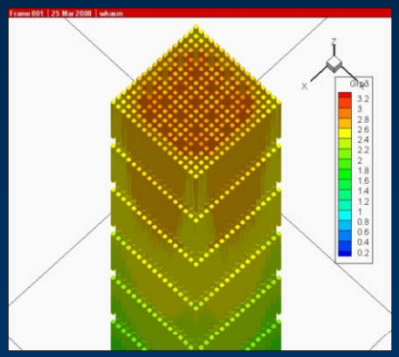
PENBURN – 3-D Parallel Burnup

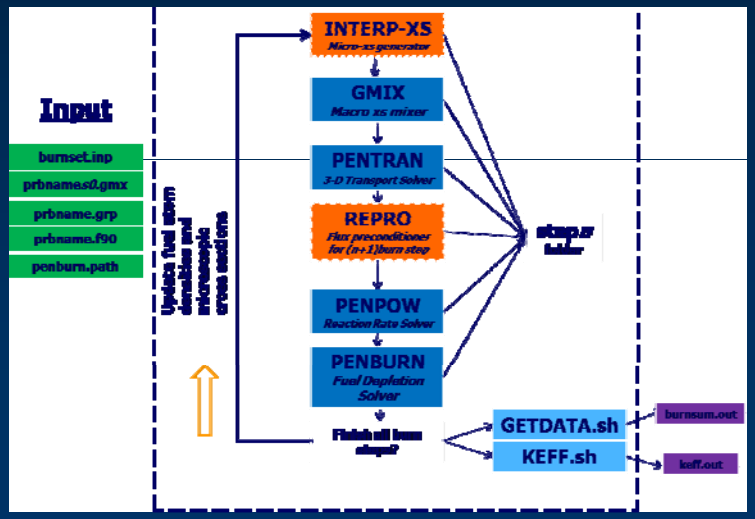
Fully attributed 3-D Transport Fuel Burnup, automated sequence

PENTRAN/PENBURN enables 3-D f.p. and actinide production tracking

Burnup dependent Cross sections derived using SCALE5.1

Proliferation monitoring, fuel cycle optimization…





$^{238}U \xrightarrow{(n,\gamma)} {}^{239}Np$

$\downarrow$ β^- $T_{1/2}$=2.35 days

$^{239}Pu \xrightarrow{(n,\gamma)} {}^{240}Pu \xrightarrow{(n,\gamma)} {}^{241}Pu \xrightarrow{(n,\gamma)} {}^{242}Pu \xrightarrow{(n,\gamma)} {}^{243}Pu$

