ISS-RAD Fast Neutron Detector (FND) Simulation and Data Unfolding- Status Report

Martin Leitgab, NASA SRAG on behalf of the NASA SRAG ISS-RAD team

Workshops on Radiation Monitoring for the International Space Station 09/10/15
Outline:

1. Introduction: Light function formalism

2. Light function calibration

3. Regularized unfolding

4. Validation on generated data

5. Summary & Outlook

graphics modified from SwRI
1. Introduction: Detection/Selection Mechanism: Boron-loaded Scintillator

- Neutrons deposit energy in plastic scintillator, some captured by $^{10}$B atoms:

**Mechanism: Boron-loaded Scintillator**

**Measurements of recoil and capture photon signals and:**

- **Recoil Pulse**: sum of light signals produced during deceleration of neutrons
- **Capture Pulse**: light produced by neutron capture on boron

**Online: Capture Amplitude Selection**

**Online: Capture Time Selection**

- Measurements of **recoil** and **capture** photon signals and:
1. Introduction: Response Spectrum Shape

- ‘Monoenergetic’ neutron calibration ($\Delta E < 5\%$) at PTB, Germany:

Data taking setup

FND on beam axis/in forward scattered field at 2.5m from target
1. Introduction: Response Spectrum Shape

- Filtered ADC spectrum in response to monoenergetic neutron fields (after background subtraction):
1. Introduction: Scintillation Light Creation/Propagation: Light Function Formalism

- Shape of response spectra dominated by factors impacting collected light:
  
  a) **Multiple scattering** of neutron with scintillator material nuclei: multiple pulses of scintillation light per neutron
  
  b) **Scintillation light quenching** (ionization quenching - Birk’s law): nonlinear amount of collected scintillation light per interaction depending on energy deposit & scattering target

Even monoenergetic neutrons create broad distribution in light deposit/FND recoil spectra.

- Approach describing scintillation light generation in multiple scattering: Light function formalism

**Literature:**
Neutron recoils on...

V.V. Verbinski et al, NIM 65 (1968) 8 ff
1. Introduction: Scintillation Light Creation/Propagation: Light Function Formalism

- Example: End-to-end FND simulation (MCNP-PoliMi and FND signal processing algorithms) for monoenergetic neutron fields at PTB (FM002 calibration)
- Spectral shape driven by number of high energy deposit neutron collisions off hydrogen:

- For result with finer energy binning than experimental data: apply light function formalism
2. Light function calibration
2. Light Function Calibration - Flowchart

- Goal: Extract continuous light function describing scintillator behavior to freely choose energy binning
- For each experimental monoenergetic data sample, start from first principles:

a) Create energy deposit files

   a.1) Generate MCNP-PoliMi energy deposits per neutron-target interaction vs. time, for experimental energies

   a.2) ‘Time-connect’ independent MCNP source events for respective Poisson-distributed event rate

b) Light function calibration

   b.1) Convert energy deposits to light yield with light function

   b.2) Apply resolution (scintillator, PMT, pulse processing electronics)

   b.3) Simulate light collection and pulse digitization in FND PMT and electronics

   b.4) Convert to channel number values using photon calibration results

   b.5) Apply FND FPGA pulse pair selection logics

   b.6) Apply chance coincidence subtraction, scale factor (efficiency not part of optimization, just product)

   Check match to experimental data

   Adjust light function and resolution

   Fill recoil spectrum

   for each energy deposit (~5M per energy)

   Check against experimental spectra

   optimization loop for each energy sample

Create recoil spectra

Create energy deposit files

Check against experimental spectra
2.a.1 Generation of Neutron Energy Deposits: MCNP-PoliMi

- Use MCNP-PoliMi package:
  
  * MCNP limitations for neutron propagation and fission/inelastic scattering simulation:
    @ only returns total energy deposition of each neutron in target volume for conversion to light
    @ photon and neutron productions in fission/inelastic collision events not correlated in time/energy/multiplicity
  
  * PoliMi package writes out each interaction of single neutrons and photons
    @ time correlation within each single history, resolution in 100 ps
    => energy-to-light conversion possible on per-interaction-basis
    @ elastic, (n,gamma) and (n,n') interactions accurately modeled/propagated
  
