Specifications for the next generation nuclear data hierarchy

WPEC Subgroup 38

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1 Introduction

One of the tasks of WPEC Subgroup 38 (SG38) is to fill out specifications for how nuclear data are to be organized inside the new hierarchy. This document is being prepared to fulfill that task.

```
All,
I went through the requirements documents and generated a list of items that need
written specifications.  Below, I list all of those items, sorted by topic area.

In the coming weeks, I will circulate a frame document that we can all use to begin
populating with our content.  I'll do the final merging and editing.  I'll also do what
I can to facilitate the negotiation between your contributions and the coding
styles/standards that we agree to.
```

```
In the lists below, an "x" in the first column indicates that a specification already
exists and is covered in Caleb's "Properties of Particles" (POP) document or Bret's
the low level data containers document (LLDC).  If there is no "x", then look to the
right for the writing assignment.  Some some topic areas are assigned completely to one
or more of you.  In other cases, individual items are assigned to you.

Completed
=========
x  Particles                                                    (Mattoon: POP)
x  General low-level                                            (Beck: LLDC)
x  Lowest level data elements                                   (Beck: LLDC)
x  List of general purpose elements                             (Beck: LLDC)
x  Text elements                                                (Beck: LLDC)



High level, no work to do
=========================
x  WPEC Subgroup 38 tasks                                       (n/a)
x  An example                                                   (n/a)
x  Main                                                         (n/a)
x  Hierarchal structures                                        (n/a)
x  Legacy data                                                  (n/a)


Rest have varying amount of GND/ENDF content developed.
```

If you want to use LaTeX's code minted environment, use it like this:

```
<grid0>
<grid1>
<grid2>
...
<gridN>
```

2 Conventions in this document

Specifications for each level of the nuclear data storage hierarchy will be presented in the following sections. A full specification for each element includes the following:
Tag: the xml `<tagname/>`
Attributes: the list of attributes that can appear inside this element.

Elements: the list of child elements that can appear inside this element. Specifications for each child element is presented in its own section.

Attributes listed in this document are required unless the flag '(optional)' is given after the attribute name. Each attribute can only appear once inside a given element. Child elements may appear multiple times. The following flags should be used to indicate how many times each child element may appear:
'(optional)' : indicates the element may appear 0 or 1 times.
'(zero or more)' : indicates the element may appear 0, 1 or multiple times.
'(one or more)' : indicates the element is required and may appear multiple times.
If none of these flags are specified, the element must appear exactly once.

Some attributes and elements may only be needed for backwards-compatibility. These are indicated by adding the 'deprecated' flag.

2.1 General Features

- Documentation
- Lists of things vs. just listing the things – depth of hierarchy vs. just looping and dealing with special cases
- Reaction designation
- `<functionDef/>`
- Placeholder hyperlinks
- Hyperlinks

3 Top of the hierarchy

All reactions involving the same combination of projectile and target can be grouped together inside a single evaluation. That evaluation, or 'reactionSuite', should clearly specify what projectile/target combination it pertains to. It should contain documentation, a list of the particles including reaction products, a list of reactions, and potentially other data.

Uncertainties and covariances may be stored alongside their central values, or they may be stored in a separate file called a 'covarianceSuite', and associated with their central values by links.

3.1 reactionSuite specifications

Tag: reactionSuite
Attributes: The following attributes are required:
projectile: Projectile particle id.
target: Target particle id.
formatVersion: Version of the format, e.g. 'GND 1.7'
projectileFrame: Options are 'lab' or 'centerOfMass'

xmlns:xlink: url for the xml 'xlink' namespace that will be used. See comments below.
other xml namespaces: (optional) additional name spaces if needed.

Elements: child elements of a reactionSuite include

representations: section listing the representations of data inside this reactionSuite
documentations: for top-level documentation applying to the entire reactionSuite
particles: for describing all particles involved in the reactionSuite, including projectile, target and reaction products.
resonances: (optional) describes resonance parameters.
reactions: (optional) list of all reactions.
sums: (optional) list of summed cross sections, multiplicities, etc.
productions: (optional) list of production reactions.
fissionComponents: (optional) list of partial fission cross sections (1st-chance, 2nd-chance, etc. FIXME: a better name might be 'partials' so we're not tied to the fission process and so we can use this for orphaned gammas and such
applicationData: (optional) list of application-specific data.
Other child elements?

