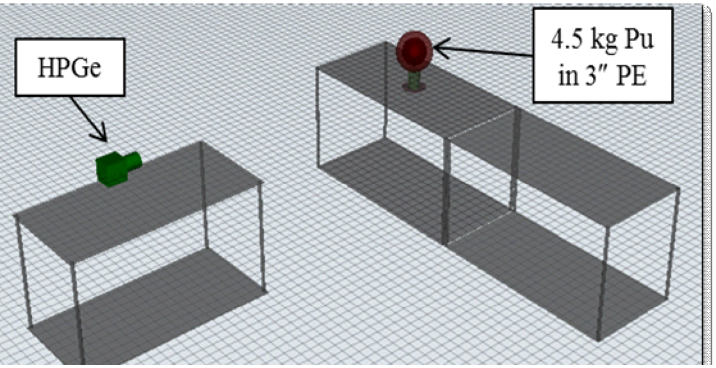
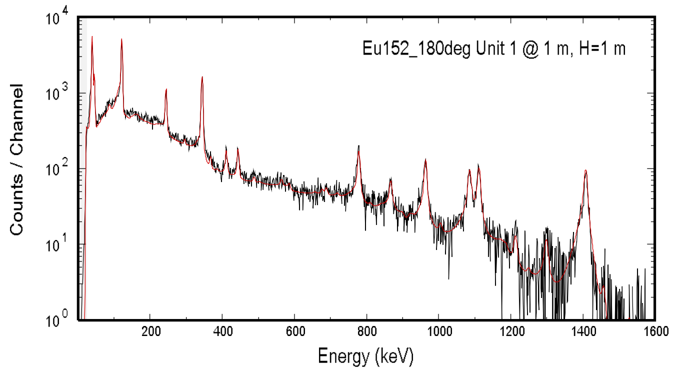
SAND2018-7719C





Rapid 1-D and 3-D Radiation Transport and Detector Response

(SAND2018-ZZZZ)

D.J. Mitchell, G.G. Thoreson, S.M. Horne, L. Harding, and S. O’Brien

September 2018

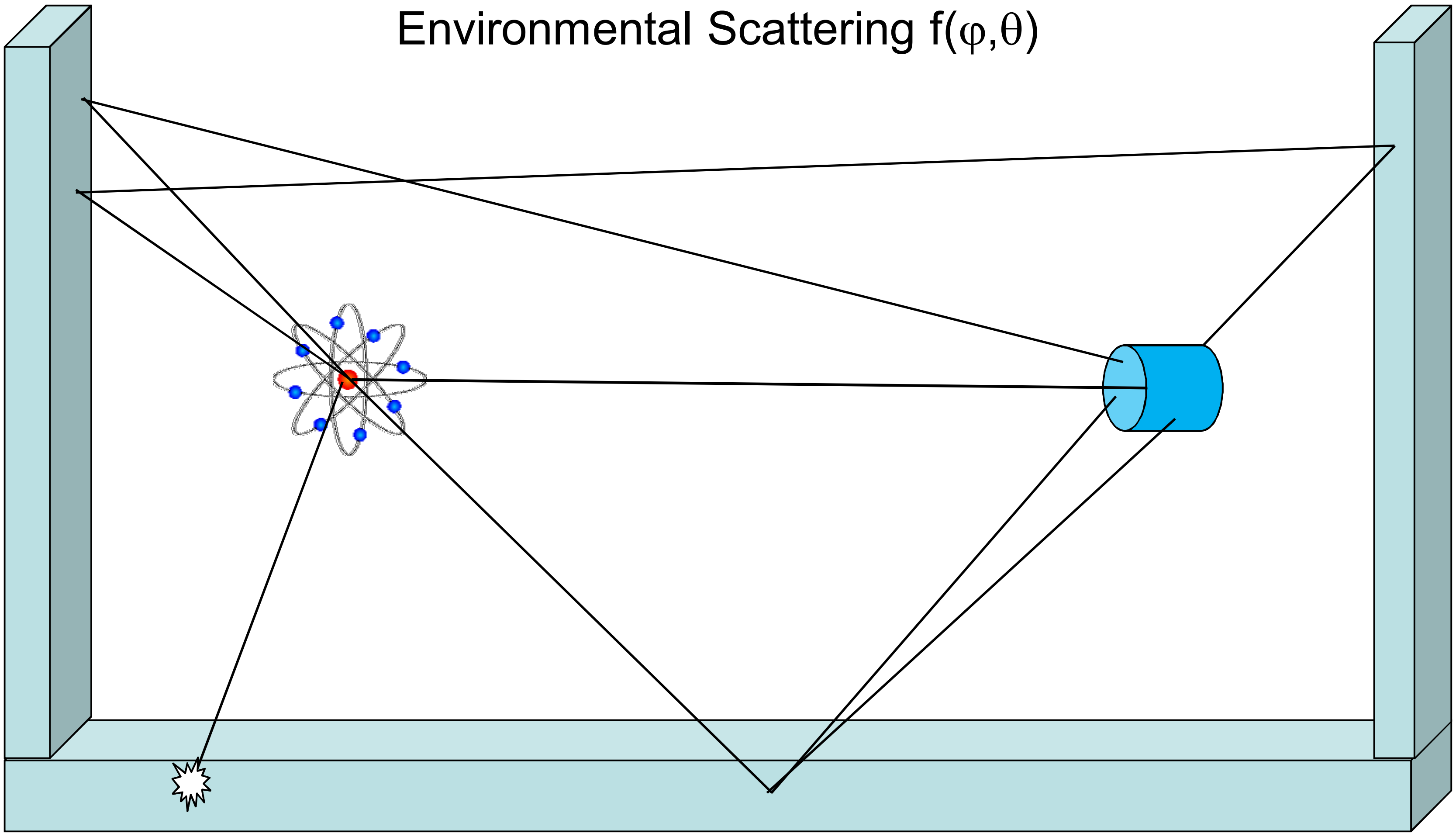
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under Contract DE-NA0003525. SAND2017-4391 C

