LA-UR-12-23282

Approved for public release; distribution is unlimited.

Title:	Use of MCNP + GADRAS in Generating More Realistic Gamma-Ray Spectra for Plutonium and HEU Objects
Author(s):	Rawool-Sullivan, Mohini Mattingly, John Mitchell, Dean
Intended for:	Nuclear Emergency Spectroscopic Analysts (NESA) 2012 meeting, 2012-07-23/2012-07-27 (Albuquerque, New Mexico, United States)

Los Alamos
NATIONAL LABORATORY
EST. 1943

Use of MCNP + GADRAS in Generating More Realistic Gamma-Ray Spectra for Plutonium and HEU Objects

Mohini Rawool-Sullivan, LANL

John Mattingly, NCSU

Dean Mitchell, SNL

Nuclear Emergency Spectroscopic Analysts (NESA) 2012 meeting, Sandia National Laboratory, Albuquerque, New Mexico, July 23 – July 27, 2012

Abstract

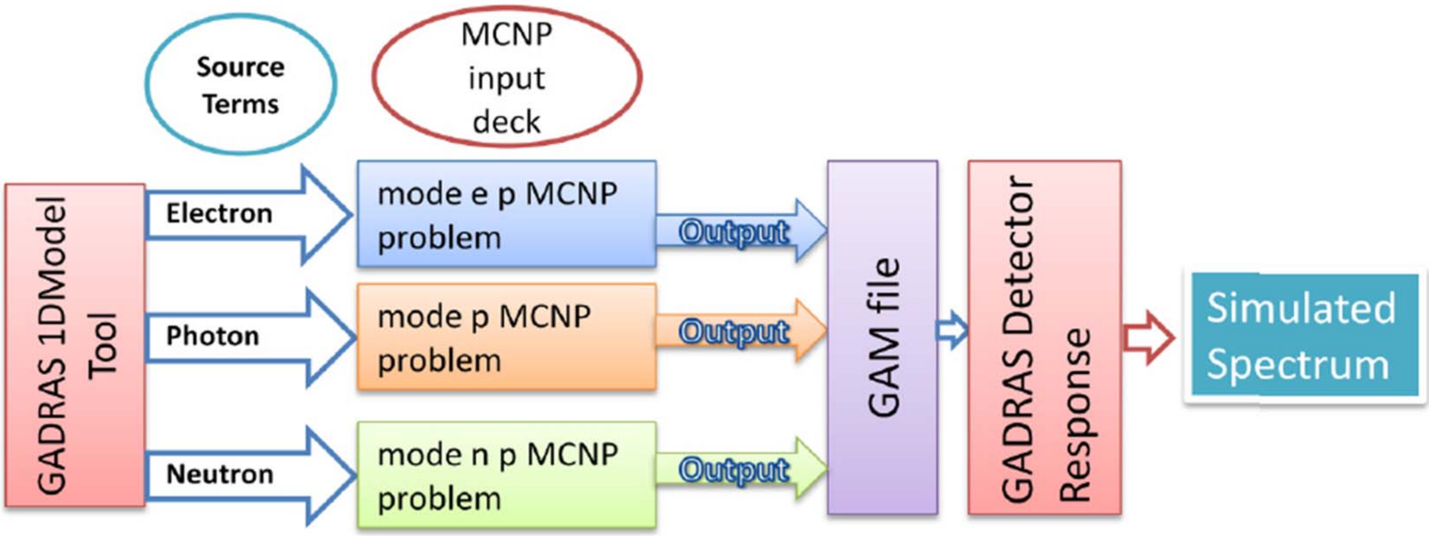
- The ability to accurately simulate high-resolution gamma spectra from materials that emit both neutrons and gammas is very important to the analysis of special nuclear materials (SNM), e.g., uranium and plutonium.
- One approach under consideration has been to combine MCNP and GADRAS
  - This approach is expected to generate more accurate gamma ray spectra for complex three-dimensional geometries than can be obtained from one-dimensional deterministic transport simulations (e.g., ONEDANT).
- This presentation describes application of combining MCNP and GADRAS in simulating plutonium and uranium spectra

Process to simulate gamma-ray spectra

- **Step 1.** An MCNP5 input deck(s) representing the appropriate neutron and gamma source terms, problem geometry, and transport medium materials is created.
  - In this presentation source terms were generated using models for neutron and gamma emissions computed by GADRAS (version 18.0.6).
- **Step 2.** MCNP5 is used to calculate the neutron and gamma leakage current for the three-dimensional source model.
  - In cases where the problem contains both neutron and gamma source terms, separate (a) coupled neutron/gamma and (b) gamma-only transport simulations are necessary to compute the gamma leakage current resulting from (1) neutron-induced gamma source terms and (2) spontaneous decay gamma source terms.
- **Step 3.** The MCNP5 neutron and gamma leakage current outputs are combined into a single leakage current file that can be read by GADRAS.

Process to simulate gamma-ray spectra continued

- **Step 4.** The gamma spectrometer response is calculated by GADRAS by folding the MCNP-calculated neutron and gamma leakage current with the detector response function.
  - This last step essentially collapses the three-dimensional source to a point, albeit with the same gamma/neutron leakage current as the original three-dimensional problem



Test Cases

- This process (hereafter referred to as MCNP+GADRAS) was used to generate a simulated gamma spectrum for benchmark measurements of two sources:

1. Two configurations of the BeRP ball, which is constructed from alpha-phase weapons-grade plutonium metal.
   - Bare
   - Bare reflected by 1.5” polyethylene
2. The Rocky Flats shells, which are constructed from highly-enriched uranium (HEU)

Step 1: MCNP5 input deck generation using GADRAS

- Test cases used here were spherically symmetric for all practical purposes
- We specified the geometry (shape) and composition (material and radioisotopic) of the source for the 1DModel tool in GADRAS.
- To ensure the 1DModel tool generates output in the required SDEF file format in MCNP, the value of the "ExportMcnpModels" setting in the "gadrasw.exe.config" needs to be set to "True"
  - This enables the 1DModel tool to export MCNP SDEF files to the GADRAS scratch folder (usually "C:\GADRAS\Temp") whenever a 1D model is saved.
- For both Rocky shells and BeRP ball only "mode n p" and mode p problems were executed using the MCNP5
  - Weak electron source

MCNP SDEF files from 1D model

File	MCNP calculation	Content	F1 tally
***modelname*.mcnp.electron.soure.txt**	**Mode e p**	**Electron source terms from beta decay**	**Photon**
***modelname*.mcnp.neutron.source.txt**	**Mode n p**	**Neutron source terms from spontaneous fission and (alpha, n) reactions**	**Neutron and photon**
***modelname*.mcnp.photon.source.txt**	**Mode p**	**Photon source terms from spontaneous nuclear (e.g., alpha, beta, etc.) decay and spontaneous fission (SF) - includes line sources from nuclear decay and continuum**	**Photon**
***modelname*.mcnp.photon.linesource.txt**	**Not used**	**Photon line source terms from nuclear decay (excludes continuum photon sources from SF)**	**Not applicable**

Step 2: Run MCNP to generate leakage current tally

- Define geometry, use appropriate SDEF, appropriate mode for about 1E10 or more particles
- Define gamma and neutron tally depending on what problem you are executing on the outermost surface of your object
- Notes about gamma tally
  - For gamma F1 tally use energy bins (or group structure) distributed by GADRAS team along with GADRAS in MCNPbins.dat
  - Gamma energy bins in MCNPbins.dat are in keV (also GADRAS GAM file also uses keV). For using these bins in MCNP you need to convert them to MeV. Also do not round off the energy bins.
- To preserve features in the gamma ray spectrum that can be resolved in a long measurement, the energy group structure in the MCNPbins.dat contains narrow bins around the locations of possible gamma rays, even those with emission yields as low as 0.0005%.

