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Title: Example on Going from SG-50 Layer 0 to Layer 3

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Example on Going from SG-50 Layer 0 to Layer 3

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I want to take you on a "hike" from layer 0 to layer 3.

Layer 0

Same data as in EXFOR entry translated into WPEC SG-50 format

Layer 1

Added information that is in literature but not in EXFOR

Layer 2

- Objective corrections – new monitors
- Highlighting missing uncertainties with template
- Outlier identified

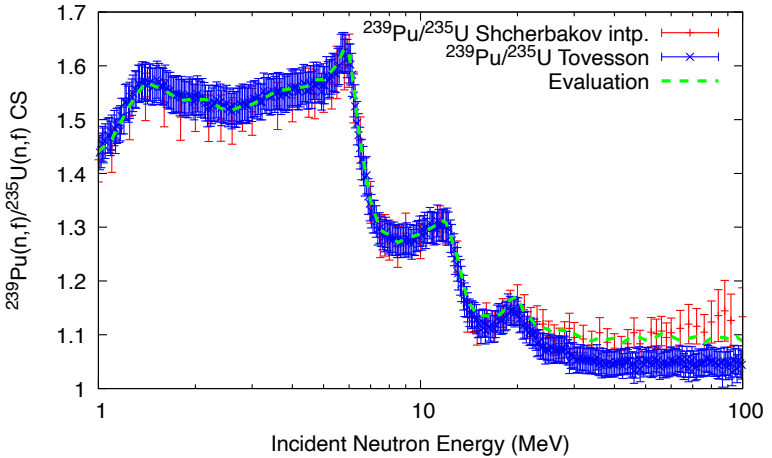
Layer 3

- Subjective corrections
- Expert judgment from evaluators
- Added uncertainties with template

I hope that makes discussions on all layers easier today.

I take ^{239}Pu/^{235}U(n,f) cross sections by Tovesson that were already highlighted as questionable by Standards.

- Tovesson et al. and Shcherbakov et al. data raised questions in the Neutron Standards evaluation -> Standards rejected Tovesson data above 13 MeV -> nice example for layer 3.
- Also some information was lost from literature when translated into EXFOR format -> nice example for layer 1.
- This is neither a criticism of experimentalists nor compilers! Both have a hard job.



Layer 0: translation from EXFOR format into layer 0.

- I started from the WPEC SG-50 requirement document and a first json file by Amanda for her observables.
- High-level comments:
  - We need a **formalized nomenclature for specific corrections to guarantee easier interpretation and allowing easier comparison between data sets**,
  - **We need a list of what features need to be saved for a particular data-type and grey the rest out**, -> otherwise you get lost in all these details.
  - We need a list of uncertainty sources and corrections expected for a specific measurement type.
  - We need well-defined containers for any values.

Layer 0: Suggestion for containers for various values.

```
▼ incident energy:
    type:                "pointwise"
  ▶ Values:              […]
    unit:                "eV"
    Uncertainty:         "unknown"
    Uncertainty unit:    "N/A"

▼ fligth path:
    Value:               10.5
    Unit:                "m"
    Uncertainty:         "unknown"
    Uncertainty unit:    "N/A"
```

Stores whether energy values are points or bin end points.

Stores uncertainty information. Do we need additional descriptors? (2nd energy group, time spread due to gamma-flash)?

Layer 0: Suggestion for correction containers.

```
corrections:
  cor1:
    correction type:                "Background"
    corrected:                      "yes"
    components included:            "All"
    correction method::             "unknown"
    code used:                      "N/A"
    energy dependent:               "yes"
    reference data:                 "N/A"
    description:                    "Systematic uncertainty for background correction  of 235U"
    values:                         "unknown"
    Unit:                           "N/A"
    Uncertainty:                    […]
    Uncertainty unit:               "%"
```

Add to requirement doc!
Need formalized nomenclature for various corrections/ unc.

Allows to store both constant and energy-dependent unc.

Correction values.

Stores unc. values of corrections.

