Benchmark and Validation Experience with the ENDF/B-VII Decay Data Sub-library

Tales From an End-User

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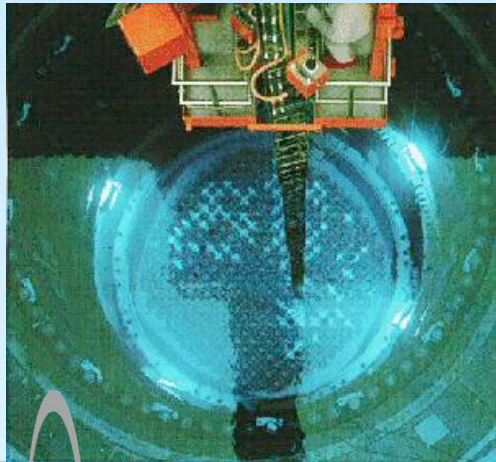Germina Ilas

Oak Ridge National Laboratory

CSEWG Validation Committee
Brookhaven National Laboratory
November 7, 2012

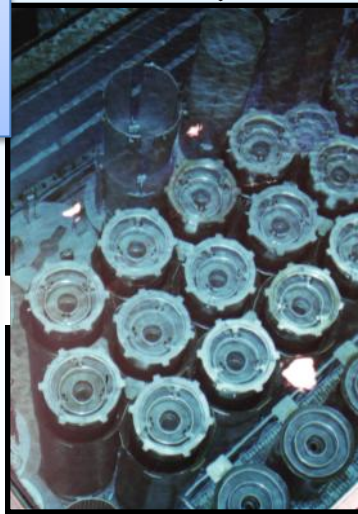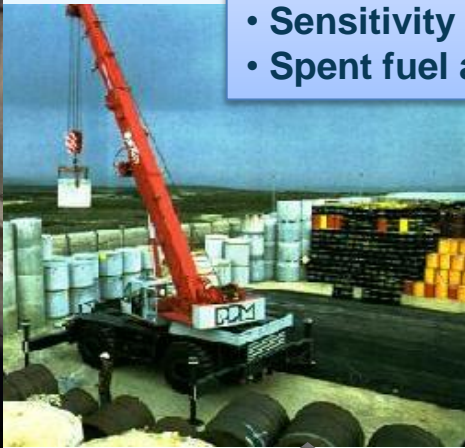Material processing and fabrication

Commercial and research reactors

SCALE is a nuclear systems modeling and simulate code used worldwide for reactor and fuel cycle applications

- **Criticality safety**
- **Radiation shielding**
- **Cross-section processing**
- **Reactor physics**
- **Sensitivity and uncertainty analysis**
- **Spent fuel and HLW characterization**

scale

Disposal

Interim storage

Reprocessing

Transportation and storage

Spent Nuclear Fuel and Source Term Analysis

ORIGEN

- <u>O</u>ak <u>R</u>idge <u>I</u>sotope <u>GEN</u>eration and Depletion code
- Irradiation and decay, batch and continuous chemical processing
- Calculates
  - Time dependent isotopic concentrations
  - Radioactivity
  - Decay heat (based on summation)
  - Radiation sources (neutron/gamma)
  - Toxicity
- Explicit simulation of 2226 nuclides
- Nuclear database for:
  - 174 actinides
  - 1149 fission products
  - 903 structural activation materials

U.S. DEPARTMENT OF ENERGY

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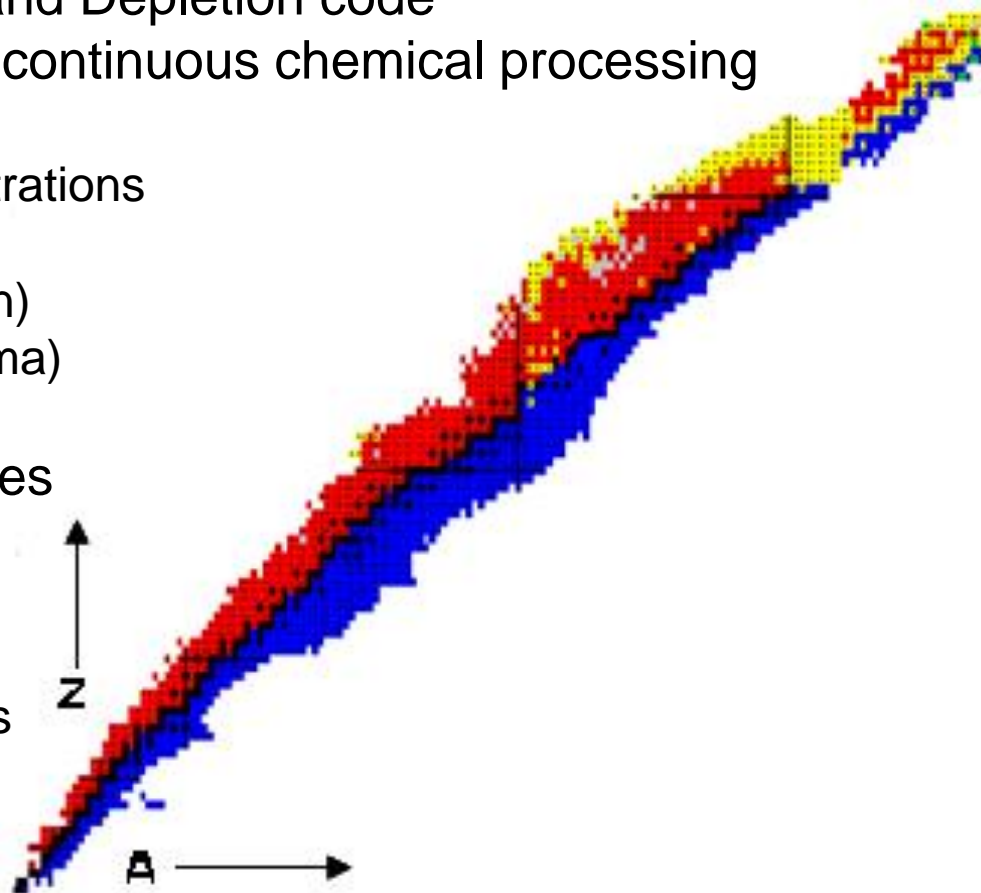
Nuclear Data Libraries

Accuracy of ORIGEN is determined by the accuracy of the nuclear data

- Decay half lives, branching fractions, energy release
  - 2226 nuclides
- Cross sections
  - ENDF/B-V, -VI, -VII
  - JEFF-3.1/A special purpose activation file
- Fission product yields
  - Energy-dependent data
- Gamma ray production data
  - X-ray and gamma ray emissions per decay
- Neutron production data
  - Alpha decay energies
  - Stopping powers
  - α,n yield cross sections
  - Spontaneous fission spectral parameters
  - Delayed neutron spectra
- Alpha and beta spectra included in next release

Isotopic validation studies

- Destructive isotopic assay data (>120 spent fuel samples)
  - SFCOMPO (OECD/NEA web database)
  - TMI-1 (GE-Vallecitos and Argonne National Laboratory)
  - Obrigheim (Karlsruhe reprocessing plant)
  - ARIANE International program
  - REBUS International program
  - MALIBU International program (SCK.CEN)
 - Spanish Fuel Program (ENUSA-CSN)

