

# Top level organization of nuclear data

*D. Brown, BNL*

**BROOKHAVEN**  
NATIONAL LABORATORY

*a passion for discovery*



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

Get ready for  
**Two Hours**  
of nuclear data

**FUN**

This talk has

**87 slides**

and the requirements document has

**31 Pages**

# Outline (roughly)

## HOUR 1

- Goals, use cases, etc.
- Preliminaries
  - low-level containers
  - designators
  - documentation
- The Top: `<evaluation>`
  - `<reactions>`
    - special two-body
    - plain old reactions
  - `<resonances>`
- The Other Top:  
`<setOfCovariance>`

## HOUR 2

- `<metaEvaluation>`
- Special cases:
  - Atomic data
  - Fission
  - Fission Product Yields
  - Large Angle Coulomb Scattering
  - Particle production
  - Thermal Scattering Law
- Odds-n-ends
- Thanks & Blame

# Goals

- The hierarchy should **reflect our understanding of nuclear reactions and decays**, and **clearly and uniquely specify all data**.
- It should support **storing multiple representations of the same quantity simultaneously** (e.g. evaluated and processed data).
- Should support **both inclusive and exclusive reaction data** (i.e., discrete reaction channels as well as sums over those channels).
- It should **eliminate redundancy where possible**.
- It should make **use of the general-purpose data containers** designed by the first SG38 project group.

# Bonus goals

**(1) Support all data and all forms in ENDF format and all ENDF-formatted libraries**

**(2) Fix (or at least document) all of the corners cut in the development of ENDF**

# Use cases to keep in mind

## ■ Particle Transport:

- All cross sections
- All outgoing energy and angle probabilities for all emitted particles for chosen reactions that are energetically possible
- Multiplicities for all emitted particles if not constant.

## ■ Isotope Burn-Up:

- cross sections and
- optionally outgoing spectra for chosen reactions that are energetically possible
- all produced particles decay so that a time dependent isotope inventory may be computed.

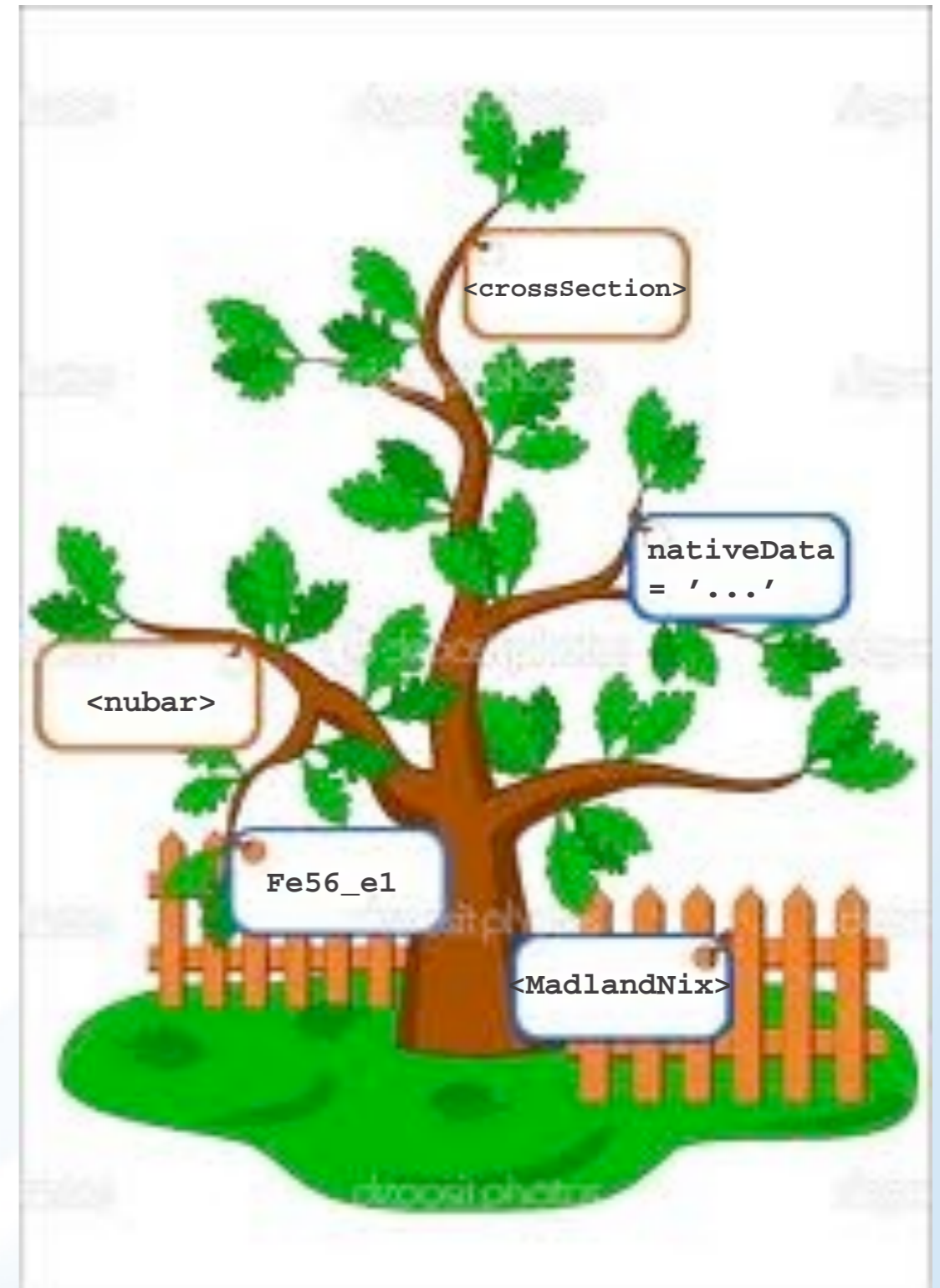
## ■ Web Retrieval: data will only most likely be visualized

# Gotchas

- **Is it a material property or a reaction property?**
  - *Answer:* It is a material property if it is independent of the excitation mechanism
  - *Examples:* mass, level excitation, BR's for decays out of a level, ...
- **Different optimal representation in different physical regimes**
  - *Example:* resonances and high energy data in same evaluation
  - *Part of solution:* `<metaEvaluation>` (an enhanced xsdir-like facility)
- **Ensuring consistency**
  - Some things we can do in the format (e.g. material database)
  - Some things need to be done in the supporting infrastructure
    - Need checking functions
    - Need fixing functions

# Notational aside(s)

- Data is viewed as a tree
- Nodes on tree are denoted `<element>`
- Attributes/member data of a node are denoted **attribute**
- Names are for discussion purposes only; *change them if you don't like them, you won't hurt my feelings*



# Caveat: In only two hours, we won't get to many details

- No talk of cross section representations
- No discussion of how to reconstruct resonances & how to connect them to the cross sections
- No talk of any parameterized data, including, but not limited to:
  - Kalbach-Mann systematics
  - Madland-Nix model
  - interpolation schemes
  - ...

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# Preliminaries: low-level containers (1)

*To be discussed in detail by M. White*

- float, int and string
- `<list>` or vector must specify type of object in the list
- `<matrix>`, must specify dimensions. May be banded, symmetric, etc.
- `<table>`, like a matrix, but the columns have labels and units and maybe even data-type information
- orthogonal function expansion, Legendre polynomials being the most obvious



# Preliminaries: low-level containers (2)

*To be discussed in detail by M. White*

- `<interp2d>`: interpolation table for univariate data, i.e.  $x$  vs.  $f(x)$
- `<interp3d>`: interpolation table for bivariate data, i.e.  $(x,y)$  vs.  $f(x,y)$
- `<interp4d>`: interpolation table for trivariate data, i.e.  $(x,y,z)$  vs.  $f(x,y,z)$
- Should we put  $\delta f(x)$  in the container too?



# Preliminaries: low-level containers (3)

*To be discussed in detail by M. White*

- **<axis>**: Where appropriate (particularly on interpolated types), we need to specify interpolation details, units, labels, etc.
  - Specify names of x, y, z, ... axes
  - Specify normalization (if any)
  - Specify units in all directions
  - Specify interpolation scheme(s) or group boundaries
  - Specify reference frame
  - If interpolation the table refers to a probability distribution function (PDF), we also must specify whether is Normal or Log-Normal



# Preliminaries: low-level containers (4)

*To be discussed in detail by M. White*

- `<text>`: marked up text, either in HTML, Markdown, or plain old text. The format must be denoted. Must allow unicode!!!!
- `<link>`, a relative or absolute URL



# Preliminaries: material designators

*Just a suggestion as C. Mattoon will discuss*

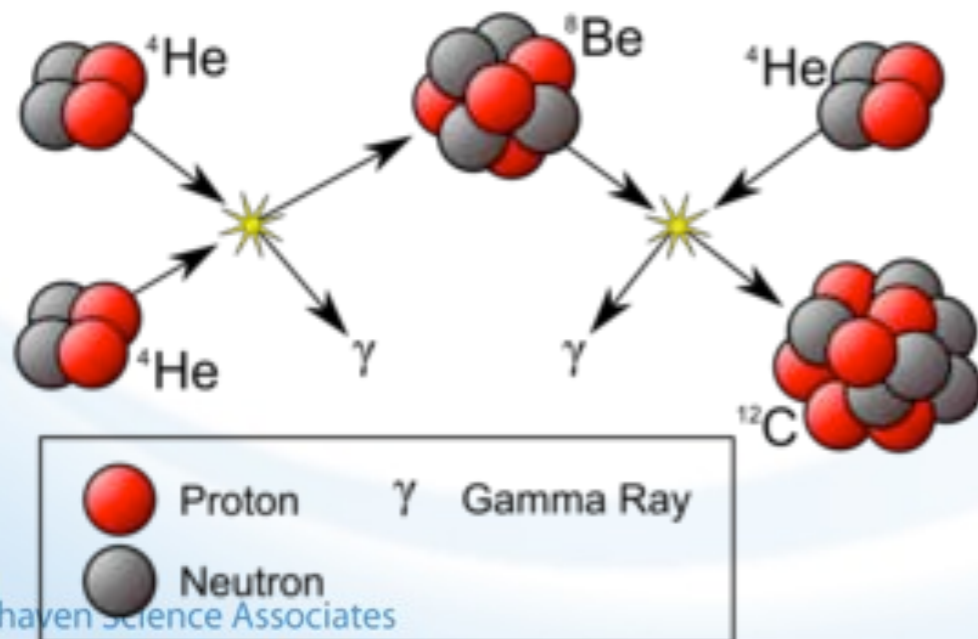
- **Aliases:** A limited number/scope of aliases for commonly used particles or to associate a level of an isotope with an isomer.
- **Compounds:** e.g. `c_Free_String_Describing_Material`, Useful for TSL data
- **Elements:** `Sym0` for atomic data
- **Isotopes:** `SymA` e.g. `Fe56`
- **Levels of an isotope:** `SymA_eN`, `V51_e1` for the first excited state. Use `SymA_c` for continuum.
- **Electronic shells of an atom:** `Sym0_eN`, e.g. `V0_e1` for the first shell. Use `Sym0_c` for continuum.



# Preliminaries: reaction designators

*Just a suggestion as C. Mattoon will discuss*

- Shared/agreed upon with EXFOR
- Not be limited to simple targets (for TSL)
- Aliases for things like `elastic`, `total_fission`, `capture`
- Need to distinguish input vs. output channels
- Allow n-body processes
- Variable multiplicity processes
- Sequential processes (esp. 2-body)
- Annotation (e.g. `compound_elastic` and `shape_elastic`)



## Triple-alpha reaction:

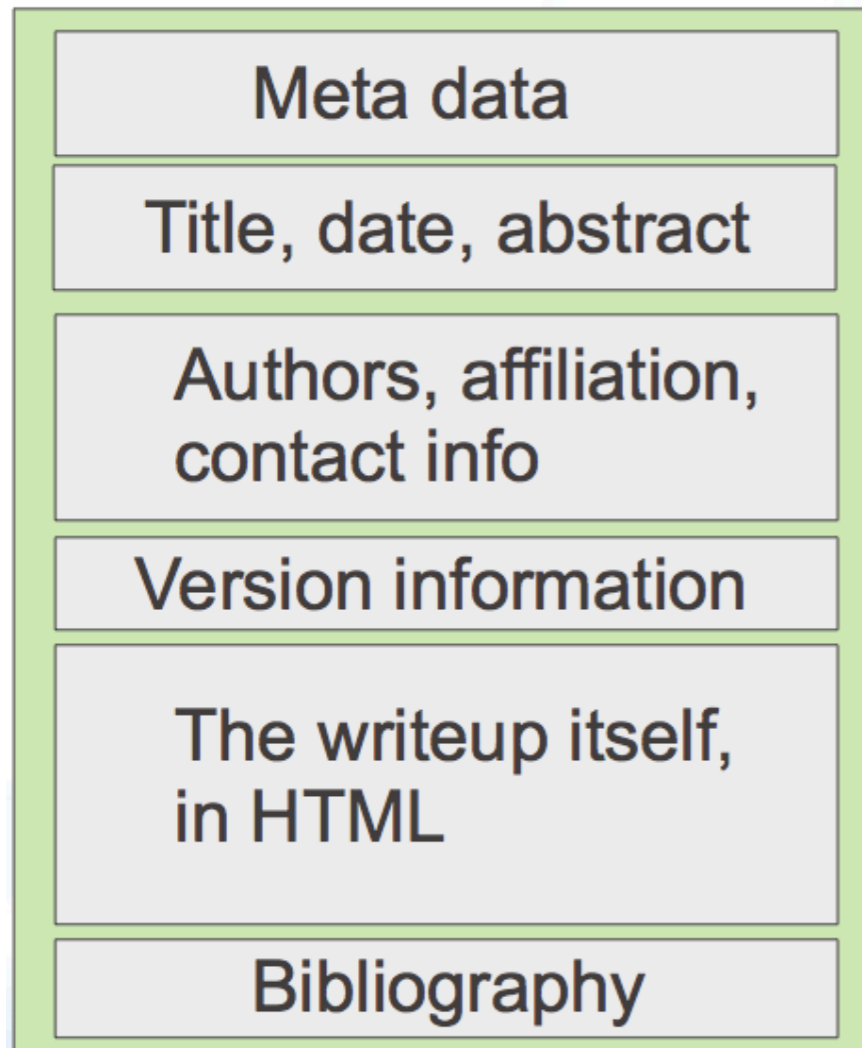


# Preliminaries:

## All data contained in `<form>` elements (*this name is from GND*)

- All the data needed to reconstruct the observable
  - Examples:
    - x-y interpolation table for a cross section
    - grouped cross sections
    - Legendre moments of an angular distribution
    - parameters of the Madland-Nix PFNS model
- There may be more than one for an observable
- Only one original data; this one may have `<link>`s to covariance data
- All derived point to original with a `nativeData` link
- The `nativeData` concept is so useful that we will use it in several places

# Preliminaries: documentation



- Allow metadata (just keywords for search engines?)
- DOI markup (using a `<link>` element)
- Have markup for title (using a `<text>` element)
- Evaluation date markup
- Library acceptance date markup (library maintainers make this up)
- Have markup for abstract (optional, using `<text>`)
- Have markup for authors (names, affiliation, email, etc.). Who is corresponding author? How should this be structured?
- Have markup for the evaluation version
- Allow free text write up (using a `<text>` element)
- Have markup for the bibliography. How should this be structured? In principal it should be shared with EXFOR.