Layer 0: Storing multiple corrections/ samples/ detectors etc. is straightforward in json.

```
corrections:
  cor1:
    correction type:                "Background"
    corrected:                      "yes"
    components included:            "All"
    correction method::             "unknown"
    code used:                      "N/A"
    energy dependent:               "yes"
    reference data:                 "N/A"
  description:                      "Systematic uncertainty for background correction  of 235U"
    values:                         "unknown"
    Unit:                           "N/A"
  Uncertainty:                      […]
    Uncertainty unit:               "%"
  cor2:
    correction type:                "Background"
    corrected:                      "yes"
    components included:            "All"
    correction method::             "unknown"
    code used:                      "N/A"
    energy dependent:               "yes"
    reference data:                 "N/A"
  description:                      "Systematic uncertainty for backgroundncorrection of 239Pu"
    values:                         "unknown"
    Unit:                           "N/A"
  Uncertainty:                      […]
    Uncertainty unit:               "%"
```

Layer 0: Some smaller comments.

- What is the difference between “observable method” and “analysis method”? Both needed?
- Bibliography:
  - how about ”authors” instead of author?
  - Added DOI #.
- Detector: Where should uncertainties go? To detector efficiency values?
- Corrections: Changed “corrected for” -> ”corrected”
- Sample:
  - changed “density methods” -> “sample density methods”
  - Took out “beam fluctuation correction” -> should go to incident flux

Layer 1: added information from literature.

Information that is missing for this data set in EXFOR:

- Uncertainties,
- How corrections were undertaken,
- Correlations between data sets.

This can be crucial information for evaluators!

Conclusion: it is important that we have a capability for evaluators to add information into layer 1 based on original literature that is critical to judge the data set and is not yet in EXFOR. -> **this database must become more interactive and allow for easy inclusion of information into existing databases.**

Layer 1: Examples on missing information in EXFOR. - Uncertainty information.

Layer 0

```
energy resolution values:
    Corrected:                  "unknown"
    Correction:                 "unknown"
    Correction unit:            "N/A"
    Uncertainty:                "unknown"
    Uncertainty unit:           "N/A"
isotopic abundances:
    0:                          "239Pu"
    1:                          "240Pu"
    2:                          "241Pu"
impurity correction:
    Corrected:                  "yes"
  ▼ Correction:
      0:                        15.05
      1:                        0.135
      2:                        0.001
  ▶ Correction unit::           […]
  ▼ Uncertainty:
      0:                        "0.1"
      1:                        "unknown"
      2:                        "unknown"
```

Layer 1

```
energy resolution values:
    Method:                     "Peak of Photofission events"
    Corrected:                  "yes"
    Correction:                 "unknown"
    Correction unit:            "N/A"
    Uncertainty:                "1.6"
    Uncertainty unit:           "ns"
isotopic abundances:
    0:                          "239Pu"
    1:                          "240Pu"
    2:                          "241Pu"
impurity correction:
    Corrected:                  "yes"
  ▼ Correction:
      0:                        15.05
      1:                        0.135
      2:                        0.001
  ▶ Correction unit::           […]
  ▼ Uncertainty:
      0:                        "0.1"
      1:                        "0.012"
      2:                        "0.0001"
```

This is important for uncertainty quantification!

Layer 1: Examples on missing information in EXFOR.
- Information on how corrections were undertaken.

Layer 0

```
cor1:
    correction type:        "Background"
    corrected:              "yes"
    components included:    "All"
    correction method::     "unknown"
    code used:              "N/A"
    energy dependent:       "yes"
    reference data:         "N/A"
  description:              "Systematic uncertainty for background correction  of 235U"
    values:                 "unknown"
    Unit:                   "N/A"
  Uncertainty:              […]
    Uncertainty unit:       "%"
```

Layer 1

```
cor1:
    correction type:        "Background"
    corrected:              "yes"
    components included:    "All"
    correction method::     "Measured (from beam), Fit (frame overlap), PHD (alphas)"
    code used:              "N/A"
    energy dependent:       "yes"
    reference data:         "N/A"
  description:              "Systematic uncertainty for background correction  of 235U"
    values:                 "unknown"
    Unit:                   "N/A"
  Uncertainty:              […]
    Uncertainty unit:       "%"
```

The information is in the journal article (layer 1) but did not make it into EXFOR (layer 0) **but is important to judge the quality of a data set**.