Step 2: continuation

- Neutron tally
  - Is used to estimate continuum
- Any group structure is okay (per SNL)
- There is no set group structure provided
- For simulated spectra shown here we used the GADRAS 79-group Kynea3 structure was used – energy range of bins was from 5E-4 eV to 19640 keV. Again note that MCNP5 needs bins in MeV.

Step 3. Generate a GAM file

- **Line 1**
  - 1st entry: model geometry (0 = spherical, 1 = cylindrical, 2 = rectilinear)
  - 2nd entry: model extent
    - Spherical geometry: not applicable, ignored
    - Cylindrical geometry: cylinder length in cm
    - Rectilinear geometry: slab surface area in cm^2
- **Line 2**
  - 1st entry: number of ray-traced photon lines (this is zero for MCNP calculations)
  - 2nd entry: number of photon energy groups (number of energies listed in the MCNPbins.dat -1)
  - 3rd entry: number of neutron energy groups (number of bins -1)
- **Photon energy groups (in ascending order by energy)**
  - 1st entry: group lower bound in keV; (do not round off energy)
  - 2nd entry: number of photons leaking into 4-pi between the lower and upper group bound; (do not round off leakage current)
- **Neutron energy groups (in descending order by energy)**
  - 1st entry: group upper bound in eV; (do not round off energy)
  - 2nd entry: number of neutrons leaking into 4-pi between the lower and upper group bound; (do not round off leakage current)

Getting MCNP photon tallies into a GAM file

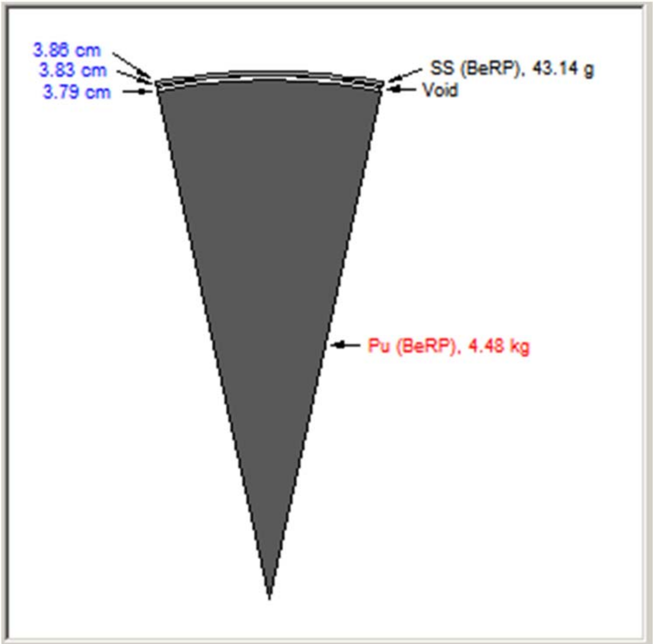
- The first two columns of gamma (or neutron) tally are needed to generate the gamma (or neutron) leakage current for the gam file.
- It should be noted that when you give energy bins in the MCNP5 you are giving an upper bound of the bin whereas in the GADRAS it is the lower bound of the bin. Thus you need to shift the second column or the column with the leakage current up by one cell if you are using excel. This applies to gamma leakage current.
- Convert gamma bins in the gamma tally table from MeV to keV.
- If you have two photon tallies – one from mode p and other from mode n p for the same object - then add together the currents corresponding to the same group structure.
- Modified columns from photon tally table were then put in the GAM file

Getting MCNP neutron tallies into a GAM file

- **The main things to note are, in contrast to the gamma current portion of the file, for neutrons**
  - group boundaries are in eV in Gadras (not keV as for gamma groups)
    - Convert energy from MeV to eV
  - group boundaries are descending (not ascending as for gamma groups)

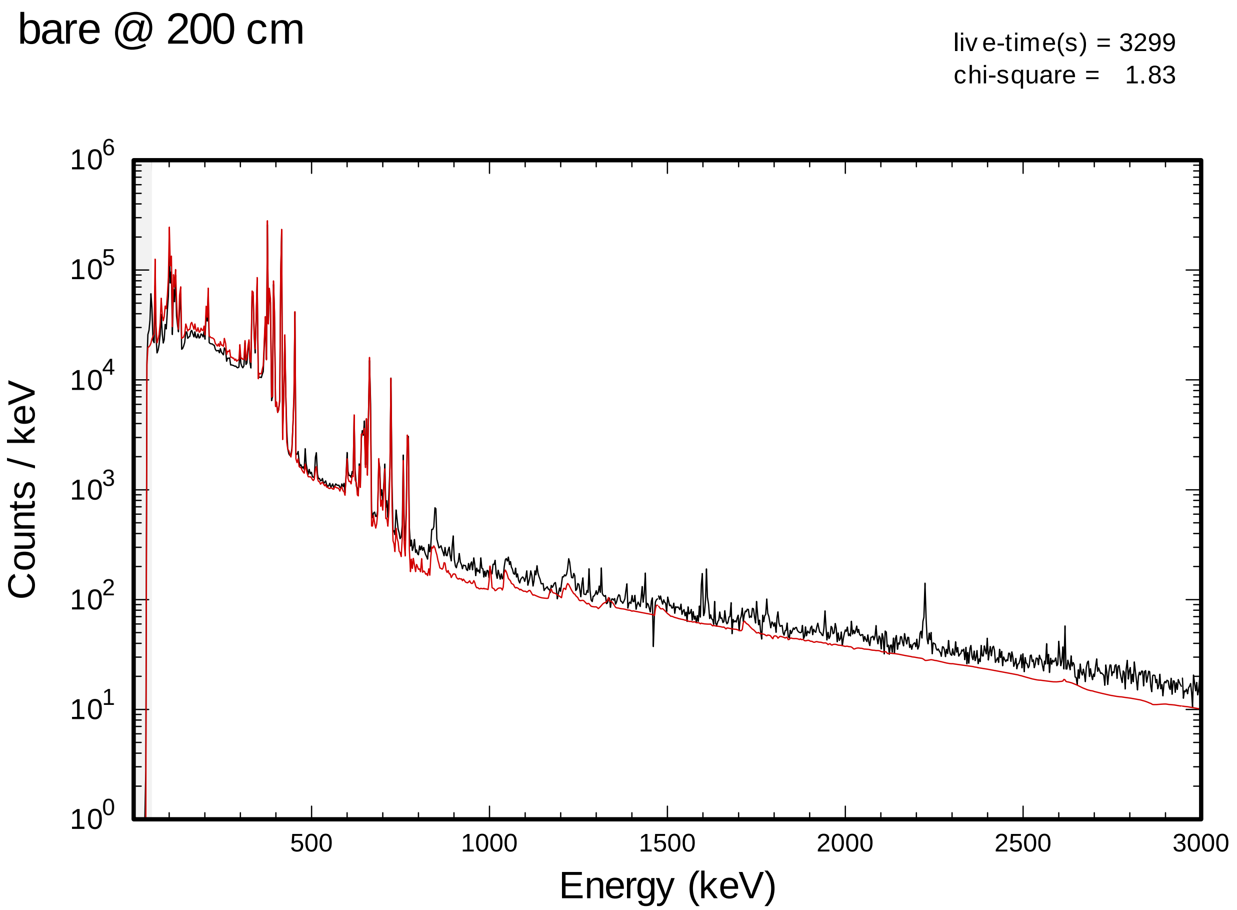
Modified columns of neutron tally were then put in the GAM file

