Improvements of Geant4 in Line Gamma-Ray Production for the Lunar and Planetary Applications

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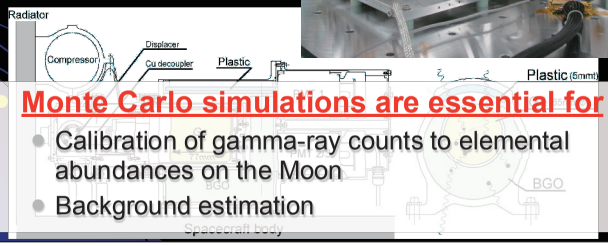
  - Physics related to planetary gamma-ray spectroscopy
- Benchmarks
- Improvements of nuclear data used in Geant4

SELENE (a.k.a. KAGUYA) mission

- Japanese lunar polar orbiter
  - Launched: Sep. 14, 2007
  - Carries 14 instruments
  - 3-axis stabilized
  - Altitude: ~100 km
  - Duration: 1 year +
- Largest lunar explorer since Apollo
- GRS observes distribution of:
  - O, Mg, Al, Si, Ca, Ti, Fe, K, Th, U

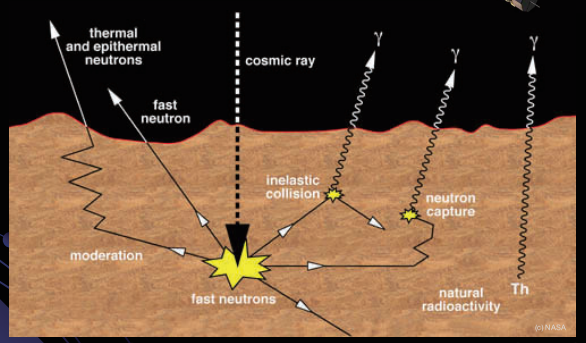
SELENE Gamma-Ray Spectrometer

- Ge: n-type, ~250 cm^3
- BGO + Plastic Anti-coincidence det.
- Cooled mechanically below 80 K



- **Monte Carlo simulations are essential for**
  - Calibration of gamma-ray counts to elemental abundances on the Moon
  - Background estimation

Gamma-Ray Emission from a Planetary Surface



1. Production of neutrons and transport ($E_{p,\,avg}$ ~ few GeV)
2. Interaction of neutrons with surface materials (~< 20 MeV)
3. Production of line gamma rays (~< 8 MeV)

Geant4 Benchmark

- ***Experiment:***
  - Apollo 17 Lunar Neutron Probe Experiment in 1972
  - Reported by Woolum et al., 1973
  - Drill core + ^{10}B detector to ~ 2 m depth
  - Measured neutron densities within the subsurface of the Moon
- ***Calculation:***
  - Geant4.9.0
  - QGSP_BERT_HP
  - G4NDL3.11
  - Scale factor of α particles: 3.8

Modeling of Galactic Cosmic Rays

- Differential 4π flux equation for GCR is calculated with:

$$J(E,\phi) = C \times \frac{E(E+2m_p c^2)(E+\chi+\phi\times\frac{Z}{A})^{-\gamma}}{(E+\phi\times\frac{Z}{A})(E+2m_p c^2+\phi\times\frac{Z}{A})}$$

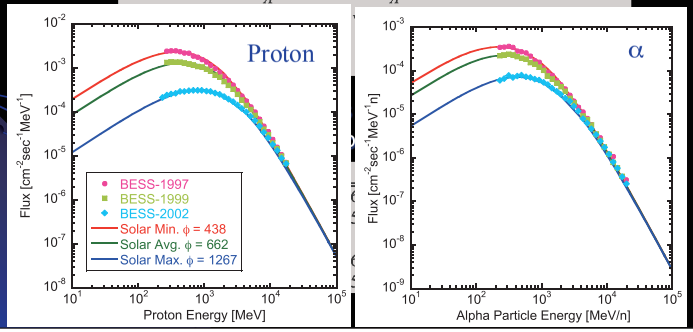
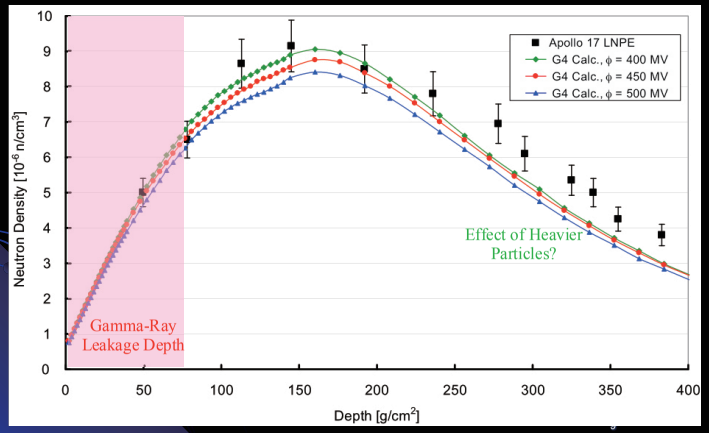