- Should we make recommendations on what should be stored?
- How to define correction method names unambiguously?

Layer 1: Examples on missing information in EXFOR. - Correlations between data sets

Layer 0

```
▼ correlation:
    entry:                  "N/A"
    correlation factor:     "N/A"
    correlation value:      "N/A"
    correlation shape:      "N/A"
```

Layer 1

```
▼ correlation:
  ▼ dataset1:
      entry:                "14271.002"
    ▼ correlation factor:
        0:                  "normalization"
        1:                  "multiple scattering"
        2:                  "background"
        3:                  "Energy"
        4:                  "Impurity"
        5:                  "Deadtime"
    ▶ correlation value:    […]
    ▶ correlation shape:    […]
  ▼ dataset2:
      entry:                "14271.005"
    ▼ correlation factor:
        0:                  "multiple scattering"
        1:                  "background"
        2:                  "Energy"
        3:                  "Deadtime"
    ▶ correlation value:    […]
    ▶ correlation shape:    […]
  ▼ dataset3:
      entry:                "14271.005"
    ▼ correlation factor:
        0:                  "multiple scattering"
        1:                  "background"
        2:                  "Energy"
        3:                  "Deadtime"
    ▶ correlation value:    […]
    ▶ correlation shape:    […]
```

The information is in the journal article (layer 1) but did not make it into EXFOR (layer 0) **but is important to do a correlated uncertainty quantification**. This is very hard to keep track off. How to automate?

Layer 1: Examples on missing information in EXFOR.

Layer 0

```
energy resolution values:
    Corrected:              "unknown"
    Correction:             "unknown"
    Correction unit:        "N/A"
    Uncertainty:            "unknown"
    Uncertainty unit:       "N/A"
```

Layer 1

```
energy resolution values:
    Method:                 "Peak of Photofission events"
    Corrected:              "yes"
    Correction:             "unknown"
    Correction unit:        "N/A"
    Uncertainty:            "1.6"
    Uncertainty unit:       "ns"
```

Comments:

- Who populates layer 1? I think evaluators.
- How do we get information added to layer 1 back to EXFOR efficiently?
- If layer 1 exists for a data set, should we hide layer 0?

Layer 2: objective corrections, highlighting missing corrections, identifying outliers.

Comments, questions:

- Should we add **automatic outlier identification** on top of the database that flags outliers?
- Should we highlight in this layer already what information we deem crucial (but is missing) for a particular datatype? How to best do that?
- How to best **highlight crucial missing uncertainties**?

-> All this information could be very helpful for evaluators.

Layer 2: suggested container for tracking changes.

```
layer2changes:
  change1:
      change:          "renormalized to newest standard"
      Old Library:     "Standard2008"
      New Library:     "Standard2018"
      Comment:         "reference for normalization not clearly stated."
```

- We need unique library identifiers.

Layer 2: suggested container for outlier identification.

```
▼ outlier:
    algorithm:          "Standards"
  ▶ energies:           […]
    unit:               "eV"
```

- We need unique identifiers for algorithm applied.
- What algorithms do we want to use?
- Do we want to compare to theory/ evaluations?
- Should SG-50 automatically apply them?
- Is an identification of the outlying data by energy ok?

Layer 2: example for tracking missing uncertainties.

```
corrections:
  cor1:                    {…}
  cor2:                    {…}
  cor3:
      correction type:     "Multiple Scattering and Attenuation"
      corrected:           "no"
      components included: "N/A"
      correction method::  "N/A"
      code used:           "N/A"
      energy dependent:    "N/A"
      reference data:      "N/A"
      description:         "N/A"
      values:              "unknown"
      Unit:                "N/A"
      Uncertainty:         "unknown"
      Uncertainty unit:    "%"
```

This missing uncertainty source was identified via templates of expected measurement unc.

Layer 2 just lists it as missing.