Bare BeRP Ball



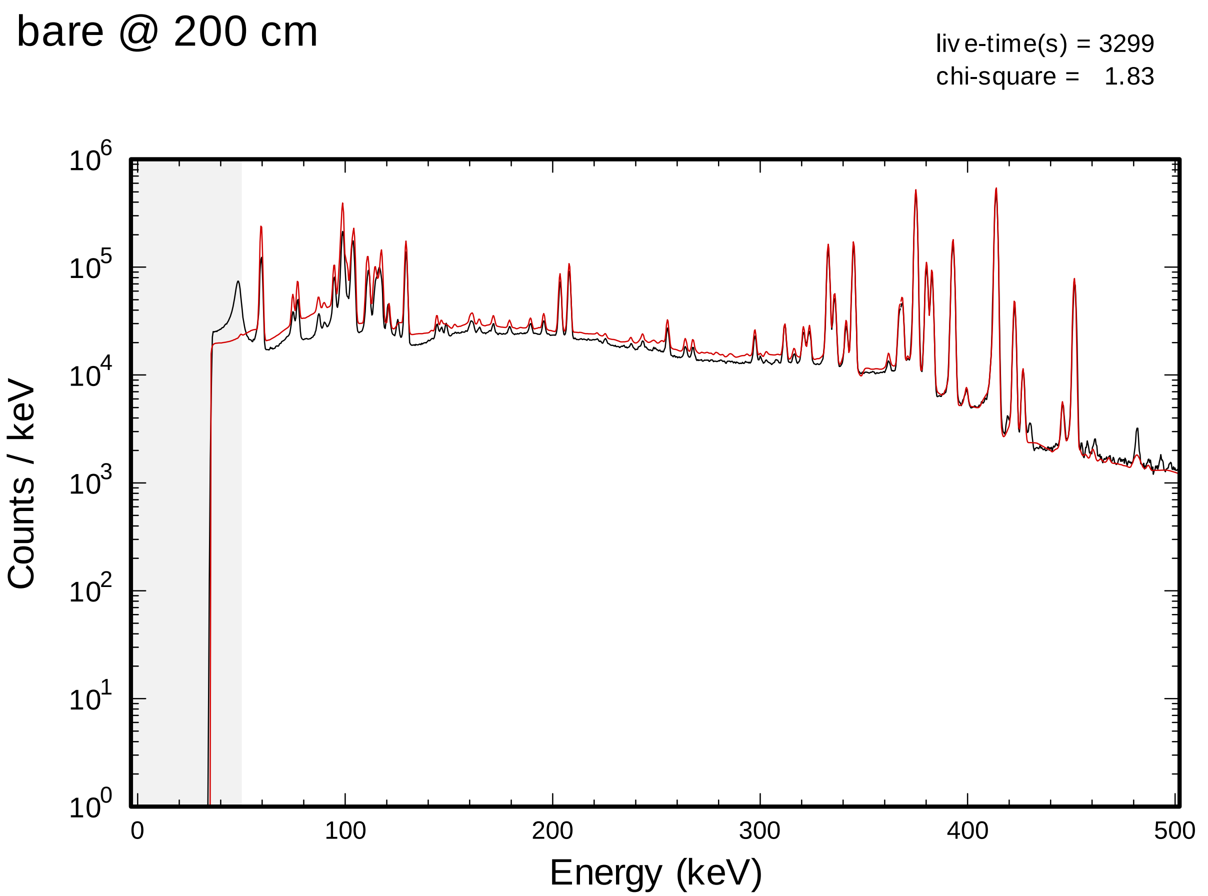
- The bare BeRP ball object features an outer cladding of stainless steel 304 that is nominally 0.0305 cm thick with a density of 7.62 g/cm^3.
- Simulated spectrum was compared with the measured data set using LANL detector K response function and corresponding GADRAS 1DModel files were provided by Mattingly.

Bare BeRP Ball Comparison between data and MCNP+GADRAS spectrum - Overall



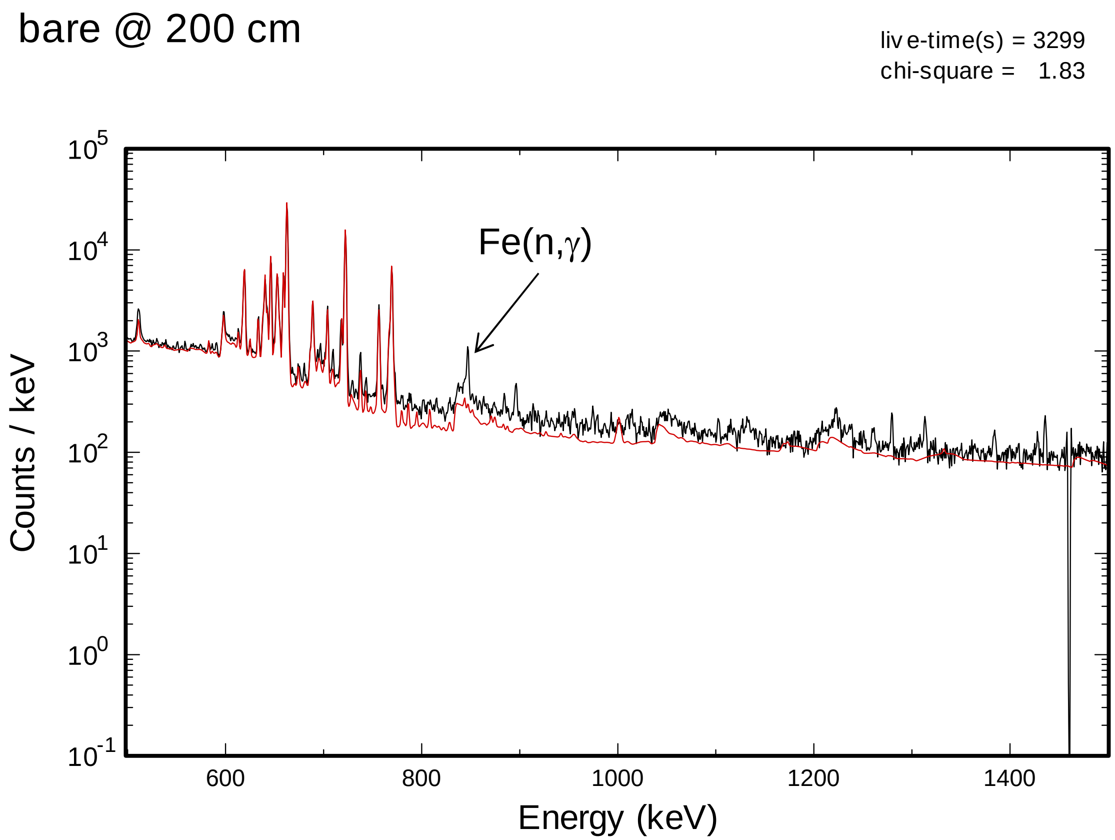
Data are in black and simulated spectrum in red

Bare BeRP Ball Comparison between data and MCNP+GADRAS spectrum – Details 0 – 500 keV