Additional comments: XML namespaces can be used to expand the types of data stored in an xml document. The 'xlink' namespace is required since different parts of nuclear data evaluations often must be linked together. Other namespaces may also be useful in the future.

According to these specifications, the 'reactions', 'sums' and 'productions' elements are all optional. This makes the format more flexible, but individual nuclear data libraries will likely want to require at least the 'reactions' and 'sums' sections.

3.2 `<metaEvaluation/>`

TODO:Dave Brown

3.3 covarianceSuite specifications

3.4 Specifications:

Tag: covarianceSuite
Attributes: The following attributes are required:
...:
Elements: child elements include
styles:

4 List of representations

A reactionSuite (and associated covarianceSuite) may contain more than one style of data, including 'evaluated', 'reconstructed', 'heated', etc. Each style has (at least) a name and a

date corresponding to when it was added to the reactionSuite. Representations may contain additional information as well.

4.1 representations:

Tag: representations
Attributes: None
Elements: **evaluated**: style corresponding to the evaluated data (rather than processed or derived data).
crossSectionReconstructed: style corresponding to cross sections (and potentially other data) derived from the evaluated resonance parameters.
heated: style corresponding to Doppler-broadened data
... other styles still to be defined

4.2 evaluated representations:

Tag: evaluated
Attributes: **name:** string identifying this representation. Must be unique among all styles in the file. Suggestion: should we specify the name, so that the evaluated style always has the name 'eval'?
library: evaluation library this file belongs to, i.e. 'ENDF' or 'JENDL'
version: library release number.
date: release date of the evaluation
temperature: target temperature, given as a string with units such as '0 K'.
Elements: None

5 Documentation sections

Attributes:
`evaluationDate` When the evaluation file was completed
`acceptanceDate` When the evaluation file was accepted
`DOI (optional, default='')` Digital Object Identifier
Elements: All child elements of the `<documentation>` element are—at their most basic level—`<text>` elements.
`title`
`listofAuthors` Each author given in child element.
`version` Free-form; project specific.
`metadata (optional)` Free-form; project specific.
`abstract (optional) <text> element`
`copyright (optional)` Free-form; project specific.

`bibliography (optional)` Set of bibitem elements used to generate a LaTeX bibliography. Each bibitem is given in a child (to bibliography) `<text>` element.

`listOfInputs` Inputs (e.g., TALYS, EMPIRE input decks) used to generate evaluation

`listOfEXFORSets` Experimental data used in models.

`writeup (optional)` Free-form; used to describe how the data was generated.

6 Dictionary of particles

7 Resonance region

Store resonance parameters, from which cross sections, cross section probability tables and potentially angular distributions can be derived.

7.1 resonances:

Tag: resonances

Attributes: reconstructCrossSection: boolean. 'true' means that resonances need to be reconstructed for a complete cross section, 'false' means resonances are provided only for self-shielding or scattering radius purposes.

Elements: The 'resonances' section contains either of the following:

scatteringRadius: only the scattering radius is specified. Used mainly for light isotopes. or

resolved: (zero or more) section containing resolved resonance parameters. Multiple resolved regions are supported but deprecated.

unresolved: (zero or one) section containing unresolved resonance parameters.

7.2 scatteringRadius:

TODO:Wim Haeck, C. Mattoon and V. Sinitsa

- `<resonances/>` (easy)
- `<spinGroup/>` (moderate)
- `<channel/>` (moderate)
- Resolved resonance region (RRR) (moderate)
- Background R matrix (moderate)
- Unresolved resonance region (URR) (moderate)
- `<backgroundReaction/>` (easy once reaction done)

```
<resonances>
  <resolved lowerE="" upperE=""
                    formalism="endfSLBW/endfMLBW/endfRM/endfLRM/SLBW/MLBW/RM"
                    width="channel/reduced" computeAngular="false/true"
```

```
                relativistic="false/true" representation="eval/multiband">
<!-- no overlapping regions allowed -->
<!-- only 1 resolved and 1 unresolved? => tag names change to
     'resolved' and 'unresolved', remove 'type' attribute -->
<!-- 'representation' attribute on a range or on the resonances element -->
  <particles />
  <!-- optional masses, target spin -->
  <channels>
    <channel label="0" name="n+O16" reaction="n+O16->O16+n" mt="2" q="0.0 eV
    <!-- default true and effective radius (can be overriden) -->
      <trueRadius />
      <!-- to be used for P and S, can be energy dependent or a constant -->
      <effectiveRadius />
      <!-- to be used for phi, can be energy dependent or a constant -->
    </channel>
    <channel label="1" name="gamma+O17" reaction="n+O16->O17+gamma" mt="102"
             q="0.0 eV" />
    <channel label="2" name="competitive" q="10.0 eV" />
    <!-- competitive channel SLBW/MLBW added as an channel -->
    <!-- how do we handle total width? -->
  </channels>
  <orbitalMomemtum l="0/1/2/3">
  <!-- add as many orbitalMomentum as needed or use NLSC? -->
    <spinGroup label="" j="2 or 3/2" parity="+/-" spin="">
    <!-- add as many spinGroup as there are possible J values? -->
    <!-- can be empty if no resonances are defined -->
      <override>
      <!-- to override defaults -->
        <channel label="">
          <trueRadius />
          <effectiveRadius />
          <!-- allows storing P, S, phi - either as constants or f(E) -->
          <penetrability />
          <shiftFactor />
          <phaseShift />
        </channel>
      </override>
      <resonanceParameters>
        <table rows="1" columns="4">
        <!-- competitive channel SLBW/MLBW added as an channel -->
          <column index="0" name="energy" unit="eV" />
```

```
            <column index="1" name="n+O16 width" unit="eV/eV^1/2" />
            <column index="2" name="gamma+O17 width" unit="eV/eV^1/2" />
            <column index="3" name="competitive width" unit="eV/eV^1/2" />
            <!-- energy | elastic | capture | competitive -->
             5000.0     0.75   0.15   0.20
            10000.0     0.70   0.20   0.15
          </table>
        </resonanceParameters>
      </spinGroup>
    </orbitalMomemtum>
    <background />
    <!-- this includes background matrices, xs and angular matrices -->
    <!-- or we put it in the channels? -->
  </resonanceRange>
  <resonanceRange lowerE="" upperE="" type="unresolved" formalism="">
    ...
  </resonanceRange>
</resonances>
```

ask Luiz: if only scattering radius is given, how do we use it?

* Do we allow overlap of ranges? * Are multiple resolved ranges deprecated? If so, 'resonanceRange' can be replaced by 'resolved' and 'unresolved' because only one can be present.

8 Cross sections

This subsection details the specifications for the various cross-section tags. They are in order of increasing dimensionality:

- `<crossSection/>`
- `<dcrossSection_dOmega/>`
- `<dcrossSection_dOmega_dE/>`

8.1 crossSection specifications

The **crossSection** tag is the most basic and most common mark up for cross sections. This section details cross sections that are a function only of incident energy: $\sigma(E)$. These are most often found in reaction elements (see 10.1) and summedReaction elements (see **??**), but also may be found as background cross sections in the resonance region (see 7).

Each cross section is assumed to be constructed from one or more interpolation regions (or given by the resonance data). This mark up contains the list of these interpolation regions. Here each region is given its own XYs and or a resonanceRegionLink. It is up to the evaluator and the processing code to ensure there is no overlap between the energy ranges of each region.

This also includes the URR probability tables since they end up hear after processing

FIXME: What about INT=6, the strange charged particle interpolation scheme?

Tag: crossSection

Attributes: The **crossSection** tag has no attributes

Elements: child elements of a crossSection are the various representations of the cross section. At least one element that describes the dependance of the cross section as a function of energy is required and that one contains the " representation='eval' " attribute.

XYs: (optional) for pointwise data. This may contain uncertainty data.

resonanceRegionLink: (optional) link to resonance data.

regions: (optional) for a cross section broken up into a series of pointwise (as XYs) regions, with different interpolations, or a hyperlink pointing to a resonance region (as sec:resonanceRegionLink).

urrProbabilityTable: (optional) URR cross section "probability table", found in processed data. It is not really a table, but that is the common name which we preserve.

documentation: (optional)