Hotcells at PSI

UO2 fuel rod segments

MOX samples at ORNL

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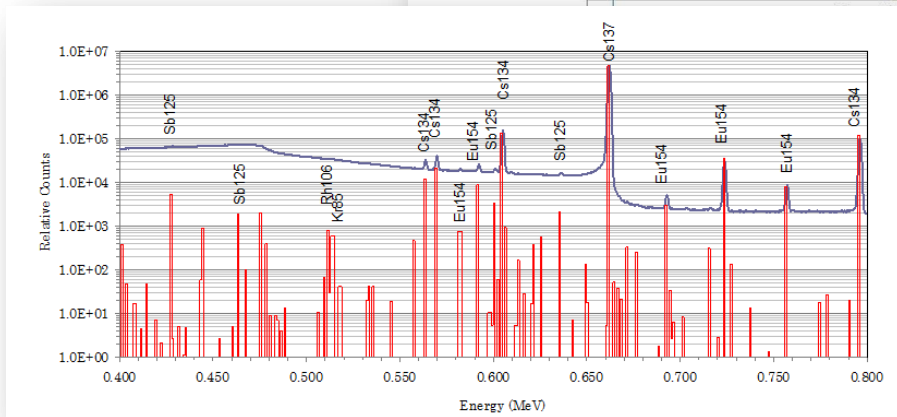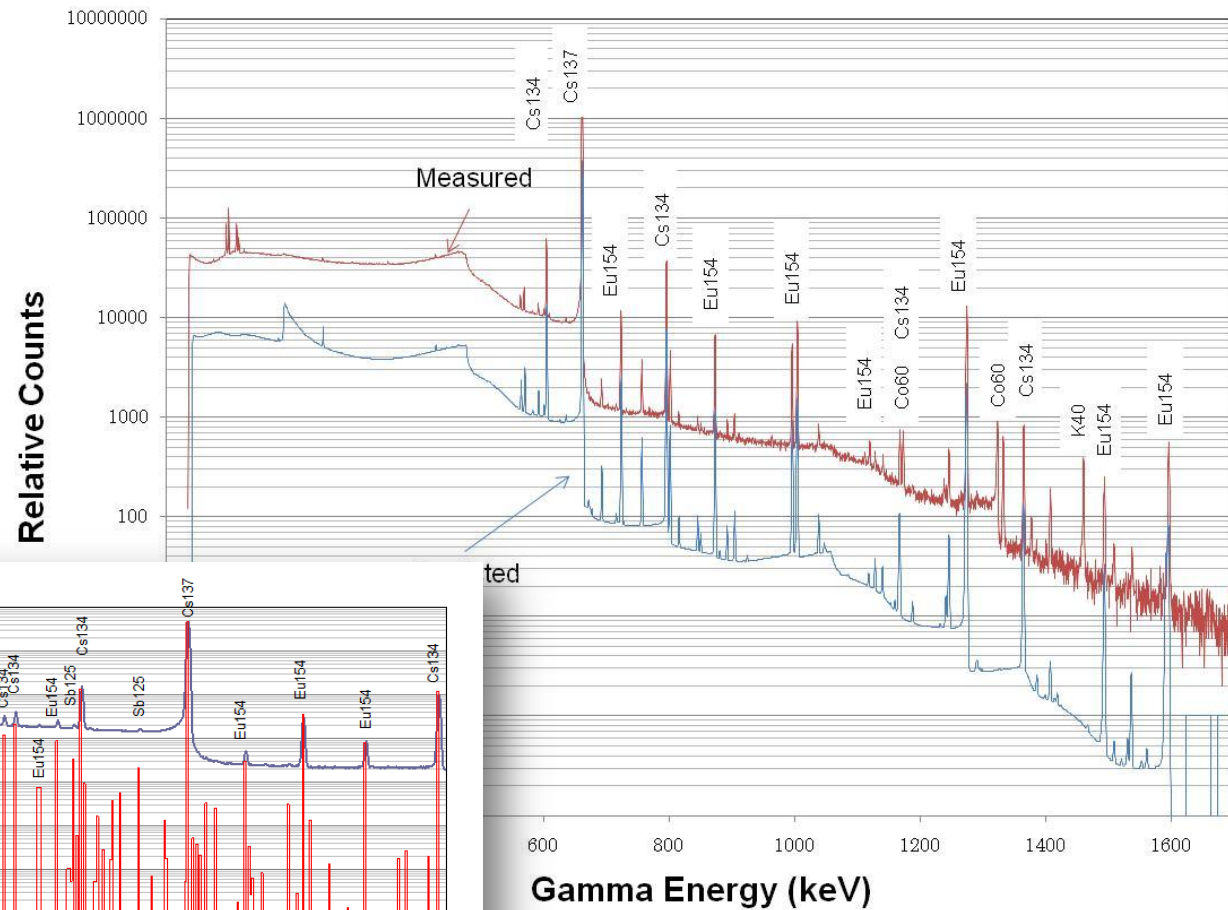
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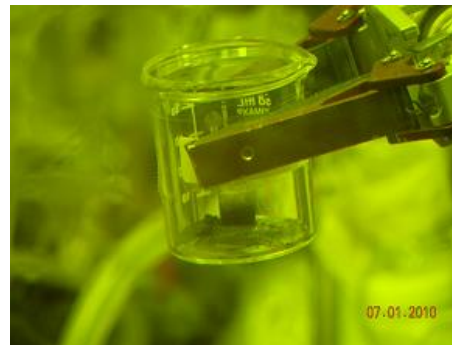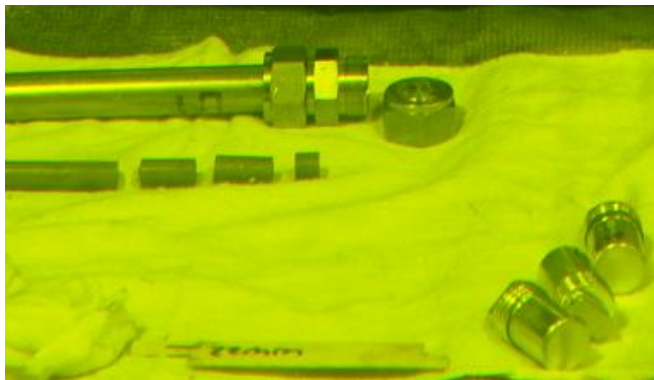
Decay heat validation studies

- Decay heat measurements
  - Calorimeter measurements of full length fuel assemblies at the Swedish Interim Spent Fuel Storage Facility CLAB
  - Burst fission experiments - short decay time ($< 10^5$ s)
  - > 80 assemblies
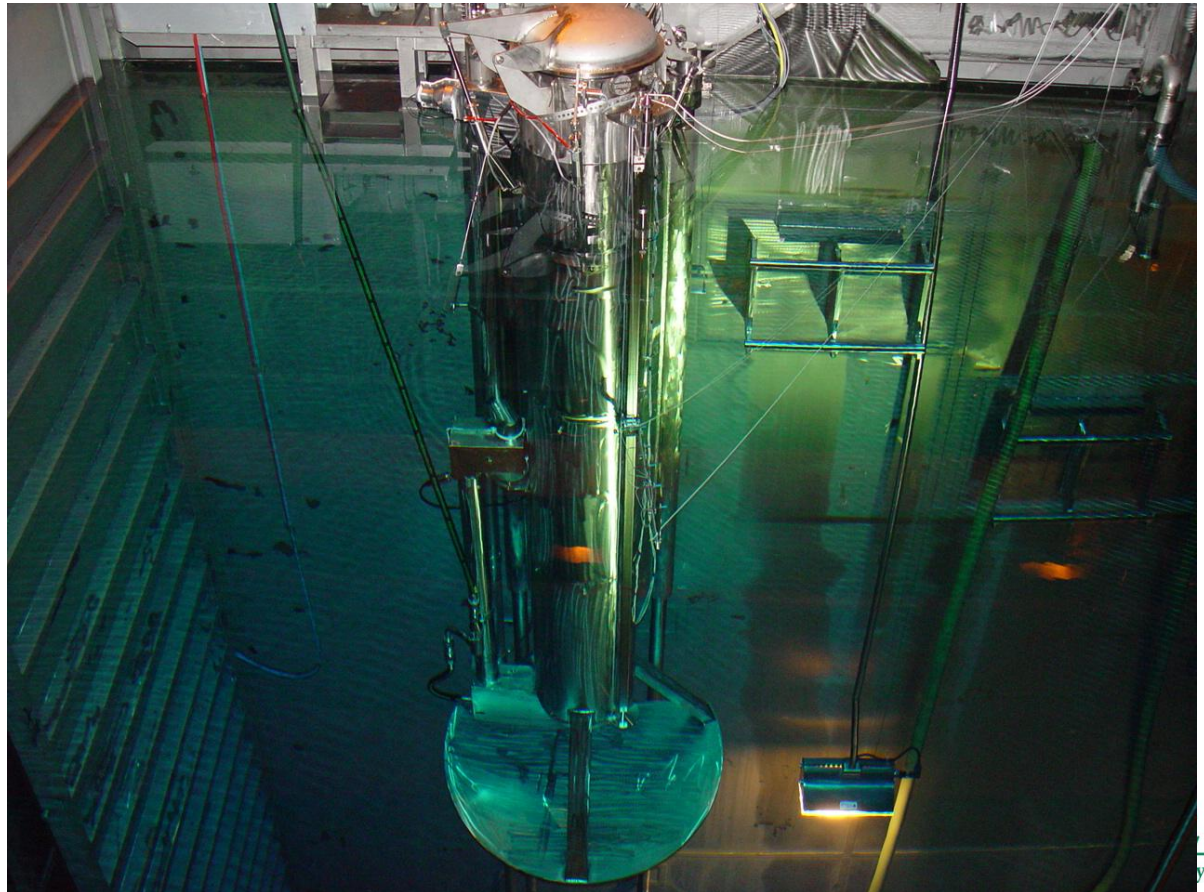
Validation of spent fuel gamma spectra

Simulated HPGe detector response

SCALE 5.0 – SCALE 6.1

2004 – 2011

Expanded Capabilities to Address a Broader Class of Problems & Sponsors

Reactor physics

Shielding analysis with automated variance reduction

Sensitivity and uncertainty analysis

High-fidelity criticality safety in continuous energy

Graphical user interfaces and visualization tools

Expanding Use

Used in 40 nations by regulators, vendors, utilities, and researchers
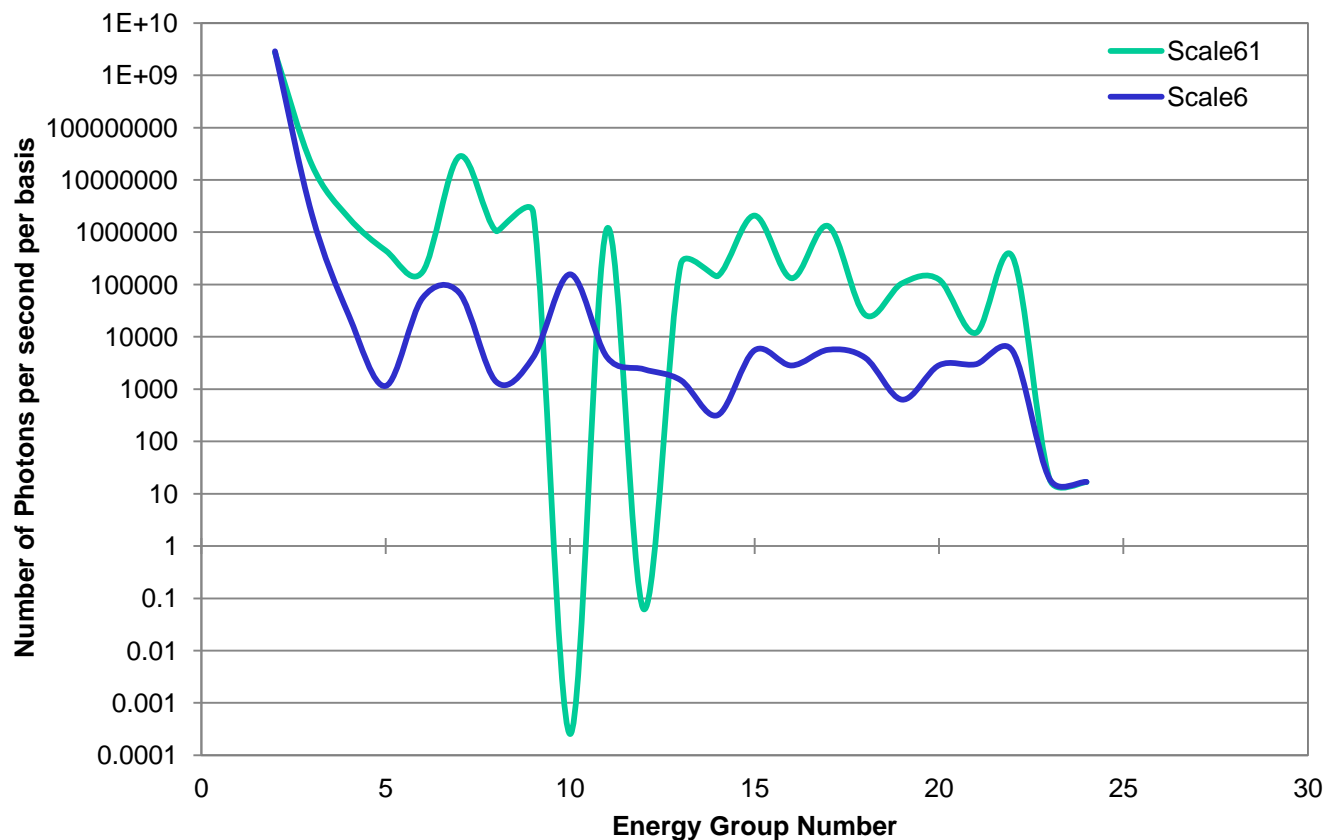
Data upgrades in SCALE 6.1