  * Generations of 1e+08 n per experimental energy in bias cone around FND

Model started by A. Bahadori (SRAG)

Energy Distributions, Neutron Source

- Neutrons into point source
- Neutrons out of point source
- Neutrons into FND
- Neutrons out of FND
- Neutrons into sphere surrounding setup
- Neutrons out of sphere surrounding setup
- Photons into point source
- Photons out of point source
- Photons into FND
- Photons out of FND
- Photons into sphere surrounding setup
- Photons out of sphere surrounding setup

0.5 MeV Neutrons
8 MeV Neutrons
2.a.2 ‘Time-connect’ Neutron Energy Deposits from MCNP-PoliMi

- Output of PoliMi: ASCII file containing interactions of neutrons and photons with target material:

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- Limitation in PoliMi: no transport of non-neutron/photon decay products of capture/fission reactions -> manually distribute recoil energy among decay products & convert to light

- To create realistic succession of neutron events in scintillator: ‘time-connect’ PoliMi events to experimental flux (30-310 /s/cm^2):

<table>
<thead>
<tr>
<th>History</th>
<th>Particle Type</th>
<th>Interaction</th>
<th>ZAID</th>
<th>Energy Deposited [MeV]</th>
<th>Absolute Time [μs]</th>
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...
2.b.1 Convert Energy Deposit to Light- Function Parameterization

- Fit to Verbinski data parameterized as: 2nd order polynomial at low deposited energy; \( \sqrt{\text{const} + E^2} \) at high energy
- Change 5 parameters to optimize match with experimental data

\[
L(x_{ED}) = \begin{cases} 
ax_{ED} + bx_{ED}^2 & \text{for } x < g \\
c + d\sqrt{e^2 + f^2x_{ED}^2} & \text{for } x \geq g, \text{ where } \quad a = \frac{df^2g}{\sqrt{e^2 + f^2g^2}} - 2bg \\
\end{cases}
\]

Neutron Light Conversion Functions

Continuity requirements for 1st and 2nd derivative
2.b.2 Apply Resolution- Implementation

- Single-point implementation of all experimental resolution contributions:
  * light production/quenching/reflections in plastic,
  * light coupling scintillator to PMT
  * PMT photon detection
  * electronic noise (PMT/amplifier) etc
- Optimize 3 parameters to match experimental data

\[ \frac{\Delta L}{L} = \left( \alpha^2 + \frac{\beta^2}{L} + \frac{\gamma^2}{L^2} \right)^{1/2} \]

\[ \begin{align*}
\text{Neutron Light Resolution, (}\Delta L/L\text{)}
\end{align*} \]

Discontinuity due to limited continuity of photon calibration function (1st order) used in conversion

Non-differentiability due to limited continuity of light function (2nd order) used in conversion
2.b.3 Light Collection/Pulse Digitization (see Michael V.’s talk)

- Convert light yields to corresponding electronics signal pulses via Gaussian function sampled by 33 MHz clock; area normalized to light yield
- Two filters create bipolar signals for peak detection and ‘moving average (sum)’ for signal height
- Time width of Gaussian chosen to match experimental signal processing pulse width (full width ~390 ns)

Recoil pulses of 2 neutrons from sample of 8 MeV neutrons @ 10 kHz

33 MHz pulse train
2. b. 4 Light to Channelnumber Conversion: Photon Calibration

- Inputs: experimental photon source and MCNP-simulated energy deposit spectra
- Perform global fit of conversion function parameters: create channelnumber spectra from generated deposited energy spectra

Channelnumber-to-light yield conversion:

\[ ED(x_{CHN}) = \begin{cases} 
  a + bx_{CHN}^c & \text{for } x < e \\
  d + bx_{CHN} & \text{for } x \geq e, \text{ where } d = a + be^c - be 
\end{cases} \]

Continuity requirement
2.b.4 Light to Channelnumber Conversion: Photon Calibration

- Result: Low light yield region prefers nonlinear (power law) shape (also seen in other literature):