An example: Here we present an example of a file whose evaluated data consists of resonances and a fast region. This data is processed in two ways: 1) into a pointwise table with a URR probability table and 2) into a grouped cross section.

```
<crossSection>
  <regions representation="eval">
```

```
    <axes> ... </axes>
      <resonanceRegionLink eMin="..." eMax="..." href="..."/>
      <XYs interpolation="lin,lin">
        <values length="6">...</values></XYs></regions>
  <regions representation="recon">
    <axes> ... </axes>
    <XYs interpolation="lin,lin">
      <values length="60">...</values></XYs>
    <urrProbabilityTable eMin="..." eMax="...">...</urrProbabilityTable>
  </regions>
  <XYs interpolation="flat" representation="grouped">
    <axes> ... </axes>
    <values length="6">...</values></XYs></regions>
</crossSection>
```

8.1.1 resonanceRegionLink specifications

This is used to establish a link from a cross section like element to a resonance region. The link establishes the energy range of the resonance region to use when reconstructing the cross section.

Tag: resonanceRegionLink

Attributes: representation: (optional) defines whether this is the 'eval' or user defined processed data. Most likely this is processed.

eMin: lower incident energy of the domain that the data is defined over

eMax: upper incident energy of the domain that the data is defined over

href: URL in xlink format of a resonance region

Elements: The **resonanceRegionLink** tag has no elements

An example:

```
<resonanceRegionLink eMin="1e-5 eV" eMax="805 keV" href="..."
    representation='eval'/>
```

8.1.2 urrProbabilityTable specifications

This is just generated URR probability tables $P(\sigma|E)$ from e.g. PURR or PURM or GRUCON. This data is generated during processing from URR parameters

FIXME: The conditional probability tables generated by GRUCON $P(\sigma_x|\sigma_{tot}, E)$ are stored where?

Tag: urrProbabilityTable

Attributes: The following attributes are required:

representation: (optional) defines whether this is the 'eval' or user defined processed data. Most likely this is processed.

eMin: lower incident energy of the domain that the data is defined over

eMax: upper incident energy of the domain that the data is defined over

Elements: child elements of a crossSectionRegions are

multiD_XYs: (optional) A 3D interpolation table (most likely a histogram) with $\{E, \sigma, P\}$ triplets where P is the probability associated with the incident energy and cross section value. The temperature is specified as part of the representation attribute of this element or the enclosing element regions element.

An example: Here we show an example of an URR probability table. As generated by PURR and PURM (up to heating of the data) the probability table is just a histogram of probabilities of the cross section at a fixed incident energy.

```
<urrProbabilityTable eMin="100 keV" eMax="805 keV" representation="recon">
  <multiD_XYs dimension="2" label="energy">
    <axes>
      <axis index="2" label="energy_in" unit="eV"/>
      <axis index="1" label="crossSection" unit="b"/>
      <axis index="0" label="P(crossSection|energy_in)" unit="1/b"/></axes>
    <XYs value="1e5" interpolation="flat"><values length="86">...</values></XYs>
    ... </multiD_XYs>
</urrProbabilityTable>
```

8.2 dCrossSection_dOmega specifications

Occasionally there is a need to store directly the $d\sigma/d\Omega$ directly in an ENDF file. This is particularly true for reactions induced by charged particles (namely electrons, protons and light nuclei as projectiles) as elastic scattering must be handled carefully. For these projectiles, the elastic scattering amplitude is the sum of a Coulomb and a nuclear term. As the Coulomb term is has singularities both at forward angles and low incident energies. Therefore, it is not possible to integrate the differential cross section $d\sigma/d\Omega$ over all angles. ENDF defines a somewhat arcane approach for dealing with charged particle elastic scattering and is detailed below in the chargedParticleElastic description (see section 8.2.1).

We comment that electron screening (especially in a plasma environment), is a serious issue with charged particle scattering and beyond the scope of this document.

That said, whenever the incident energy and the outgoing particle angle completely determine the kinematics of a reaction, this mark up could be used. This includes all elastic and inelastic two-body reactions.