# DOI's are unique id's on a publication/dataset; doi.org resolves them to URLs



The screenshot shows the homepage of doi.org. At the top left is the 'doi' logo. Below it is a navigation bar with links: HOME | HANDBOOK | FACTSHEETS | FAQs | RESOURCES | USERS | NEWS | MEMBERS AREA. The main content area is divided into two columns. The left column is titled 'The DOI® System' and contains a collage of images representing various digital and physical media (clapperboard, camera, laptop, microscope, satellite dish, tablet). Below the images is text explaining the International DOI Foundation (IDF) and the DOI system. The right column features a 'Resolve a DOI Name' section with a text input field containing '10.1016/j.jnds.2011.11.002' and a 'SUBMIT' button. Below this is a 'DOI.ORG® In the News' section with several blue hyperlinks to news articles. At the bottom of the page, there is a footer with the text: 'Updated 9 April 2013 | DOI®, DOI.ORG® and shortDOI® are trademarks of the International DOI Foundation.'

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Type or paste a DOI name (e.g., 10.1000/182) into the text box below.

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## Nuclear Data Sheets

Volume 112, Issue 12, December 2011, Pages 2887–2996  
Special Issue on ENDF/B-VII.1 Library

### ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data

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# osti.gov and datacite.org want DOI's on all nuclear data in US; likely by end of FY14



## ■ DOI's are unique id's on a publication/dataset

- NNDC will generate them for NNDC-generated data
- If CSEWG & USNDP OK, we will assign DOI's for all US nuclear databases
- We decide on URL scheme
- We provide a permanent URL to a dataset, datacite.org maintains the DOI->URL redirect
- We promise to maintain URL's forever (or provide tombstone)

## ■ This is a very good thing

- Gives proper credit to evaluators
- Generates citations (always good for performance appraisals)

# How does this affect us?

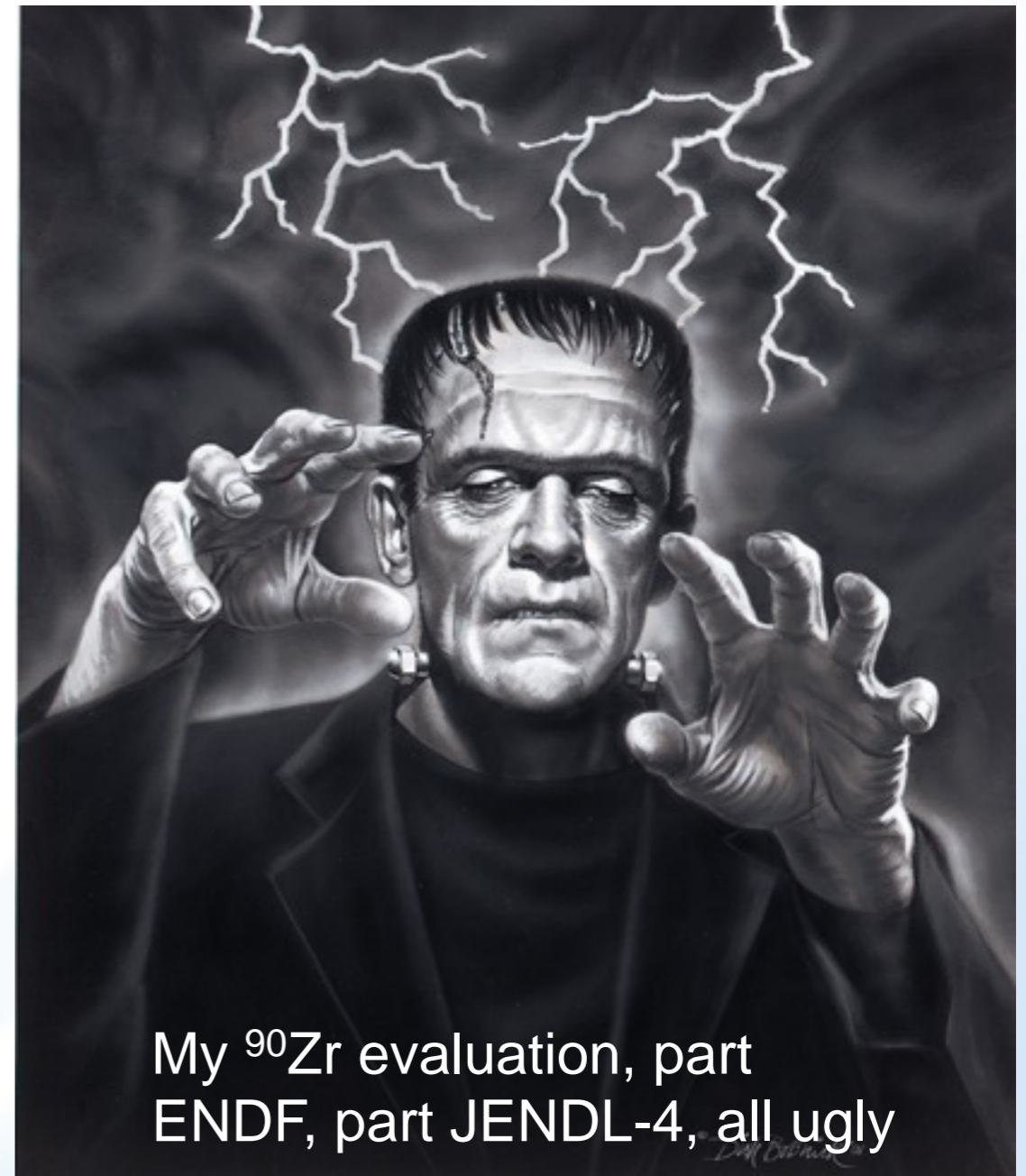


- **ENDF borrows from other libraries**

We'd like to be able to give proper credit; e.g a JAEA DOI for a JENDL-4.0 derived evaluation rather than an NNDC DOI

- **What about partial evaluations?**

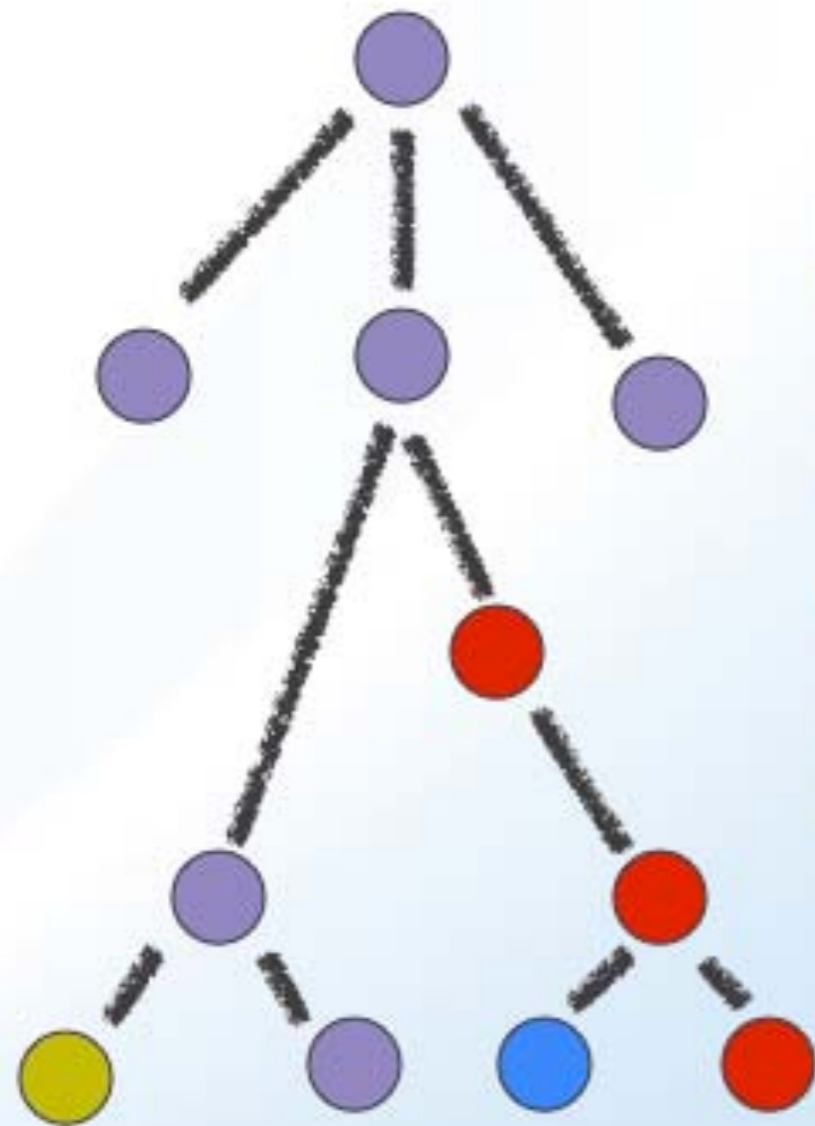
Fine grained DOI's (i.e. on evaluation parts) allow us to make Frankenevaluations with proper attribution.



My  $^{90}\text{Zr}$  evaluation, part ENDF, part JENDL-4, all ugly

# Preliminaries: documentation

Frankenevaluation (built from other evaluations);  
DOI's for each unique contribution, linked to URL of contribution



*Four DOIs,  
each linked to  
URL of top  
node of  
individual  
contribution*

Therefore,  
<documentation>  
is a legal element  
that may appear in  
numerous levels in  
the hierarchy

# Outline (roughly)

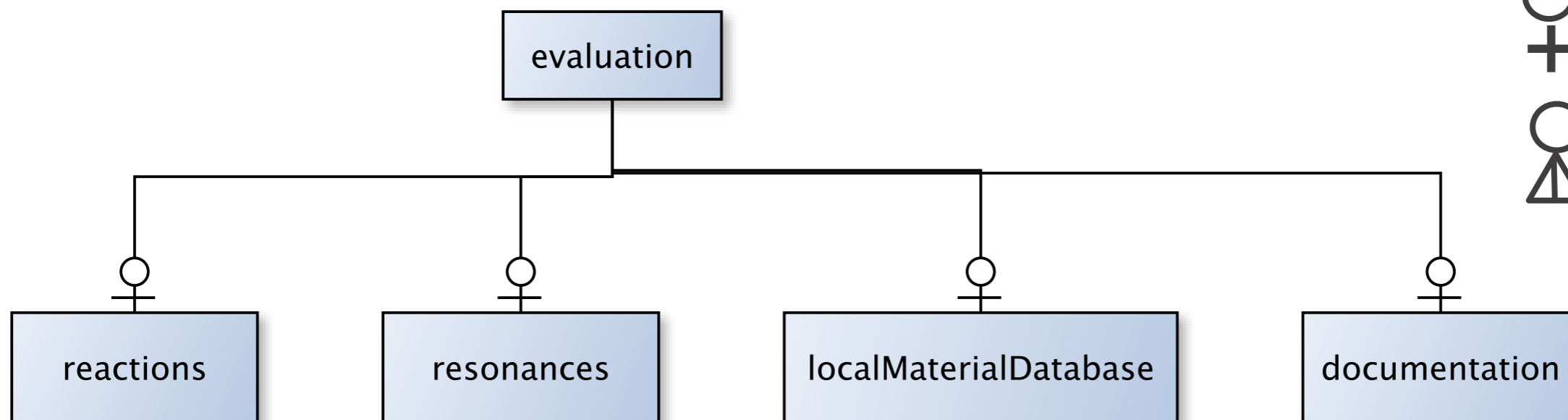
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# The top level: an <evaluation>



+ = 1  
○ = 1 or 0  
⊕ = Any num.