3-D Radiation Transport and Detector Response Approaches

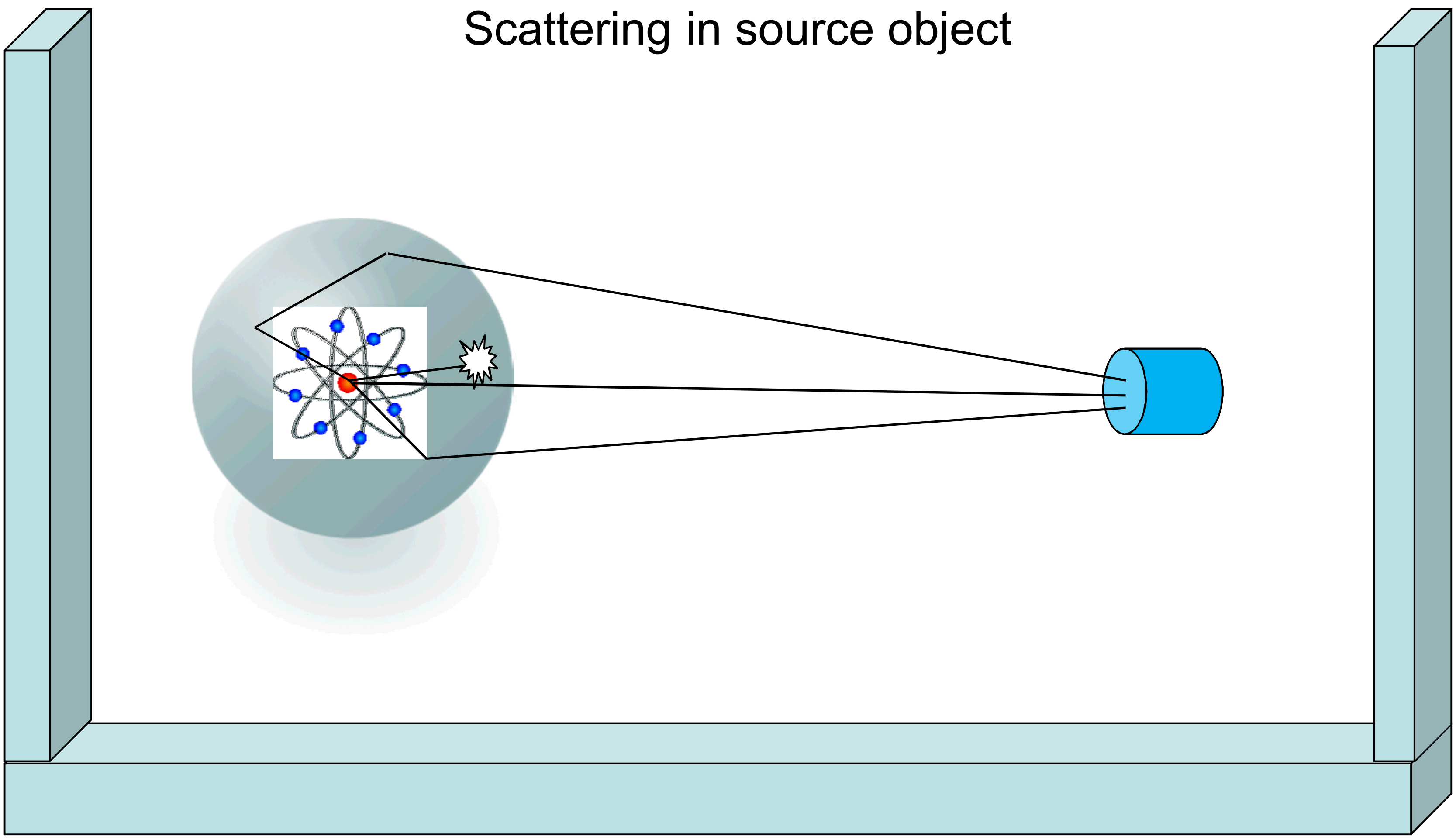
- **Monte Carlo**
  - Accurate and accommodates virtually any source configurations
  - Calculations take days to weeks or require massive parallel processing
  - Variance reduction reduces computation time, but even knowledgeable operators make mistakes
  - Can accelerate by coupling with external detector response function
- **Discrete Ordinates**
  - Accurate, but not quite as flexible as Monte Carlo
  - Calculations can be faster than Monte Carlo, but not always
- **Gamma Detector Response and Analysis Software (GADRAS)**
  - 1-D: ~ 1 s
  - 3-D: < 1 minute

  } ~ 10^5 times faster
  - Accurate, but not as flexible as Monte Carlo or 3-D discrete ordinates