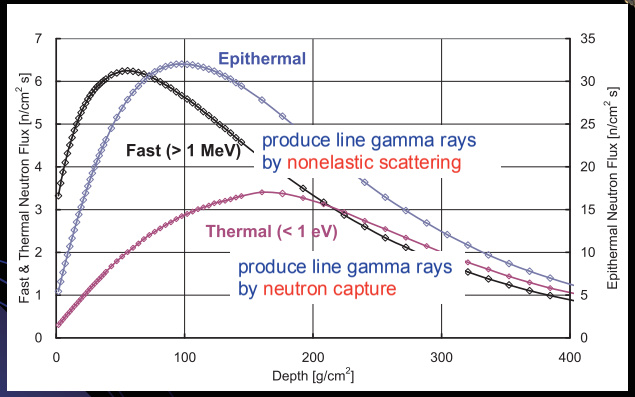
Table 5. Weight Fractions of Elements Used in Various Lunar Studies

Element	McKinney et al., 2006 [1972]	[1991]	Reedy [1978]	Data From LNPE Borehole Analysis 0–22 cm 1.76 g/cm^3	22–71 cm 2.11 g/cm^3	71–224 cm 1.78 g/cm^3	>224 cm 1.79 g/cm^3
H			4.0266E-5				
C			1.0066E-4				
N			1.0066E-4				
O	4.2321E-1	4.1929E-1	4.3286E-1	4.17392E-1	4.15573E-1	4.22977E-1	4.26358E-1
F			1.0066E-4				
Na			3.5233E-3	2.92297E-3	3.13559E-3	3.07497E-3	3.45504E-3
Mg	4.8435E-2	4.7799E-2	4.0266E-2	6.16153E-2	6.02596E-2	6.15627E-2	6.09114E-2
Al	7.3649E-2	7.2299E-2	1.1073E-1	6.06144E-2	5.97684E-2	7.38401E-2	7.54983E-2
Si	1.9895E-1	2.0260E-1	2.0133E-1	1.90261E-1	1.89552E-1	1.96678E-1	2.02181E-1
P			6.0399E-4				
S			7.0465E-4				
Cl			2.0133E-5				
Ar			1.0066E-4				
K			1.2080E-3	7.26238E-4	7.89646E-4	9.20113E-4	1.63182E-3
Ca	8.6578E-2	8.9899E-2	1.0066E-1	7.54095E-2	7.66773E-2	8.02016E-2	7.70691E-2
Ti	4.5701E-2	4.3599E-2	1.4093E-2	5.14365E-2	4.90522E-2	3.37976E-2	3.19830E-2
Cr			1.0066E-3	2.87170E-3	3.09015E-3	2.64148E-3	2.54547E-3
Mn			8.0532E-4	1.76362E-3	1.77817E-3	1.51862E-3	1.45811E-3
Fe	1.2483E-1	1.2450E-1	9.0598E-2	1.34964E-1	1.40303E-1	1.22768E-1	1.16880E-1
Ni			4.0266E-4				
Br	2.0075E-7						
Sr			1.8120E-4				
Y			6.0399E-5				
Zr			2.5166E-4				
Cd	4.0059E-08						
Ba			2.0133E-4				
La			1.0066E-5				
Nd			1.7113E-5				
Sm	1.8205E-6		7.0465E-6	8.33423E-6	7.74688E-6	7.34285E-6	1.05062E-5
Eu	8.5929E-7		5.0332E-7	1.81644E-6	1.78208E-6	1.54526E-6	1.69973E-6
Gd	5.2492E-6	1.7000E-5	8.0532E-6	1.09969E-5	1.05765E-5	9.81784E-6	1.35473E-5
Lu			5.0332E-7				
W	7.1622E-8						
Th			1.9126E-6	9.44947E-7	8.02150E-7	1.38193E-6	3.00648E-6
U			5.0332E-7				

Neutron Production & Transport



Neutron Flux within the Lunar Surface



- Rate of nuclear reactions by neutrons:
  - Consistent with ENDF-VII cross sections

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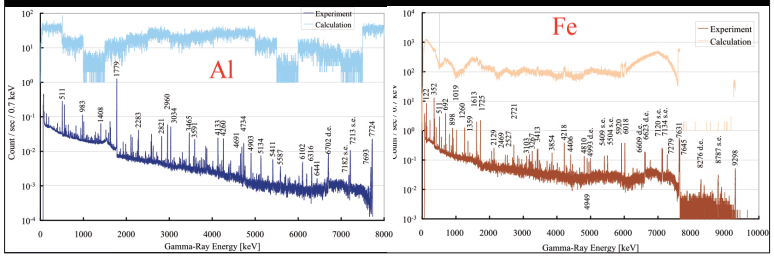
Gamma-Ray Production (1): Neutron Capture

- Line gamma rays:
  - *VERY* unsatisfactory for most of nuclides
    - Energies & Intensities
  - Need improvement...