$\downarrow$ β^- $T_{1/2}$=13.2 year

^{241}Am

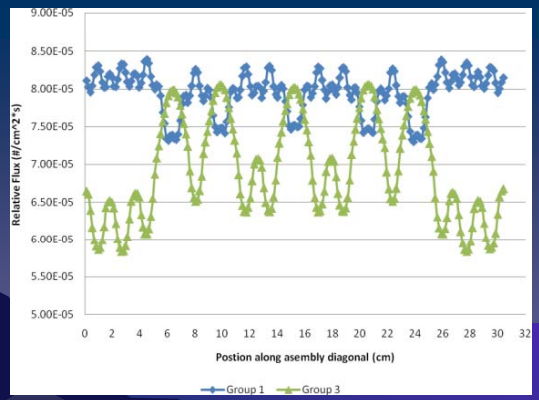
$\downarrow$ β^- $T_{1/2}$=4.98 hr

$^{243}Am \xrightarrow{(n,\gamma)} {}^{244}Am$

$\downarrow$ β^- $T_{1/2}$=10.1 hr

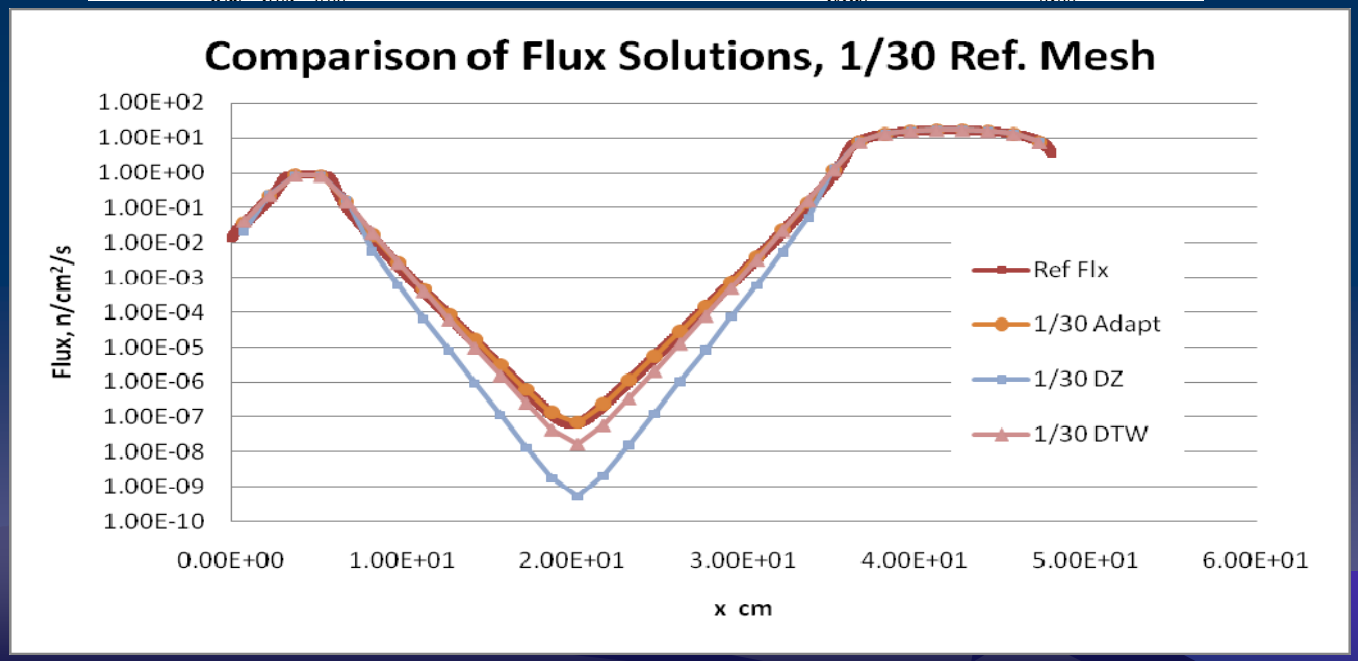
^{244}Cu

α $T_{1/2}$=17.6 yr



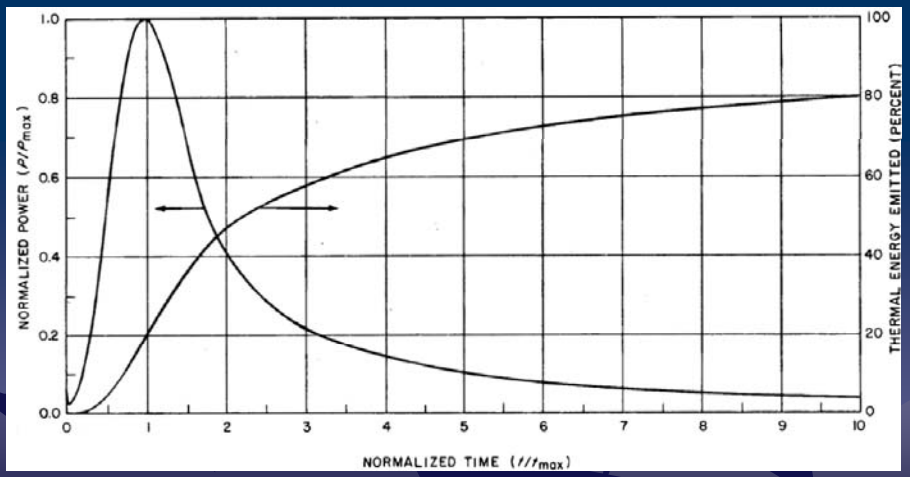
Algorithm Development: Adaptive Differencing Schemes in Computational Transport

- Sn Code adapts to optimal algorithm based on physics
- New, efficient schemes for optimized transport solutions

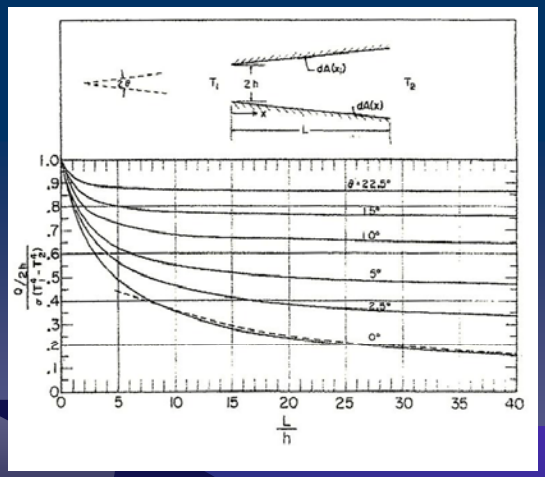


Simulations Supporting Nuclear Forensics

- Consider thermal radiation damage due to an IND
  - Thermal radiation through street canyons, passages
    - Thermal degradation modeling
    - Adiabatic and non-adiabatic wall models
  - Plane walled "canyon" gaps linked via isothermal environments



Thermal NW Pulse, Scaled Time



Canyon Radiative Transfer

Summary

- **University of Florida**
  - *Nuclear and Radiological Engineering Department (NRE)*
  - *Florida Institute of Nuclear Detection and Security (FINDS)*
- **Broad Scope of Detailed Computational Simulation Research for Government, Science, and Industry**
  - Non-proliferation and Radiation Detection
  - Spectrometry / System Optimization
  - Nuclear Power / 3-D/Large Scale Reactor Physics Simulation
  - Code and Algorithm development
  - Forensics Research
- **Leverage Computational methods to minimize cost, maximize effectiveness**
  - **Advanced Education and Training for future engineers**

Questions?