Monte Carlo Approach for Transport / Response

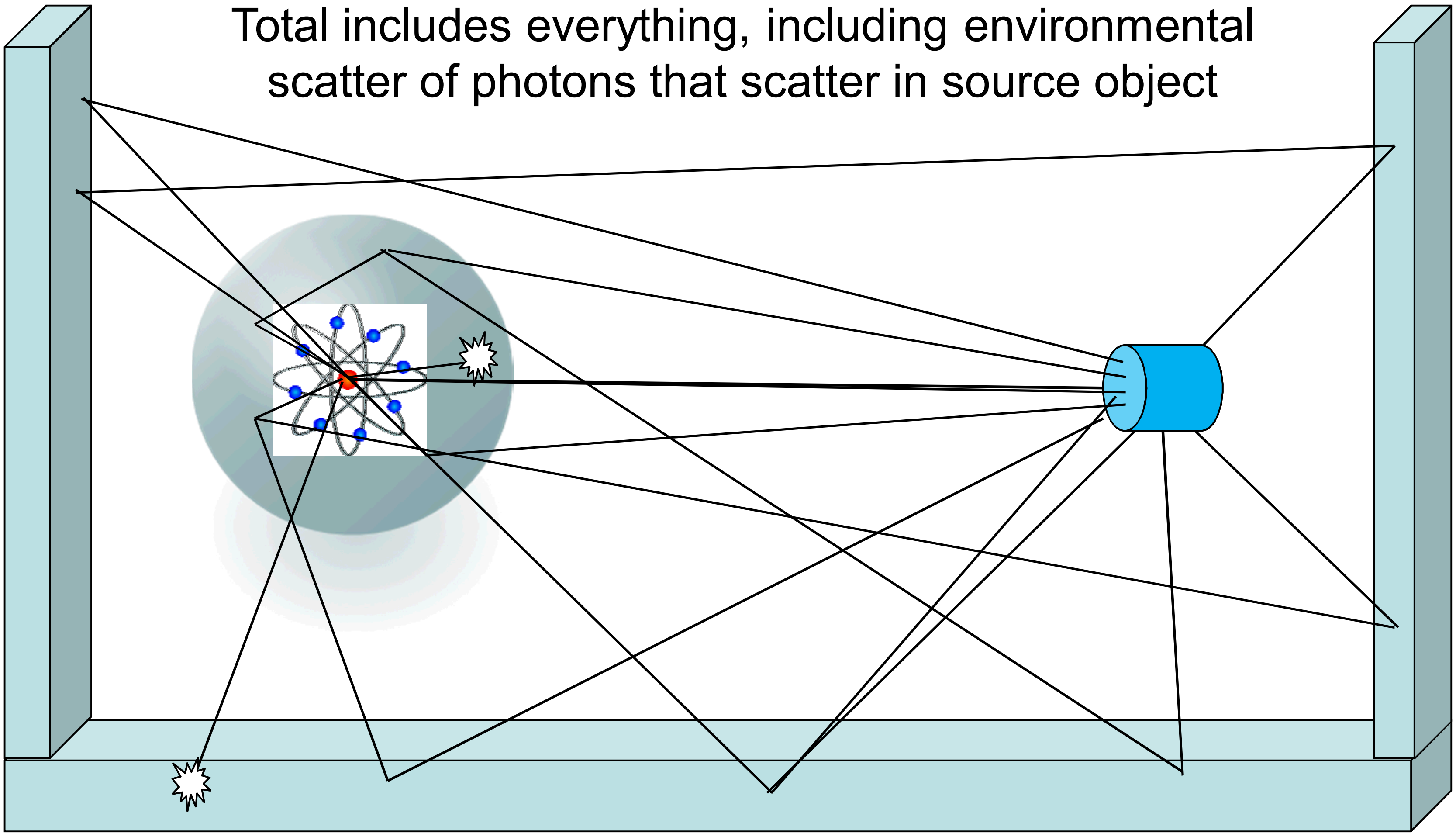


Monte Carlo Approach for Transport / Response



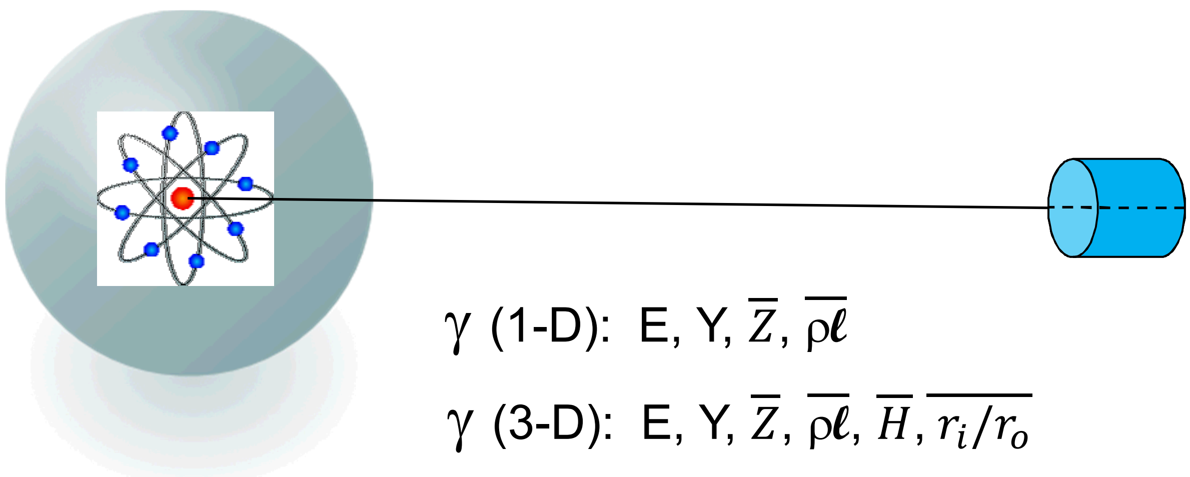
Monte Carlo Approach for Transport / Response

Total includes everything, including environmental scatter of photons that scatter in source object



GADRAS Approach for Transport / Response

- One ray-trace calculation for each source volume element determines entire spectral response
  - Scatter continua interpolated from pre-computed databases for source objects and environment
  - Intrinsic detector continuum (i.e., scatter out of detector) from DRF



γ (1-D): E, Y, $\overline{Z}$, $\overline{\rho\ell}$

γ (3-D): E, Y, $\overline{Z}$, $\overline{\rho\ell}$, $\overline{H}$, $\overline{r_i/r_o}$

