Decay Data and Processing in GNDS

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Nov 6, 2024

LLNL-PRES-2000758
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

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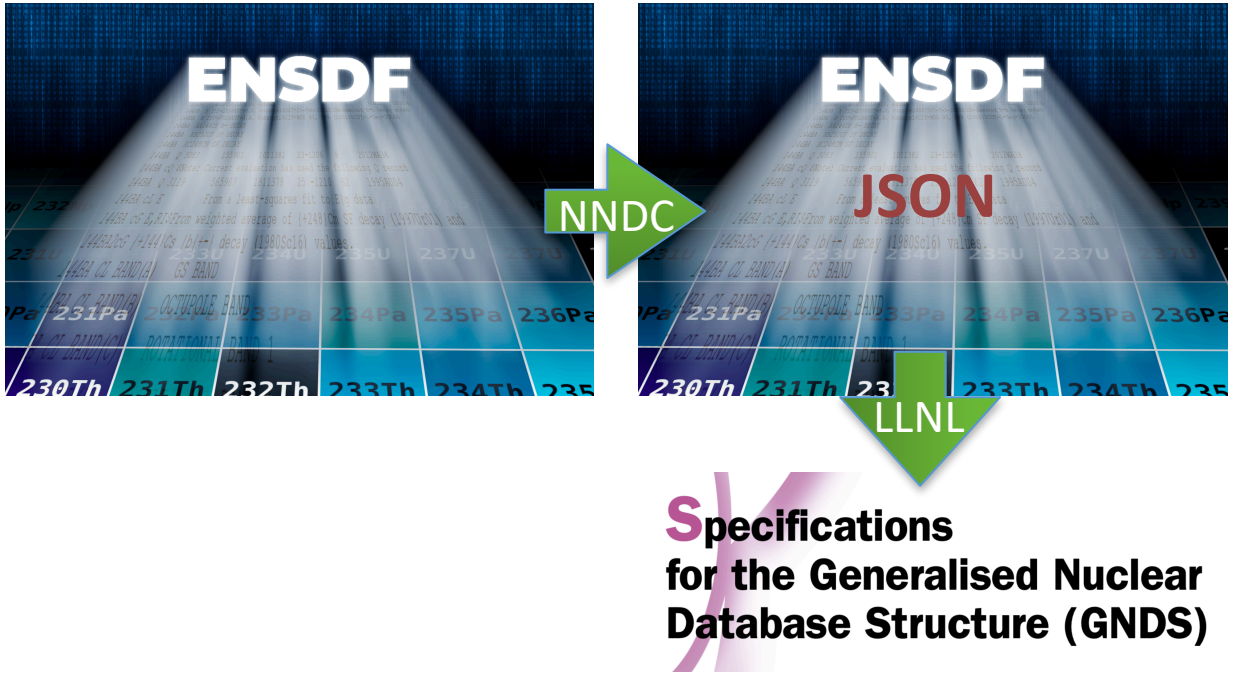
Overview

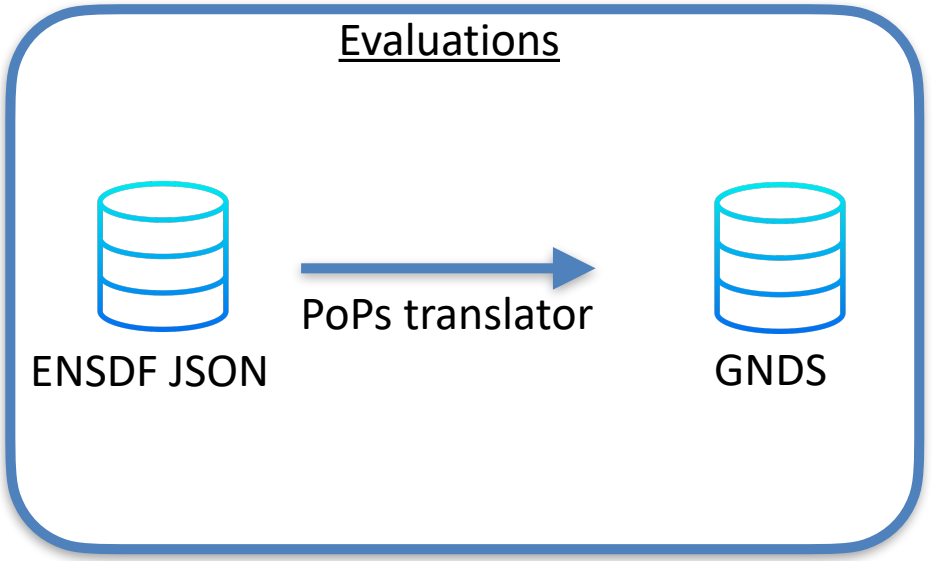
In this talk, I would like to

- Suggest how to store decay data while preserving cascade information
- Introduce the GNDS specification changes proposed on NEA GitLab server
- Introduce processing capabilities coming in FUDGE