- ENDF/B-VII.0 decay data
- ENDF/B-VII.0 fission yields with energy dependent implementation
- New gamma emission libraries based on NuDat 2.0 (gamma evaluations not included in VII.0)
- ENDF/B-VII.0 cross sections used for isotopic depletion

Isotopic validation – ENDF/B-V and -VII
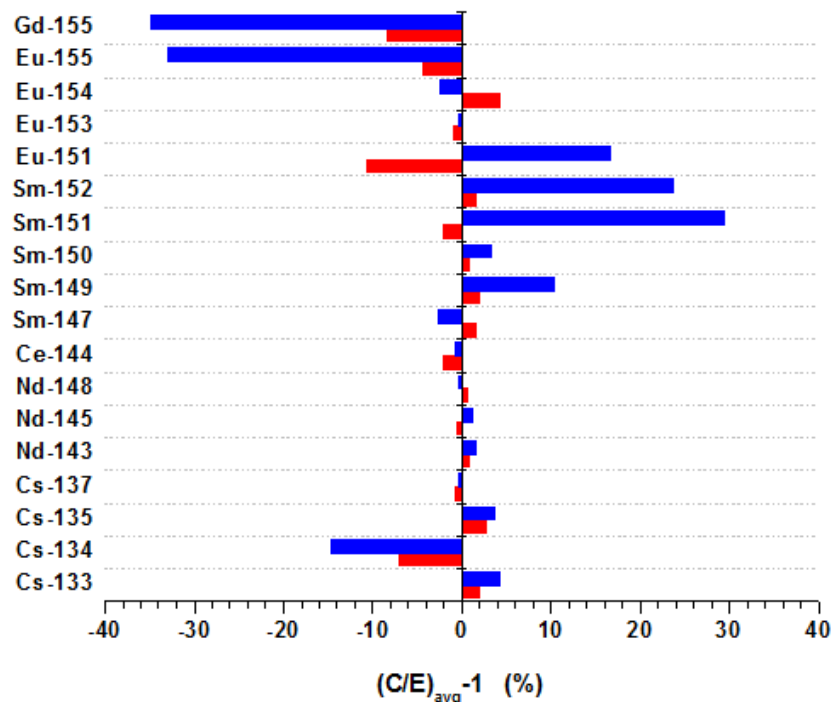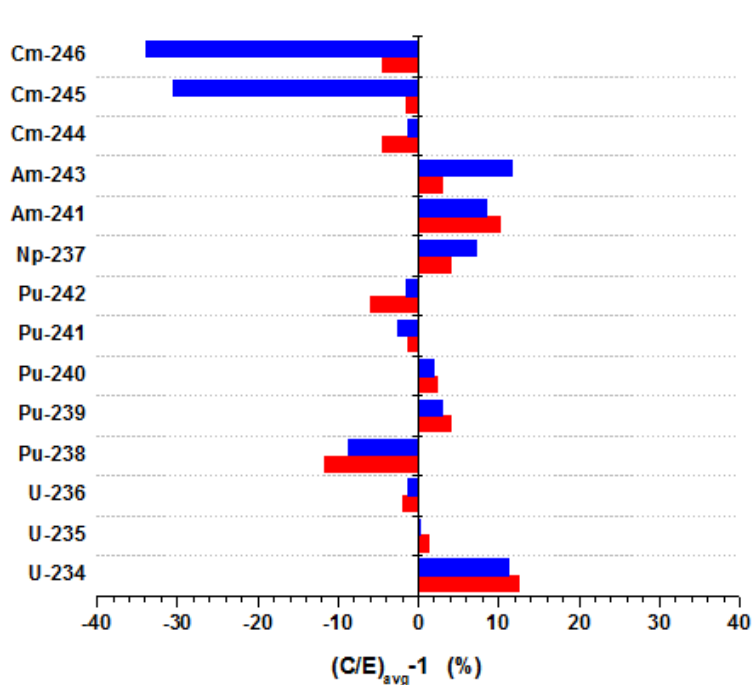
Errors in gamma spectrum for HEU decay

Errors identified in ENDF/B-VII.0 actinide decay data

- ^{234}Th beta decay daughter incorrectly assigned as ground state ^{234}Pa instead of isomer ^{234m}Pa

- Further review of data in ENDF/B-VI, -VII.0, and recently released –VII.1 identified other widespread problems in actinide data
  - Systematic errors in decay energy release values (γ, β, α)
  - ^{240}U beta decay daughter also incorrectly assigned
  - ^{207}Bi decay mode incorrect
  - ^{238}U spontaneous fission fraction x100 too large
  - ^{215}Po beta branch missing
  - ^{234}Th beta branch missing (100% to isomeric level missing)
  - ^{240}Cm has spontaneous fission (does not exist)
  - ^{254}Es decay scheme incorrect

- Similar problems identified in the fission product decay data

Implementation of ENDF/B-VII.1 decay sublibrary

- Updated decay data with ENDF/B-VII.1
  - New decay modes
    - (b-2n), (b-3n), (b-4n) included
  - Removal of nuclides with $T_{1/2}$ < 1 ms
    - ^{115m}Sb, ^{153m}Gd, ^{199m}Au
  - Additional metastable levels in new evaluations
    - ^{72m}Ga, ^{73m}Ge, ^{90m}Zr, ^{90m}Nb, ^{141m}Nd, ^{172m}Lu, ^{177m}Lu, ^{197m}Au, ^{246m}Am, ^{129m}Sb
  - Changes in isotope set required regeneration of ORIGEN fission yield library
  - Also regeneration of the ORIGEN gamma ray library

Implementation of ENDF/B-VII.1 gamma data

- ENDF/B-VII.1 replaced gamma data from NuDat 2

- Gamma spectra following ^{235}U fission compared from 1 s to 30 years after fission

- Most differences attributed to
  - Missing decay modes in NuDat
  - Continuum evaluations in ENDF/B-VII.1 vs lines
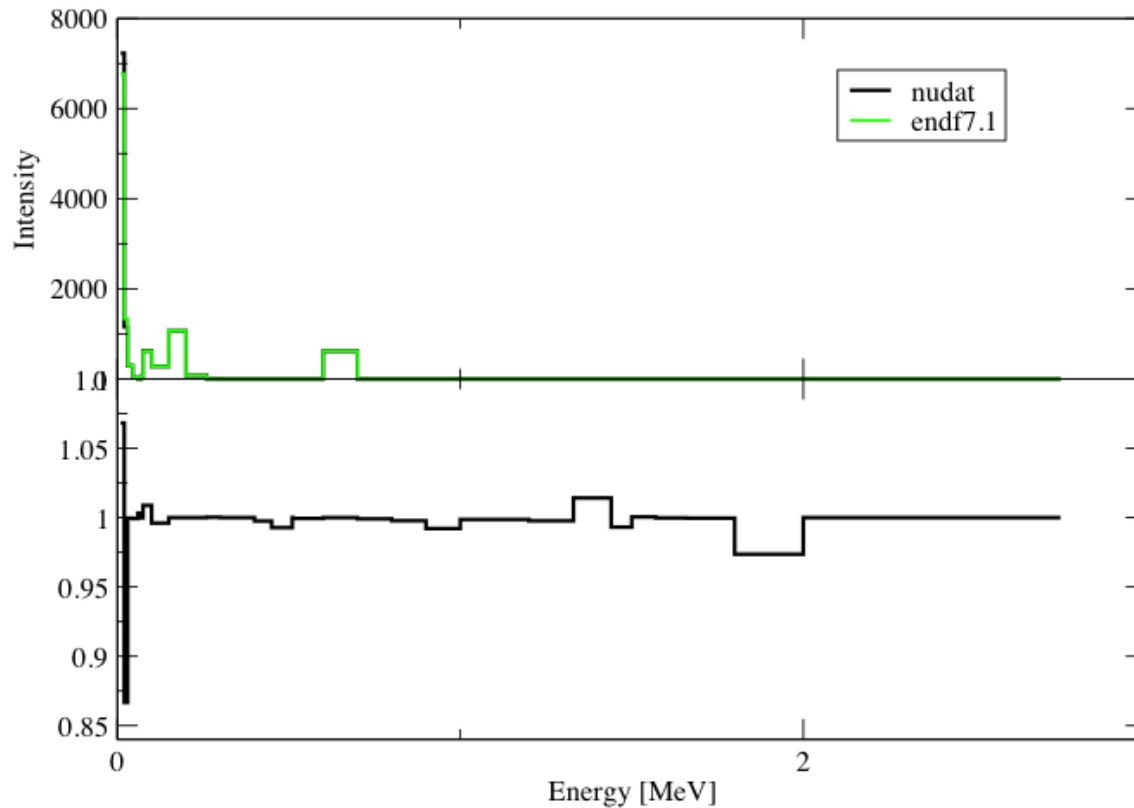 - Changes in evaluation
  - Changes in half lives