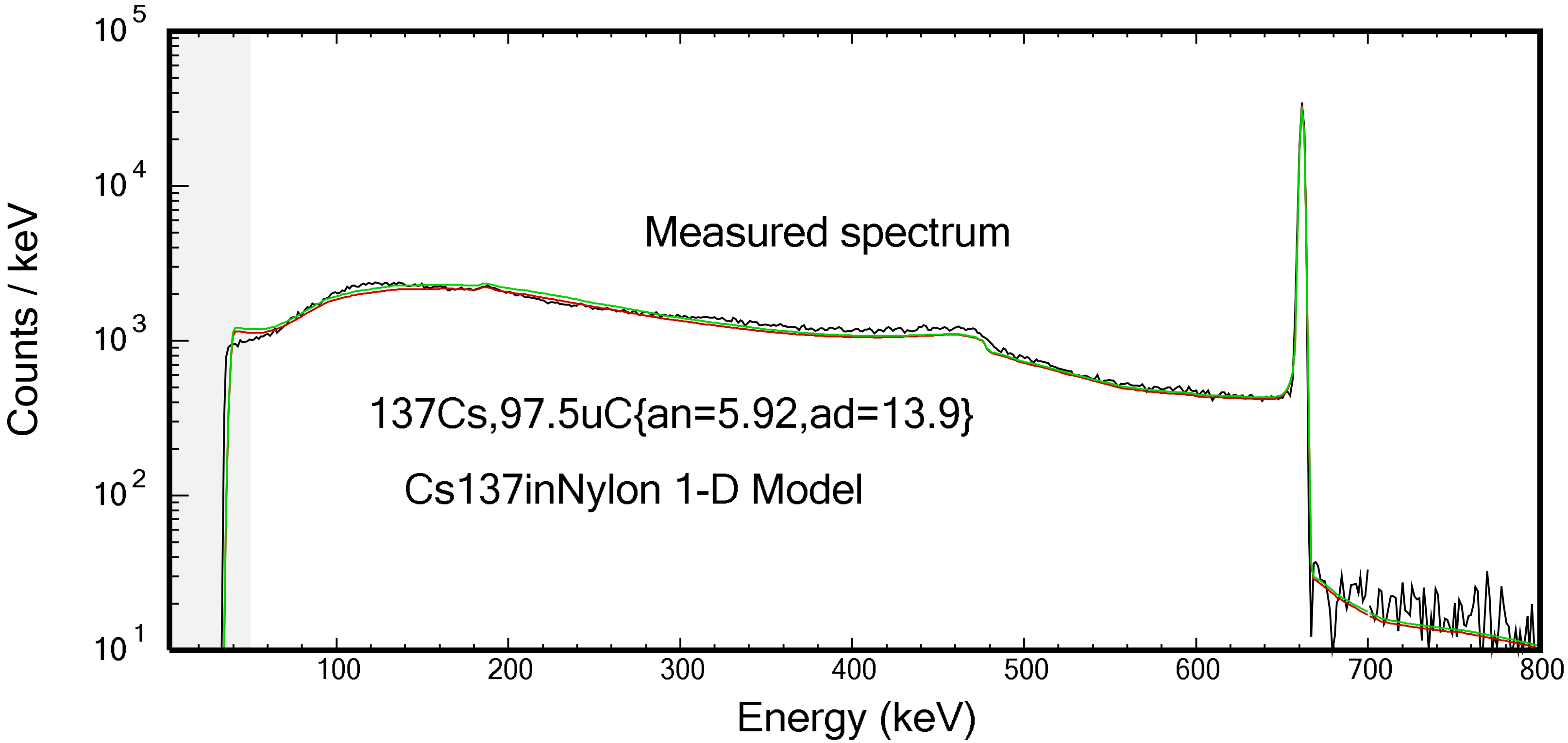
1-D Method Combines DO and RT Calculations

- **Discrete ordinates (Partisn) calculation yields 4π leakage**
  - Few wide energy groups enable rapid solutions, accurate continua
- **Ray-trace (RT) calculations**
  - Reproduces abrupt changes in continua at photopeak energies
  - Only E and Y normally tallied by most ray-trace codes
  - GADRAS output augmented to include Z and $\rho\ell$
  - Database of pre-computed scatter calculations interpolated based on E, Y, Z, and $\rho\ell$
- **Residuals obtained by stripping ray-trace from discrete ordinates compensate for ray-trace continuum errors**
  - Otherwise, spectrum for source surrounded by lead then polyethylene would be the same as spectrum with shielding materials reversed

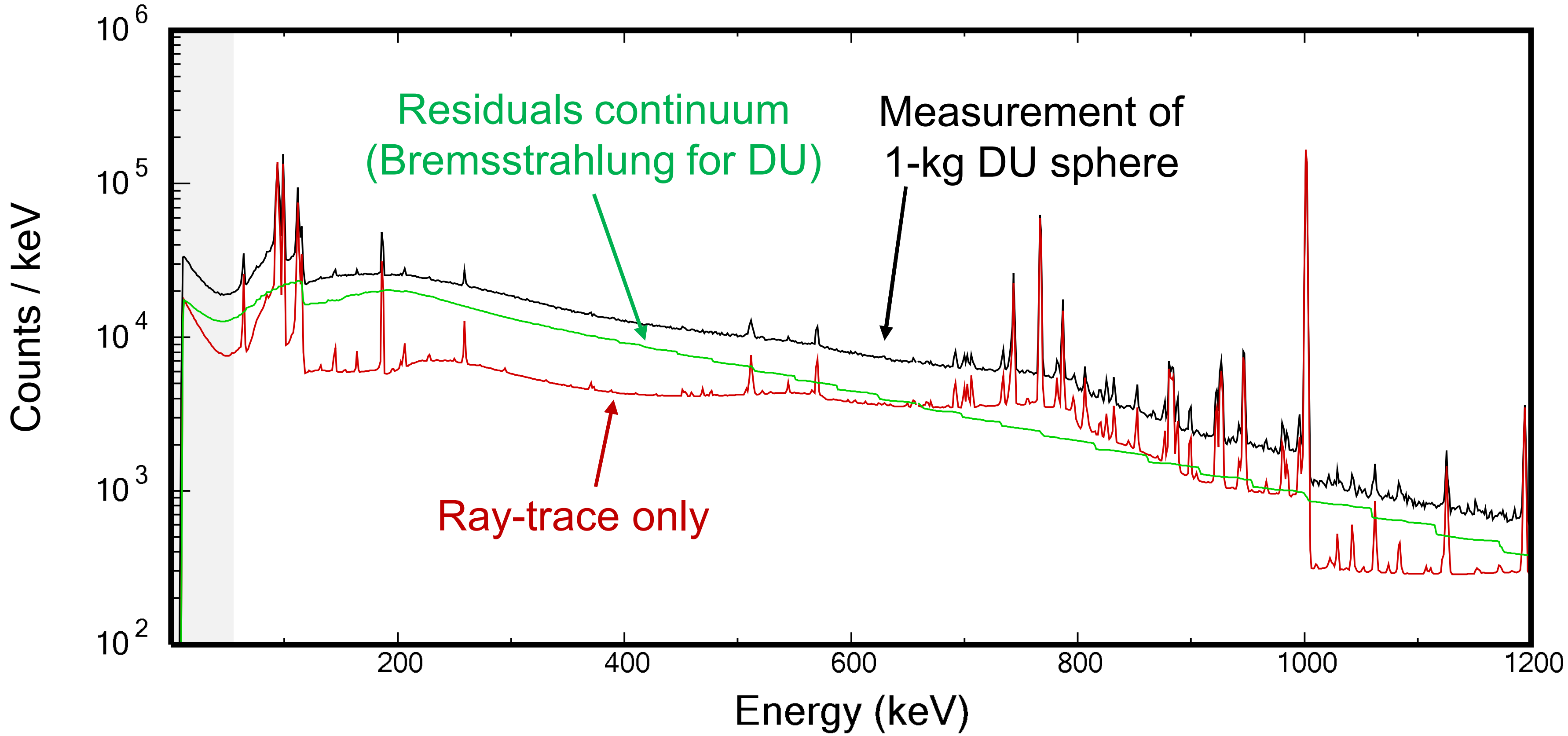
D. J. Mitchell et al., "Gamma-ray Response Functions for Scintillation and Semiconductor Detectors", *Nuclear Instruments and Methods in Physics Research Section A*, Vol. 276(3), p. 547-556 (1989)