Improvements

- No modification to source codes
  - Too much effort
  - Updated too often (for me)
- Modify nuclear data
  - Cross sections, branching ratios, ...
  - Read source codes and "good" XS like ^{28}Si
  - Implement data open for public
    - IAEA, Reedy and Frankle 2002, ENDF-VII, JENDL-3.3, ...

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"Good" Nuclear Data
G4NDL / Capture / FS / 14_28_Silicon

```
      1  repFlag   27.7370  targetMass          (Atomic Mass values relative to neutrons)
     46  nDiscrete                              (Number of Gamma-Ray Lines)
      2  disType   0.847220E+07  energy  2 isoFlag   (Gamma-Ray Energy)
      1  tabulationType                         (# of Energy-Ratio Pair)
      2  nDiscrete2  1  nIso
0.100000E-04 0.216670E-01 0.200000E+08 0.216670E-01
                                          (Gamma Intensity per Capture)
---
      2        0.493400E+07        2
      1
      2        1
0.100000E-04 0.650000      0.200000E+08 0.650000
---
      2        0.353900E+07        2
      1
      2        1
0.100000E-04 0.701520      0.200000E+08 0.701520
---
      2        0.209290E+07        2
      1
      2        1
0.100000E-04 0.195360      0.200000E+08 0.195360
```

$^{28}Si(n, \gamma)^{29}Si$

0.172 [barn]

	Eγ [keV]	XS [barn]
^{28}Si	**4933.889**	**0.1120**
^{28}Si	**3538.966**	**0.1190**
^{28}Si	**2092.902**	**0.0331**

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G4NDL / Capture / FS / 26_56_Iron

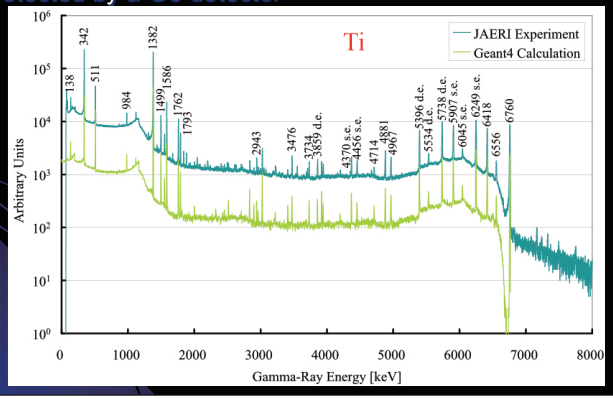
```
1 55.4545
      1
      1     0.          85
      1
     85         2
0.100000E-04 2.57220    1000.00    2.57220    10000.0    2.70730
 30000.0     2.81470    100000.    2.90110    300000.    2.99960
 500000.     3.14460    700000.    3.28320  0.100000E+07 3.12670
0.125000E+07 3.14190  0.150000E+07 3.20400  0.175000E+07 3.27060
0.200000E+07 3.34200  0.212280E+07 3.35130  0.225000E+07 3.29740
0.250000E+07 3.31910  0.270620E+07 3.35860  0.299540E+07 3.43460
0.301370E+07 3.44560  0.312570E+07 3.47350  0.317660E+07 3.44920
0.317960E+07 3.45020  0.343110E+07 3.50200  0.345050E+07 3.50790
0.350750E+07 3.52130  0.351150E+07 3.52300  0.364370E+07 3.56530
0.366430E+07 3.57190  0.366630E+07 3.57340  0.367240E+07 3.57720
0.381600E+07 3.62900  0.382410E+07 3.63250  0.382820E+07 3.63380
0.389950E+07 3.65630  0.392590E+07 3.66580  0.409940E+07 3.71640
0.412240E+07 3.72330  0.417440E+07 3.73780  0.419470E+07 3.74160
...
```