We translate data from ENSDF JSON data to GNDS to see what needs to be revised in GNDS

- We focused on the decay and adopted level data that are translated into ENSDF JSON by the modernization project
- We translated the evaluation into the current GNDS format and found a lot of data types are not supported.
- We proposed several changes to the GNDS specifications full data integrity.



Eval to eval translation is necessary for specification revisions

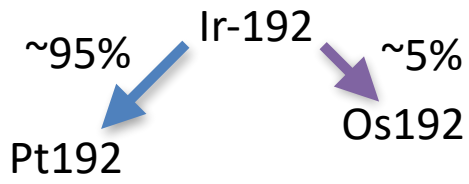
- ENDF Decay Sublibrary is the only complete library for decay data in GNDS specification.
- However, decay data are organized to store the ground state to ground state* transition.
- In this collapsed form, the coincident information is lost.
- ENSDF JSON preserves the cascade information by having tables of levels, gammas, betas, …
- We performed an eval to eval translation to see what is the best form to store the decay data.

ENDF-VIII.1/decay/dec-077_Ir_192.endf.gnds.xml

```
<decayMode label="0" mode="beta-">
  <probability>
    <double label="BR" value="0.9513">
      <uncertainty> …
  <Q> …
  <decayPath>
    <decay index="0">
      <products>
        <product label="e-" pid="e-"/>
        <product label="nu_e-_anti" pid="nu_e-_anti"/>
        <product label="Pt192" pid="Pt192"/></products></decay></decayPath>
  <spectra>
    <spectrum label="gamma" pid="photon"> …
    <spectrum label="beta-" pid="e-"> …
    <spectrum label="discrete electron" pid="e-"> …
    <spectrum label="x-ray" pid="photon"> …
<decayMode label="1" mode="beta+ or e.c.">
```

* or metastable to metastable

A level by level approach may be easiest to understand




```
<decayData>
  <decayModes>
    <decayMode label="0" mode="beta-">
      <probability>
        <double label="BR" value="0.479809596">
          <uncertainty> …
      <decayPath>
        <decay index="0">
          <products>
            <product label="e-" pid="e-"/>
            <product label="nu_e-_anti" pid="nu_e-_anti"/>
            <product label="pt192_e3" pid="pt192_e3"/></products></decay></decayPath>
      <spectra> …
    <decayMode label="1" mode="beta-">
      <probability>
        <double label="BR" value="0.414208284">
          <uncertainty> …
      <decayPath>
        <decay index="0">
          <products>
            <product label="e-" pid="e-"/>
            <product label="nu_e-_anti" pid="nu_e-_anti"/>
            <product label="pt192_e4" pid="pt192_e4"/></products></decay></decayPath>
      <spectra> …
    <decayMode label="2" mode="beta-">
      <probability>
        <double label="BR" value="0.05600112">
          <uncertainty> …
      <decayPath> …
      <spectra> …
    <decayMode label="3" mode="beta-"> …
    <decayMode label="4" mode="beta-"> …
    <decayMode label="5" mode="beta-"> …
```

```
<decayMode label="6" mode="beta+ or e.c.">
  <probability>
    <double label="BR" value="6.699998928e-3">
      <uncertainty> …
  <decayPath>
    <decay index="0">
      <products>
        <product label="nu_e-" pid="nu_e-"/>
        <product label="os192_e3" pid="os192_e3"/></products></decay></decayPath>
  <spectra> …
<decayMode label="7" mode="beta+ or e.c.">
  <probability>
    <double label="BR" value="0.039299993712">
      <uncertainty> …
  <decayPath>
    <decay index="0">
      <products>
        <product label="nu_e-" pid="nu_e-"/>
        <product label="os192_e4" pid="os192_e4"/></products></decay></decayPath>
  <spectra> …
<decayMode label="8" mode="beta+ or e.c.">
  <probability>
    <double label="BR" value="9.399998496e-4">
      <uncertainty> …
  <decayPath>
    <decay index="0">
      <products>
        <product label="nu_e-" pid="nu_e-"/>
        <product label="os192_e5" pid="os192_e5"/></products></decay></decayPath>
  <spectra> …
```