γ-spectrum ^{235}U fission – 0.5 seconds
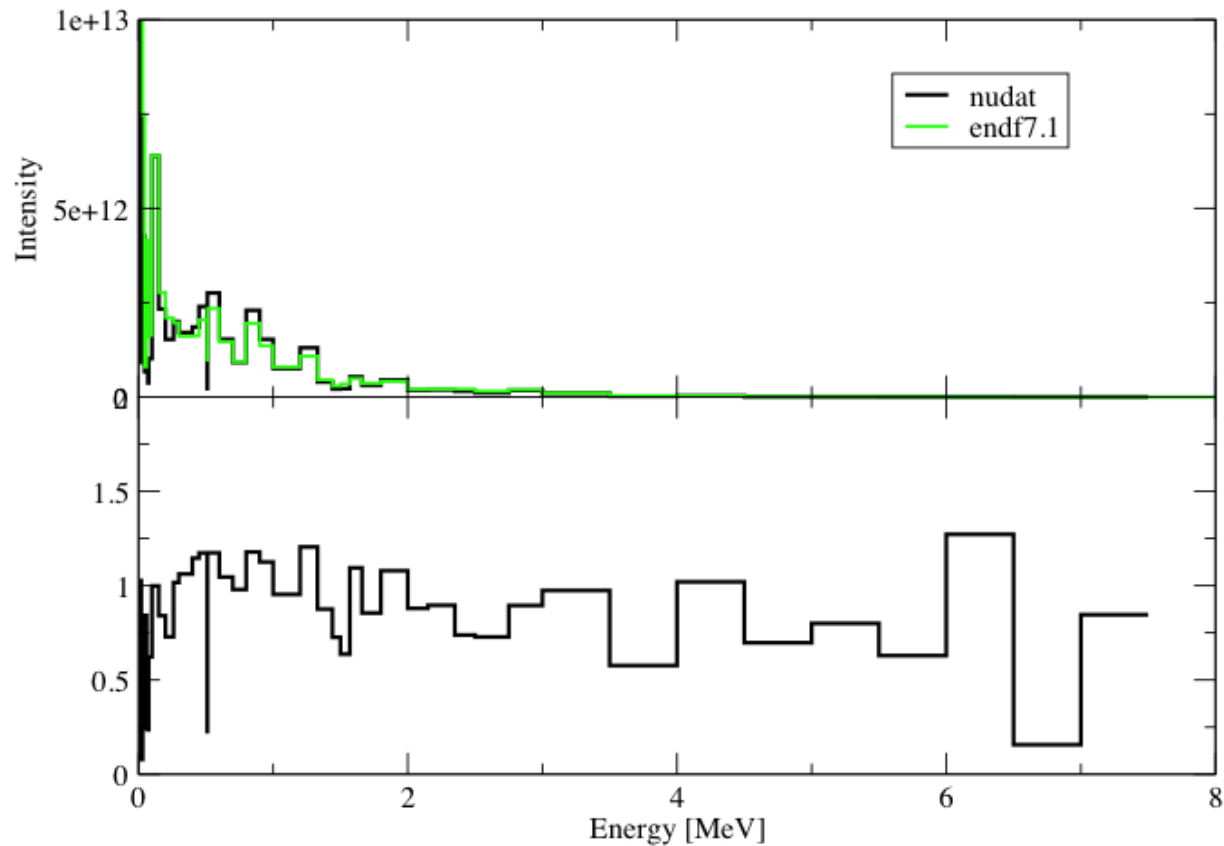
γ-spectrum ^{235}U fission – 1.5×10^4 seconds
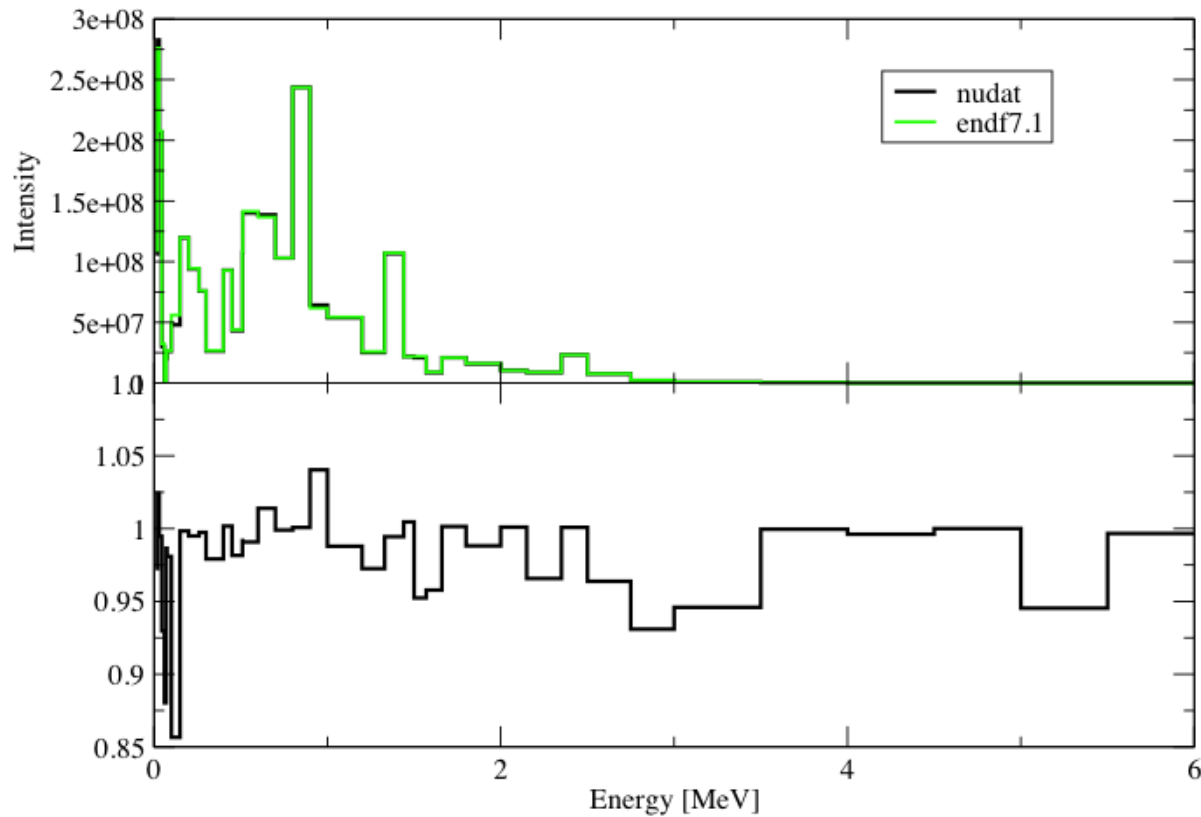
γ-spectrum ^{235}U fission – 2.0 x 10^9 seconds

# ENDF/B-VII benchmark and validation tests
Decay sublibrary

- Actinide decay series

  - Thorium series (4n) – ^{232}Th

  - Neptunium series (4n+1) – ^{237}Np

  - Radium series (4n+2) – ^{238}U

  - Actinium series (4n+3) – ^{235}U

- Energy release following fission (<10^5 s after fission)
  - ^{235}U, ^{238}U (fast), ^{239}Pu, ^{241}Pu, ^{233}U, ^{232}Th (fast)