- **One temperature only; one projectile; one target material**
- **<localMaterialDatabase>** Fulfills need to override default material information with what is in a file (esp. for older evaluations) -- *will not cover, see C. Mattoon*
- **<reactions>** is the base of most kinds of reaction data
- **<resonances>** are for anything explicitly described by the R matrix (basically ENDF MF=2, MT=151)

# How to organize: Energy-major or Reaction-major?

## Energy-major is good?

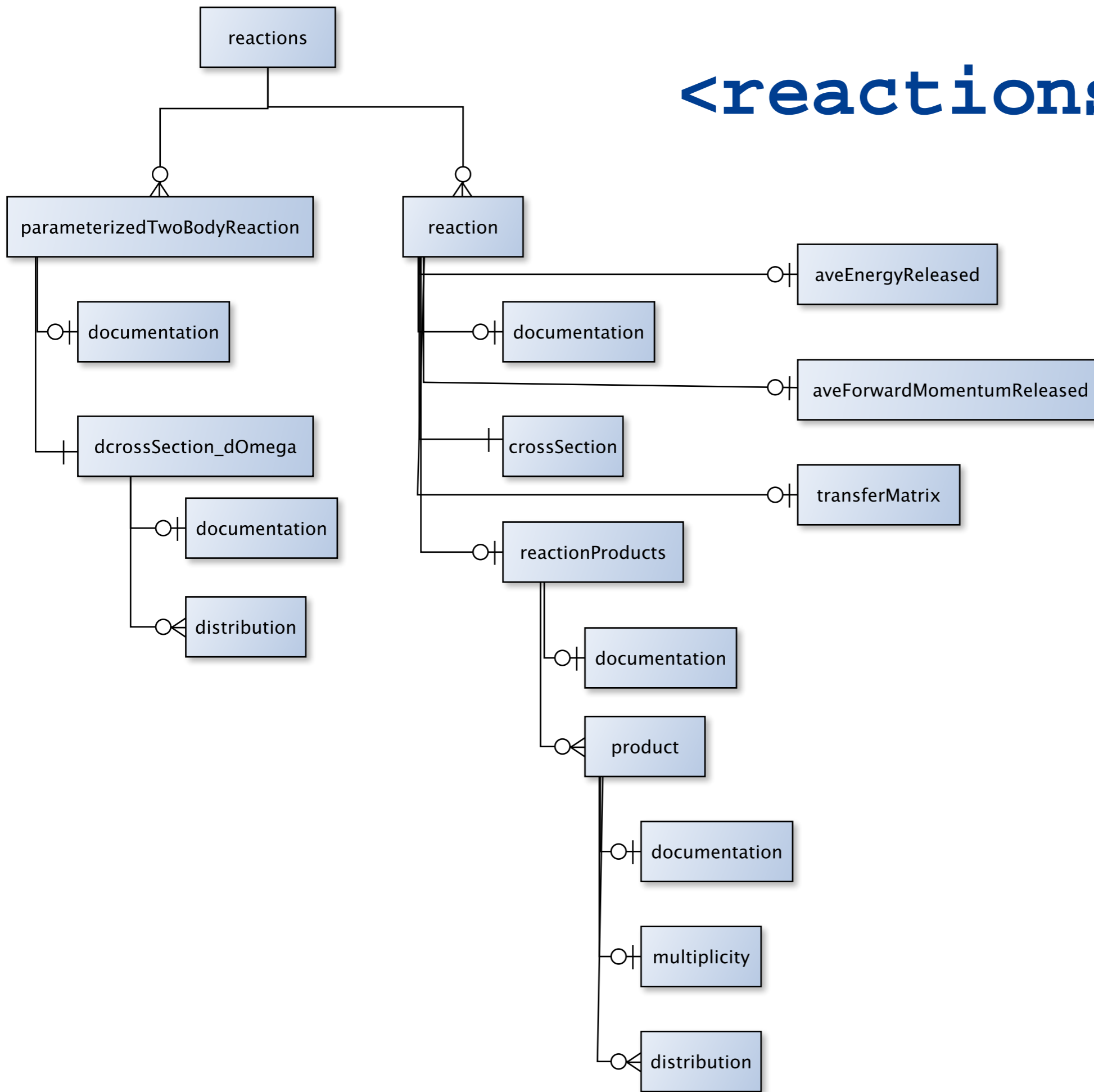
- Natural output of a reaction model such as EMPIRE or TALYS
- Energy-major is natural for sampling in Monte Carlo transport
- One can see at a glance what channels open and compete with one another
- Helps eliminate background cross sections in the resonance region

**On the balance,  
I recommend  
reaction-major**

## Energy-major is bad?

- Very difficult to plot say a cross section as a function of incident energy
- Very difficult to compare to experimental data
- Requires major refactoring of Monte Carlo codes are needed to get benefits
- Difficult to diagnose unphysical discontinuities as a function of incident energy
- Hard for deterministic codes to use
- Not familiar to users as legacy ENDF data is stored with the reaction-major arrangement

# <reactions>



+ = 1  
○ = 1 or 0  
⊕ = Any num.

# What do we need to know about to designate a reaction?

<reaction> or  
<parameterizedTwoBodyReaction>

- reaction designator
- kinematics type
- relativistic/non-relativistic flag
- ENDF MT (if appropriate)

**Should there be a shared <channel> markup?**

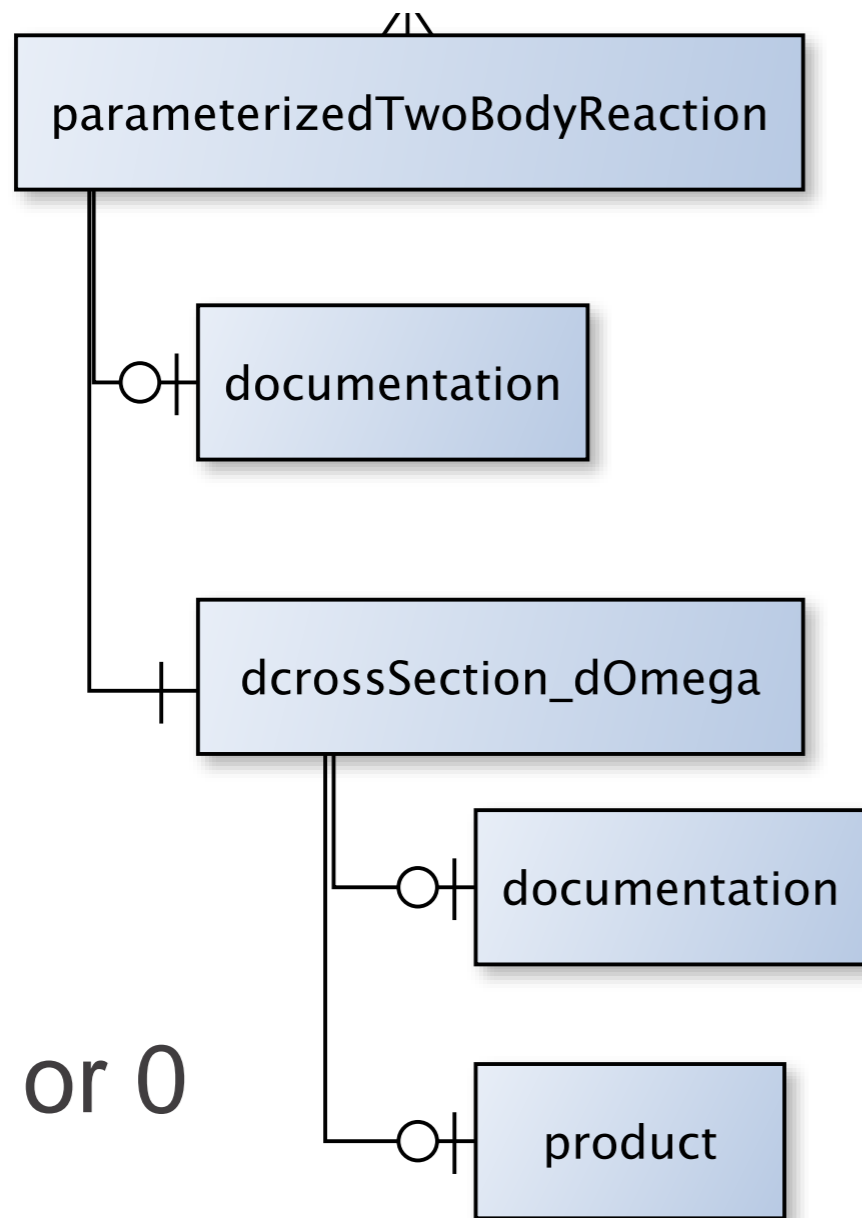
<resonances> (only 2 body)

- reaction designator
- kinematics type
- relativistic/non-relativistic flag
- ENDF MT (if appropriate)
- $s, l, J, \Pi$
- other user-definable quantum numbers (e.g.  $K$ )
- boundary parameter  $B_c$
- channel radius information
- sign of reduced width

# Specifying the kinematics with a kinType

kinType	Description
two-body	only two products are emitted per channel, the products are correlated, and only the center-of-mass angular distribution is needed in order to calculate the double-differential distribution
uncorrelated	the products are uncorrelated from each other, and a complete double-differential distribution is required in order to describe each product
activation	no outgoing particle distributions are needed since this is just activation data

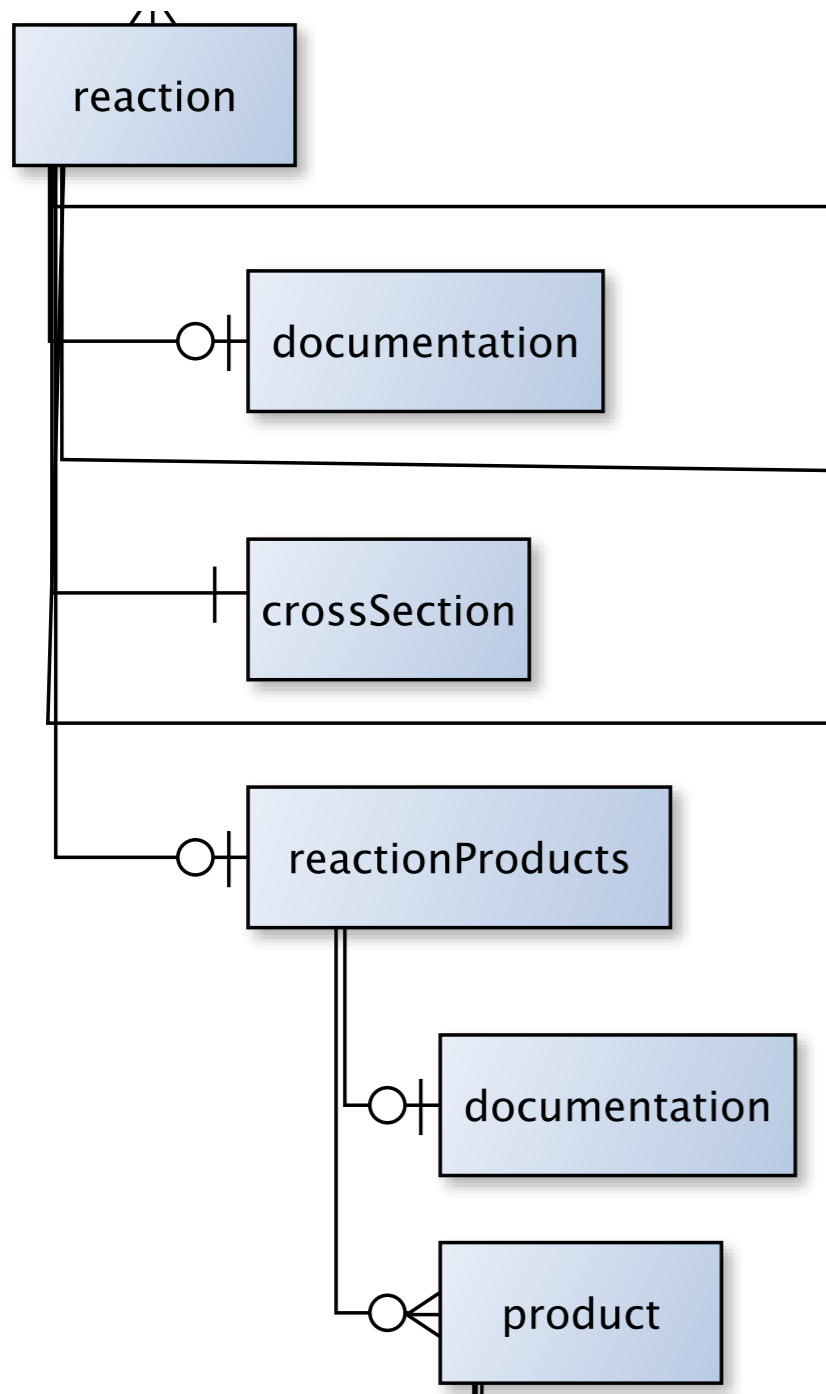
# Left branch: The `<parameterizedTwoBodyReaction>`



$+$  = 1  
 $\circ$  = 1 or 0  
 $+$   
 $\circ$   
 $\triangle$  = Any num.

- Two-body kinematics
- Store  $d\sigma(E)/d\Omega$  as parameterized data
- Sometimes it is the only way,
  - e.g. Large Angle Coulomb Scattering (LACS) data
- `<products>` element contains data `<form>`s (deep down)
- Used in a variety of special cases:
  - atomic scattering using Klein-Nishina formula
  - Thermal Scattering Law (TSL)
  - LACS

# Right branch: Familiar <reaction> tree



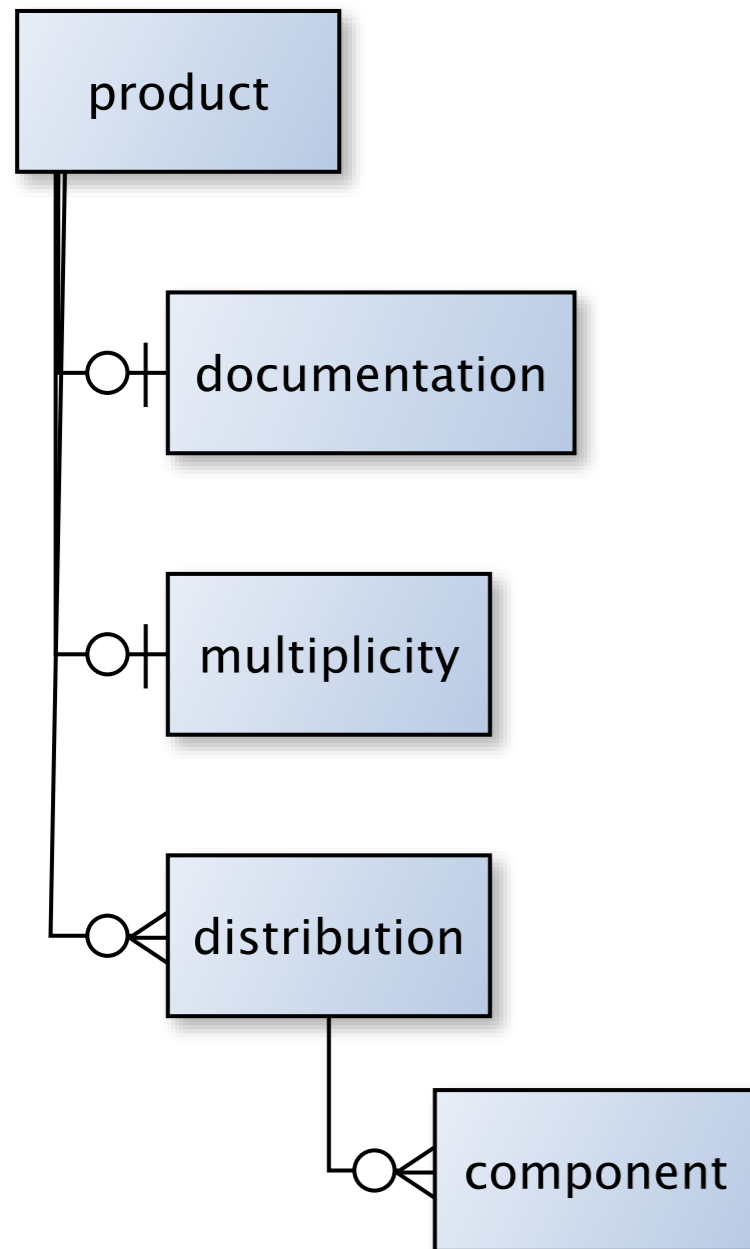
- Two-body reactions:

$$\frac{d\sigma(E)}{d\Omega} = \frac{1}{2\pi} \sigma(E) P(\mu|E)$$

- Everything else:

$$\frac{d\sigma(E)}{d\Omega dE'} = \frac{1}{2\pi} \sigma(E) P(\mu, E'|E)$$

# <product> element holds everything about a product

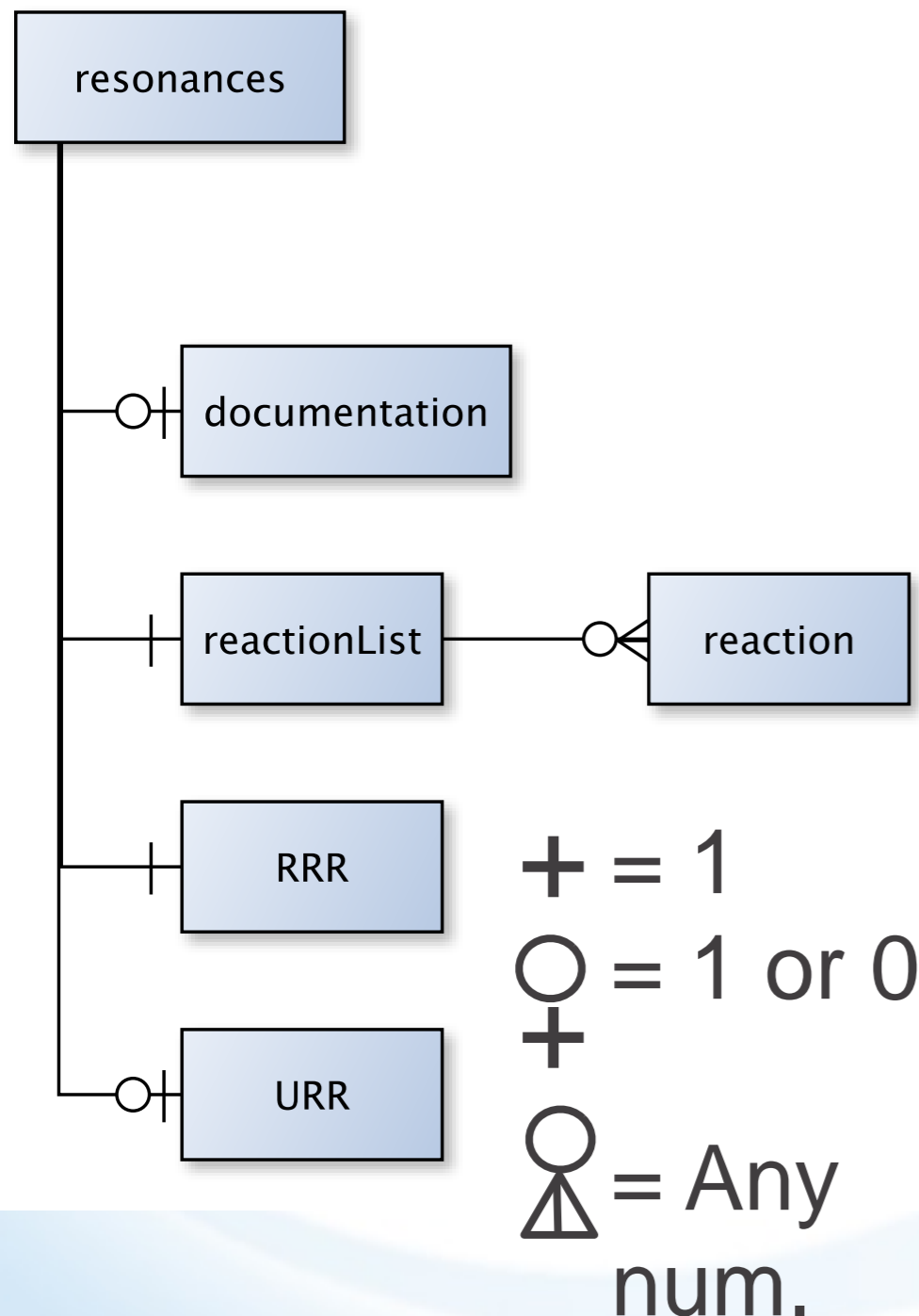


- Multiplicity may be just an `int` and be obvious ( $n, 2n$ )
- May be interpolation table (for nubar data)
- May want to rename for e.g. nubar
- May want  $P(\nu)$  for fission
- The distributions are divided into components; they are listed on the next slide

# A <distribution> collects all the possible representations of an observable together

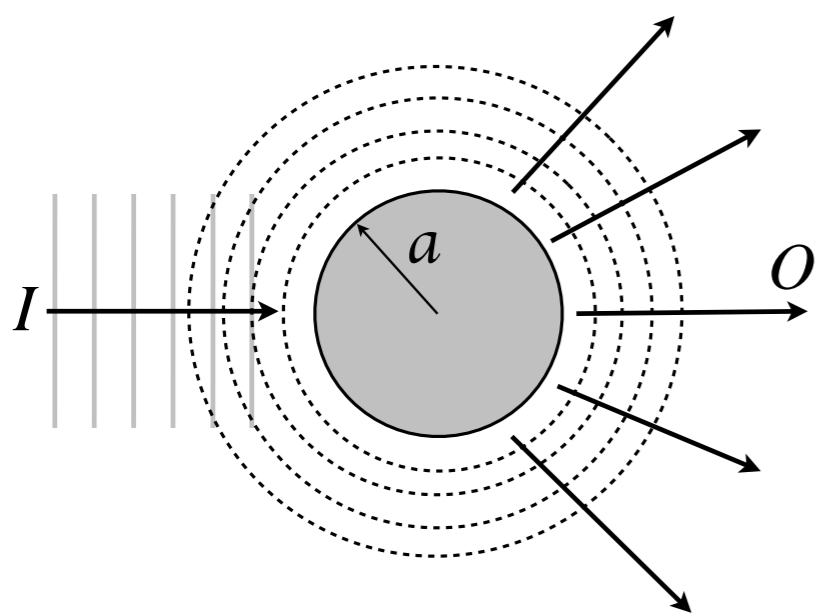
<component>	<form>	ENDF equivalent
angular	pointwise	MF4 LTT2
	Legendre	MF4 LTT1
	isotropic	MF4 LTT0
	recoil	MF6 LAW4
energy	pointwise	MF5 LF1
	Evaporation Spectrum	MF5 LF9
	Maxwellian	MF5 LF7
	Watt Spectrum	MF5 LF11
	Madland-Nix	MF5 LF12
	N-Body Phase Space	MF6 LAW6
energy-angular	Kalbach-Mann	MF6 LAW1 LANG2
angular-energy	pointwise	MF6 LAW7
uncorrelated	combination of 'angular' and 'energy'	MF4 and MF5

# <resonances>



- Standard ENDF MF=2, MT=151 (*but improved*)
- <reactionList>: the list of channels/reactions in this element
- <RRR> are the resolved resonances
- <URR> are average resonance data
- Based on R matrix theory, so helps to have some background

# R matrix background



$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_{\lambda} - E}$$

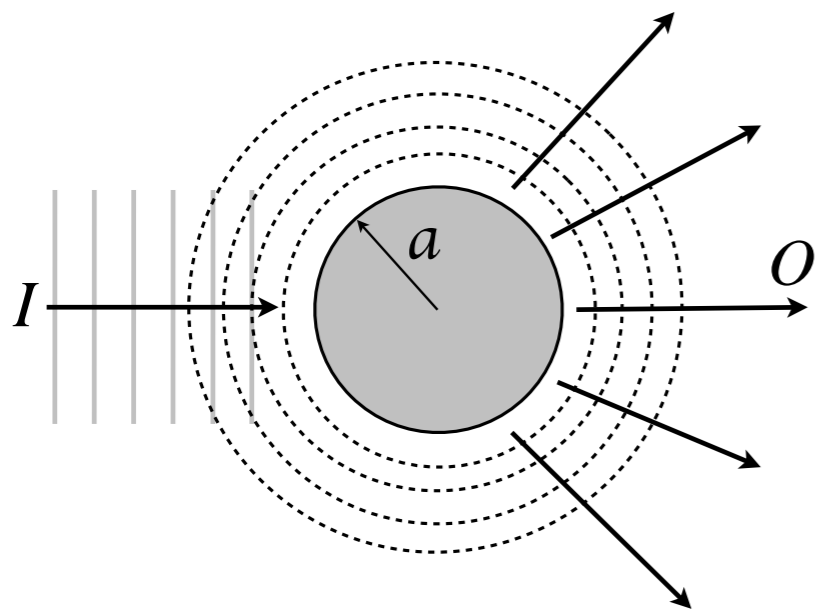
$$U_{cc'} = e^{-i(\varphi_c + \varphi_{c'})} \sqrt{P_c} \sqrt{P_{c'}} \times \{ [\mathbf{1} - \mathbf{R}(\mathbf{L} - \mathbf{B})]^{-1} [\mathbf{1} - \mathbf{R}(\mathbf{L}^* - \mathbf{B})] \}_{cc'}$$

Given by the WF

Boundary parameter

- Divide the universe with a spherical box.
- Outside box, use two-particle “free” wave functions
- Somewhere inside the box is the reaction zone; we don’t care about the details. Can write those details as the Green’s function solution of Schoedinger’s equation.
- The R matrix is the Green’s function.
- “Everything” can be written in terms of R; with it we can compute the scattering matrix U, so we have  $d\sigma/d\Omega$ .

# R matrix background



$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_{\lambda} - E}$$

$$U_{cc'} = e^{-i(\varphi_c + \varphi_{c'})} \sqrt{P_c} \sqrt{P_{c'}} \times \{[\mathbf{1} - \mathbf{R}(\mathbf{L} - \mathbf{B})]^{-1} [\mathbf{1} - \mathbf{R}(\mathbf{L}^* - \mathbf{B})]\}_{cc'}$$

- “Everything” can be written in terms of R; with it we can compute the scattering matrix U:

$$\sigma_c \equiv \sum_{c'} \sigma_{cc'} = 2\pi \lambda_c^2 (1 - \Re U_{cc})$$

$$\sigma_{cc'} = \pi \lambda_c^2 g_c |\delta_{cc'} - U_{cc'}|^2$$

$$\frac{d\sigma_{\alpha, \alpha'}(E)}{d\Omega} = \frac{1}{k^2 (2i + 1)(2I + 1)} \sum_{s, s'} \sum_{L=0}^{\infty} B_L(\alpha s, \alpha' s'; E) P_L(\mu)$$

$U_{cc'}$  is in there, but you do NOT want to see the equation

# R matrix background

- R matrix theory works for any two particles
- R matrix theory is exact
- R matrix theory is elegant

# R matrix background

- R matrix theory works for any two particles
- R matrix theory is exact
- R matrix theory is elegant

The original developers of ENDF should be tried for crimes against humanity for what they did to the R matrix

# Reiterating what we need for a channel

## <resonances> (only 2 body)

- reaction designator
- kinematics type
- relativistic/non-relativistic flag
- ENDF MT (if appropriate)
- $s, l, J, \Pi$
- other user-definable quantum numbers (e.g.  $K$ )
- boundary parameter  $B_c$
- channel radius information
- sign of reduced width

# RRR

- ENDF gives a lot of possible approximations and modifications to the R matrix; not all of these are faithful to R matrix theory
- ENDF provides a lot of tricks to help repair damage bad approximations cause
- ENDF also doesn't store  $\gamma_{\lambda c}$ ; it stores  $\Gamma_{\lambda c} = 2P_c \gamma_{\lambda c}^2$ . Should we store the partial widths?
- **We will need to grandfather in all of the ENDF approximations, no matter how bad they are.**
- **We will need to grandfather in all the ENDF tricks to fix the ENDF approximations, no matter how bad they are.**

# RRR

- The RRR doesn't need a complicated format, but it needs a complete one. All we need is a <table>:

$E_\lambda$	$\Gamma_{\lambda\text{tot}}$	$\Gamma_{\lambda\text{c0}}$	$\Gamma_{\lambda\text{c1}}$	$\Gamma_{\lambda\text{c2}}$	...
eV	eV	eV	eV	meV	...
1.23	9.433	0	2.33E-03	7.1	...
1.46	4.833	0	2.33E-03	4.6	...
3.45	1.78	1.78	0	0	...
...	...	...	...	...	...

- Must also store
  - background corrections to R matrix
  - background kludges to cross sections
  - approximation flags
  - overridden values of scattering radius, penetrability, shift, ...
  - outgoing distributions if not calculable from RR parameters?

# URR

- We don't know the resonances (they are unresolved)
- We assume
  - the resonance energies are distributed according to random matrix theory
  - the widths of the resonances are distributed with  $\chi^2$  distributions
- ENDF further assumes the resonances were given in SLBW
- With these assumptions, can compute
  - average cross sections
  - probability distributions for cross sections, e.g.  $P(\sigma|E)$  using NJOY's PURR module

# URR

- **Need: degree of freedom for each channel**
- **Need: table with:**
  - incident energy
  - average level spacing
  - average width for each channel
- **Need interpolation scheme for average parameters**
- **Should we also put a flag for the approximation (to allow other than SLBW)?**
- **Should we provide a spot for PURR probability distributions?**