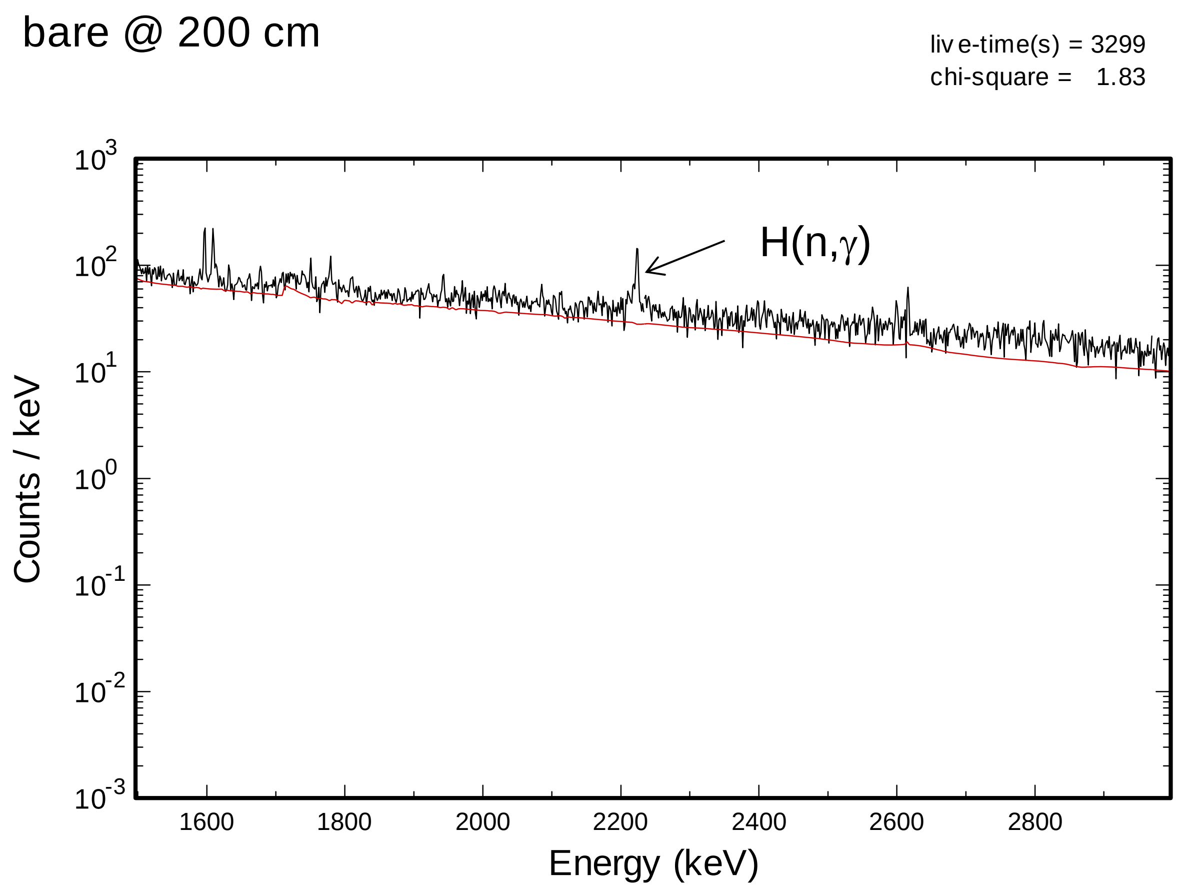
Data are in black and simulated spectrum in red

Bare BeRP Ball Comparison between data and MCNP+GADRAS spectrum – Details 500 – 1500 keV



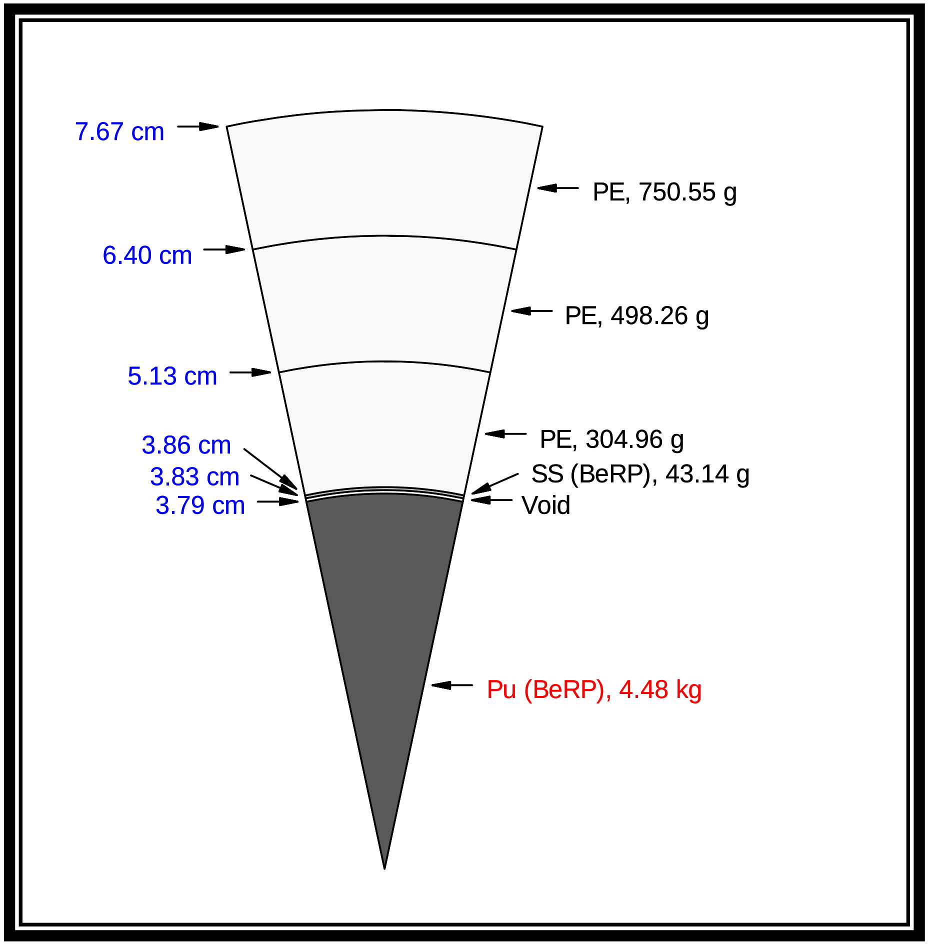
Data are in black and simulated spectrum in red

Bare BeRP Ball Comparison between data and MCNP+GADRAS spectrum – Details 1500 – 3000 keV