Tag: dCrossSection_dOmega

Attributes: The following attributes are required:

representation: (optional)

documentation: (optional)

Elements: child elements of a crossSection are

chargedParticleElastic (optional)

resonanceRegionLink: (optional) link to resonance data.

regions: (optional) for a cross section broken up into a series of regions, with different interpolations, or a hyperlink pointing to a resonance region (see 8.1.1).

multiD_XYs: (optional) a pointwise table of $\{E, \mu, d\sigma/d\Omega\}$ values. This may be used in lieu of a chargedParticleElastic table.

documentation: (optional)

Examples:

In the following example, we show a charged particle reaction given as a link to a resonance region at low energies and as a chargedParticleElastic set of tables at higher energies. Upon reconstruction, the entire cross section is written in a single chargedParticleElastic spanning all energies.

```
<dCrossSection_dOmega>
  <regions representation="eval">
    <axes> ... </axes>
      <resonanceRegionLink eMin="10 eV" eMax="2 MeV" href="..."/>
      <chargedParticleElastic eMin="2 MeV" eMax="30 MeV">
        ...</chargedParticleElastic></regions>
  <chargedParticleElastic eMin="10 eV" eMax="30 MeV" representation="recon">
    ...</chargedParticleElastic>
</dCrossSection_dOmega>
```

8.2.1 chargedParticleElastic specifications

Container for the table of double differential nuclear+interference $d\sigma/d\Omega$. The pure Coulomb term is the analytic Rutherford cross section and not repeated here.

Tag: chargedParticleElastic

Attributes: The following attributes are required:

eMin: (optional) ??

eMax: (optional) ??

representation: (optional)

documentation: (optional)

muCutOff: (optional) ??

Elements: child elements of a crossSection are

fakeCrossSection: (optional)

fakeAngular: (optional)

8.3 dcrossSection_dOmega_dE specifications

Needed for charged particle scattering, photo-atomic and thermal neutron scattering, but in many of these cases, there are arcane parametric forms.

Elastic TSL scattering could have been included in the dcrossSection_dOmega mark up above, but as the kinematics are quite different than traditional elastic scattering, it was felt that it would be better if all the TSL formats were collected together in one common markup and in one place in the manual.

Tag: dcrossSection_dOmega_dE

Attributes: The following attributes are required:

??: (optional) ??

Elements: child elements of a crossSection are

coherentPhoton: (optional)
incoherentPhoton: (optional)
tslNeutronCoherentElastic: (optional)
tslNeutronIncoherentElastic: (optional)
tslNeutronInelastic: (optional)
documentation: (optional)

Examples:

- Photo-atomic scattering
- TSL, graphite has both coherent and incoherent
- TSL, water has just incoherent

8.3.1 coherentPhoton specifications

Coherent scattering term in photo-atomic scattering, meant to be added to incoherent term

8.3.2 incoherentPhoton specifications

Incoherent scattering term in photo-atomic scattering, meant to be added to coherent term

8.3.3 tslNeutronCoherentElastic specifications

8.3.4 tslNeutronIncoherentElastic specifications

8.3.5 tslNeutronInelastic specifications

9 Products and product lists

9.1 Product

A `product` is a particle that is the result of a reaction. More than one particle of the same type can be released in a single reaction (e.g., $(n, 2n)$). Thus a multiplicity—how many are produced—must be defined for each product.

For the `<product>` element:

Attributes:

`name` The name of a particle. The name of the particle must correspond to the name of a particle in the particle database.

Elements:

`multiplicity` One or more elements describing the multiplicity of the product.

`distributions` One or more elements describing the energy/angle distribution of the product. The number of distribution elements must be the same as the number of multiplicity elements.

`discrete` (optional) Describes a discrete gamma particle. Only used when `name="gamma"`

`primary` (optional) Describes a spectrum of gamma particles. Only used when `name="gamma"`

`prompt` (optional) Describes prompt fission neutron. Only allowed with fission reaction.

`delayed` (optional) Describes delayed fission neutron. Only allowed with fission reaction.

```
<product name="gamma">
  <discrete label="a" energy="... eV" originationLevel="31376.0 eV">
    <multiplicty>...</multiplicity>
    <distribution>...</distribution>
  </discrete>
  <discrete label="b" energy="... eV" ...>...</discrete>

  <!--- other discrete elements -->

  <primary label="cd" energy="... eV">
    <multiplicty>...</multiplicity>
    <distribution>...</distribution>
  </primary>
</product>
```

```
<product name="n">
  <prompt>  <!-- only allowed for fission reaction -->
    <multiplicty>...</multiplicity>
```

```
    <distribution>...</distribution>
  </prompt>

  <!-- only allowed for fission reaction -->
  <delayed label="a" decayRate="0.13271 1/s">
    <multiplicty>...</multiplicity>
    <distribution>...</distribution>
  </delayed>
  <delayed label="b" decayRate="0.030881 1/s">
    <multiplicty>...</multiplicity>
    <distribution>...</distribution>
  </delayed>
  <!-- additional delayed elements -->
</product>
```

9.2 Products

There are three "types" of product lists:

- reaction
- orphaned
- decay

Each type has the same structure; a constant for the Q-value, one or more child `<product>` elements, and optional `<documentations>` child element.