# Outline (roughly)

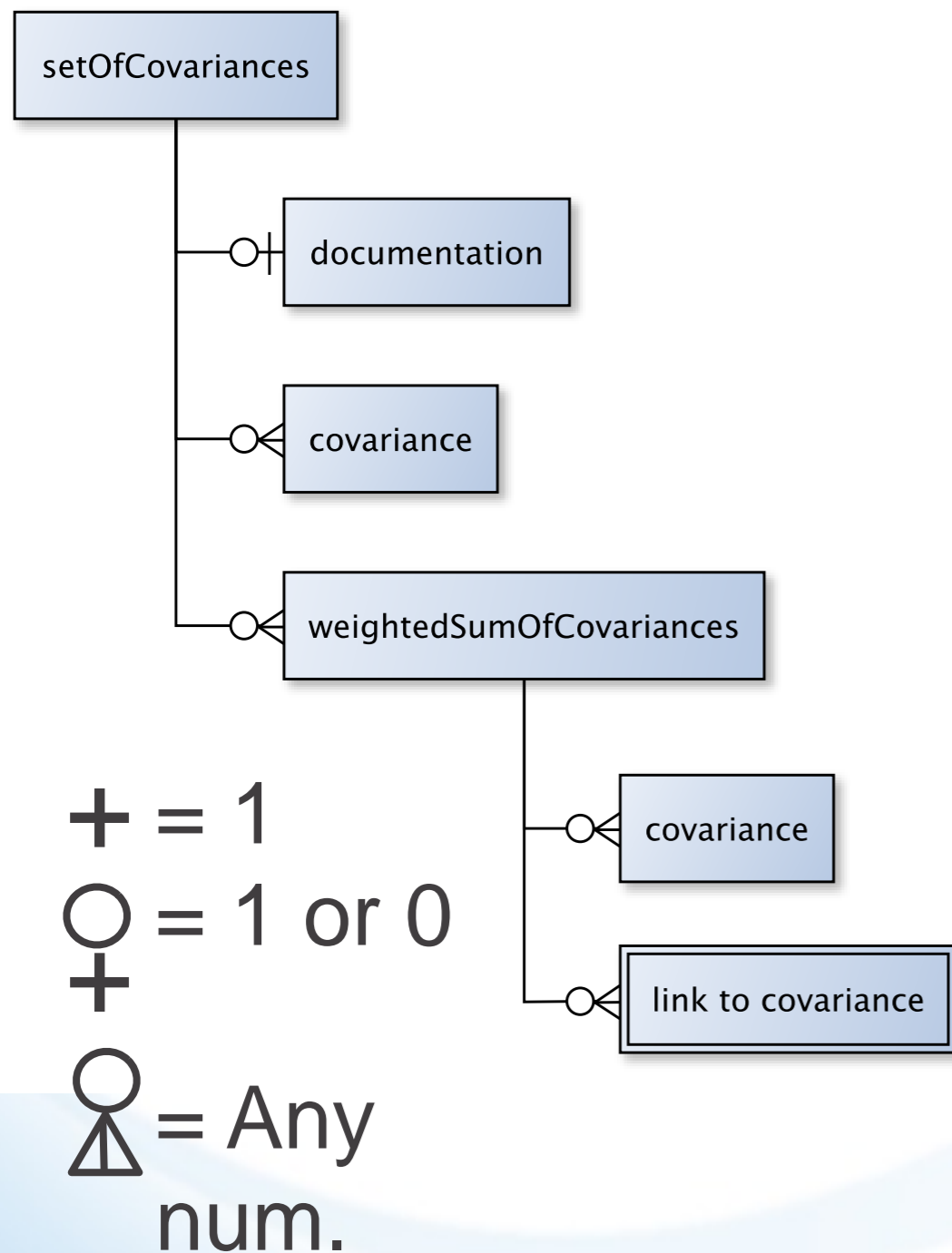
## HOUR 1

- Goals, use cases, etc.
- Preliminaries
  - low-level containers
  - designators
  - documentation
- The Top: `<evaluation>`
  - `<reactions>`
    - special two-body
    - plain old reactions
  - `<resonances>`
- The Other Top:  
`<setOfCovariance>`

## HOUR 2

- `<metaEvaluation>`
- Special cases:
  - Atomic data
  - Fission
  - Fission Product Yields
  - Large Angle Coulomb Scattering
  - Particle production
  - Thermal Scattering Law
- Odds-n-ends
- Thanks & Blame

# The Other Top Level: <setOfCovariances>

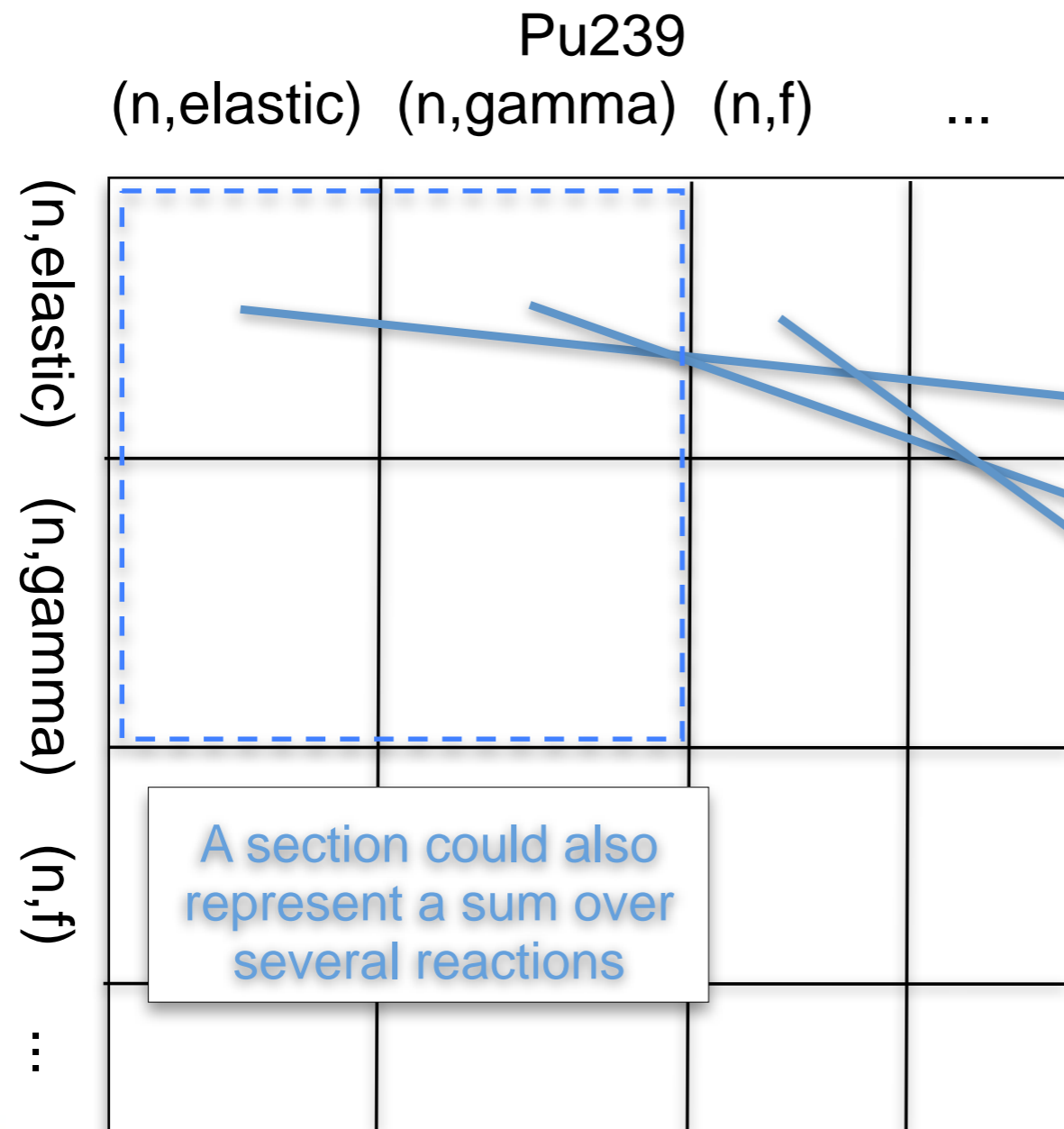


- Covariances can be big
- They can encode correlations across material, reaction, observable

*However*

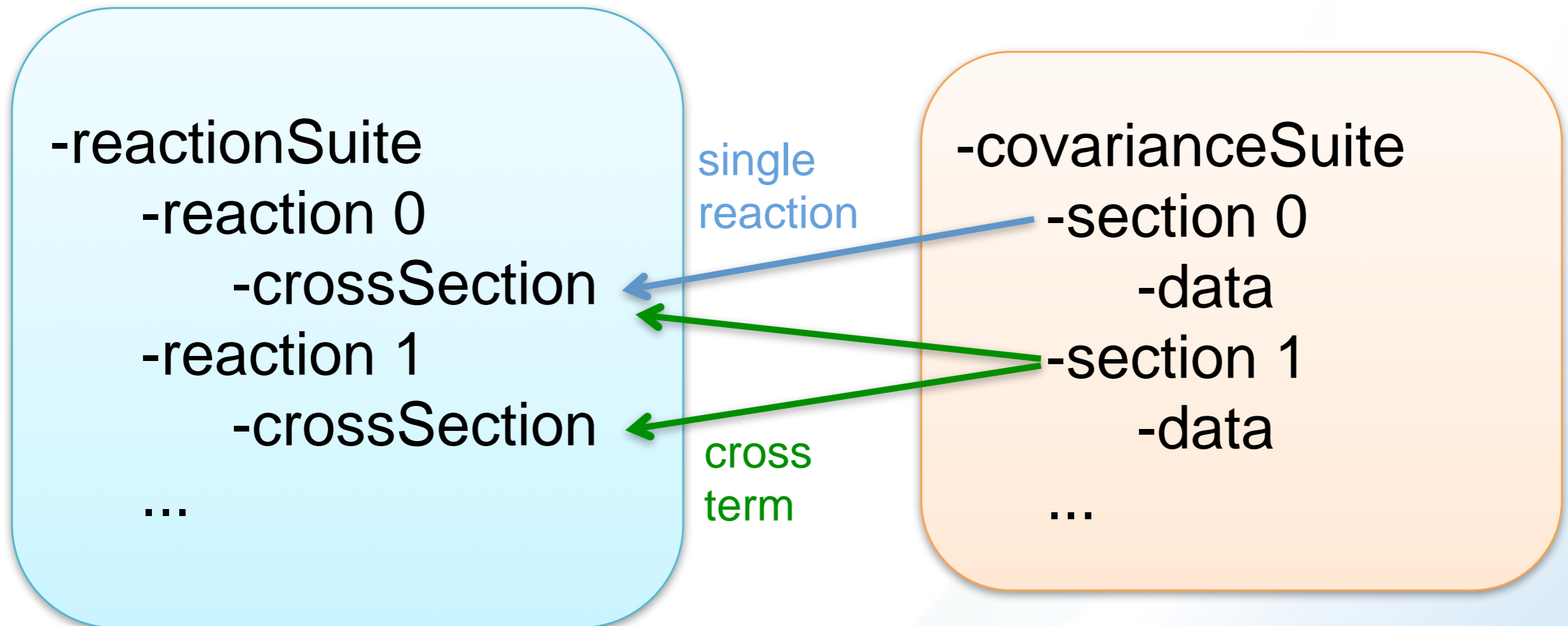
- They are **just matrices**
- You just have to know how to **pack them**
- **<setOfCovariances> is easy way to group them**

# View covariances using block matrix construction



-covarianceSuite  
-section 0  
-data  
-section 1  
-data  
-section 2  
-data  
...