1-D Method ^{137}Cs in 12-cm Thick Nylon Sphere

- **Example: ^{137}Cs in 13.9 g/cm^2 nylon**
  - Computed ray-trace spectrum is almost identical to measurement
  - Residuals are negligible, so compensation is not required



1-D Method Applied to Depleted Uranium



Sum of ray-trace and residuals continuum yields accurate reproduction of measurement

Differences Between 1-D and 3-D Scatter Calculations

- **1-D**
  - Approximation for scatter from ray-trace is adequate because discrete ordinates leakage calculation compensates for errors in ray-trace
  - Scatter spectrum = f(E, Y, Z_{eff}, $\rho\ell_{eff}$)
- **3-D**
  - Discrete ordinates calculations do not correspond to 1-D source models, so gross leakages cannot be used to compensate for ray-trace errors
  - Scatter spectrum derived from ray-trace calculation must be accurate
  - Scatter spectrum = f(E, Y, $\overline{Z}$, $\overline{\rho\ell}$, $\overline{H}$, $\overline{r_i/r_o}$)

hydrogen fraction ($\overline{H}$)

metric used to mix scatter libraries ($\overline{r_i/r_o}$)

3-D Computation of Effective Atomic Number, $\overline{Z}$

Old 1-D Approach

$$\overline{Z} = \frac{\sum_{k=1}^{n} Y(k) \sum_{i=k+1}^{n} Z(i)\rho l(i)}{\sum_{k=1}^{n} Y(k) \sum_{i=k+1}^{n} \rho l(i)}$$

New 3-D Approach

$$\overline{Z} = \frac{\sum_{k=1}^{v} Y(k) \int_0^L dx\, Z(x)\rho(x)\, e^{-\mu(x)(L-x)}}{\sum_{k=1}^{v} Y(k) \int_0^L dx\, \rho(x)\, e^{-\mu(x)(L-x)}}$$

voxels replace shells

integrated instead of summed

transmission through external materials

where:

- *n* is the number of source shells
- *v* is the number of source voxels
- *Y(k)* is the gamma-ray leakage originating in shell or voxel k
- *Z(x)* is the mean atomic number at location *x*
- *ρ(x)* is the density at location *x*
- *μ(x)* is the total cross section at location *x* (g/cm^2)
- *S(k)* is the shell corresponding to voxel *v*
- *L* is the distance along vector to the detector face
- *p* is an empirical term (*p*=0 yields old approach, *p*=1 more weighting external shells)

3-D Computation of Effective Hydrogen Fraction, $\overline{H}$

Old 1-D Approach	**New 3-D Approach**
Not used	$\overline{H} = \frac{\sum_{k=1}^{v} Y(k) \int_0^L dx\, H(x)\rho(x)\, e^{-\mu(x)(L-x)}}{\sum_{k=1}^{v} Y(k) \int_0^L dx\, \rho(x)\, e^{-\mu(x)(L-x)}}$

- The hydrogen concentration is important because hydrogen has twice as many electrons per unit mass as any other element, so the relative scatter probability is also twice as great
- $\overline{H}$ is computed using the same weighting as $\overline{Z}$

3-D Computation of Effective Areal Density, $\overline{\rho l}$

Old 1-D Approach:

$$\overline{\rho l} = \frac{\sum_{k=1}^{n} Y(k) \sum_{i=k+1}^{n} \rho l(k)}{\sum_{k=1}^{n} Y(k)}$$

New 3-D Approach:

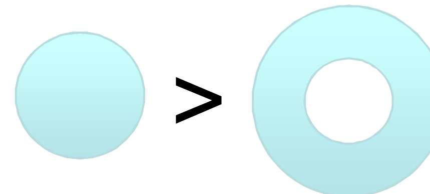
$$\overline{\rho l} = \frac{\sum_{k=1}^{v} Y(k) \int_0^L dx\, \rho(x) \frac{\mu_s(x)/\mu(x)}{\overline{\mu_s}/\overline{\mu}} \left[1 - B(x)\left(1 - \frac{e^{-\mu(r)r}}{e^{-\overline{\mu}x}}\right)\right]}{\sum_{k=1}^{v} Y(k)}$$

where:

- $\mu_s(x)$ is the scatter cross section at location x
- $\overline{\mu_s}$ is the scatter cross section evaluated at $\overline{Z}$
- $\overline{\mu}$ is the total cross section evaluated at $\overline{Z}$
- $B(x)$ is the probability of photon backscatter probability computed by integrating the Klein-Nishina formula from 90° to 180° divided by the total integral

3-D Computation of Shield Shape Metric $\overline{r_i/r_o}$

- More scattered photons are emitted for a point source at the center of a solid sphere than if a gap exists between the source and the same thickness of shielding material
- The ratio of the inner to outer radius is a metric used to interpolate scatter database



$\overline{r_i/r_o} = \quad 0 \qquad\qquad 0.3$

Old 1-D Approach: Not used

New 3-D Approach:

$$\overline{\left(\frac{r_i}{r_o}\right)} = \frac{\text{effective mean inner radius}}{\text{effective mean outer radius}} = \frac{R_o - \dfrac{\overline{\rho l}}{\bar{\rho}}}{R_o - \dfrac{\sum_{i=1}^{\infty} e^{-(i-1)}\left(r(i\lambda) - i\bar{\lambda}\right)}{\sum_{i=1}^{\infty} e^{-(i-1)}}}$$