Attributes:

`kinematicType` (optional)

- `two-body` (default)
- `uncorrelated`
- `correlated`
- `fission`

Elements:

`constant` An element that contains the Q-value for the reaction. The `name` attribute for this element must be `"Q"`; i.e., `<constant name="Q" .../>`

`product` One or more `<product>` child element.

`documentations` `(optional)` Element describing documentation specific to the list of products.

Some of the child `<product>` elements may be unstable and decay further. The decay products of the unstable product are not given here, but are given explicitly in the particle database.

```
<products kinematicType="two-body">
  <constant name="Q" value="-7861.0 eV"/>
```

```
  <product name="n">...</product>
  <product name="Pu239_e1">...</product>
</products>
```

9.3 Distributions and distribution lists

TODO:Bret Beck & Caleb Mattoon

- `<distributions/>` (moderate, so many of them!) – Bret & Caleb
- `<multiplicity/>` (easy, but includes nubar) – Bret

10 Reaction-related descriptions

TODO:Bret Beck, Caleb Mattoon, Dave Brown

- `<reactions/>` (in GND, mostly done)
- `<summedReactions/>` (in GND, mostly done)
- `<productionReactions/>` (in GND, mostly done)
- `<derivedReactions/>` (in GND, mostly done)
- `<reaction/>` (in GND, mostly done)

10.1 Reaction

10.2 List of reactions

10.3 List of summed reactions (e.g. total cross section, total gamma multiplicity)

10.4 List of production reactions

11 Covariances

Nuclear data evaluations are incomplete unless they include estimates of the uncertainties on values and the covariances between those values. Covariances may be given for various quantities, including reaction cross sections, outgoing product multiplicities, outgoing product energy (or angle) distributions and resonance parameters. Covariances may also link two different quantities (e.g., cross sections for two different reactions or for reactions on different targets).

Items to address in this section:

- Where to put covariance data
- Cross–covariance linkage
- `<grid/>` (Beck: LLDC)
- Multidimensional `<grid/>` use
- `<covariance/>` and `<correlation/>`
- `<matrixData/>`
- `<weightedSumOfCovariances/>`
- `<matrixSandwich/>`
- `<sensitivity/>`

11.1 section

Covariance data are stored inside a 'covariance' element. This may be stored inside the 'reactionSuite' hierarchy together with the associated central values (cross section, multiplicity, etc.). It may also be stored in a separate list of covariances, in which case it must contain links to the corresponding central values.

For the `<covariance>` element:

Attributes:

label: string identifying this covariance section. If the section is inside a covariance-Suite, label must be unique among all sections.

id: do we still need this? It's supposed to be descriptive, but if so it's not really an id...

Elements:

rows: (required unless the covariance is stored along with central values) defines what data lie along the rows of the covariance

columns: (required unless the covariance is stored along with central values) defines what data lie along the columns of the covariance

followed by one of the following:

covarianceMatrix: Used when the entire covariance can be captured in a single matrix. The matrix may be relative or absolute.

correlationMatrix: For when the correlation is stored instead of the covariance, fitting in a single matrix.

weightedSumOfMatrices: For when the full matrix is broken up into separate sections that must be added together (potentially weighted by different coefficients).

GLSqrSumOfMatrices: Used when the covariance has several sources (systematic, normalization, etc.) that should be combined as $cov_{total} = (\sum_{source\ k}(cov_k)^{-1})^{-1}$

11.2 covarianceMatrix

An individual covariance matrix can be stored using the 'gridded' data container, along with a 'type' that could be 'absolute' or 'relative'. It may also need a unique label (to permit linking in case it appears inside a 'weightedSumOfMatrices' or 'GLSqrSumOfMatrices' as defined below.

```
<covarianceMatrix label="0" type="relative" style="eval">
  <gridded dimension="2">
    <axes>
      <axis index="2" label="row_energy_bounds" unit="eV"
                      gridStyle="boundaries">
        <values length="...">...</values></axis>
      <axis index="1" label="column_energy_bounds" unit="eV"
                      gridStyle="link">
        <link xlink:href="../axis[@index='2']/values"/></axis>
      <axis index="0" label="matrix_elements" unit=""/>
    </axes>
    <array shape="10,10" symmetry="lower">
      <values length="55">...</values>
    </array>
  </gridded>
</covarianceMatrix>
```