# Blocks of a covariance have to be associated with the data in the `<form>` elements

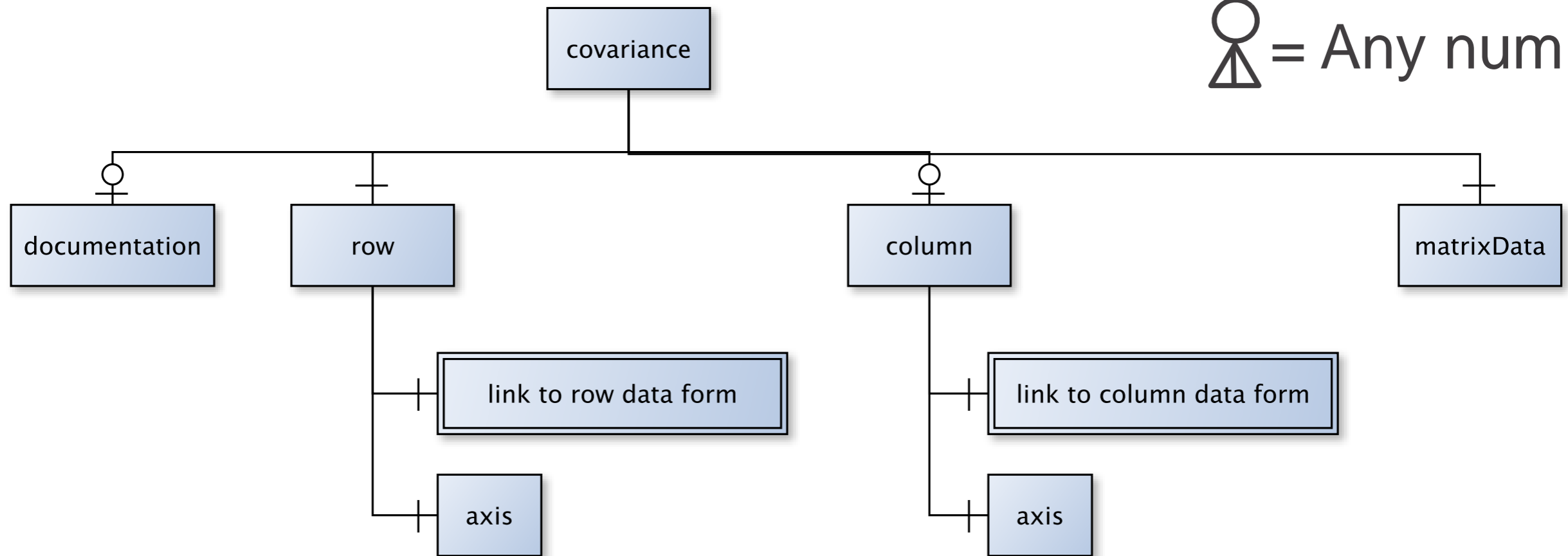


## ■ Why?

- `<form>`s have the data
- `<covariance>` are the covariance on the data

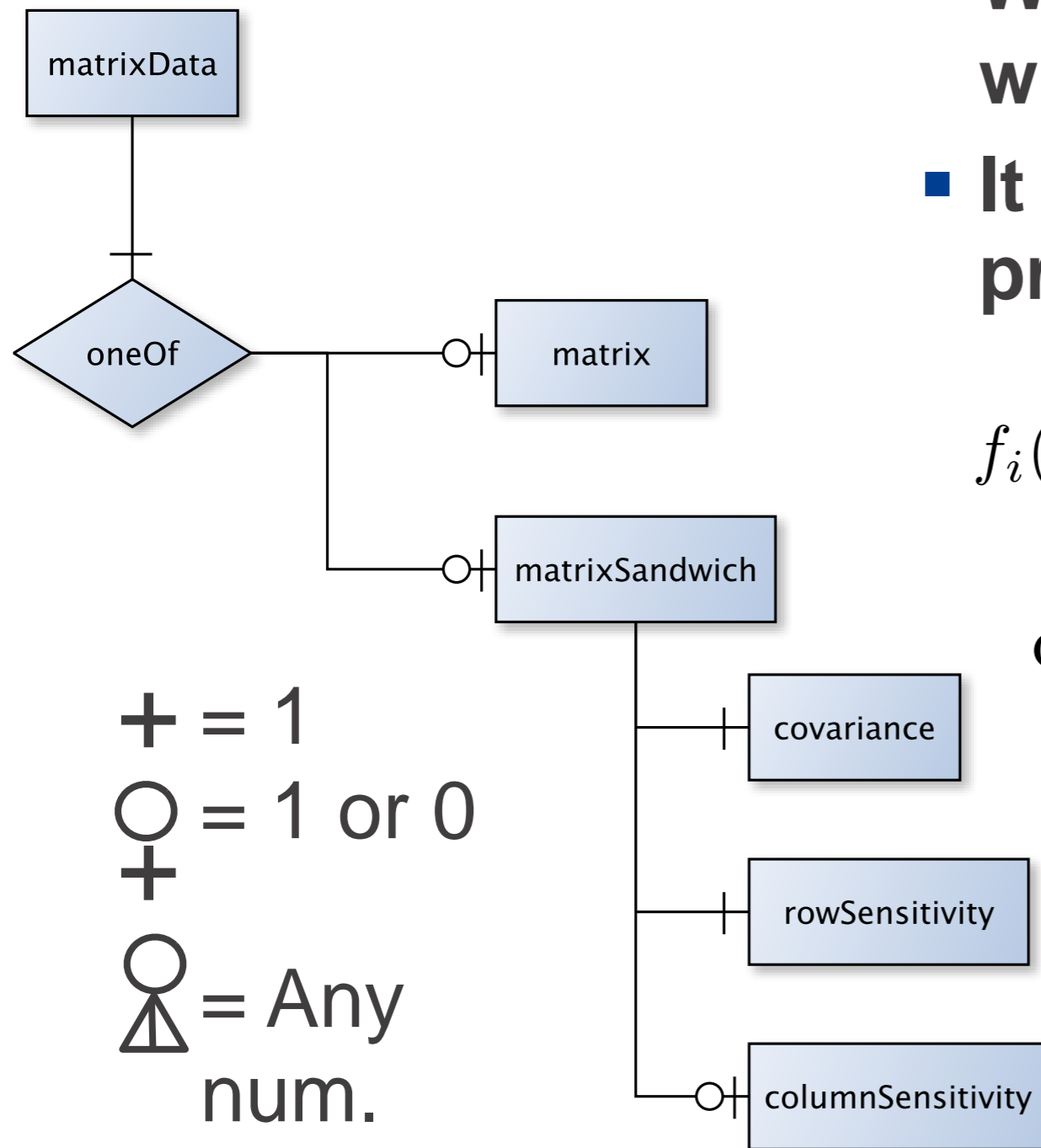
# covariance

+ = 1  
○ = 1 or 0  
+ = 1 or 0  
○ = Any num.  
△ = Any num.



- Need `<row>` to describe the `<form>` ↔ `<covariance>` mapping
- If cross-correlation, need `<column>` too
- The matrix itself is in `<matrixData>`

# matrixData



- We understand <matrix>, but what is a <matrixSandwich>?
- It is just sandwich rule for propagating covariance:

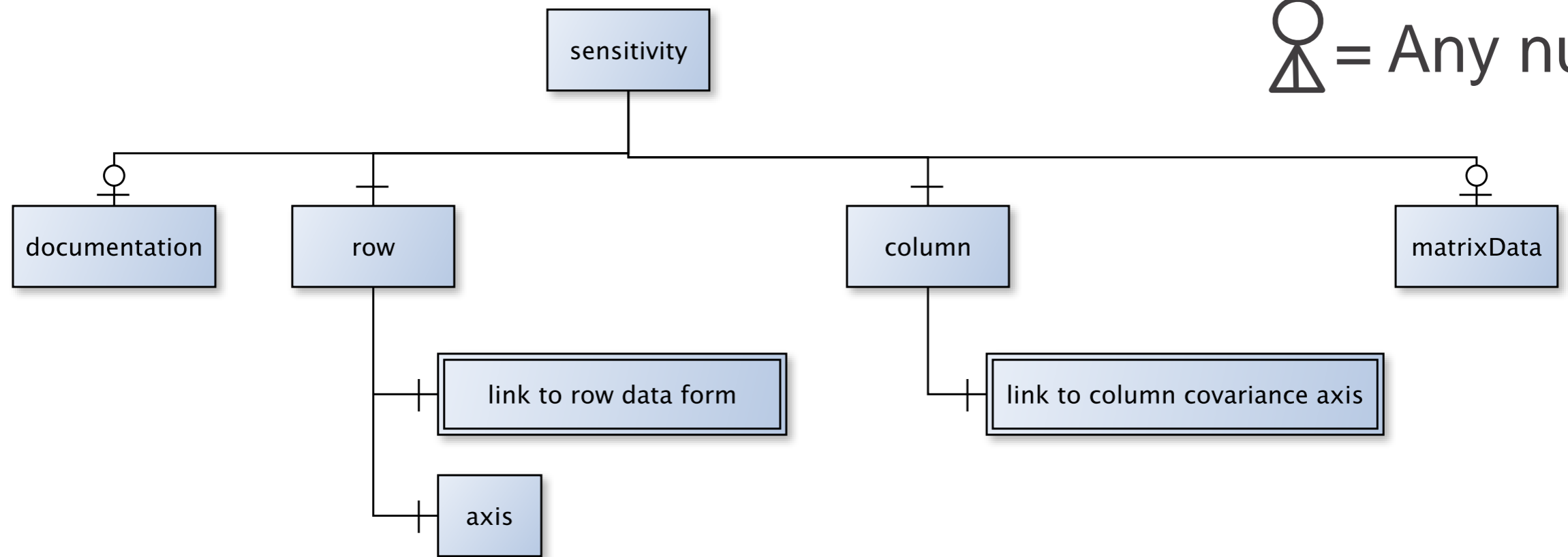
$$f_i(\vec{x}) \approx f_i(\langle \vec{x} \rangle) + \sum_j \frac{\partial f_i(\langle \vec{x} \rangle)}{\partial x_j} (x_j - \langle x_j \rangle)$$

$$\text{COV } f_{ij} = \sum_{i' j'} \text{SENS}_{ii'} \text{COV } x_{i' j'} \text{SENS}_{j' j}$$

- For cross-correlations, need two sensitivity matrices

# sensitivity

+ = 1  
○ = 1 or 0  
⊕ = Any num.  
⊙ = Any num.



- Sensitivity can be given by equation (e.g. RRR)
- Or can be a matrix
- <row> links to data form
- <column> links to parameter covariance
- Both row and column must be specified

# Outline (roughly)

## HOUR 1

- Goals, use cases, etc.
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- The Top: `<evaluation>`
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  - `<resonances>`
- The Other Top:  
`<setOfCovariance>`

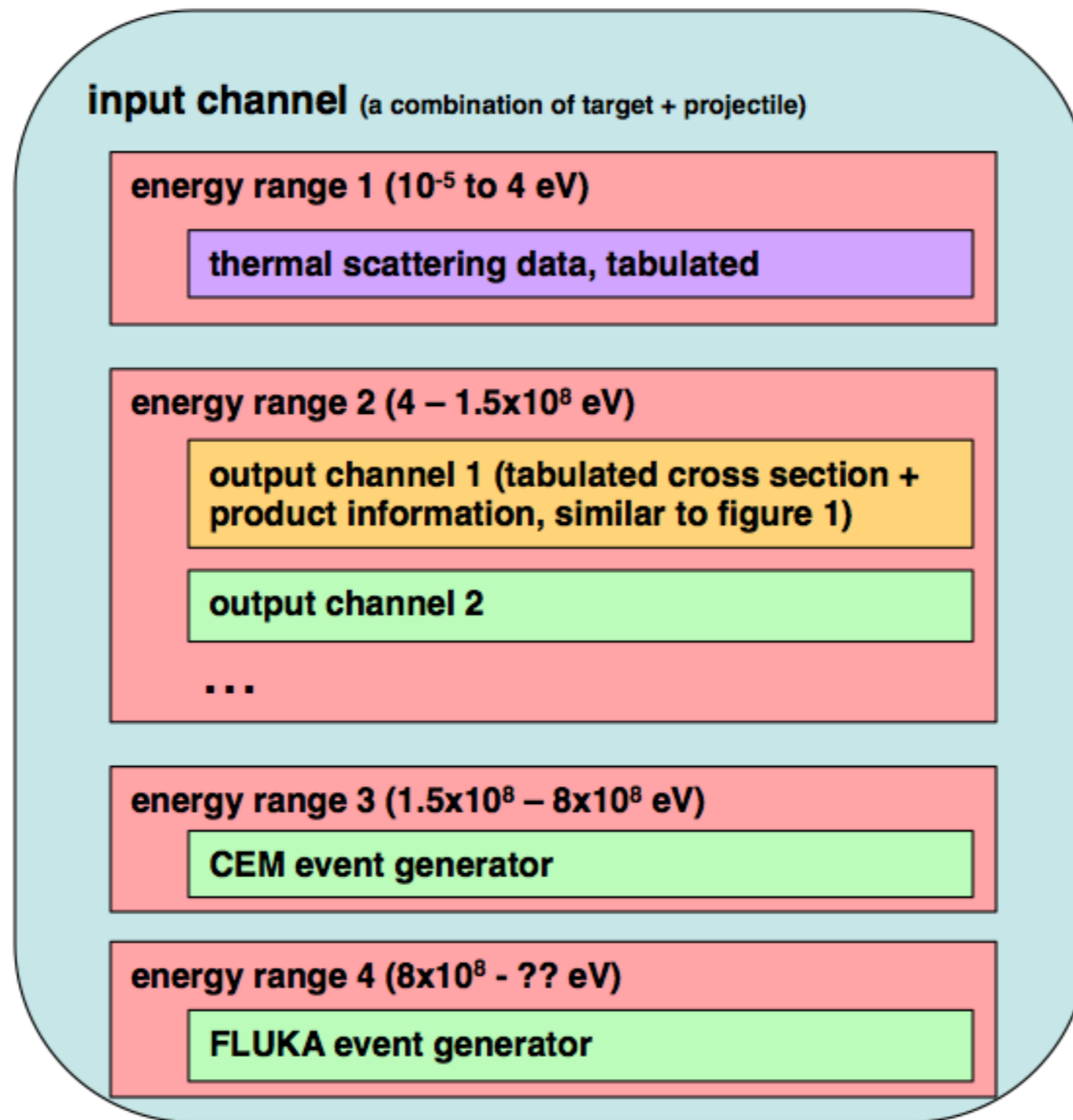
## HOUR 2

- `<metaEvaluation>`
- Special cases:
  - Atomic data
  - Fission
  - Fission Product Yields
  - Large Angle Coulomb Scattering
  - Particle production
  - Thermal Scattering Law
- Odds-n-ends
- Thanks & Blame

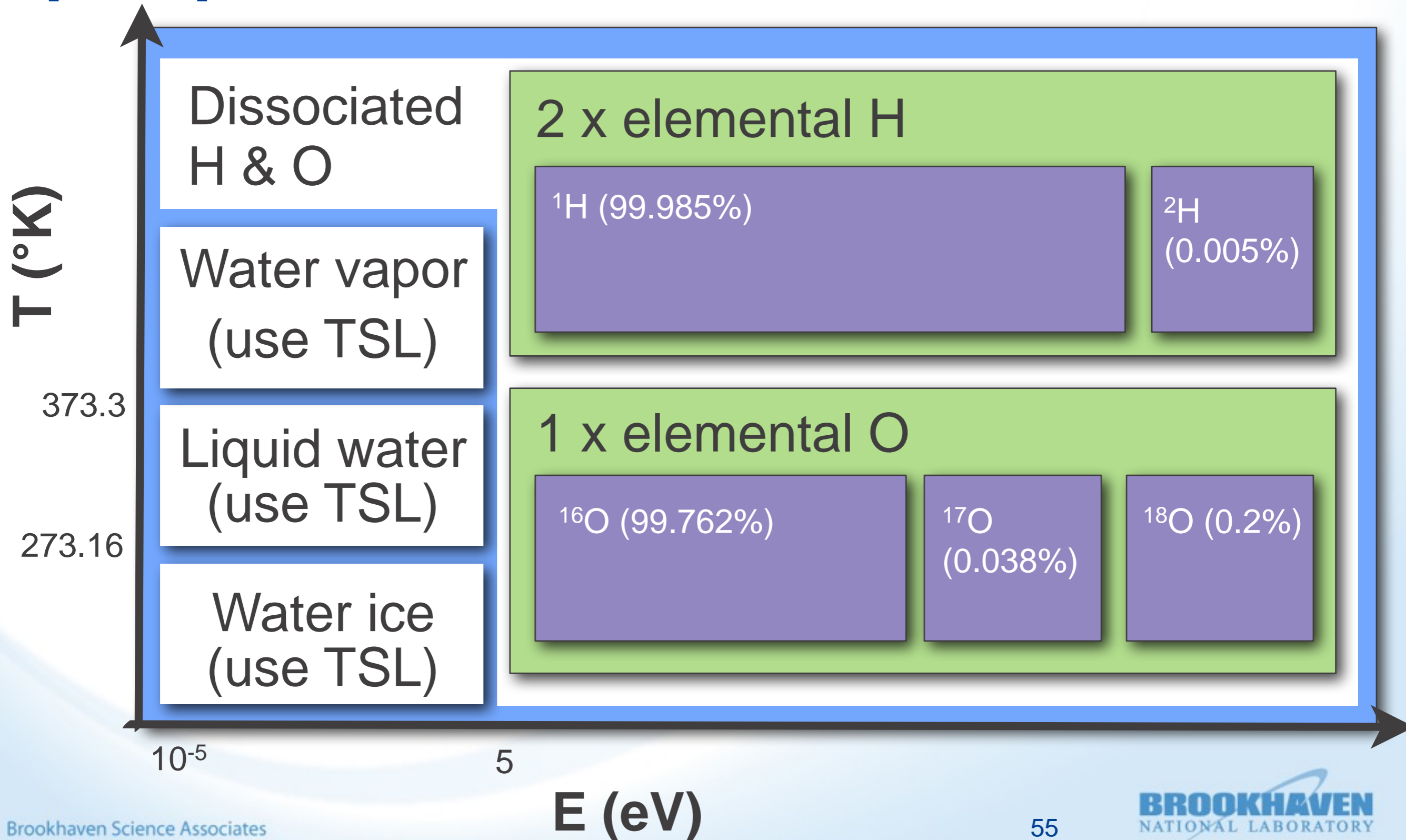
# Gluing together evaluations: <metaEvaluation>

- **An xsdir-like facility is used by many institutions to glue together evaluations**
  - In LANL's MCNP code system, the xsdir file allows one to connect the thermal neutron scattering data with the neutron nuclear reaction data and even various high energy models such as CEM.
  - The LLNL transport codes AMTRAN and Mercury both allow one to define target macros to describe the material in a zone.
  - AECL, there is another, similar, facility to connect thermal neutron scattering data at different temperatures and even different phases of the target material.
- **There are other uses for connecting evaluations:**
  - Defining elemental evaluations
  - Grouping data on same target, but heated to different temperatures
  - Defining generic fission fragments through a weighted average of fission fragment evaluations
  - Putting together the parts of a TSL evaluation at fixed temperature, but including all the scatterers.
  - ...