- Spent fuel assembly calorimeter measurements

- Spent fuel isotopic assay measurements
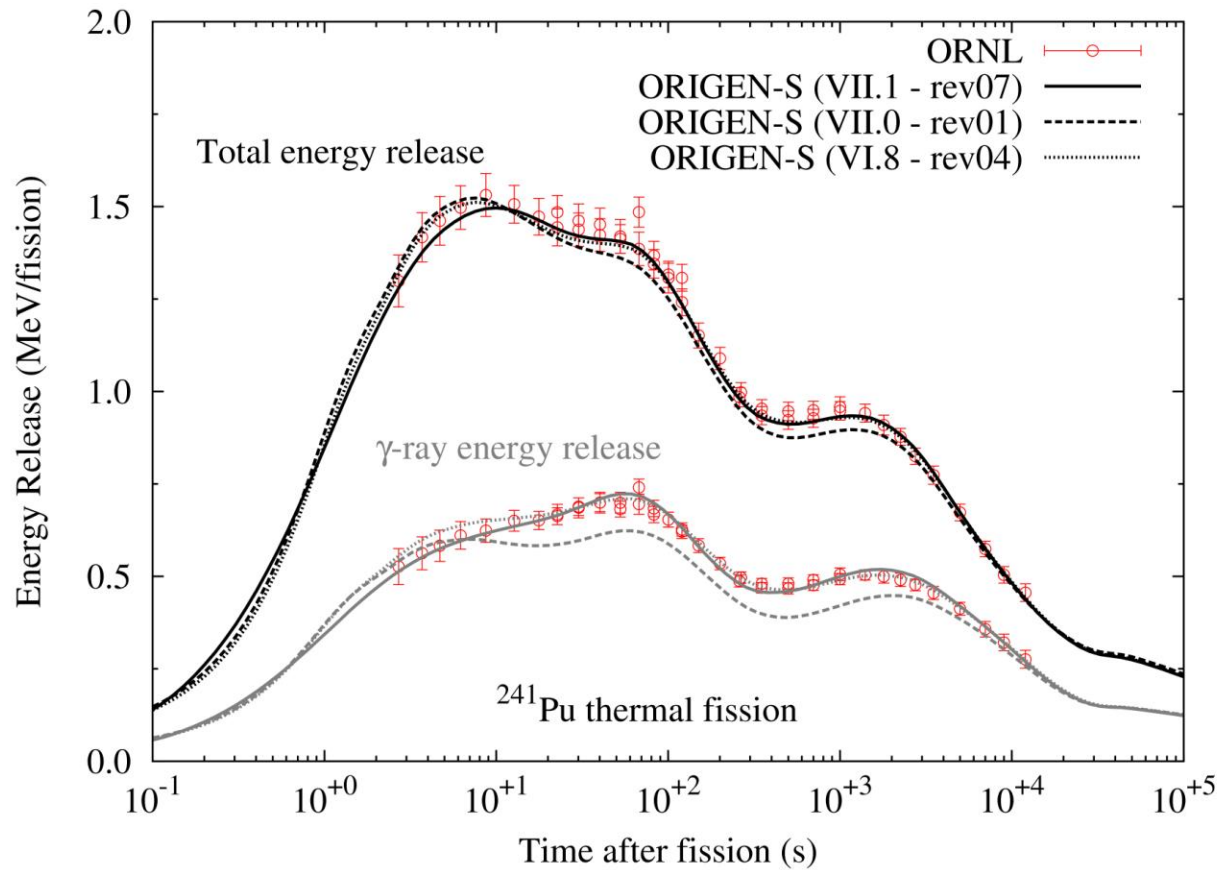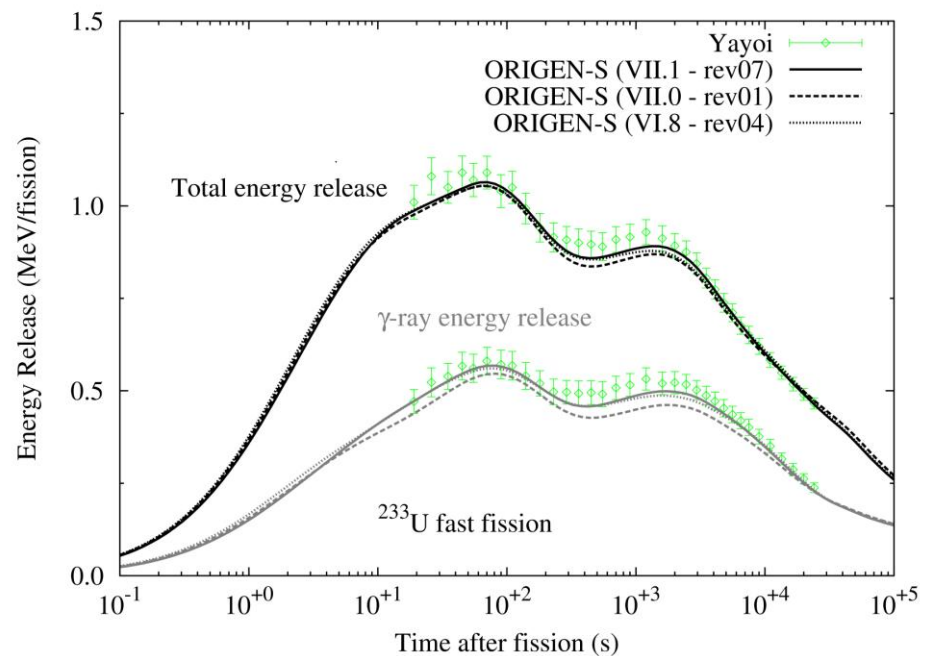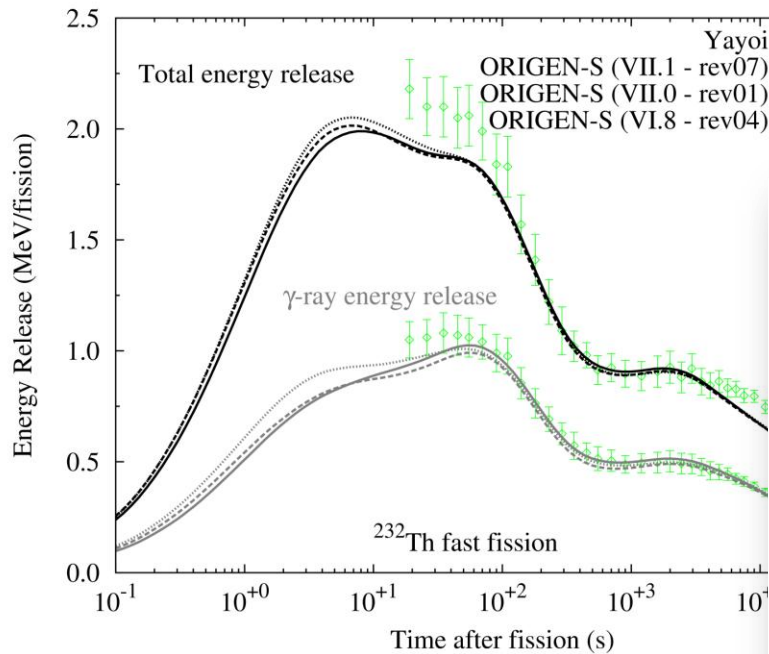
^{235}U fission
