Recent updates to the top-level hierarchy, review draft requirements document

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Hopefully we've captured your input see https://www.oecd-nea.org/science/wpec/sg38/top_level_hierarchy.pdf

Requirements for a next generation nuclear data format

OECD/NEA/WPEC SubGroup 38*

(Dated: April 1, 2015)

This document attempts to compile the requirements for the top-levels of a hierarchical arrangement of nuclear data such as is found in the ENDF format. This set of requirements will be used to guide the development of a new set of formats to replace the legacy ENDF format.

CONTENTS

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Latest version on SG38 GForge site https://ndclx4.bnl.gov/svn/sg38 and https://ndclx4.bnl.gov/gf/project/sg38/

Status of requirements coverage

- **ENDF/B-VII.1 has 14 sublibraries**
  - [x] neutron incident
  - [x] charged particle incident: p, d, t, 3He
  - [x] photonuclear
  - [x] neutron standards
  - [x] thermal neutron scattering
  - [x] photo-atomic, electro-atomic
  - [x] NFY
  - [ ] decay,
  - [ ] SFY
  - [ ] atomic relaxation,

- **Other easily envisioned future sub libraries**
  - [x] More charged particles: all Z<=6
  - [x] A structure-lite library
  - [x] muons, pi0 (cosmic rays)
  - [x] GFY, PFY, DFY, TFY, HFY, AFY, …
  - [x] heavy-ion projectiles
  - [x] activation

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This is also covered, but by a separate document

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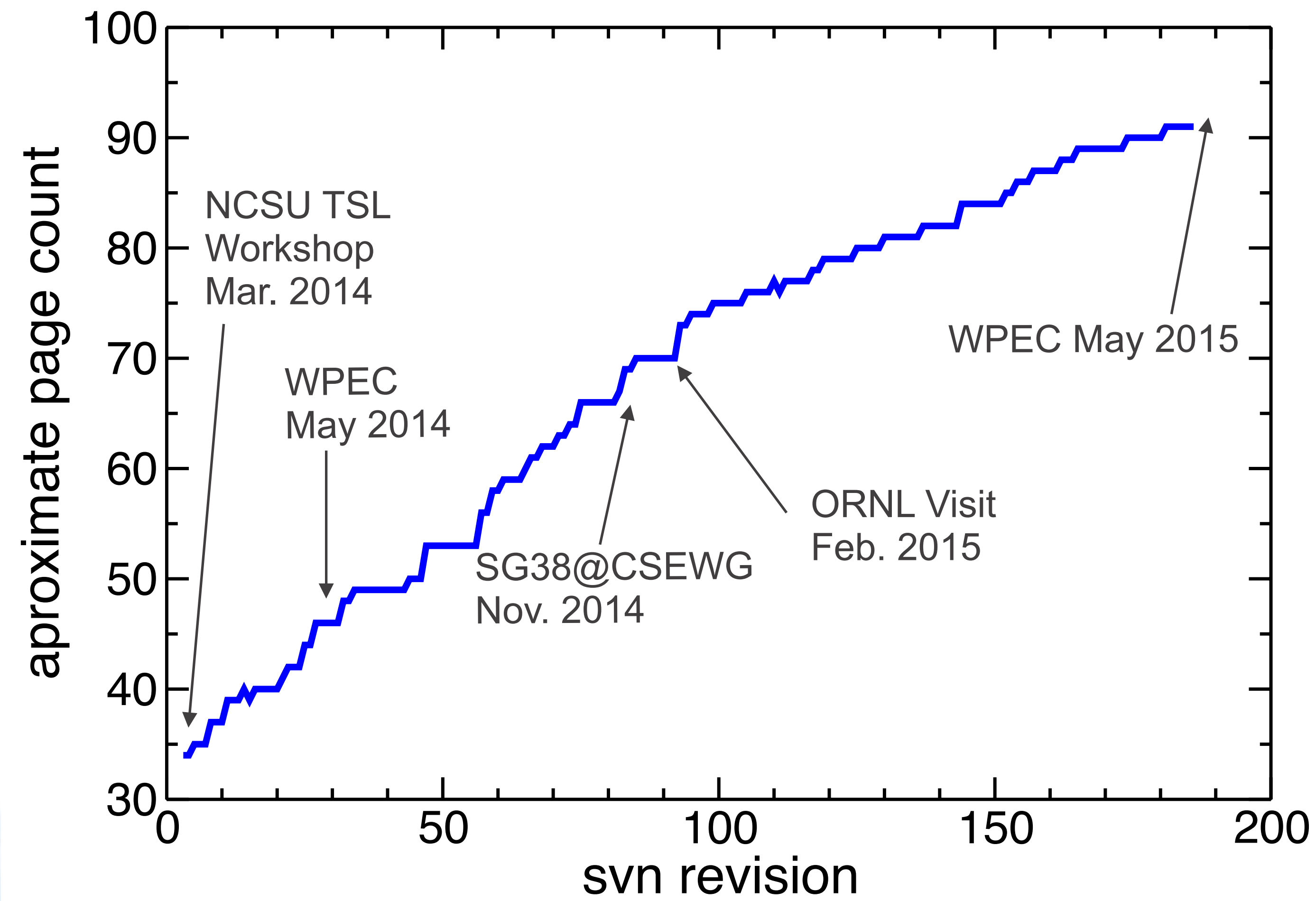
We switched to GForge for versioning of requirements after SG38 Tokai Meeting (early 2014)