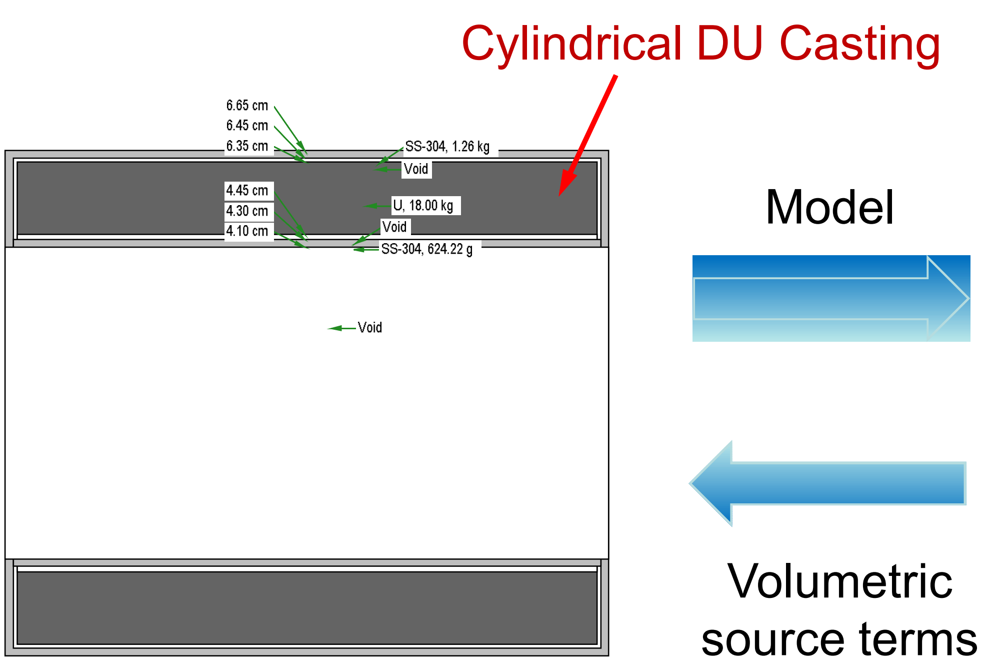
- R_o is distance between a source voxel and last material element along vector to the detector surface
- λ is the mean free path
- $\bar{\lambda}$ is the mean free path evaluated at $\overline{Z}$ and $\overline{\rho l}$
- $r(i\lambda)$ is the radius corresponding to i mean free paths inward from R_o

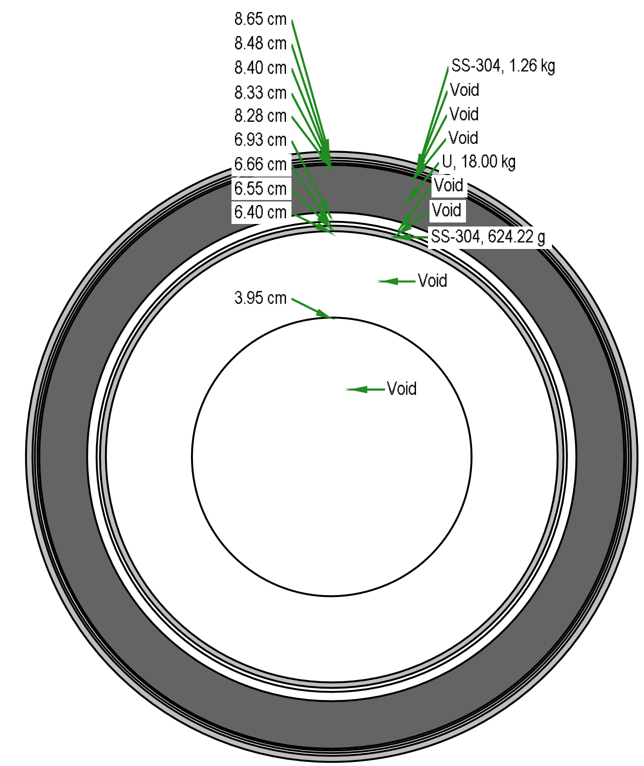
3-D: Six Parameters Define Scatter Spectrum

- E Gamma-ray energy
- Y Gamma-ray leakage
- $\overline{Z}$ Mean effective atomic number
- $\overline{\rho l}$ Mean effective areal density
- $\overline{H}$ Mean effective hydrogen fraction
- $\overline{r_i/r_o}$ Mean effective ratio of inner to outer radius of intervening material

Spherical Equivalent for Volumetric Source Terms

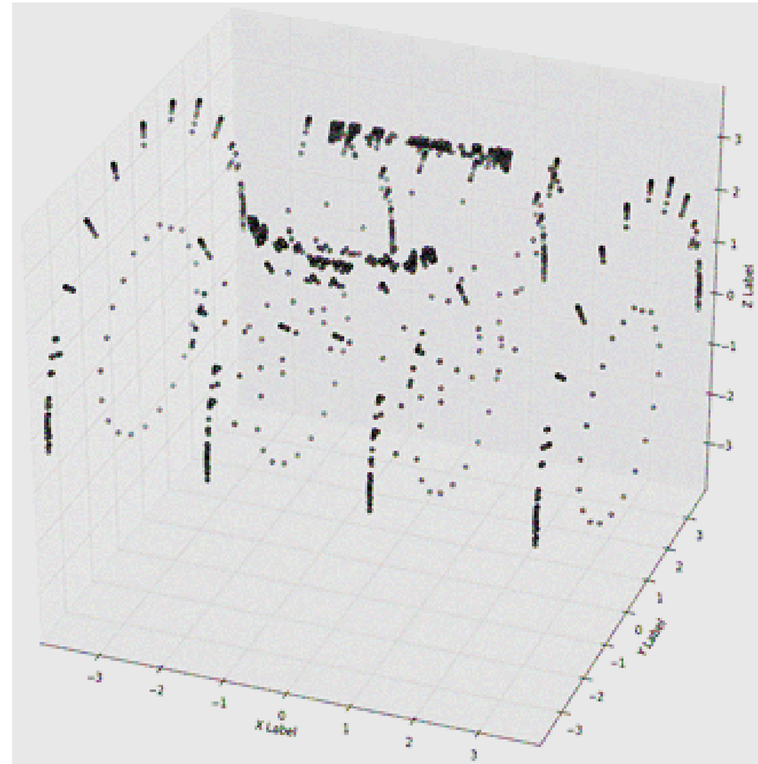
- Volumetric source terms determined for geometries by 1-D deterministic solvers for spherical equivalent source
- Surface areas and masses of each layer are preserved as much as possible
- Source-terms are transformed back onto the original to get volumetric source terms