Global red. chisq. = 695 / 490 = 1.42
Red. chisq. for single plots:
- Co-57: 27/31 = 0.86
- Ba-133: 63 / 35 = 1.80
- Na-22 a): 53 / 32 = 1.67
- Cs-137: 108 / 70 = 1.54
- Mn-54: 69 / 80 = 0.86
- Co-60: 211 / 160 = 1.32
- Na-22 b): 164 / 100 = 1.64
2.6.5 FND Pulse Pair Selection *(see Michael V.’s talk)*

- Apply same selection as FND FPGA
- Algorithm considers three latest detected pulse amplitudes (moving averages) and time intervals between them (zero crossing of bipolar signal)

- **Pulse selection logics**: accept A, B as pulse pair:

  I) \( SH_B \) in capture signal window & &
  II) \( \Delta t_{AB} \) in capture time window & &
  III) \( \Delta t_{AB} < \Delta t_{BC} \) | |

  \( SH_C \) outside of capture signal window | | \( \Delta t_{BC} \) outside of capture time window )
2.b.6 Background/Chance Coincidence Subtraction

- Poisson time correlation between recoil and capture pulses for B10 capture event allow to subtract backgrounds

- Oversubtraction ensures all backgrounds subtracted; rejected neutron pairs recovered via efficiency correction

- Performed in both experimental and simulated samples for consistency
2. Preliminary Calibration Results - Recoil Spectra Match

- Deviations for low channel numbers at mid to high energies - further analysis to be done to identify missing process/incorrect treatment of neutron interactions; resolution to be adjusted as well.
3. Regularized Unfolding

[Graphics modified from SwRI]
3.1 Unfolding Procedure: Regularized SVD Unfolding

- Uncertainties on data distributions and response matrix
  => use regularized, singular vertex decomposition-based unfolding algorithm (ROOT: TSVDUnfold)

- **Advantages:**
  * correct treatment of uncertainty-equipped input quantities (detector response matrix, input distribution)
  * full uncertainty propagation; fast

- **Limitations:**
  * ‘strength’ of regularization described by free parameter, needs to be determined from simulation and pre-launch data (systematic uncertainty)
  * dependence on input distribution (to be studied)

general problem formulation:

\[ \hat{A} x^{ini} = b^{ini}, \quad \sum_{i=1}^{n_b} \left( \sum_{j=1}^{n_x} \hat{A}_{ij} x_j - b_i \right)^2 = \min \]

but: \( \Delta b \neq 0 \)

rescaling and regularization:

\[ \sum_{i=1}^{n_b} \left( \frac{\sum_{j=1}^{n_x} \hat{A}_{ij} x_j - b_i}{\Delta b_i} \right)^2 = \min. \quad (\hat{A} x - b)^T B^{-1} (\hat{A} x - b) = \min \]

regularization parameter: chosen from rank of response matrix/problem

-> need response matrix for given recoil channel/number and chosen neutron energy binning
3.2 Neutron Energy Binning

- Neutron energy binning:
  * low and high limits: approach from detector side:
    @ lower limit: 200 keV (electronics lower pulse cutoff/arming threshold)
    @ upper limit: 8.5 MeV (corresponding pulses start to saturate 12-bit ADC)
  * bin width:
    @ FND orbit data histograms hardcoded to 512 channel width (29 bins)
    @ light function nonlinearity: first recoil bin contains most of all < 1 MeV neutrons
    @ choose second bin such that contains majority of peak for 1.2 MeV
=> 12 bins, bin width 0.7 MeV

- Boundary effects:
  * Neutrons < 200 keV contribute to low bins of recoil distributions (finite detector resolution, fixed-amplitude capture signals)
  * Neutrons > 8.5 MeV contribute to all bins in recoil spectra (scattering, capture signals)

  -> include under- and overflow bins in neutron energy:

* reason to believe that low energies correctly modeled
* fidelity of simulation/physics models for energies > 8.5 MeV not as high -> additional systematic uncertainties
3.3 Response Matrix Assembly