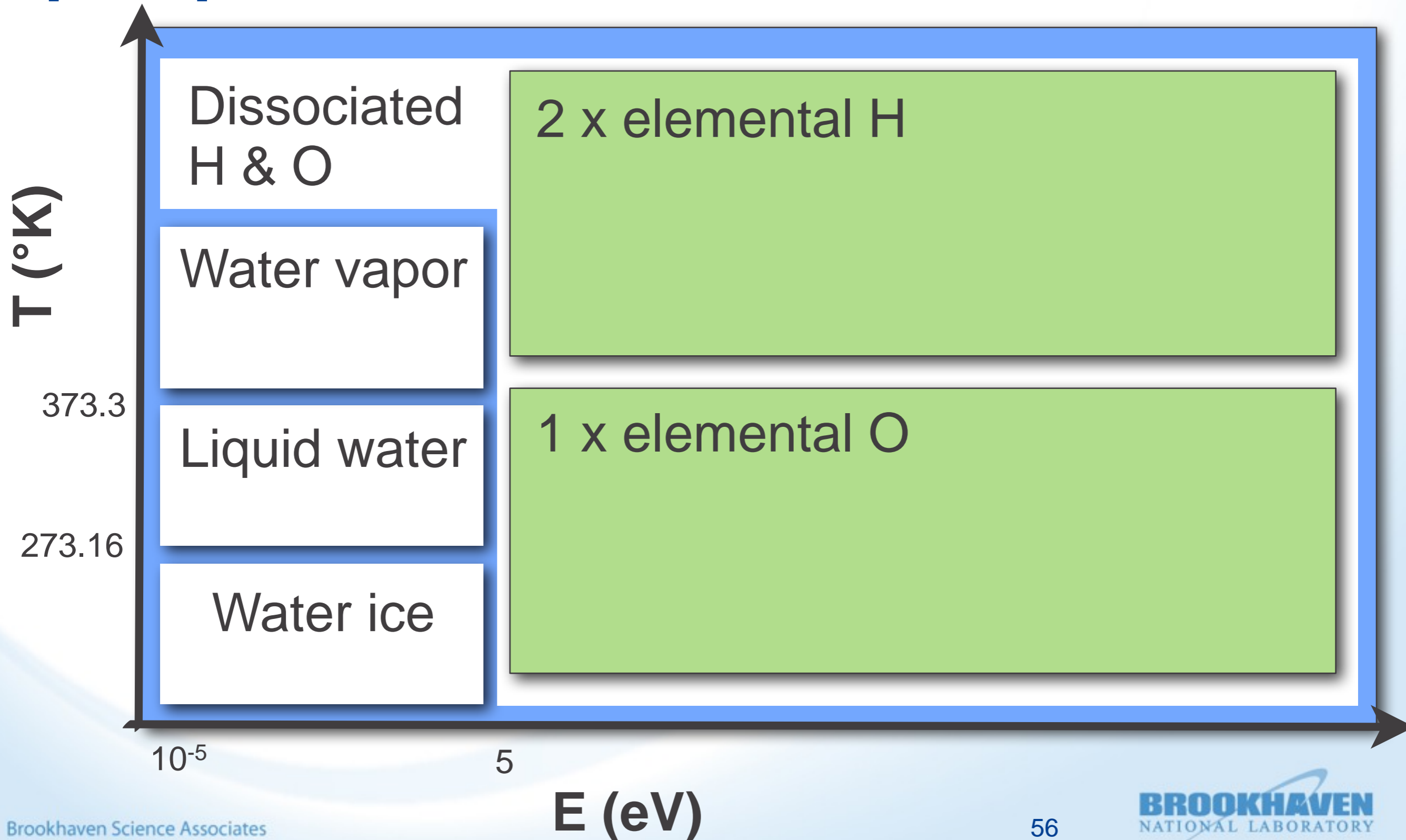
# Once we allow very energetic projectiles, we need to consider model-switching



# Think about water from a neutron's perspective



# ... versus water from an electron's perspective



# Defining a metaTarget

```
<metaTarget name="water" projectile="n">
  <documentation>...</documentation>
  <axes>
    <axis index="0" label="temperature_bounds" unit="K" interpolation="linear,flat"
    length="4">
      0.0 273.16 373.16 1e9</axis>
    <axis index="1" label="incident_energy_bounds" unit="eV"
    interpolation="linear,flat" length="3">
      1e-5 5 1e9 </axis>
  </axes>
  <referredTargets>
    <referredTarget index="0" name="Water ice" xlink:type="simple" xlink:href="..."
    axisCoords="0,0" stoichiometricFraction="1.0"/>
    <referredTarget index="1" name="Liquid water" xlink:type="simple" xlink:href="..."
    axisCoords="1,0" stoichiometricFraction="1.0"/>
    <referredTarget index="2" name="Dissociated water" xlink:type="simple"
    xlink:href="..." axisCoords="2,0" stoichiometricFraction="1.0"/>
    <referredTarget index="2" name="Dissociated water" xlink:type="simple"
    xlink:href="..." axisCoords="0,1" stoichiometricFraction="1.0"/>
    <referredTarget index="2" name="Dissociated water" xlink:type="simple"
    xlink:href="..." axisCoords="1,1" stoichiometricFraction="1.0"/>
    <referredTarget index="2" name="Dissociated water" xlink:type="simple"
    xlink:href="..." axisCoords="2,1" stoichiometricFraction="1.0"/>
  </referredTargets>
</metaTarget>
```

# Defining a metaTarget

names it and  
defines the valid  
projectile

```
<metaTarget name="water" projectile="n">
```

```
<documentation>...</documentation>
```

```
<axes>
```

```
<axis index="0" label="temperature_bounds" unit="K" interpolation="linear,flat"  
length="4">
```

```
0.0 273.16 373.16 1e9</axis>
```

```
<axis index="1" label="incident_energy_bounds" unit="eV"  
interpolation="linear,flat" length="3">
```

```
1e-5 5 1e9 </axis>
```

```
</axes>
```

```
<referredTargets>
```

```
<referredTarget index="0" name="Water ice" xlink:type="simple" xlink:href="..."  
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```

```
<referredTarget index="1" name="Liquid water" xlink:type="simple" xlink:href="..."  
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```

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<referredTarget index="2" name="Dissociated water" xlink:type="simple"  
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```

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<referredTarget index="2" name="Dissociated water" xlink:type="simple"  
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<referredTarget index="2" name="Dissociated water" xlink:type="simple"  
xlink:href="..." axisCoords="2,1" stoichiometricFraction="1.0"/>
```

```
</referredTargets>
```

```
</metaTarget>
```

# Defining a metaTarget

gotta say where we got it from

```
<metaTarget name="water" projectile="n">
  <documentation>...</documentation>
  <axes>
    <axis index="0" label="temperature_bounds" unit="K" interpolation="linear,flat"
      length="4">
      0.0 273.16 373.16 1e9</axis>
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      xlink:href="..." axisCoords="0,1" stoichiometricFraction="1.0"/>
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      xlink:href="..." axisCoords="1,1" stoichiometricFraction="1.0"/>
    <referredTarget index="2" name="Dissociated water" xlink:type="simple"
      xlink:href="..." axisCoords="2,1" stoichiometricFraction="1.0"/>
  </referredTargets>
</metaTarget>
```

# Defining a metaTarget

defines regions of  
validity of  
metaTarget parts

```
<metaTarget name="water" projectile="n">
```

```
<documentation>...</documentation>
```

```
<axes>
```

```
<axis index="0" label="temperature_bounds" unit="K" interpolation="linear,flat"  
length="4">
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```
0.0 273.16 373.16 1e9</axis>
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<axis index="1" label="incident_energy_bounds" unit="eV"  
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1e-5 5 1e9 </axis>
```

```
</axes>
```

```
<referredTargets>
```

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xlink:href="..." axisCoords="2,0" stoichiometricFraction="1.0"/>
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xlink:href="..." axisCoords="1,1" stoichiometricFraction="1.0"/>
```

```
<referredTarget index="2" name="Dissociated water" xlink:type="simple"  
xlink:href="..." axisCoords="2,1" stoichiometricFraction="1.0"/>
```

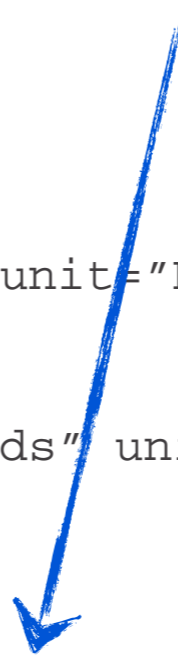
```
</referredTargets>
```

```
</metaTarget>
```

# Defining a metaTarget

defines the  
metaTarget parts

```
<metaTarget name="water" projectile="n">
  <documentation>...</documentation>
  <axes>
    <axis index="0" label="temperature_bounds" unit="K" interpolation="linear,flat"
      length="4">
      0.0 273.16 373.16 1e9</axis>
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  <referredTargets>
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      axisCoords="0,0" stoichiometricFraction="1.0"/>
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      axisCoords="1,0" stoichiometricFraction="1.0"/>
    <referredTarget index="2" name="Dissociated water" xlink:type="simple"
      xlink:href="..." axisCoords="2,0" stoichiometricFraction="1.0"/>
    <referredTarget index="2" name="Dissociated water" xlink:type="simple"
      xlink:href="..." axisCoords="0,1" stoichiometricFraction="1.0"/>
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      xlink:href="..." axisCoords="1,1" stoichiometricFraction="1.0"/>
    <referredTarget index="2" name="Dissociated water" xlink:type="simple"
      xlink:href="..." axisCoords="2,1" stoichiometricFraction="1.0"/>
  </referredTargets>
</metaTarget>
```



# Notes on metaTarget concept

- `referredTarget` points to a `reactionSuite` or another `metaTarget`
- `stoichiometricFraction` tag lets you specify, say, chemical or isotopic make-up if multiple `referredTargets` are allowed
- `stoichiometricFraction` better add up to 1!
- outside of parameter ranges in axis tags, the `metaTarget` does not exist
- `metaTarget` only valid for listed `projectile`
- need to make sure every region in `axes` covered by a `referredTarget`
- `metaTargets` are often reusable across different libraries

# Outline (roughly)

## HOUR 1

- Goals, use cases, etc.
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  - designators
  - documentation
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  - `<reactions>`
    - special two-body
    - plain old reactions
  - `<resonances>`
- The Other Top:  
`<setOfCovariance>`

## HOUR 2

- `<metaEvaluation>`
- Special cases:
  - Atomic data
  - Fission
  - Fission Product Yields
  - Large Angle Coulomb Scattering
  - Particle production
  - Thermal Scattering Law
- Odds-n-ends
- Thanks & Blame

# Special case: Atomic data

- Includes electromagnetic (electrons & gammas) interactions with electronic orbitals of an atom
- Most needs we have already addressed:
  - **variable yields of electrons and gammas**
  - **binding energies of shells (material database issue)**
  - **tabulated energy transferred to atom (need a special `<form>` in the `<distribution>`)**
- but...

# Special case: Atomic data

- For (in)coherent photon scattering, it is more efficient and appropriate to use parameterized form of two body reactions in a `<parameterizedTwoBodyReaction>`

- Incoherent scattering:

$$\frac{d\sigma_{\text{incoh}}(E, E', \mu)}{d\mu} = S(q; Z) \frac{d\sigma_{KN}(E, E', \mu)}{d\mu}$$

- Coherent scattering:

$$\frac{d\sigma_{\text{coh}}(E, E', \mu)}{d\mu} = \pi r_0^2 (1 + \mu^2) \left\{ [F(q; Z) + F'(E)]^2 + F''(E)^2 \right. \\ \left. \dots \right.$$

- **Atomic form factors should go in there own special `<dcrossSection_dOmega>` `<form>`**

# Special case: Fission

- In my mind, this is a regular channel, even though in reality it is a large collection of channels leading to an even larger number of decay products.
- We have all the parts in the top level to support it, but there are things we can do to make life easier:
  - Allow reaction aliases “total\_fission”, “1st\_chance\_fission”, “2nd\_chance\_fission”, etc. Probably reaction designator annotations can help with this.
  - Allow fission to be broken out by chance, but ensure sum rules obeyed.
  - Allow FPY data
  - Allow prompt, delayed and total nubar. Ensure sum rules obeyed.
  - Allow PFNS using tables or Madland-Nix model
  - Allow P(nu) data
  - Break out delayed data by time group and put each group's delayed nubar with the groups DFNS and time constant
  - Allow the emission of neutrons, gammas, fission fragments (FF), electrons, neutrinos
  - Allow all ejected particles to have variable multiplicities and energy-angle spectra
  - Allow for semi-derived data such as energy release broken out into components

# Special case: Fission Product Yield

- Held discussions with R. Mills at last WPEC-SG37 meeting in Paris
- Results presented to the SG and was well received
- That talk now follows

# Brainstorming GND Markup for Fission Product Yields

*David Brown*

*NNDC, Brookhaven National Laboratory*

**BROOKHAVEN**  
NATIONAL LABORATORY

*a passion for discovery*



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

# The Generalized Nuclear Data (GND) format is a possible replacement for the ENDF format

- Under active development under auspices of WPEC/SG-38
- Lead by D. McNabb, outgrowth of earlier LLNL (US) project
- Initial focus was neutron and charged particle transport data
- Now looking to other ENDF format/data, in particular, FPY formats

# Fission Product Yield tables give the number of nuclides of a given type, post-fission

- **Independent Fission Product Yields (IFPY)**

These are the fragments immediately after fission and de-excitation from prompt neutron and gamma emission

- **Cumulative Fission Product Yields (CFPY)**

These are the fragments after they are allowed to undergo all (beta and other) decays

- If you think about it, if you know all possible decays of all fission products, you can construct a matrix that relates the IFPY and CFPY.