Gamma de-excitation can be tracked using the label of the decay daughter

Decay data of Ir192

```
<decayMode label="6" mode="beta+ or e.c.">
  <probability>
    <double label="BR" value="6.699998928e-3">
      <uncertainty>…
  <decayPath>
    <decay index="0">
      <products>
        <product label="nu_e-" pid="nu_e-"/>
        <product label="os192_e3" pid="os192_e3"/></products></decay></decayPath>
```

Decay data of Os192

```
<nuclide id="Os192_e3">
  <nucleus id="os192_e3" index="3">
    <spin>
      <fraction label="eval" value="4" unit="hbar"/></spin>
    <parity>
      <integer label="eval" value="1"/></parity>
    <halflife>…
    <decayData>
      <decayModes>
        <decayMode label="0" mode="IT">
          <probability>
            <double label="BR" value="1.">
              <uncertainty>
                <standard>
                  <double value="5.69476082005e-3"/></standard></uncertainty></double></probability>
          <decayPath>
            <decay index="0">
              <products>
                <product label="gamma" pid="gamma"/>
                <product label="os192_e1" pid="os192_e1"/></products></decay></decayPath>
          <spectra>…
    <energy>
      <double label="eval" value="580.28" unit="keV">
        <uncertainty>
          <standard>
            <double value="8.e-4"/></standard></uncertainty></double></energy></nucleus></nuclide>
```

```
<nuclide id="Os192_e1">
  <nucleus id="os192_e1" index="1">
    <spin>
      <fraction label="eval" value="2" unit="hbar"/></spin>
    <parity>
      <integer label="eval" value="1"/></parity>
    <halflife>
      <double label="eval" value="288." unit="ps">
        <uncertainty>
          <standard>
            <double value="4."/></standard></uncertainty></double></halflife>
    <decayData>
      <decayModes>
        <decayMode label="0" mode="IT">
          <probability>
            <double label="BR" value="1.">
              <uncertainty>
                <standard>
                  <double value="2.99925018745e-3"/></standard></uncertainty></double></probability>
          <decayPath>
            <decay index="0">
              <products>
                <product label="gamma" pid="gamma"/>
                <product label="os192" pid="os192"/></products></decay></decayPath>
          <spectra>…
    <energy>
      <double label="eval" value="205.79442" unit="keV">
        <uncertainty>
          <standard>
            <double value="9.e-5"/></standard></uncertainty></double></energy></nucleus></nuclide>
```

Changes proposed to decayMode

- Several physical quantities are missing from the specifications as they are not needed in the translation of the ENDF Decay Sublibrary
- However, to perform an eval to eval translation, we need to specify how they should be stored
- We propose to include `hindranceFactor` and `logft` in `decayMode`

Specifications for `decayMode`

Node name: `decayMode`
Attributes: The list of additional allowed attributes is:
- `label` [`XMLName`, **required**] Unique label for this decay mode.
- `mode` [`decayType`, **required**] Type of decay, e.g. 'electroMagnetic', 'beta+', etc.

Child nodes: The list of additional allowed child nodes is:
- `probability`: [**required**, must appear one time] Probability that this decay mode occurs. Probability of all 'decayMode' nodes should sum to 1.0.
- `internalConversionCoefficients`: [optional, when present, must appear one time] Proportional to the probability that the decay proceeds through internal conversion.
- `photonEmissionProbabilities`: [optional, when present, must appear one time] Probability that photons are emitted as part of the decay.
- `Q`: [optional, when present, must appear one time] Decay Q-value.
- NEW `hindranceFactor`: [optional, when present, must appear one time] hindrance factor of the decay mode.
- NEW `logft`: [optional, when present, must appear one time] Log ft value of the decay mode.
- `decayPath`: [optional, when present, must appear one time] Lists specific decay products including excited states where possible.
- `spectra`: [optional, when present, must appear one time] Contains a list of outgoing energy spectra for various types of decay products.

Changes proposed to spectrum

- We propose to store beta spectrum as `continuum` instead of `discrete`
  - Allow storing endpointEnergy or averageEnergy
  - Allow storing an XYs1d as a reconstruction of the beta spectrum
- This can
  - Reflect the three body nature of the decay
  - Facilitate processing after the translation

Specifications for `continuum`

Node name: `continuum`
Attributes: The list of additional allowed attributes is:
NEW
`type` [`UTF8Text`, optional] Type of transition for beta. For example, 'allowed', 'first-forbidden', etc.
Child nodes: The list of additional allowed child nodes is:
NEW `endpointEnergy`: [optional, when present, must appear one time] Emitted particle endpoint energy.
NEW `averageEnergy`: [optional, when present, must appear one time] Emitted particle average energy.
`XYs1d`: [optional, when present, must appear one time] Continuum energy spec--trum stored as a 1-dimensional function.