Data are in black and simulated spectrum in red

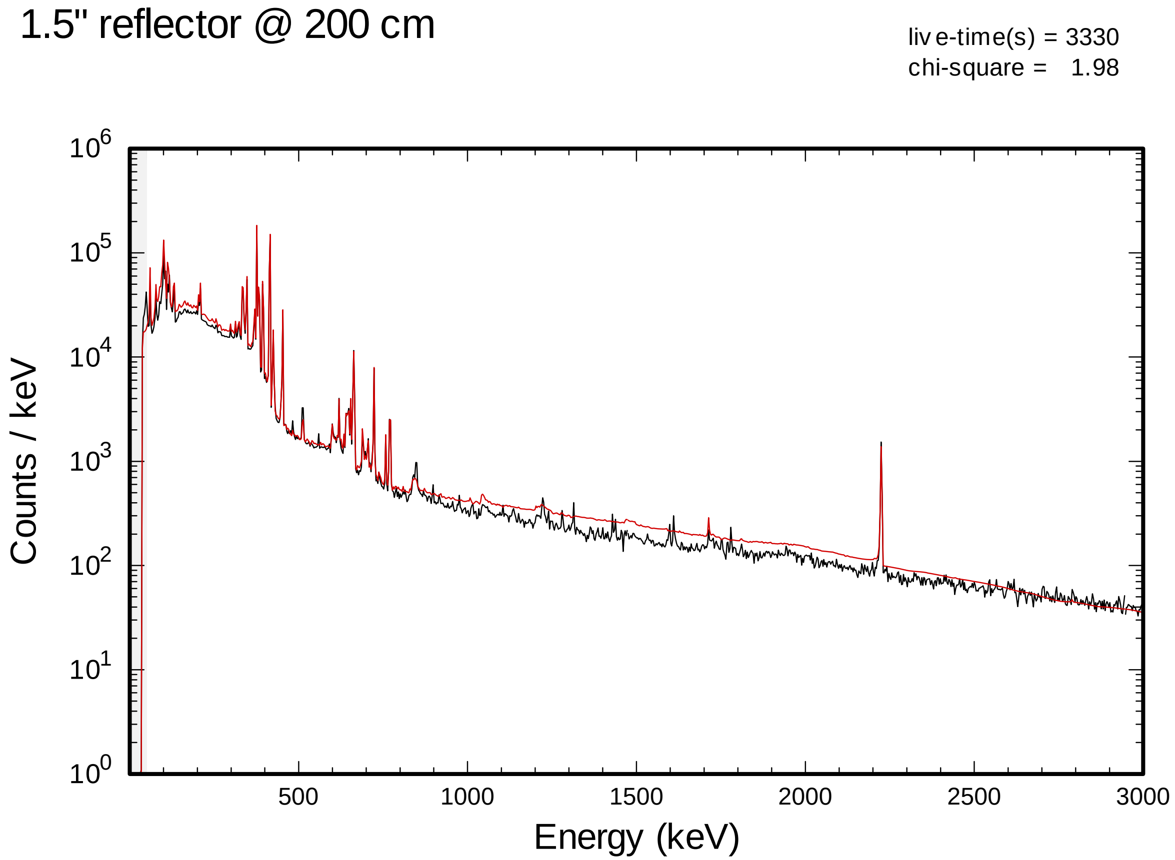
BeRP ball with 1.5” high density poly



LANL
Detector K

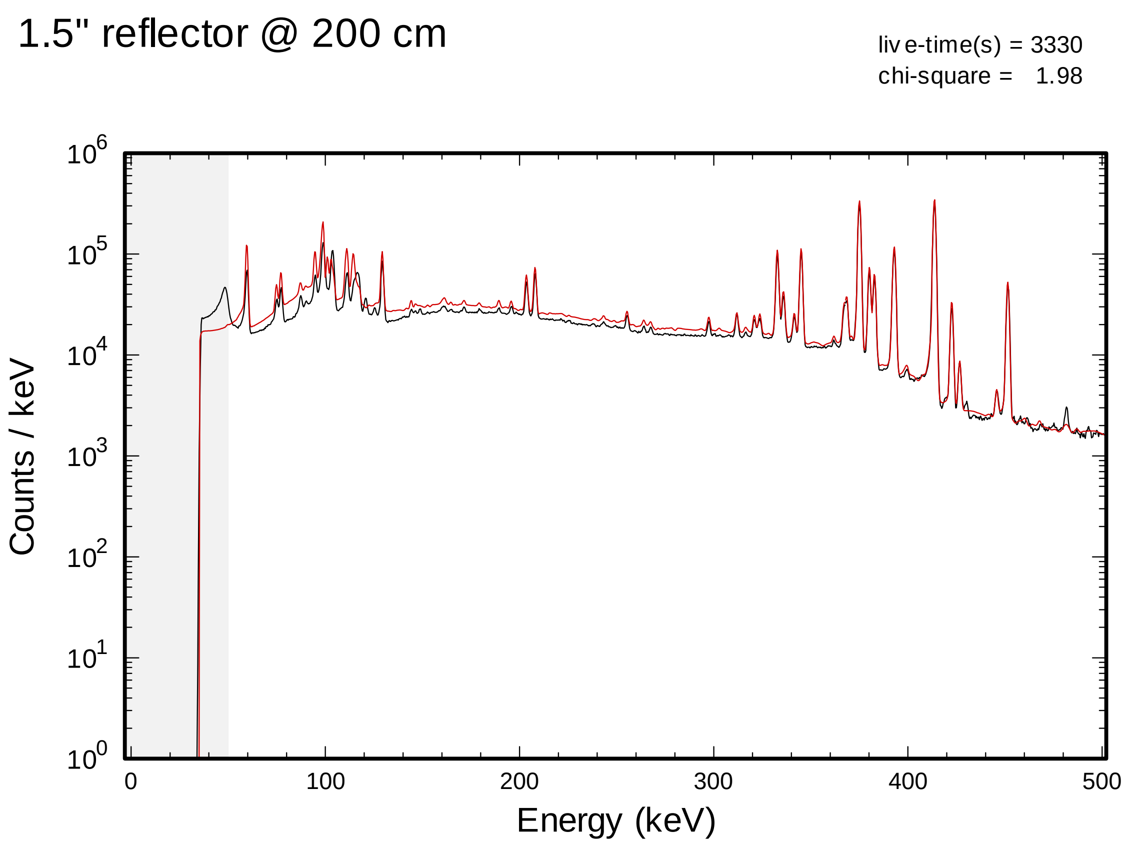
LA-UR-12-23282 Rev. 3

BeRP ball with 1.5” high density poly comparison



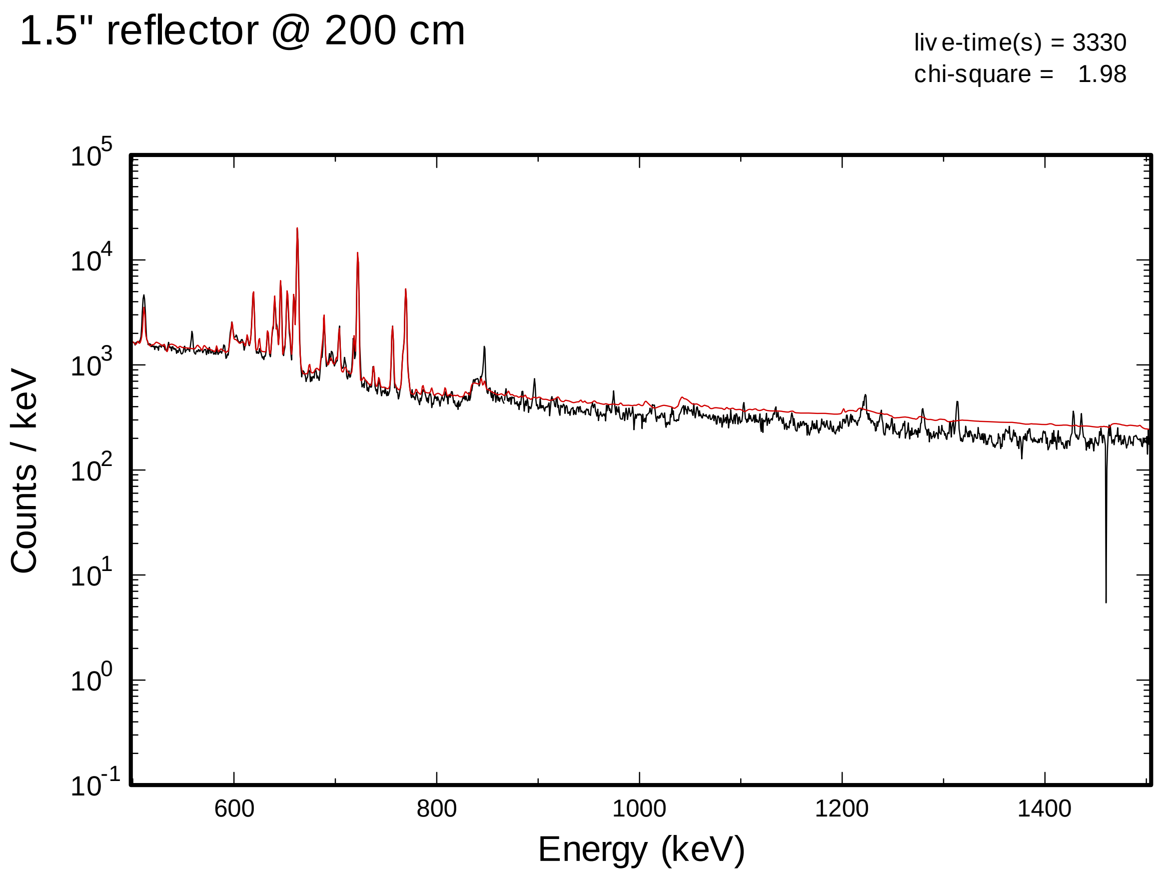
Data are in black and simulated spectrum in red