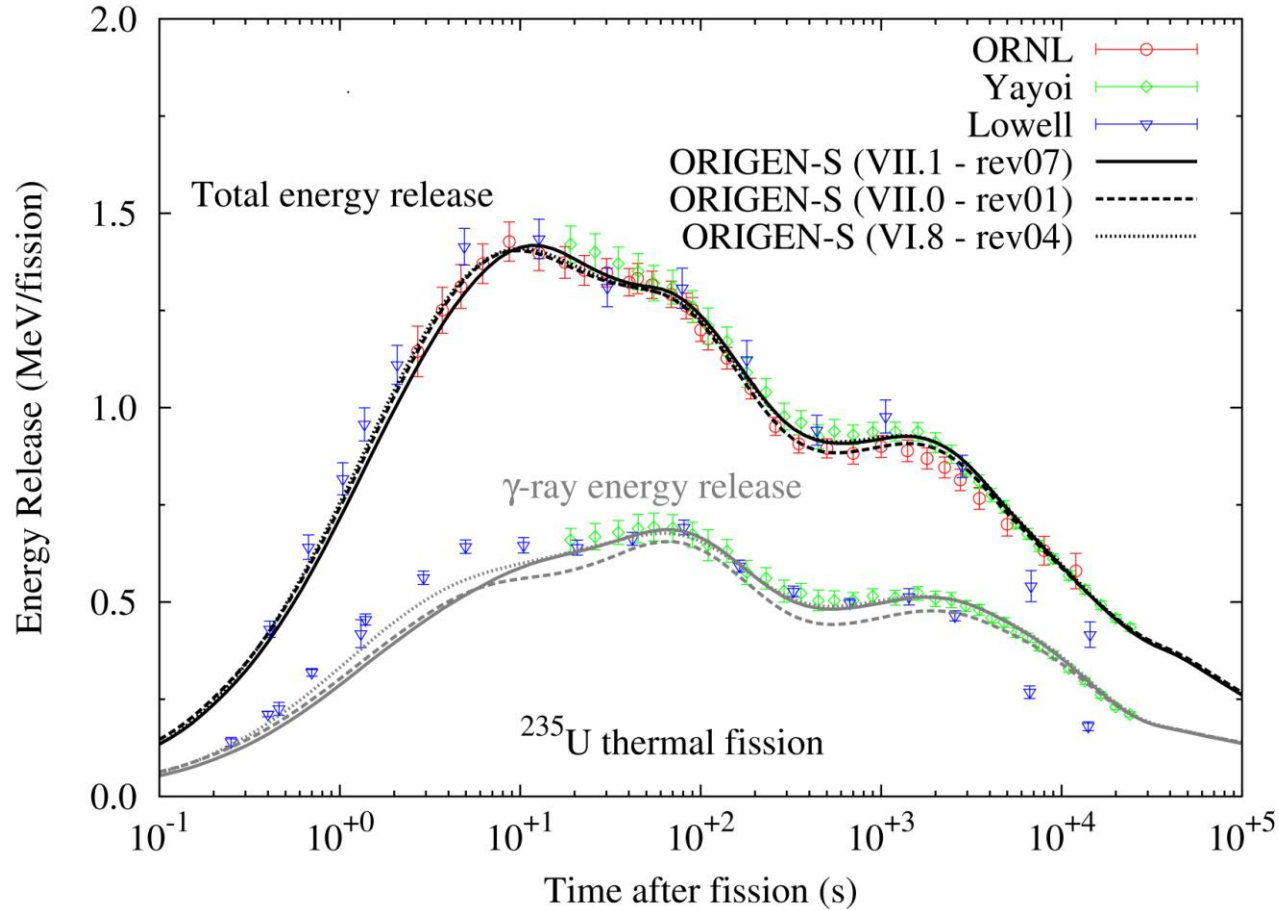
^{238}U fast fission
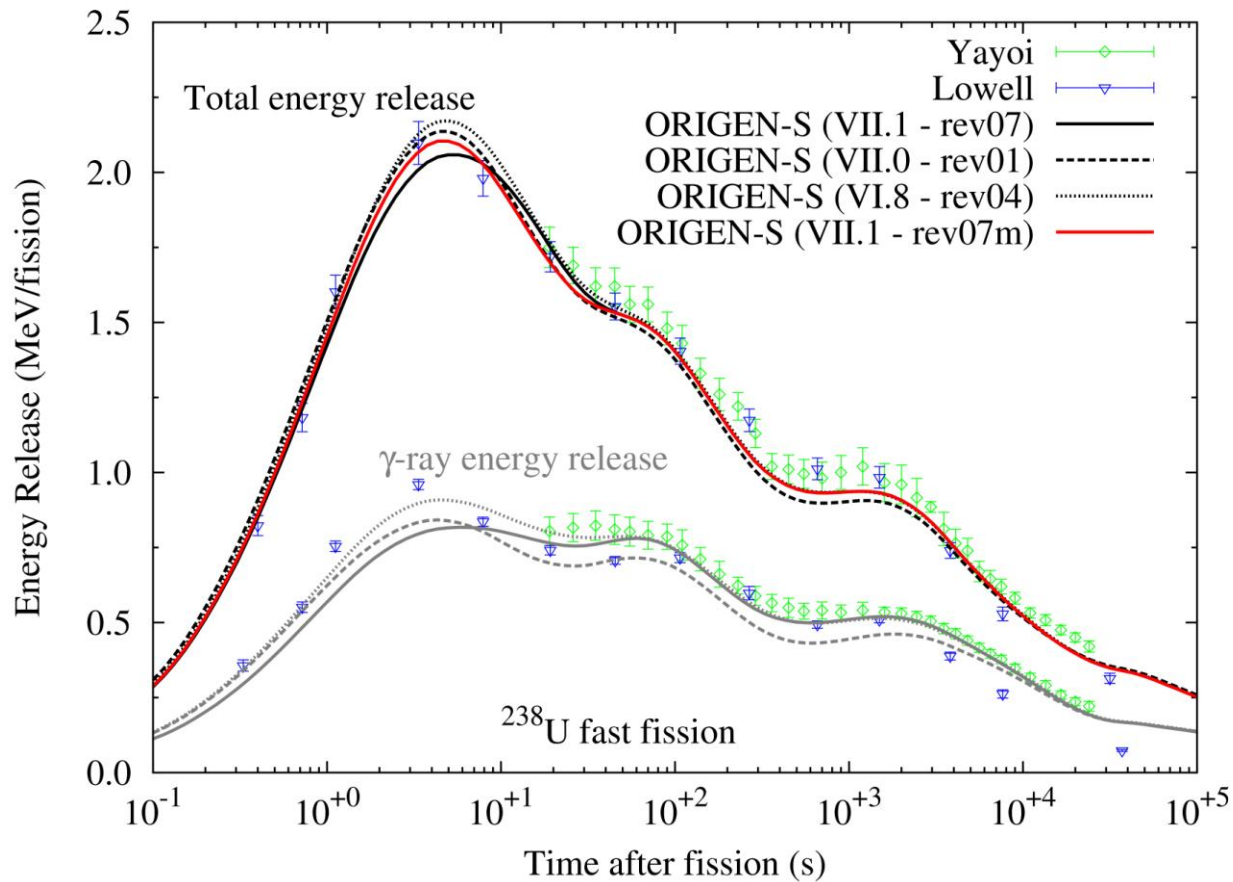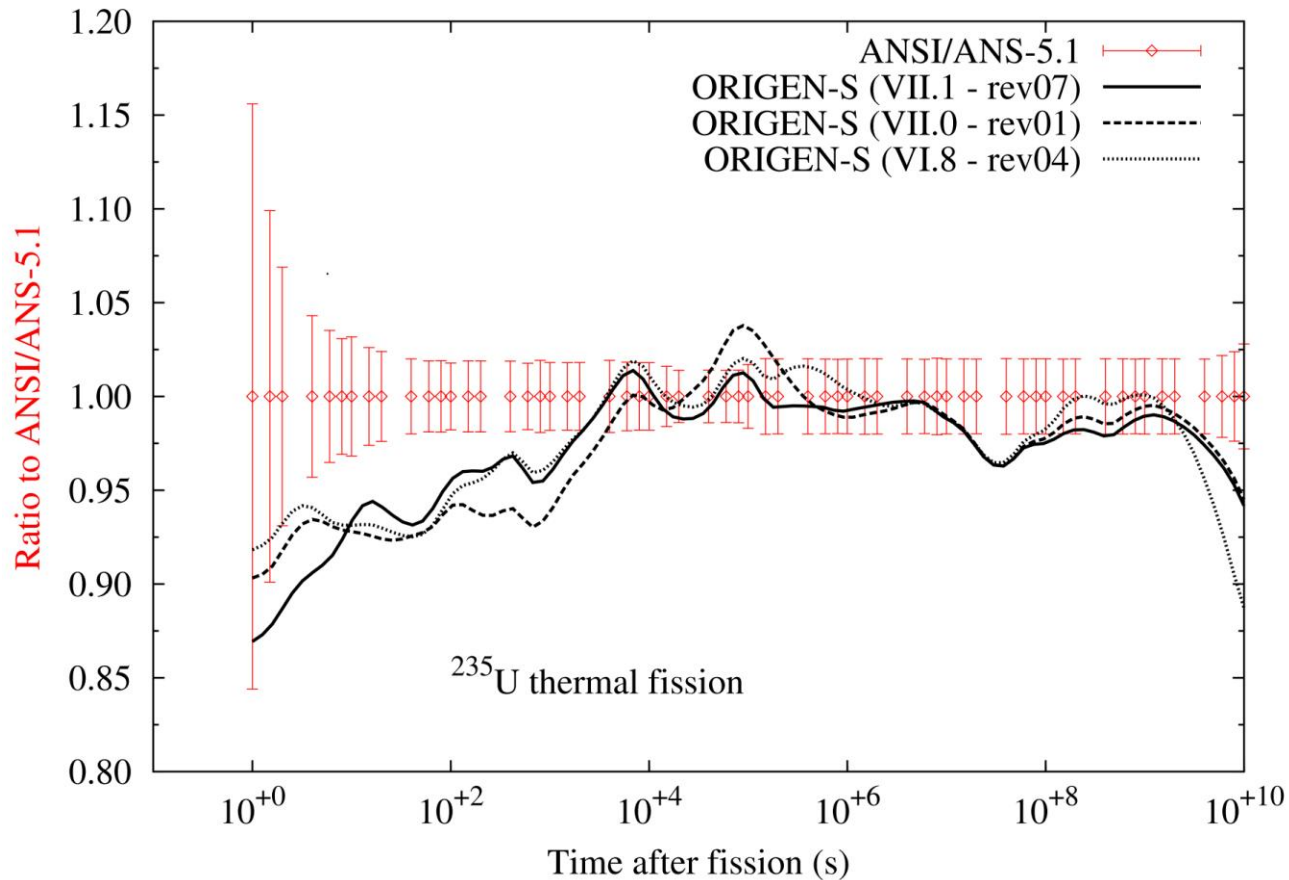
^{239}Pu fission
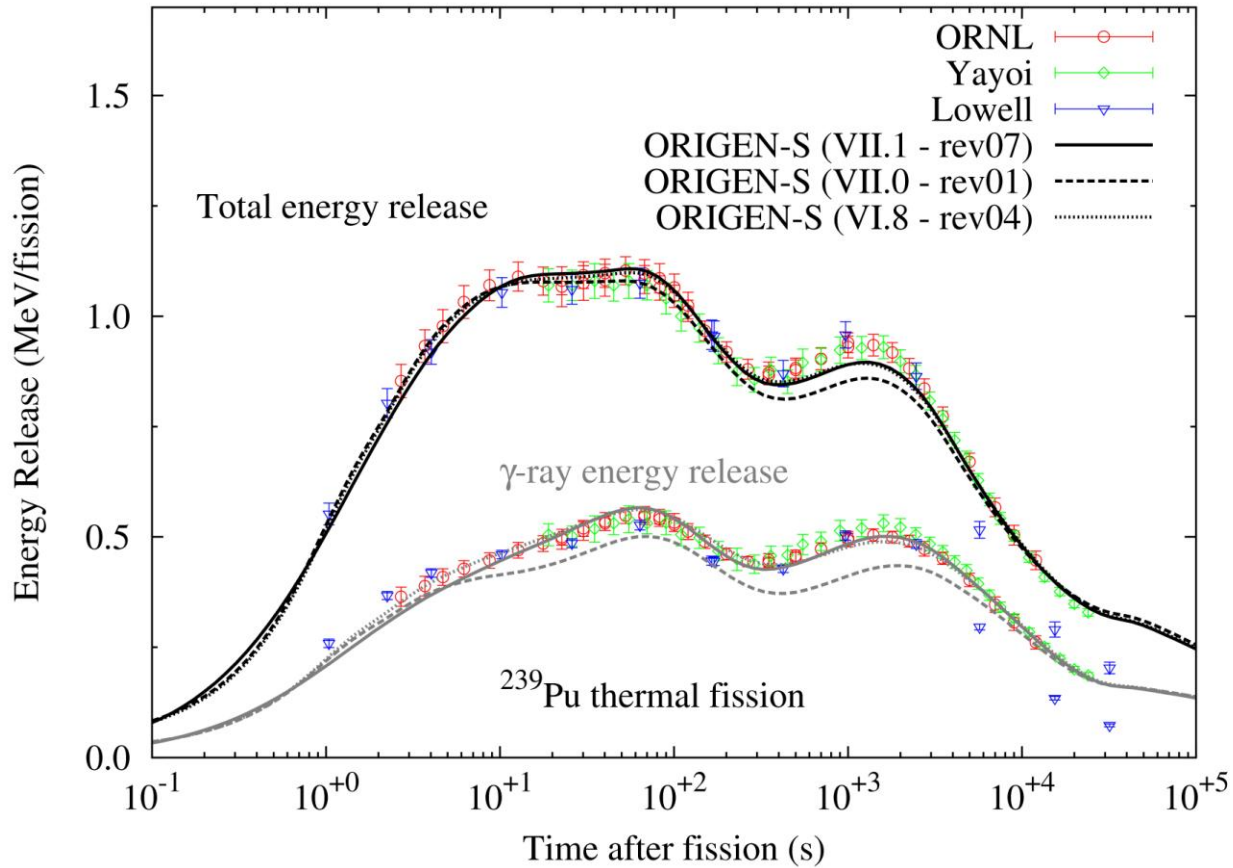
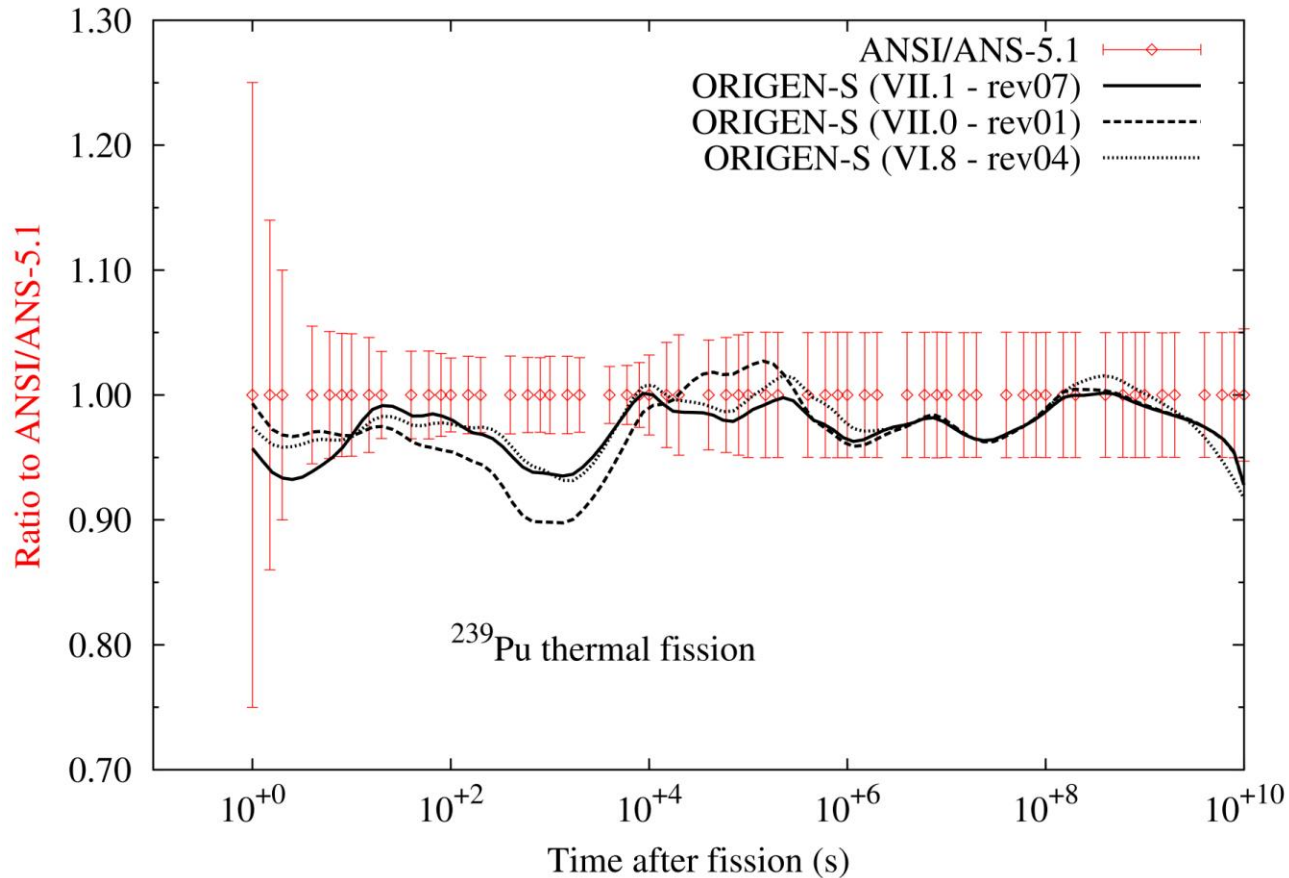# ²⁴¹Pu fission