$^{56}Fe(n, \gamma)^{57}Fe$

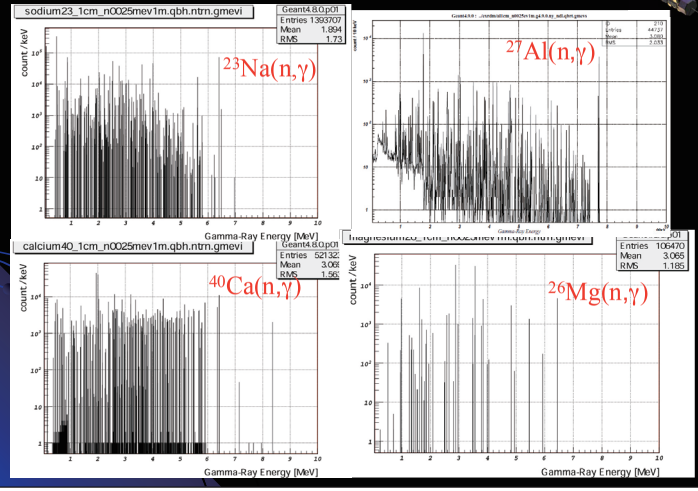
- We have gained full control of cross sections and branching ratios for (n,γ) gamma rays

Improved (n,γ) Gamma-Ray Spectra

- Thermal neutrons irradiated to a 1-cm-thick target
- Detected by a Ge detector

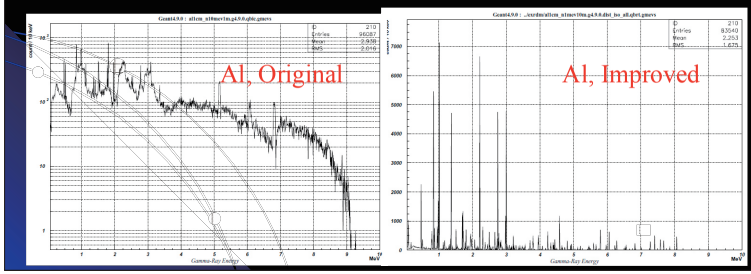


Emission Spectra of Other Major Nuclides

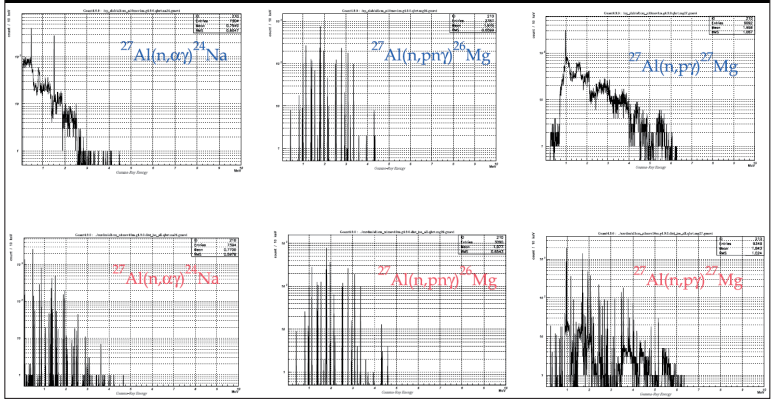


Gamma-Ray Production (2): Nonelastic Scattering

- Line gamma rays:
  - Unsatisfactory for most of nuclides in terms of energies & Intensities
- Modified data for distribution of neutron energy and/or angle
  - "dataType": theXsection & theAngularDistribution are fine.
  - Other dataType's, often theEnergyAngData interupts line gammas

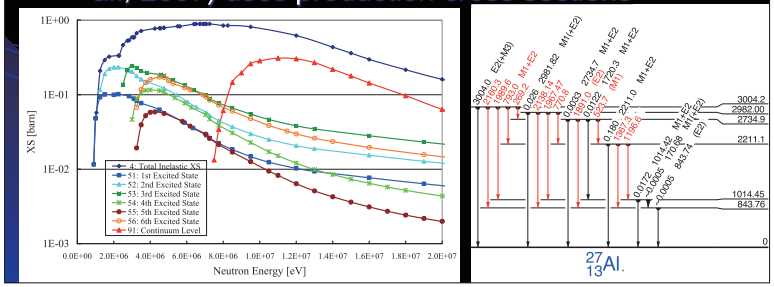


Emission Spectra from Other Reactions



Problem in Improving G4NDL

- Evaluated nuclear data (as well as G4NDL) incorporates excitation cross sections
  - "Continuous Level" exists
- Planetary gamma-ray people use (c.f. Kim et al., 2007) uses production cross sections



We appreciate more information.

- Structure of nuclear data
  - Should be open, easy to read
  - Data format
    - To convert "public" data to G4NDL style
  - Sources from which data are retrieved
- Manuals
  - What neutron_hp really can do, how it does, …
  - How it treats de-excitation from "continuous" energy levels
- Activation, rdm
- Evaluation by users?

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