XML Example(s) of `continuum`

```
<continuum
        type="...">
    <endpointEnergy>...</endpointEnergy>
    <averageEnergy>...</averageEnergy>
    <XYs1d>...</XYs1d></continuum>
```

Proposed changes to integer and fraction

- ENSDF spinParity assignments can be tentative.
- A spin is stored as `fraction` and a parity is stored as `integer`
- We propose `spin` and `parity` nodes to allow and encourage future evaluations to make use of a new quantity named "`confidence`"

```
"spinParity": {
    "values": [
        {
            "twoTimesSpin": 3,
            "isTentativeSpin": true,
            "parity": "+",
            "isTentativeParity": true
        },
        {
            "twoTimesSpin": 5,
            "isTentativeSpin": true,
            "parity": "+",
            "isTentativeParity": true
        }
    ]
},
```

ENSDF JSON

```
<fraction
        label="..."
        unit="..."
        value="..."
        confidence="...">
</fraction>
```

```
<integer
        label="..."
        unit="..."
        value="..."
        confidence="...">
</integer>
```

GNDS

We develop processing capabilities in FUDGE

- We aim to provide information such as
  - Q values
  - Beta Spectra
  - Coincident information for gamma rays
- These are derived from the evaluations.

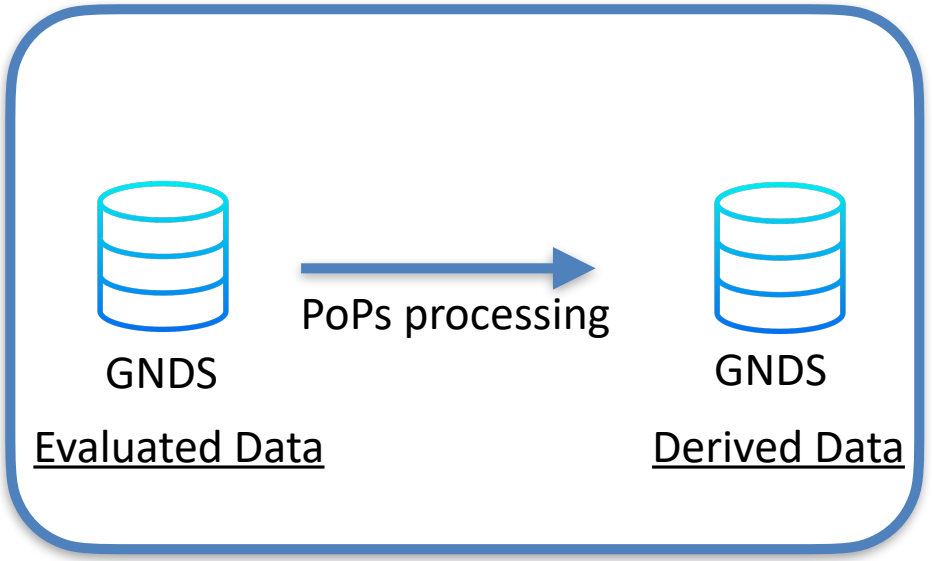


Illustration: 137Cs -> 137Ba ground state to 2nd excited state transition

- We are developing processing codes that can insert an XYs1d into the continuum node
- These derived data will be stored in under a different style.

```
<styles>
<evaluated> … </evaluated>
<betaSpectrumReconstructed, label="betaSpectrumReconstructed"
, derivedFrom="eval"> … </betaSpectrumReconstructed>
```

```
<XYs1d label="betaSpectrumReconstructed">
…
… </XYs1d>
```

```
<spectra>
    <spectrum label="ba137_e2" pid="ba137_e2">
        <discrete>
            <energy value="661.659" unit="keV">
                <uncertainty>
                    <standard>
                        <double value="0.003"/>
                    </standard>
                </uncertainty>
            </energy>
        </discrete>
    </spectrum>
    <spectrum label="beta-" pid="e-">
        <continuum type="first-forbidden-unique">
            <intensity value="94.7">
                <uncertainty>
                    <standard>
                        <double value="0.2"/>
                    </standard>
                </uncertainty>
            </intensity>
            <averageEnergy label="eval" value="174.32" unit="keV">
                <uncertainty>
                    <standard>
                        <double value="0.06"/>
                    </standard>
                </uncertainty>
            </averageEnergy>
        </continuum>
    </spectrum>
```