11.3 correlationMatrix

We may also wish to store uncertainties and correlations separately:

```
<covarianceMatrix label="0" type="uncertaintyAndCorrelation" style="eval">
  <uncertainty>
    <XYs>...</XYs></uncertainty>
  <gridded dimension="2">...</gridded>
</covarianceMatrix>
```

11.4 weightedSumOfMatrices

Covariances can be composed by adding and/or subtracting other covariances. For example, the covariance for the total cross section can be composed by adding together the covariances for all partial cross sections. It could also be composed by adding together two or more smaller matrices in different energy ranges.

```
<covarianceMatrix label="0" style="eval">
  <add weight="1.0">
    <covarianceMatrix>...</covarianceMatrix></add>
  <add weight="1.0">
    <link xlink:href="..."/></add>
  <add weight="-1.0">
    <link xlink:href="..."/></add>
</covarianceMatrix>
```

11.5 GLSqrSumOfMatrices

Covariances may also need to be composed in a Generalized Least Squares mode, where they add as inverse matrices rather than directly:

$$cov_{total} = (\sum_{source\ k} (cov_k)^{-1})^{-1}$$

```
<covarianceMatrix type="GLSqrSumOfMatrices" label="0" style="eval">
  <add>
    <covarianceMatrix>...</covarianceMatrix></add>
  <add>
    <link xlink:href="..."/></add>
  <add>
    <link xlink:href="..."/></add>
</covarianceMatrix>
```

11.6 Covariance for normalized distribution

Add special tag to indicate: "Do Not Sum"

11.7 Covariances for model parameters

Covariances may be given between model parameters. In nuclear data this especially occurs for resonance parameters. The 'gridded' data container supports using model parameters instead of energy intervals to define the matrix elements.

ADD: instructions for 'unpacking' parameters into this matrix.

```
<modelParameterCovariance label="0" type="relative" style="eval">
  <gridded dimension="2">
    <axes>
      <axis index="2" label="row_energy_bounds" unit="eV"
                      gridStyle="parameters">
        <parameters>
          <link xlink:href="/reactionSuite/resonances/resolved"/>
        </parameters></axis>
      <axis index="1" label="column_energy_bounds" unit="eV"
                      gridStyle="link">
        <link xlink:href="../axis[@index='2']/parameters"/></axis>
      <axis index="0" label="matrix_elements" unit=""/>
    </axes>
    <array shape="12,12" symmetry="lower">
      <values length="78">...</values>
    </array>
  </gridded>
</covarianceMatrix>
```

12 Special Cases

12.1 Simple cases

TODO: Bret Beck, Caleb Mattoon, Dave Brown

- Atomic reaction data (in GND, mostly done)
- Charged particle scattering (easy, just unfamiliar)
- Fission (easy, issues familiar)
- Photo-atomic data (in GND, mostly done)
- Radiative capture (just easy)
- Spallation (in GND, mostly done)

12.2 Fission product yields

TODO: Robert Mills, Dave Brown, Morgan White

- Fission Product Yields (FPYs) (need to review requirements)

12.3 Thermal Neutron Scattering

TODO: Ayman Hawari, Dave Brown, & Jessie Holmes (all moderate)

- Thermal scattering kernel
- Gaussian self-part scattering kernel
- Coherent Elastic Scattering
- Incoherent Elastic Scattering
- Short Collision Time Approximation

13 Derived Data For Applications

TODO: Lots of people, see below

- Average kinetic energy and forward momentum (easy) – Bret
- Mubar (easy) – Dave
- CDFs (easy) – Fausto
- URR probability tables (moderate) – Mirielle & Jean-Christoph Sublet??
- Grouped transport data (moderate) – Bret & Morgan
- Production data (easy) – Dave
- DPA and KERMA (probably easy) – Fausto
- Transfer matrices (moderate) – Bret

References

[1] XML Linking Language (XLink) Version 1.1. See: http://ww.w3.org/TR/xlink11