BeRP ball with 1.5” HDPE 0-500 keV comparison



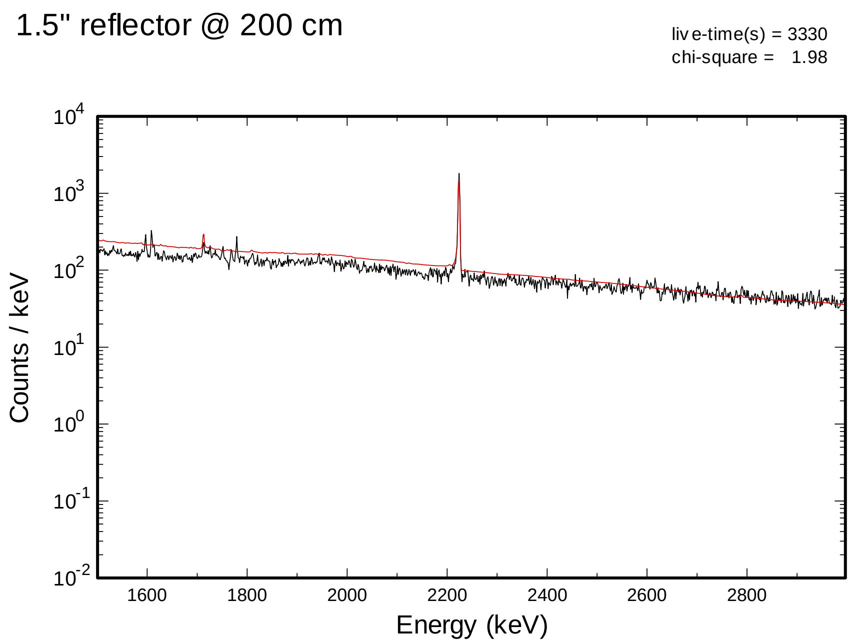
Data are in black and simulated spectrum in red

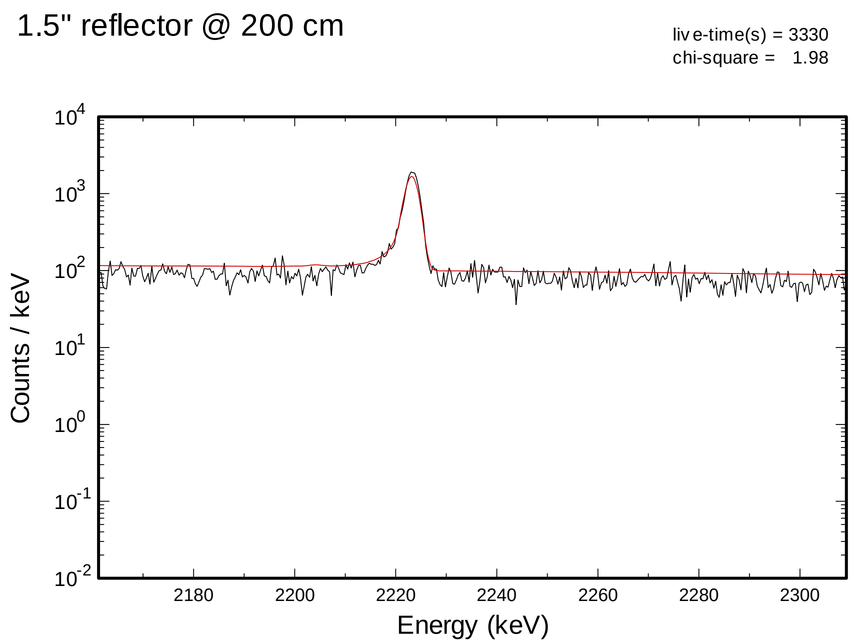
BeRP ball with 1.5” HDPE 500-1500 keV comparison



Data are in black and simulated spectrum in red

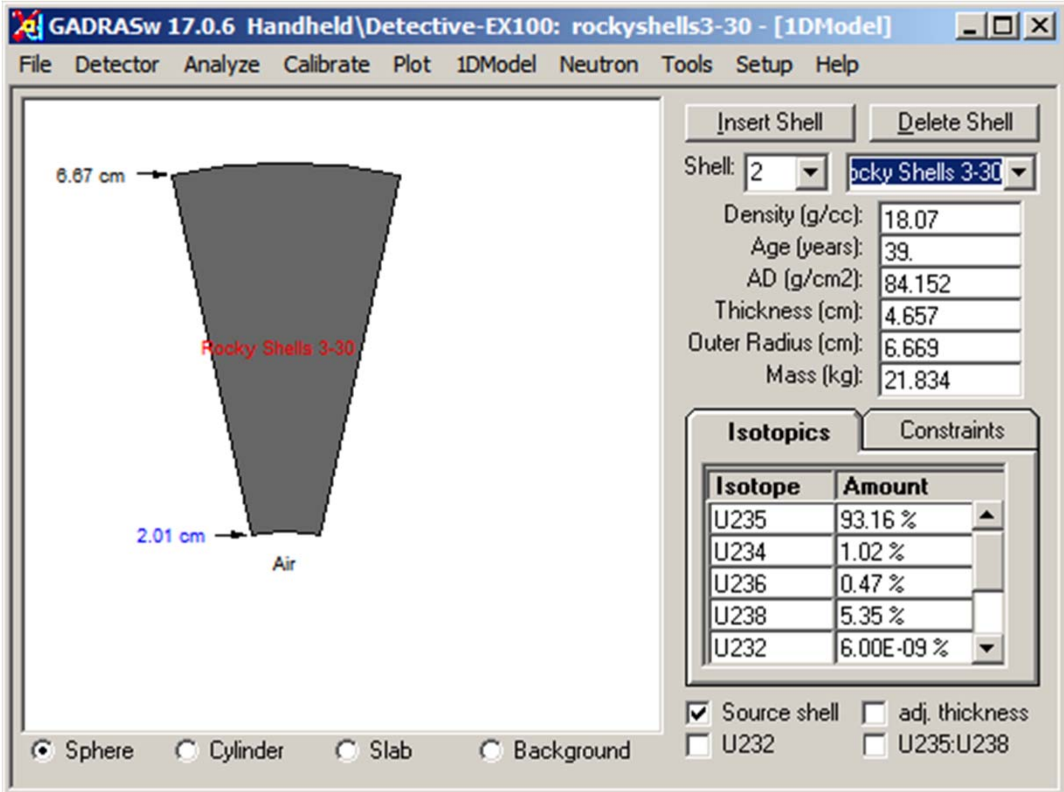
BeRP ball with 1.5” HDPE 1500-3000 keV comparison