- Choose ‘input spectrum’ close to expected truth:
  * Koshiishi et al, published 2007 (data from 2001);
  * three data points filled for energies [100 MeV; 10 GeV) from simulation
- Integral orbit averaged flux (black line):
  * thermal to 200 keV: ~0.6 n/cm^2/s, > 8.5 MeV: 0.6 n/cm^2/s
  * total ~3.0 n/cm^2/s

H. Koshiishi et al, Rad. Meas. 42 (2007), 1510ff
3.3 Response Matrix Assembly

- Generated energies from thermal to maximum energies to have representative neutron spectra of each kinematic region (MCNP-PoliMi)
- Scale relative statistics/time for each neutron energy analysis bin according to measured orbit averaged fluxes reported in Koshiishi et al, to be close to expected environment
3.3 Response Matrix Assembly

- Response recoil spectra for chosen neutron binning; fluxes acc. to Koshiishi et al
- Underflow contributions only in first channelnumber bin: 12%
- Overflow neutron energies contribute to all channelnumber bins: dominates highest two bins; >10% contribution to bins >11000; few % down to first bin
- -> unfolding removes contributions

![Reconstructed Yields from Generated Neutrons](image-url)

- Underflow bin contributions limited to first channelnumber bin
- Overflow bin contributes to all recoil bins

![Rel. Response Contribution of Neutron Energy Bins per Recoil Bin](image-url)
3.3 Response Matrix Assembly
- Line and row integrals of response matrix;
- Recoil channel number distribution represents simulation of detector response to on orbit spectrum from 0.1 meV to 10 GeV measured by Koshiishi et al + simulation

Increasing flux and falling efficiency compensate
Bin width in Koshiishi et al data changes from 1 MeV to 2 MeV

likely: hard photons from Gd capture coincidental with other neutrons
4. Validation on generated data
4.1 Validation on Generated Monoenergetic Data

- MCNP-PoliMi-generated monoenergetic energies encountered at PTB
- Apply energy resolution of FND light function calibration, simulated efficiencies
- Tuning necessary for single energies - resolution mismatch

Efficiencies, resolution used to create truth histograms

Efficiencies from Simulation
Exp PTB 2015
Fit to Sim Eff

Neutron Energy Resolution, Converted

Non-differentiability due to limited continuity of light function (2nd order) used in conversion

Pre Unfolding Recoil Spectra, 2.5 MeV

Post Unfolding, Eff. Corr Neutron Spectra, 2.5 MeV, kregidx 13

Pre Unfolding Recoil Spectra, 8 MeV

4.1 Validation on Generated Monoenergetic Data

- Extreme case: combine all single energies in one reconstructed histogram, unfold;
- Differences <~25% for most part
4.2 Validation on Generated Data- AmBe

- Built-in MCNP-Polimi AmBe spectrum, generated inside simulated source as volume source
- Deviations to ISO AmBe spectrum ~30%, but benchmarking rather for functional relation to original true spectrum
4.2 Unfolding Benchmarking - Generated AmBe Data

- Largest deviations 18%, general undershoots truth (possibly normalization tuning necessary)
5. Plan Ahead

- **Improve match** of calibration to experimental data and of unfolding to generated data; unfold experimental data

- Systematic studies: other unfolding algorithms

- Study FND **response and recoil spectrum contributions** of **mixed radiation field** on ISS: protons, alphas, photons (simulations/ experimental measurements: TRIUMF, NSRL)
Backup
2c) Direct Mapping/Conversion Spectral Match Test

- Created ‘truth’ distributions from ISO for AmBe and Cf sources:
  apply detector resolution, direct mapping binning and energy range selection (0.5-8 MeV)
* Cf ISO binning mostly too wide for smearing to have effect;

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<th>ISO AmBe and Cf Neutron Spectra, Binnings &amp; FND Resolution</th>
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<td><img src="image1" alt="Graph of ISO AmBe and Cf Neutron Spectra, Binnings &amp; FND Resolution" /></td>
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<td><strong>ISO Raw</strong></td>
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<td><strong>FND Energy Resolution</strong></td>
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<td><strong>Direct Mapping Binning</strong></td>
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<td><img src="image4" alt="Graph of ISO AmBe and Cf Neutron Spectra, Binnings &amp; FND Resolution" /></td>
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<tr>
<td><strong>FND ‘Truth’, Energy Range 0.5-8 MeV</strong></td>
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</table>
2c) Direct Mapping/Conversion Spectral Match Test