^{234}Th and ^{233}U fission
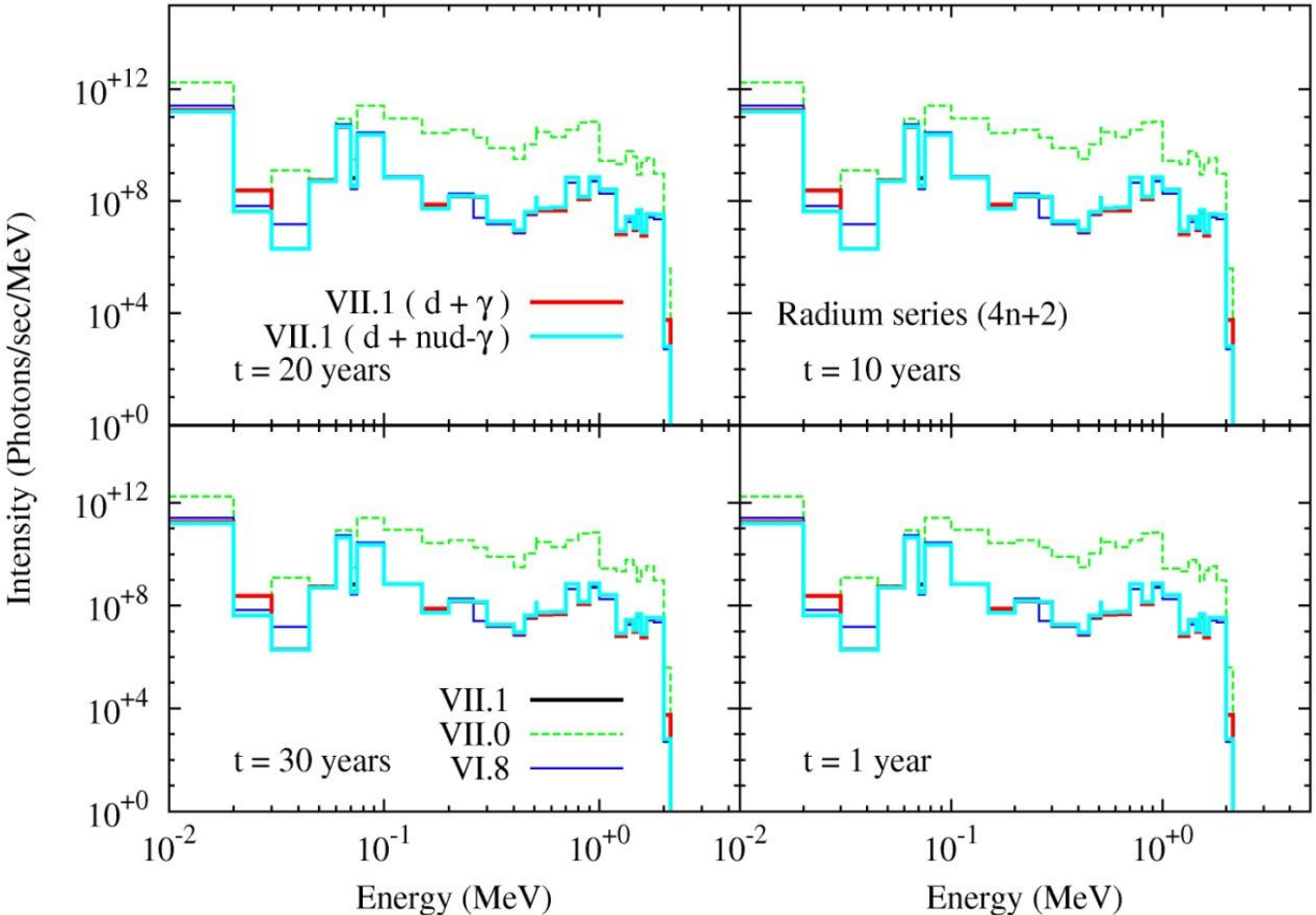
^{235}U fission (comparison with ANSI/ANS-5.1)
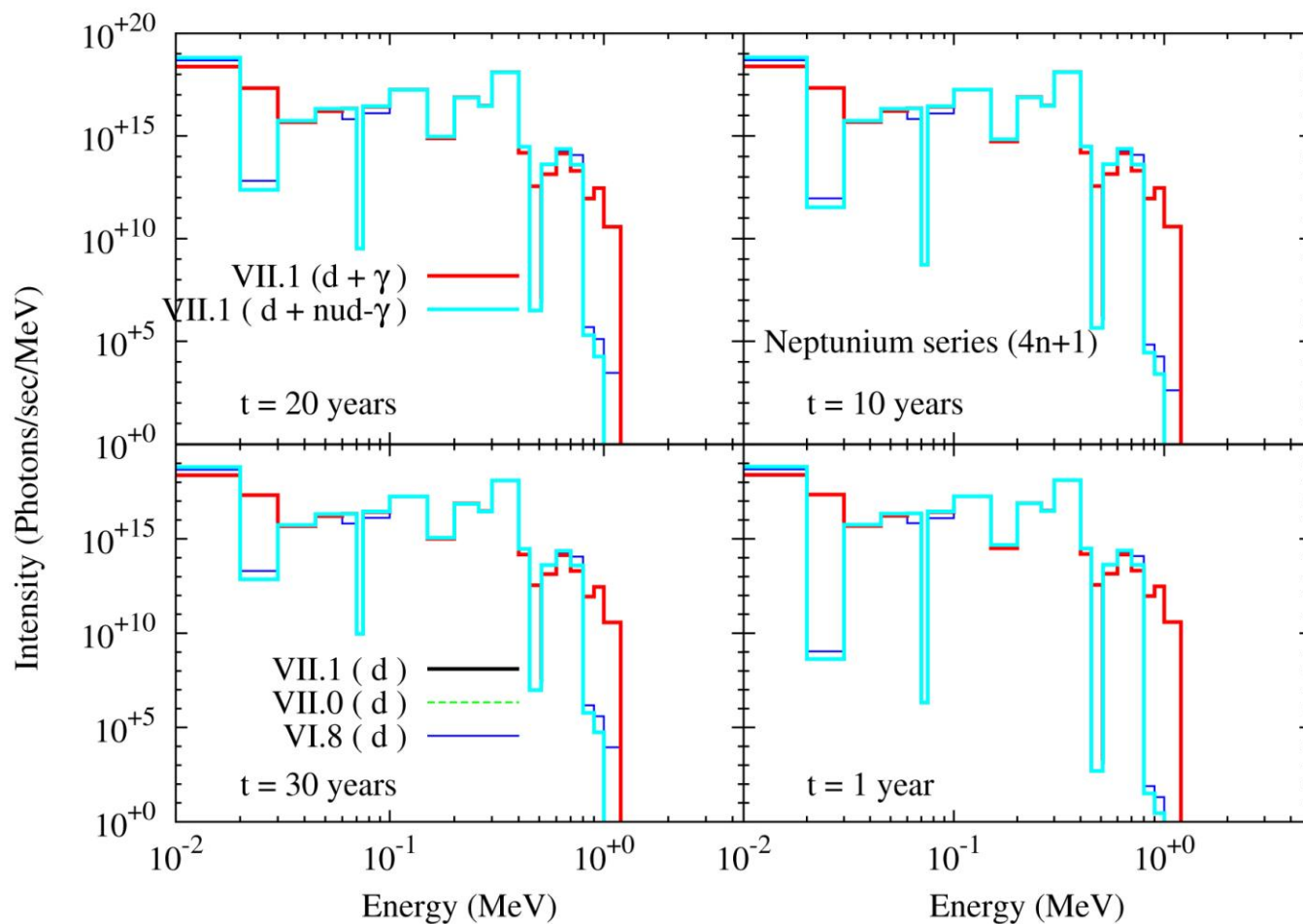
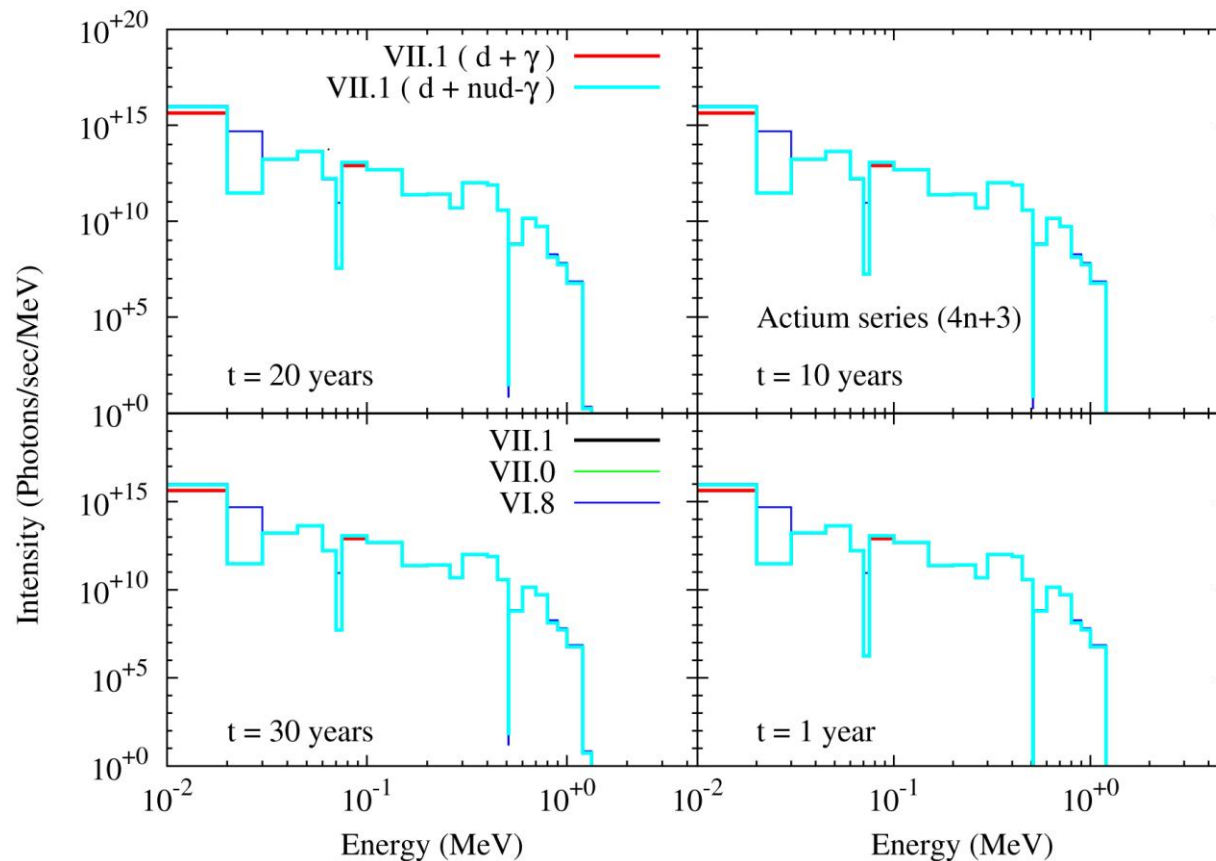# ²³⁹Pu fission (comparison with ANSI/ANS-5.1)
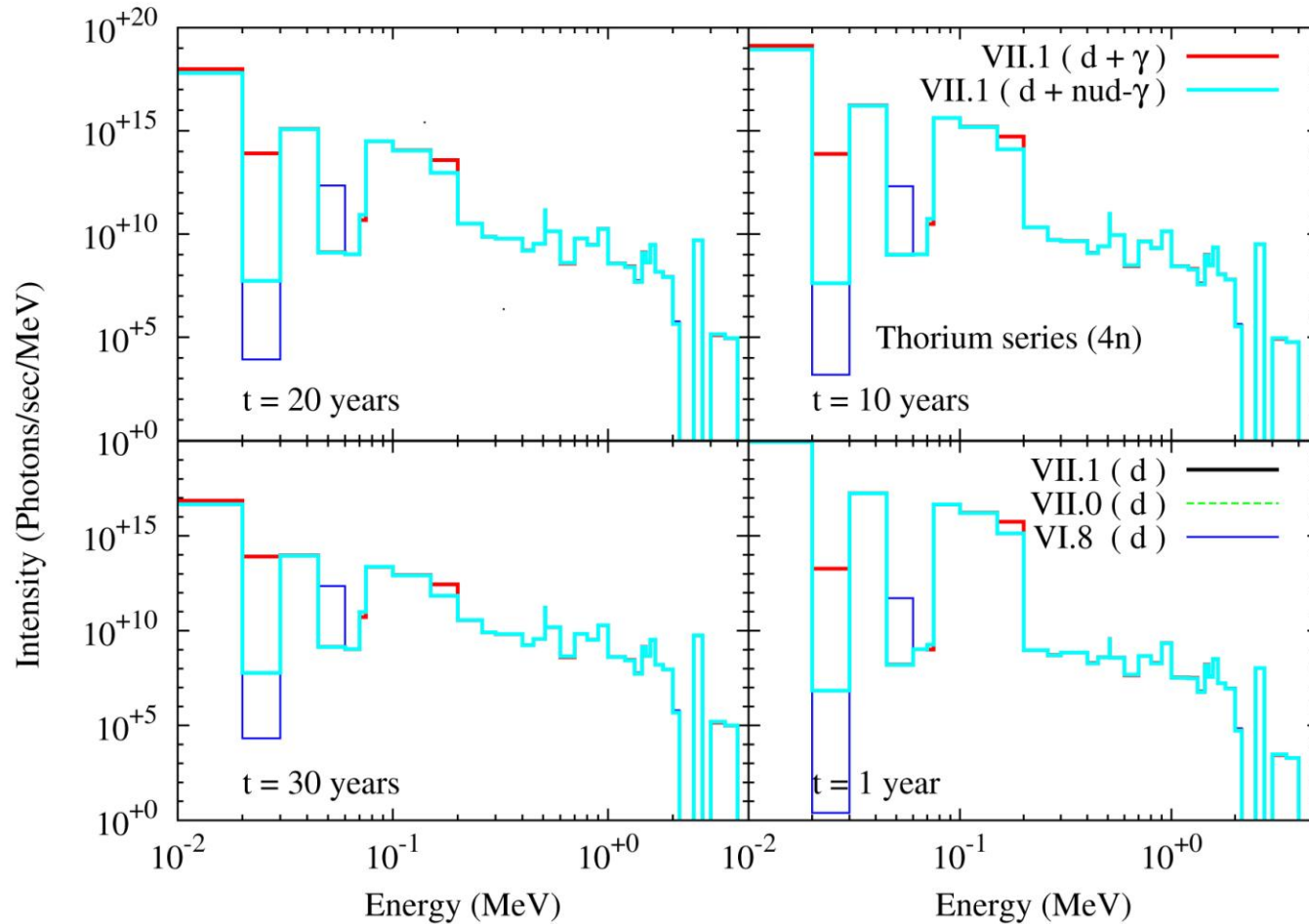
Radium decay series (4n+2)

Neptunium decay series (4n+1)

Actinium decay series (4n+3)

Thorium decay series (4n)

Summary

- Serious errors identified in ENDF/B-VII.0 actinide and fission product decay data – developers not fully aware of the problems (current notice of errors may not be adequate)

- ENDF/B-VII.1 has been fully integrated into ORIGEN

- Experience with ENDF/B-VII.1 decay sublibrary has been very good – decay data and gamma ray data

- Systematic testing of ENDF/B using benchmarks should be extended to include the decay sublibrary – data are widely used and <u>quality is important</u>

- Benchmarks developed by ORNL represent a good starting point for decay sublibrary testing – expand in collaboration with other organizations to cover isotopes important to a broad range of potential applications

Questions?