Data are in black and simulated spectrum in red

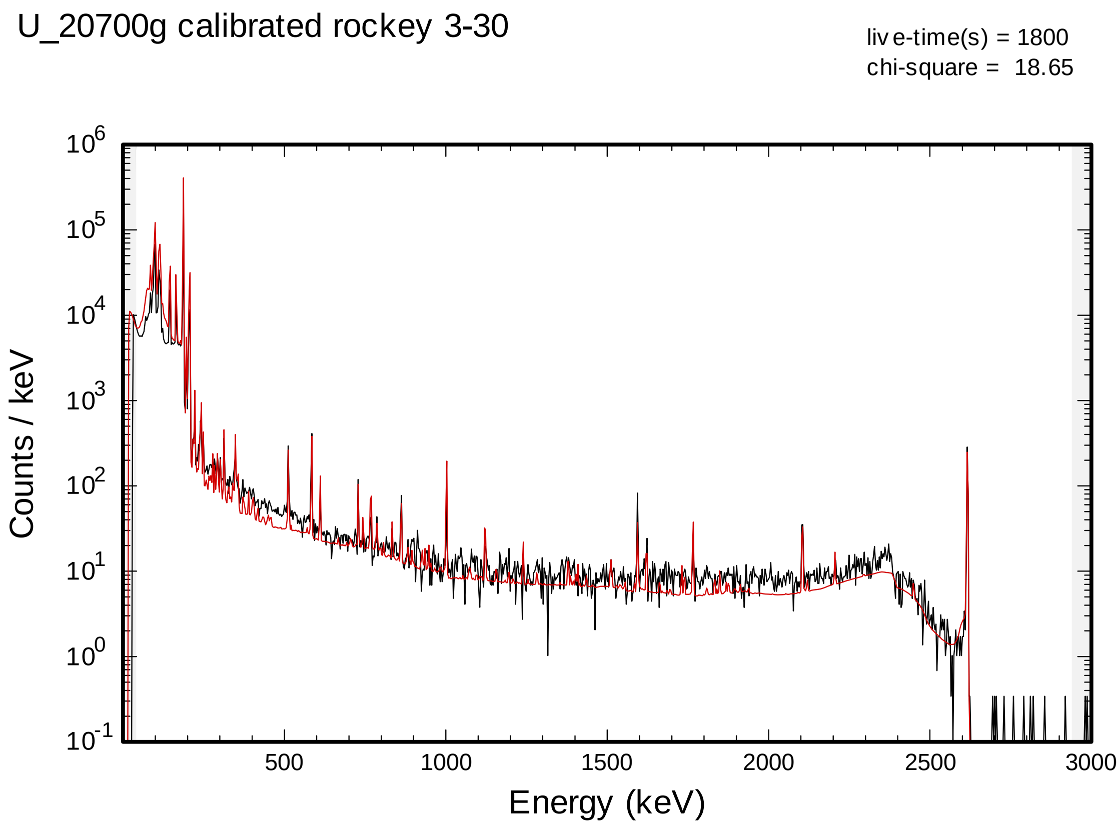
Rocky Flat 3-30 shells



Detective EX-100

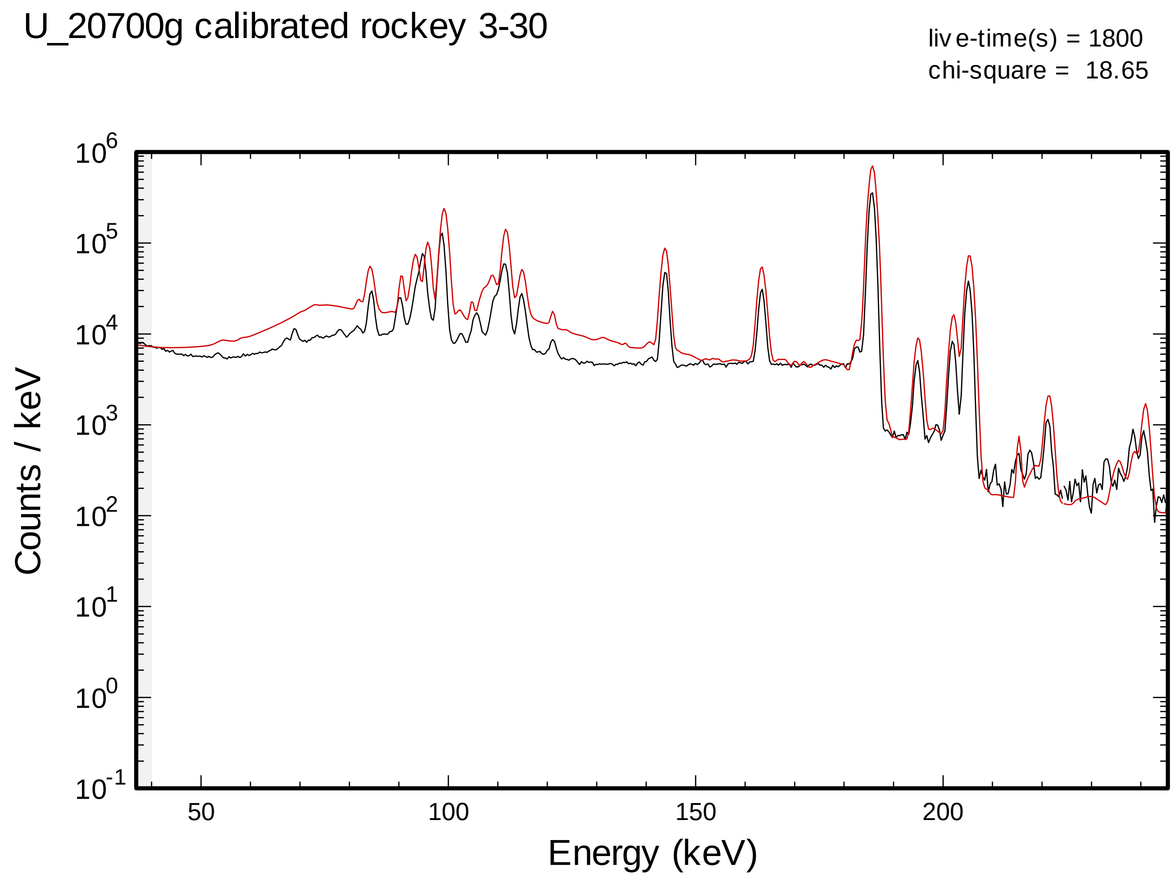
Data was collected by Jesson Hutchinson, NEN-2, LANL