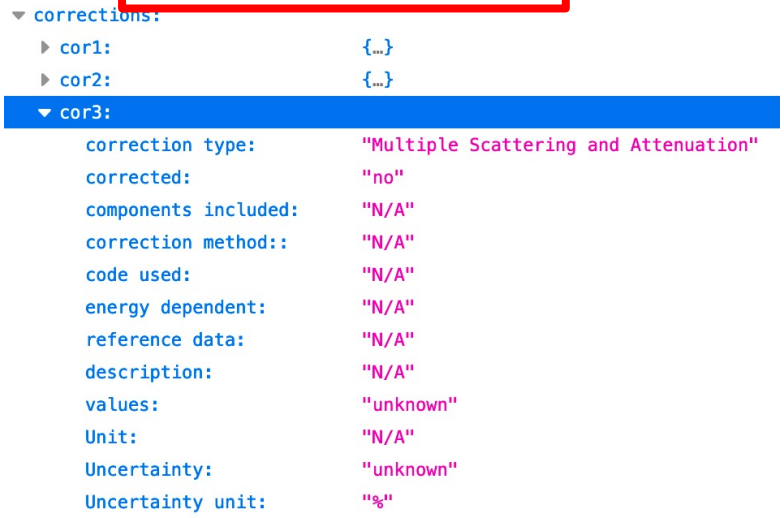
Layer 3 will give stand-in values.

Layer 3: expert judgment, subjective corrections, added uncertainties with templates.

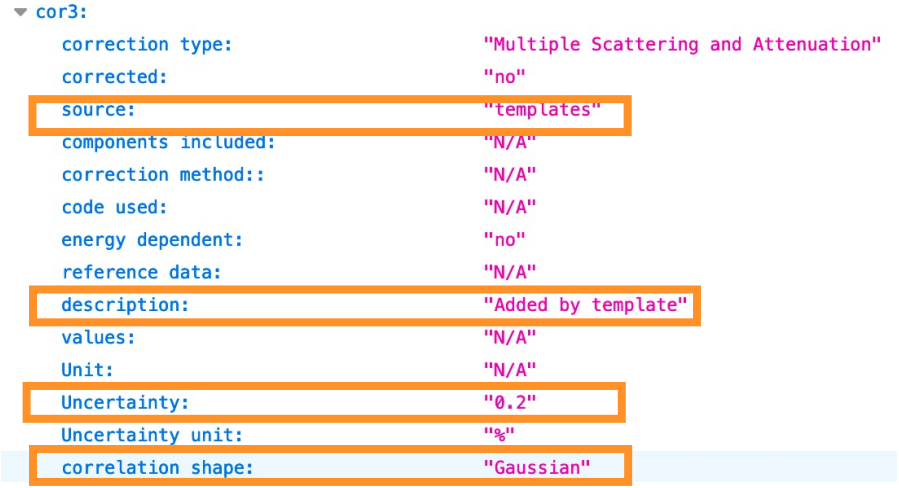
- How to best store expert judgment and subjective corrections? -> If we store the raw data every evaluator used the database will become very big -> how about storing correction factors and cut-offs (in energy or angles) applied by evaluators on top of the original data?
- Do we want to add a capability to estimate total covariances on top of layer? (information incomplete in all previous layers).
- Should we document for which evaluations these data were used?

Layer 3: example on added uncertainties with templates.

Layer 1



Layer 2



Need:

- Source descriptor (template, expert judgement, reference to other EXFOR entry, etc.)
- Correlation shape for complete cov. Estimate.

Layer 3: example on expert judgment and subjective corrections.

```
▼ layer3changes:
  ▼ change1:
      change:        "data treated as shape"
    ▶ Comment:       "Data are treated as shap…self in the evaluation."
      use:           "Standards 2018"
  ▼ change2:
      change:        "data rejected above 13 MeV."
    ▶ Comment:       "Data systematically lowe…od through discussions."
      Status:        "Further investigation needed."
▶ outlier:           {…}
```

For discussion: How to best store that? For each use-case one data set as used in the evaluation or only storing correction factors???

Thank you for your attention!

- Initial draft of requirement document covers a lot already.
- Json works well for this.
- Suggestions for data containers, layer 2 and layer 3 additions made.
- We should involve evaluators heavily in what information is needed in these data files!
- We need to discuss how to distill the information to the one that is essential.