3-D Calculations: Adaptive Mesh

- **Good results obtained by subdividing source shells into large number of spatial groups**
  - There is a computation time penalty if large number of groups
- **The problem is approached by applying an adaptive mesh**
  - Starts with crude mesh
  - Reduce the size of regions over which rapid changes occur
  - Meshes are computed for several energy groups to maintain accuracy with fewest spatial groups

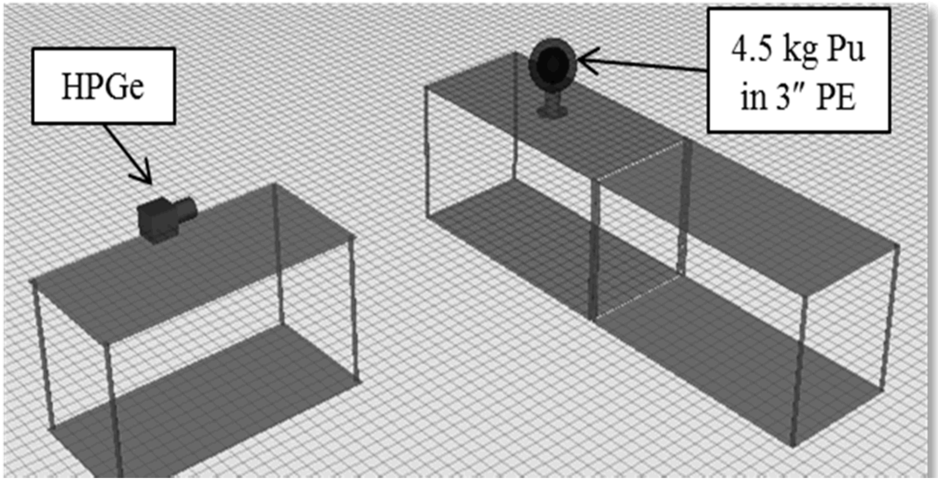


Adaptive mesh points for a plutonium cylinder beneath a shadowing sphere (60-keV energy group)

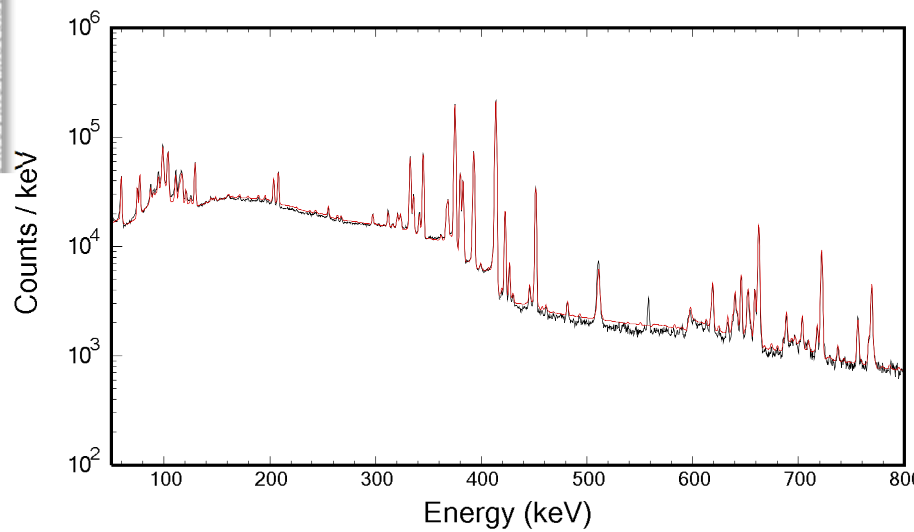
Method Validation

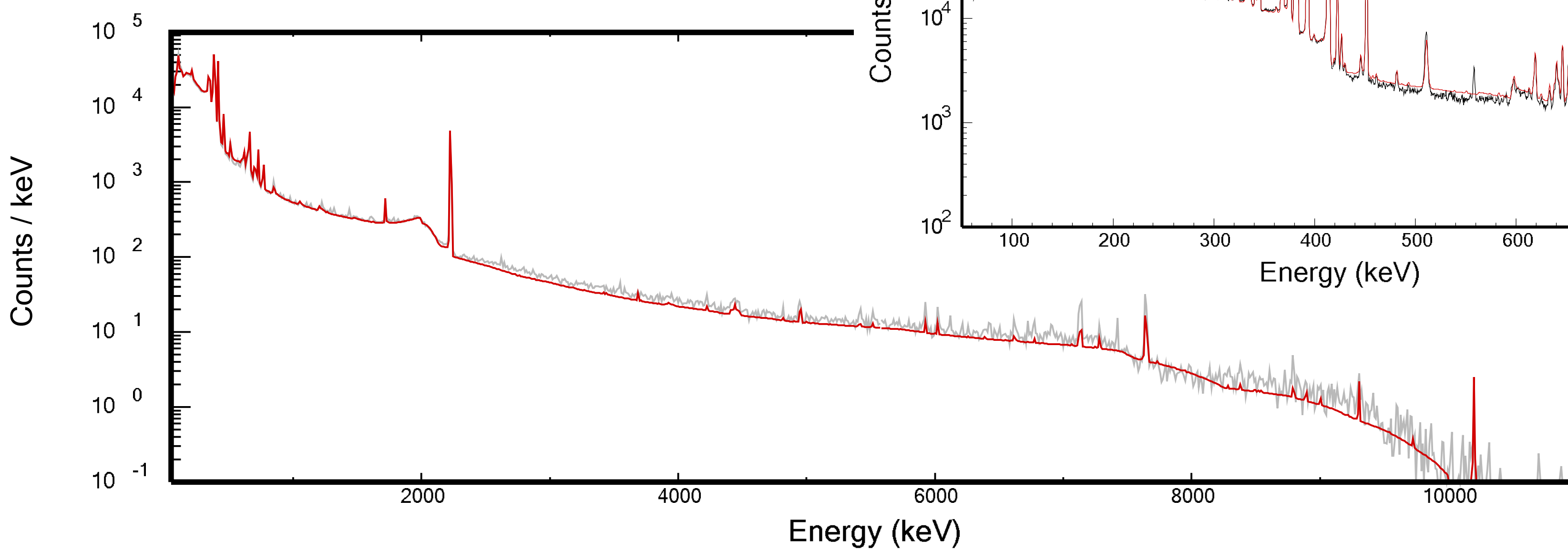
- Accuracy of calculations have been evaluated for numerous source and detector configurations, including: spheres, cylinders, slabs, cones, and combinations of these primitive models
- Examples follow:

3-D Benchmark Test (Pu in PE)



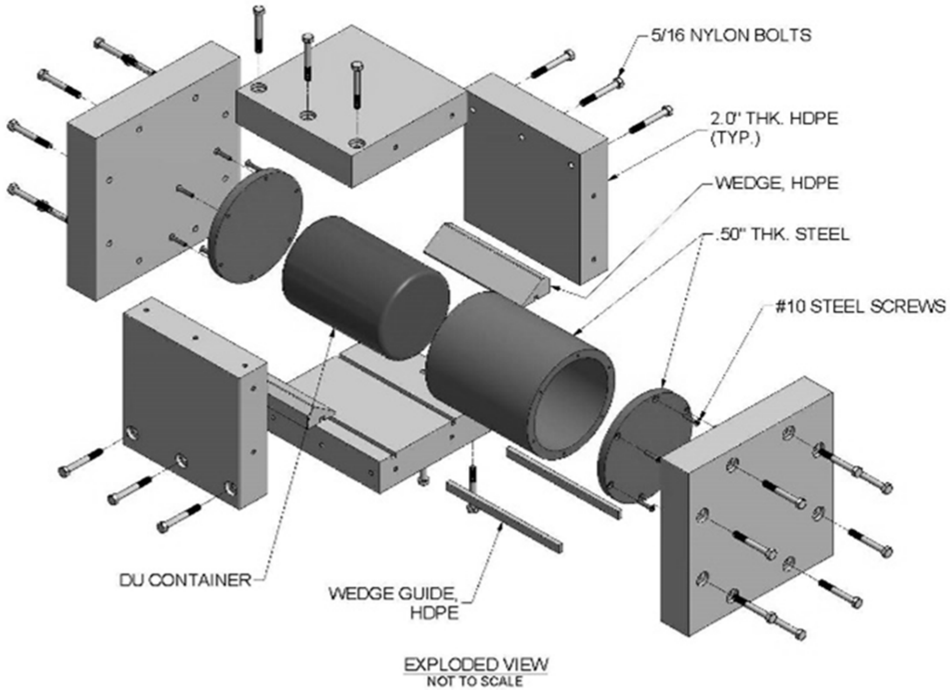
- 4.5 kg Pu in 3” PE sphere
- Neutron capture γ from table
- Computation time: **30 s**

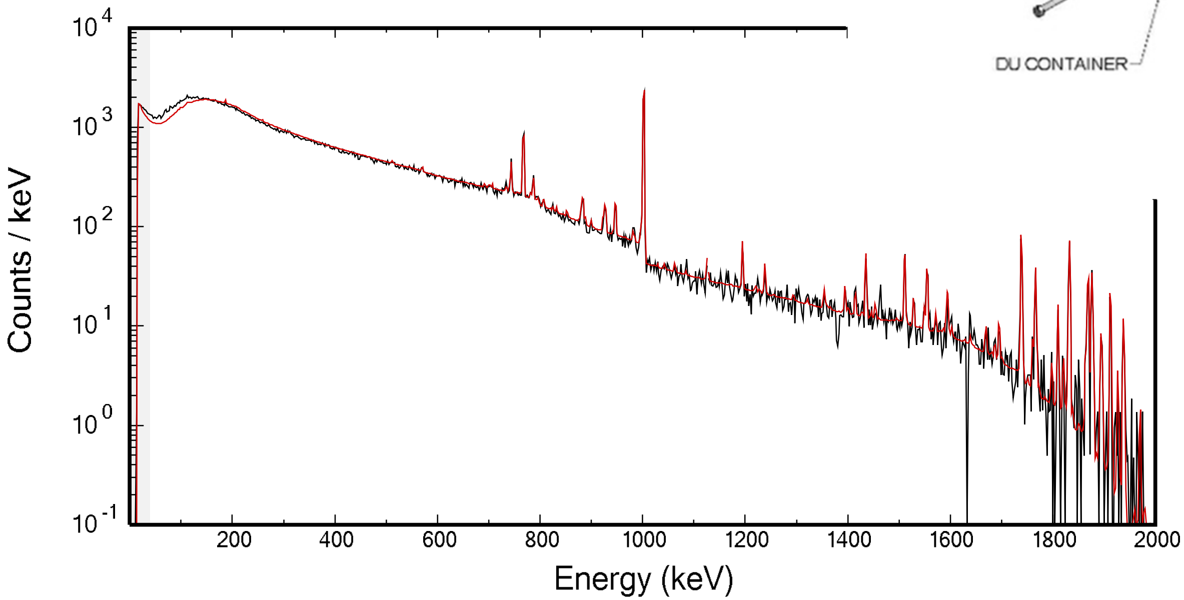




3-D Benchmark Test (DU Casting in Steel and PE)

- Source is 18-kg DU casting
- Inside 0.5-inch-thick steel cylinder
- Inside 2-inch-thick PE box
- Computation time: **35 s**





Computational Validation Ongoing

- **Computed spectra are accurate for all but a few configurations**
- **Calculations are inaccurate for the following cases:**
  - 3-D configurations if gamma-ray emission is highly asymmetric
  - Measurement with collimated detectors pointed away from radiation source
    - The current method associates origin of scattered photons with location of original gamma rays as opposed to scattering material
- **Photograph to right shows test configuration used as part of "DNDO 1-D vs. 3-D" project**
  - Impact of voids and streaming paths included in the evaluation

Summary

- **This presentation describes a computational method that enables radiation transport and accurate detector response for 3-D source models in < 1 minute**
  - Incorporated into the Gamma Detector Response and Analysis Software (GADRAS)
- **The approach utilizes pre-computed continua for the detector response and scattered radiation**
- **The method is accurate for numerous configurations of radioactive and shielding materials**
  - Research is ongoing to improve accuracy for a problematic cases

Extras

Flowchart of Transport Process (< 1 minute)