- Both A. Sonzogni and R. Mills have codes that can compute this matrix from the decay sublibrary
- Implies only one of IFPY and CFPY needed

# There are two MT's in ENDF that use the same FPY format. MT=454 is IFPY and MY=459 is CFPY.

## 8.3.1 Formats

The structure of a section always starts with a HEAD record and ends with a SEND record. Sets of fission product yield data are given for one or more incident energies. The sets are ordered by increasing incident energy. For a particular energy the data are presented by giving four parameters (ZAFP, FPS, YI, and DYI in MT=454 and ZAFP, FPS, YC, and DYC in MT 459) for each fission product state. The data are first ordered by increasing values of ZAFP. If more than one yield is given for the same (Z,A) the data are ordered by increasing value of the state designator (FPS). The structure for a section is:

```
[MAT, 8, MT/ ZA, AWR, LE+1, 0, 0, 0]HEAD
[MAT, 8, MT/ E1, 0.0, LE, 0, NN, NFP/ Cn(E1) ]LIST
[MAT, 8, MT/ E2, 0.0, I, 0, NN, NFP/ Cn(E2) ]LIST
[MAT, 8, MT/ E3, 0.0, I, 0, NN, NFP/ Cn(E3) ]LIST
-----
[MAT, 8, 0 /0.0, 0.0, 0, 0, 0, 0]SEND
```

where MT=454 for independent yield data, and MT=459 for cumulative yield data. There are (LE+1) LIST records.

**fudge/legacy/convert/endfFileToGND.py**  
**has readMF8 function**

# This is what the ENDF parameters mean (part 1)

**NFP** Number of fission product nuclide states to be specified at each incident energy point (this is actually the number of sets of fission product identifiers fission product yields). ( $NFP \leq 2500$ ).

**ZAFP** (Z,A) identifier for a particular fission product. ( $ZAFP = (1000Z + A)$ ).

**FPS** State designator (floating-point number) for the fission product nuclide (FPS = 0.0 means the ground state, FPS=1.0 means the first excited state, *etc.*)

**YI** (MT=454), independent yield for a particular fission product prior to particle decay.

**DYI** (MT=454)  $1\sigma$  uncertainty in YI.

**YC** (MT=459) cumulative yield.

**DYC** (MT=459)  $1\sigma$  uncertainty in YC.

# This is what the ENDF parameters mean (part 2)

$C_n(E_i)$  Array of yield data for the  $i^{th}$  energy point. This array contains NFP sets of four parameters in the order ZAFP, FPS, YI, and DYI in MT=454 and ZAFP, FPS, YC, and DYC in MT=459.

**NN** Number of items in the  $C_n(E_i)$  array, equal to  $4 \times \text{NFP}$ .

$E_i$  Incident particle energy of the  $i^{th}$  point (eV).

**LE** Test to determine whether energy-dependent fission product yields given:

LE=0 implies no energy-dependence (only one set of fission product yield data given);

LE>0 indicates that (LE+1) sets of fission product yield data are given at (LE+1) incident particle energies.

**I<sub>i</sub>** Interpolation scheme (see paragraph on Two-dimensional Interpolation Schemes in Section 0.5.2) to be used between the  $E_{i-1}$  and  $E_i$  energy points.

# Where can we put this and how?

- **Both IFPY and CFPY are reaction data.**  
They should be part of a <reactionSuite> in the fission <reaction>.
- **Do we need to store the matrix?**  
Currently no easy way to tell if IFPY and CFPY are internally consistent.
- **How do we store dY?**  
IFPY and CFPY both have Y and dY. GND currently doesn't have a provision for uncertainties along side the data.
- **What about full covariances?**  
Neither GND nor ENDF have provisions for them. In GND it is not hard to make a spot for them. Is there test data to use?

# GND version should be part of the total fission <reaction>, even if rest of reaction unpopulated with data

```
1 <?xml version="1.0" encoding="UTF-8"?>
2 <reactionSuite projectile="n" target="Pu239" format="gnd version 1.2" temperature="0 K" xmlns:xlink="http://ww
3 <styles> ☐ ☐ ☐ </styles>
5 <documentations> ☐ ☐ </documentations>
40 <particles> ☐ ☐ </particles>
43 <reaction label="45" outputChannel="n[multiplicity:'energyDependent', emissionMode:'prompt'] + n[emissionMod
... [total fission]" date="2006-09-01" ENDF_MT="18" fissionGenre="total">
44 <crossSection nativeData="resonancesWithBackground"> ☐ ☐ </crossSection>
65 <outputChannel genre="NBody" Q="1.98902e8 eV">
66 <fissionEnergyReleased nativeData="polynomial"> ☐ ☐ </fissionEnergyReleased>
77 <fissionProductYields nativeData="independentFissionProductYields" conversionMatrixGiven="true">
78 <independentFissionProductYields numNuclides="780"> ☐ ☐ </independentFissionProductYields>
95 <cumulativeFissionProductYields numNuclides="920"> ☐ ☐ </cumulativeFissionProductYields>
11 <fissionYieldConversionMatrix> ☐ ☐ </fissionYieldConversionMatrix>
28 </fissionProductYields>
29 <product name="n" label="n" multiplicity="energyDependent" emissionMode="prompt"> ☐ ☐ </product>
94 <product name="n" label="n__a" multiplicity="energyDependent" decayRate="0.013271 1/s" emissionMode="del
35 <product name="n" label="n__b" multiplicity="energyDependent" decayRate="0.030881 1/s" emissionMode="del
76 <product name="n" label="n__c" multiplicity="energyDependent" decayRate="0.11337 1/s" emissionMode="dela
29 <product name="n" label="n__d" multiplicity="energyDependent" decayRate="0.2925 1/s" emissionMode="delay
82 <product name="n" label="n__e" multiplicity="energyDependent" decayRate="0.85749 1/s" emissionMode="dela
35 <product name="n" label="n__f" multiplicity="energyDependent" decayRate="2.7297 1/s" emissionMode="delay
88 <product name="gamma" label="gamma" multiplicity="energyDependent"> ☐ ☐ </product></outputChannel></react
12 </reactionSuite>
13
```


# GND version should be part of the total fission <reaction>, even if rest of reaction unpopulated with data

```
1 <?xml version="1.0" encoding="UTF-8"?>
2 <reactionSuite projectile="n" target="Pu239" format="gnd version 1.2" temperature="0 K" xmlns:xlink="http://ww
3 <styles> ☐ ☐ </styles>
5 <documentations> ☐ ☐ </documentations>
40 <particles> ☐ ☐ </particles>
43 <reaction label="45" outputChannel="n[multiplicity:'energyDependent', emissionMode:'prompt'] + n[emissionMod
... [total fission]" date="2006-09-01" ENDF_MT="18" fissionGenre="total">
44 <crossSection nativeData="resonancesWithBackground"> ☐ ☐ </crossSection>
65 <outputChannel genre="NBody" Q="1.98902e8 eV">
66 <fissionEnergyReleased nativeData="polynomial"> ☐ ☐ </fissionEnergyReleased>
77 <fissionProductYields nativeData="independentFissionProductYields" conversionMatrixGiven="true">
78 <independentFissionProductYields numNuclides="780"> ☐ ☐ </independentFissionProductYields>
95 <cumulativeFissionProductYields numNuclides="920"> ☐ ☐ </cumulativeFissionProductYields>
11 <fissionYieldConversionMatrix> ☐ ☐ </fissionYieldConversionMatrix>
28 </fissionProductYields>
29 <product name="n" label="n" multiplicity="energyDependent" emissionMode="prompt"> ☐ ☐ </product>
94 <product name="n" label="n__a" multiplicity="energyDependent" decayRate="0.013271 1/s" emissionMode="del
35 <product name="n" label="n__b" multiplicity="energyDependent" decayRate="0.030881 1/s" emissionMode="del
76 <product name="n" label="n__c" multiplicity="energyDependent" decayRate="0.11337 1/s" emissionMode="dela
29 <product name="n" label="n__d" multiplicity="energyDependent" decayRate="0.2925 1/s" emissionMode="delay
82 <product name="n" label="n__e" multiplicity="energyDependent" decayRate="0.85749 1/s" emissionMode="dela
35 <product name="n" label="n__f" multiplicity="energyDependent" decayRate="2.7297 1/s" emissionMode="delay
88 <product name="gamma" label="gamma" multiplicity="energyDependent"> ☐ ☐ </product></outputChannel></react
12 </reactionSuite>
13
```

Proposed

From ENDF

# In ENDF, both Y and dY stored, can we do that in an XY? Can we put multiple <data>'s in a <linear> block?

```
<independentFissionProductYields numNuclides="780">
  <linear xData="XYs" length="6" accuracy="0.001" hasUncertainty="true">
    <axes>
      <axis index="0" label="energy_in" unit="eV" interpolation="linear,flat" frame="lab"/>
      <axis index="1" label="yield" unit="" frame="lab"/></axes>
    <data nuclide="Nd146_e0">
      1e-05 3.45996e-13 2.21437e-13
      0.0253 3.45996e-13 2.21437e-13
      500000.0 4.01972e-13 2.57262e-13
      2000000.0 4.01945e-13 2.57245e-13
      14000000.0 5.452814e-09 3.489803e-09
      20000000.0 5.452814e-09 3.489803e-09
    </data>
    <data nuclide="...">  </data>
  </linear>
</independentFissionProductYields>
```

# The optional matrix that couples the IFPY and the CFPY can be stored here too

```
<fissionYieldConversionMatrix>
  <!-- Each row of this matrix corresponds to a nuclide in the independentFissionProductYields and
  each column of this matrix corresponds to a nuclide in the cumulativeFissionProductYields.
  The ordering of nuclides is arbitrary, but it is more convenient if they match the ordering
  in the independentFissionProductYields and cumulativeFissionProductYields elements.

  Do we really need the URL and the xlink here?-->
  <rowParameters>
    <parameter name="Nd146_e0" xlink:href="../../../independentFissionProductYields/linear/data[]"/>
  ...</rowParameters>
  <columnParameters>
  ...</columnParameters>
  <matrix rows="780" columns="920" form="asymmetric" precision="6">
    0.000000e+00  ....
    0.000000e+00  6.367300e-04  ....
    ....
  </matrix></fissionYieldConversionMatrix>
```

Should this be energy dependent?

Is this the best way?

# On the issue of covariances...

## ■ For the individual yields

- It makes sense to have covariance for either IFPY or CFPY, then derive other
- Simple covariance format can be created using existing GND covariance markup

## ■ Cross nuclide covariances

- Simple covariance format can also be created using existing GND covariance markup

## ■ Covariance on conversion matrix?

- Requires better covariances on data in decay sublibrary
- If care about nuclei after heat death of universe, then  $T_{1/2}$ 's drop out. In real life, there are long lived isotopes that don't finish beta decaying by the time of the CFPY. Uncertainty propagation tough here since parameter dependence nonlinear.

# Special case: Large Angle Coulomb Scattering

- Quantum mechanically, charged particle elastic scattering is a sum of Coulomb and Nuclear amplitudes:

$$A = A_{\text{Coulomb}} + A_{\text{nuclear}}$$

- The elastic differential cross section is then:

$$\frac{d\sigma_{el}(E)}{d\Omega dE'} = \frac{d\sigma_{\text{Coulomb}}(E)}{d\Omega dE'} + \frac{d\sigma_{int}(E)}{d\Omega dE'} + \frac{d\sigma_{nucl}(E)}{d\Omega dE'}$$

- But, the Coulomb term is divergent:

$$\frac{d\sigma_{\text{Coulomb}}(E)}{d\Omega dE'} \propto \frac{\eta^2}{k^2(1-\mu)^2}$$

- This is analytic, so we don't store it, but...

# Special case: Large Angle Coulomb Scattering

- The interference term carries the square-root of these divergences
- Workarounds:
  - Start the ``nuclear+interference'' data tables at  $E \gg 0$  where nuclear effects become noticeable.
  - Cut-off the ``nuclear+interference'' term at small angles.
    - At small angles, Coulomb scattering dominates and must be handled in particle transport separately with techniques such as condensed history.
    - ENDF data uses 10 degrees as a cut-off (if I remember correctly), but it is not documented anywhere I can find.
- Recommend:
  - `<parameterizedTwoBodyReaction>` for LACS data
  - `<dcrossSection_dOmega>` for LACS data
  - `<form>` for ``nuclear+interference'' data
  - A spot for the cut-off angle

# Special case: Particle production

- Basically ENDF's MT=5
- Above roughly ~20 MeV (for neutrons, higher for charged particles), the number of emitted particles explodes.
- We could try to list them all. Or we could give up and assume the emitted particles have an energy dependent multiplicity.
- The facility for both already exist.
- **Would be nice to have a reaction alias e.g. "spallation"**

# Special case: Thermal Scattering Law

- Neutrons scattering off material with energy low enough that their de Broglie wavelength bigger than atomic spacing, either coherently or incoherently scatter off surface
- 3 Cases:
  - coherent elastic (off ordered substances)
  - incoherent elastic (hydrogenous solids)
  - incoherent inelastic (famous  $S\alpha\beta$  data)
- **In all cases parameterized form of  $d\sigma/d\Omega$ , so use**
  - `<parameterizedTwoBodyReaction>` and `<dcrossSection_dOmega>`
  - **Parameterizations for elastic cases in ENDF manual**
  - **Parameterization for inelastic case sort of in ENDF manual**

# Special case: Thermal Scattering Law

- Requested to support covariance data in TSL
- For elastic, tables small and can be handled with `<link>` from `<form>` to `<covariance>`
- For inelastic,  $S_{\alpha\beta}$  table is 3d object, covariance would be immense
- In practice, generate  $S_{\alpha\beta}$  using photon spectrum  $\rho(\omega)$  of material and structure factor  $S(q)$  in NJOY's LEAPR module
  - Both  $\rho(\omega)$  and  $S(q)$  are 2d tables that can have covariance
  - Would need to "encode" LEAPR somehow

# Outline (roughly)

## HOUR 1

- Goals, use cases, etc.
- Preliminaries
  - low-level containers
  - designators
  - documentation
- The Top: `<evaluation>`
  - `<reactions>`
    - special two-body
    - plain old reactions
  - `<resonances>`
- The Other Top:  
`<setOfCovariance>`

## HOUR 2

- `<metaEvaluation>`
- Special cases:
  - Atomic data
  - Fission
  - Fission Product Yields
  - Large Angle Coulomb Scattering
  - Particle production
  - Thermal Scattering Law
- Odds-n-ends
- Thanks & Blame

# Odds-n-ends

- Derived data for transport
  - Transfer matrices
  - Average energy release (or KERMA)
  - Average forward momentum deposited in medium
  - mubar (average scattering angle)
  - mubar covariance
- ENDF sum rules
  - sum of parts equal total cross section
  - similarly for MT=3
  - nubar
- Should decay information be in the reaction somehow?