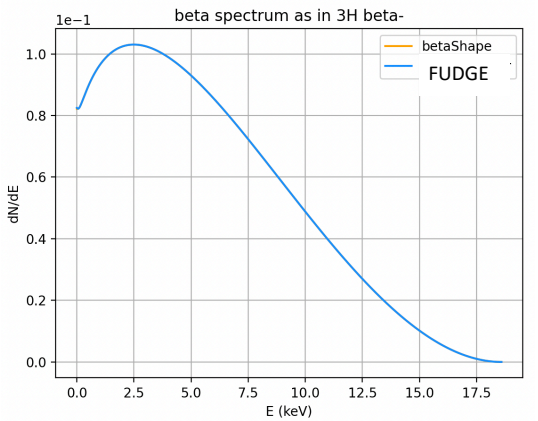
Simple processing capability to provide reasonable spectra

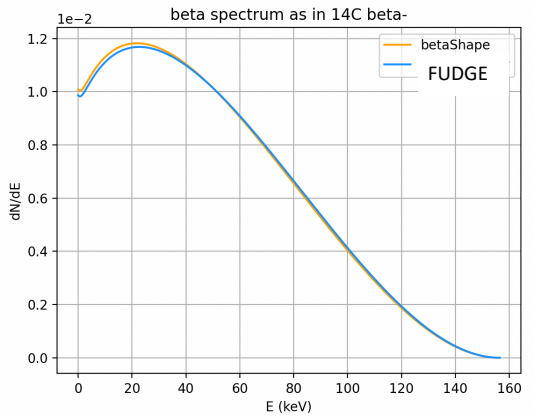
$$\frac{dN}{dW} \propto pWq^2 F(Z,W)C(W)S(Z,W)R(Z,W)$$

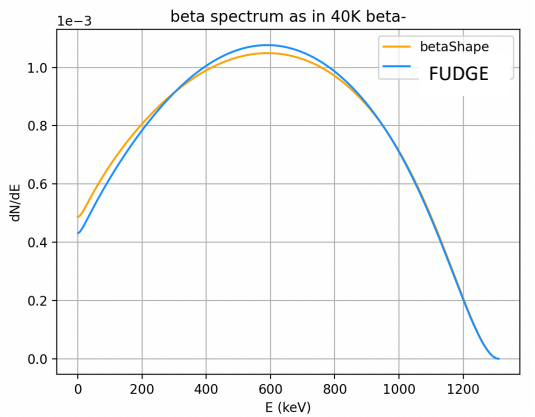
Fermi Shape Screening Radiative

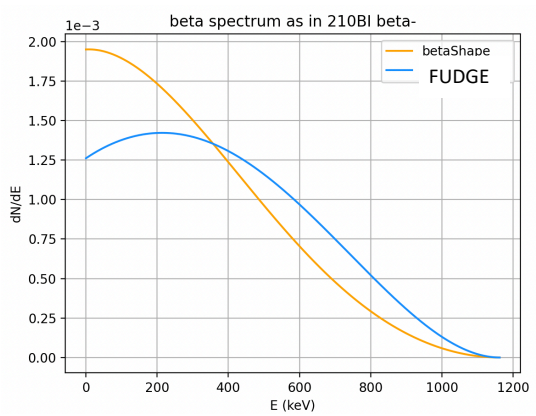
Implemented

Not Implemented









averageEnergy
FUDGE: 5.6959 keV
betaShape: 5.6955 keV
ENSDF: 5.6817 keV

averageEnergy
FUDGE: 49.39 keV
betaShape: 48.92 keV
ENSDF: 49.47 keV

averageEnergy
FUDGE: 588.33 keV
betaShape: 583.98 keV
ENSDF: 560.18 keV

averageEnergy
My calculation: 390.6 keV
betaShape: 317.6 keV
ENSDF: 389.0 keV

Current Status and Future Developments

- We translate the ENSDF JSON decay and adopted levels records to modify the GNDS specifications to pressure data integrity
- Several revisions to the GNDS specifications presented
- We are developing processing capabilities in FUDGE
- We look for opportunity to perform the highly non-trivial ENSDF to ENDF Decay Sublibrary processing within GNDS

Acknowledgements

- We thank the NNDC for sharing their pre-release ENSDF JSON files with us.
- Their data sheets can be downloaded here

  https://www.nndc.bnl.gov/ensdf-json/

- And be visualized here

  https://www.nndc.bnl.gov/ensdfschema/

- VC is supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics (Nuclear Data) and the United States Nuclear Data Program.