- Scale ‘truth’ histograms with PTB reported (adjusted) neutron flux
- Comparison with GAS analysis results statistics-limited to <~ 5 MeV (only spotty shadow cone and background subtraction data at higher chn bins):
  @ Expected: Low energy spectrum overestimated, medium/high energy spectrum underestimated
  @ AmBe spectrum shows structure in ISO-truth, not reflected in DBM spectrum: deviations +45% to -41%;
  @ Cf spectrum closer (statistics limited): overestimate at low bins ~22%, medium energy bins large uncertainties, in part consistent;
- Conclusion: Direct Mapping/Conversion analysis method by design shows limitations in reproducing neutron energy spectra.
4.1a Simulation of Neutron Energy Deposits: MCNP-PoliMi

- for all materials use ENDF-VII library at 300 K, assembled in 2005; max energy 20 MeV, 500-3500 energies depending on material
4.1a Simulation of Neutron Energy Deposits: MCNP-PoliMi

- for all materials use ENDF-VII library at 300 K, assembled in 2005; max energy 20 MeV, 500-3500 energies depending on material
6) Low Energy Nonlinear Light Output in Literature

Energy deposit -> Light Yield -> Channelnumber

FND Channelnumber to Energy Deposit Conversion

FND Fit Result


Assumed linear

Literature a)

Literature b)

Literature c)

http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=4696573
http://pasj.asj.or.jp/v63/sp3/63s303/63s303-frame.html
http://iopscience.iop.org/0031-9155/59/16/4621/article

FND Fit Result: A ~ C^(1.02)
4. Scintillation Light Creation/Propagation: Light Function Formalism

**MCNP-PoliMi Scintillator Simulations**

![Histogram of Number of Interactions per Neutron with B-10 Capture]

- 5.46e+05 eV
- 1.24e+06 eV
- 1.93e+06 eV
- 2.62e+06 eV
- 3.31e+06 eV
- 4.01e+06 eV
- 4.70e+06 eV
- 5.39e+06 eV
- 6.08e+06 eV
- 6.77e+06 eV

**Exp. Recoil of 8 MeV Monoenergetic**

![Graph of Recoil Channel Number vs. Recoil Energy]
### 3.1 Unfolding Procedure: Regularized SVD Unfolding


**general problem formulation:**

$$\hat{A} x^{\text{ini}} = b^{\text{ini}}, \quad \sum_{i=1}^{n_b} \left( \sum_{j=1}^{n_x} \hat{A}_{ij} x_j - b_i \right)^2 = \min$$

with SVD:

$$\hat{A} = U S V^T$$

$$z = V^T x \quad d = U^T b$$

$$x = V z = V S^{-1} d = V S^{-1} U^T b = \hat{A}^{-1} b \quad \hat{A}^{-1} = V S^{-1} U^T$$

**but: delta b != 0**

$$\sum_{i=1}^{n_b} \left( \frac{\sum_{j=1}^{n_x} \hat{A}_{ij} x_j - b_i}{\Delta b_i} \right)^2 = \min, \quad (\hat{A} x - b)^T B^{-1} (\hat{A} x - b) = \min$$

**rescaling and regularization:**

$$\begin{align*}
(\hat{A} w - \tilde{b})^T (\hat{A} w - \tilde{b}) + \tau \cdot (C w)^T C w &= \min
\end{align*}$$

**regularization parameter: chosen from rank of response matrix/problem**
2) Neutron Efficiency Results, ADC Saturation

- Efficiencies from PTB datasets: Rel. uncertainties 2-3%;

![Efficiency graph](image)

- ADC saturation for high pulse heights

![Clipping graph](image)
2) Preliminary Fit Result to Capture Pulse Distributions

- Experimental data not corrected for beam background/room return
2) Preliminary Simulation Result for Delta t Capture Distribution

- Experimental data not corrected for beam background/room return