Rocky Flat 3-30 shells MCNP+GADRAS spectrum



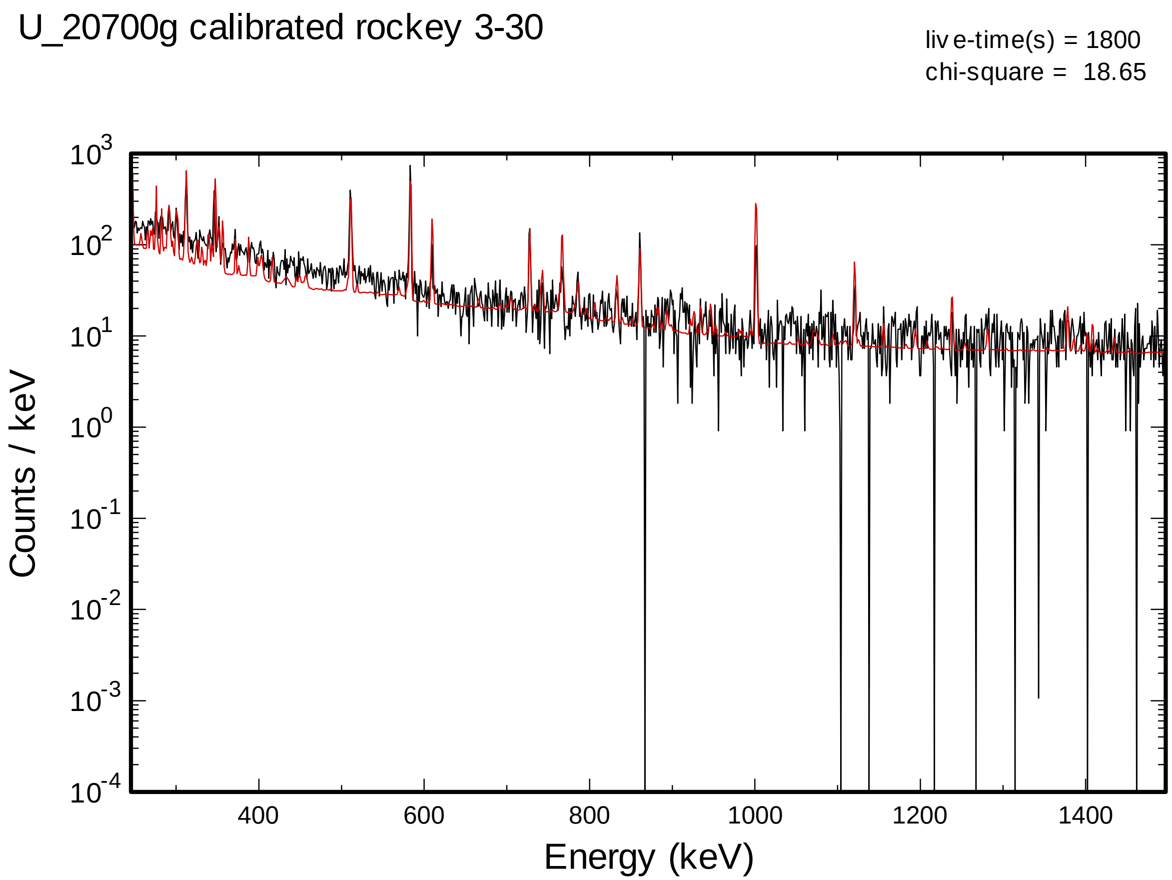
Data are in black and simulated spectrum in red

Rocky Flat 3-30 shells– Details from 40 keV – 250 keV



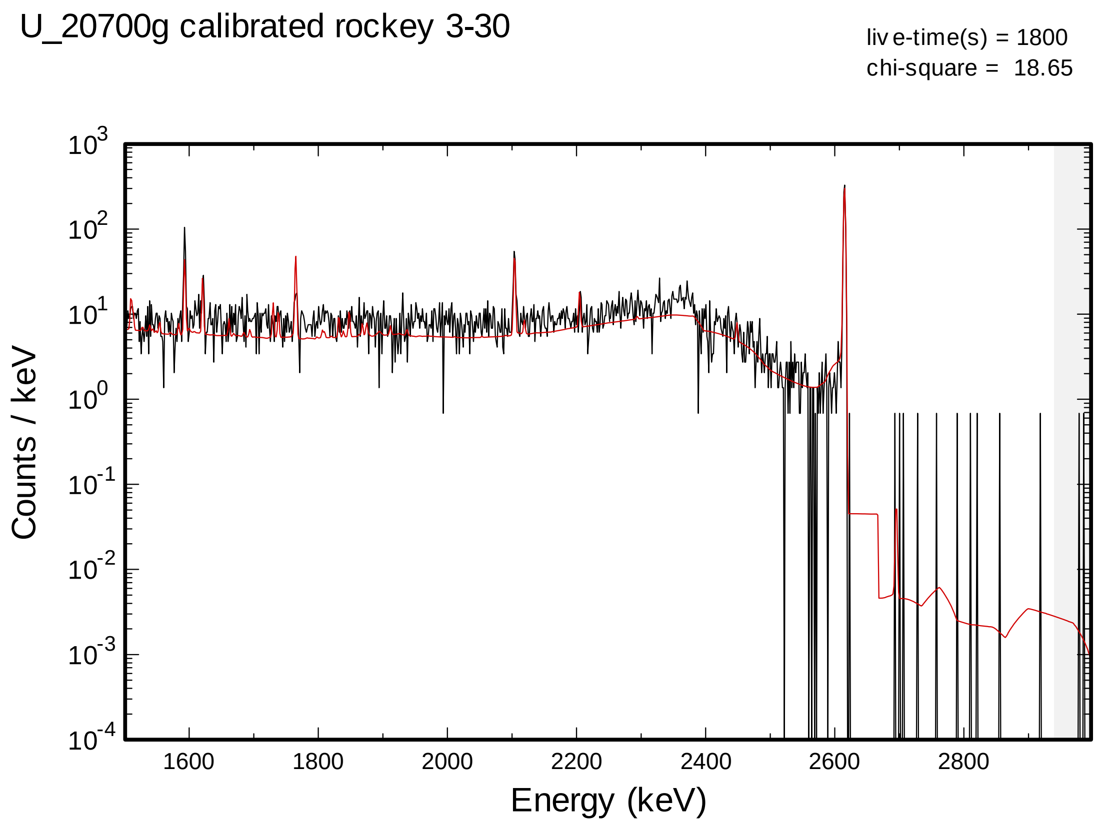
Data are in black and simulated spectrum in red

Rocky Flat 3-30 shells– Details from 250 – 1500 keV



Data are in black and simulated spectrum in red

Rocky Flat 3-30 shells– Details from 1500 – 3000 keV



Data are in black and simulated spectrum in red

Conclusions

- **The approach presented here does make it possible to simulate more complex three-dimensional geometries.**
- **You can put in your own source terms if you wish**
- **In bare BeRP and HEU cases GADRAS + MCNP continua are generally lower than data. In HDPE reflected BeRP continuum is higher than data**
  - The mismatch of the gamma continuum by MCNP is still being studied
- **For BeRP measurement there was a steel table on which the experimental set-up was sitting - generated Fe(n,γ). The source term for Fe(n,γ) was not included in our simulations.**
- **The concrete floor in the room gave gamma rays from H(n,γ) in bare BeRP spectrum and in Rocky Shells spectrum - these source terms were not included.**
- **For better accuracy all source terms need to be included.**