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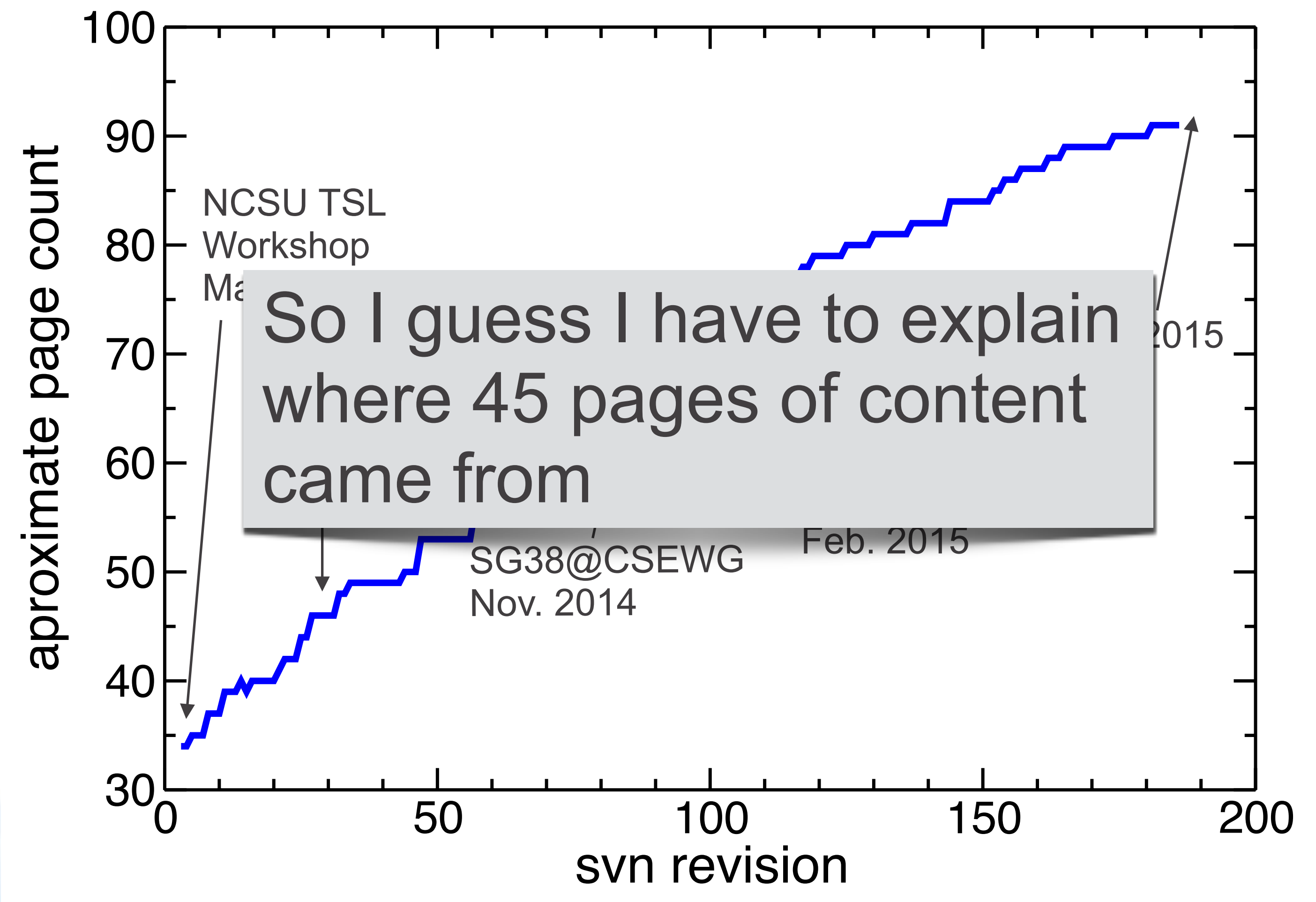

Notable meetings (i.e. meetings that resulted in us doing a lot of writing)

- **SG 37 meeting 2013**
  - got lots of good FPY feedback
- **Mar 2014 meeting at NCSU**
  - got lots of TSL feedback
- **SG 38 meeting before Nuclear data week @ BNL**
  - Lots of fixes from meeting
  - Lots of particle property/decay feedback
  - Backlog of fixes from previous meeting(s)
- **ORNL mini-meeting in March**
  - got lots of RR & covariance feedback
- **Work with R. Cullen to learn atomic data**

Major changes

- **Move covariance/ uncertainty data to be near data**
  - A very popular request
- **Function prototyping**
  - Morgan's request
- **Resonance region fixes**
- **Expanded derived data discussion**
  - Transport data
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Covariance data should go where it is most useful

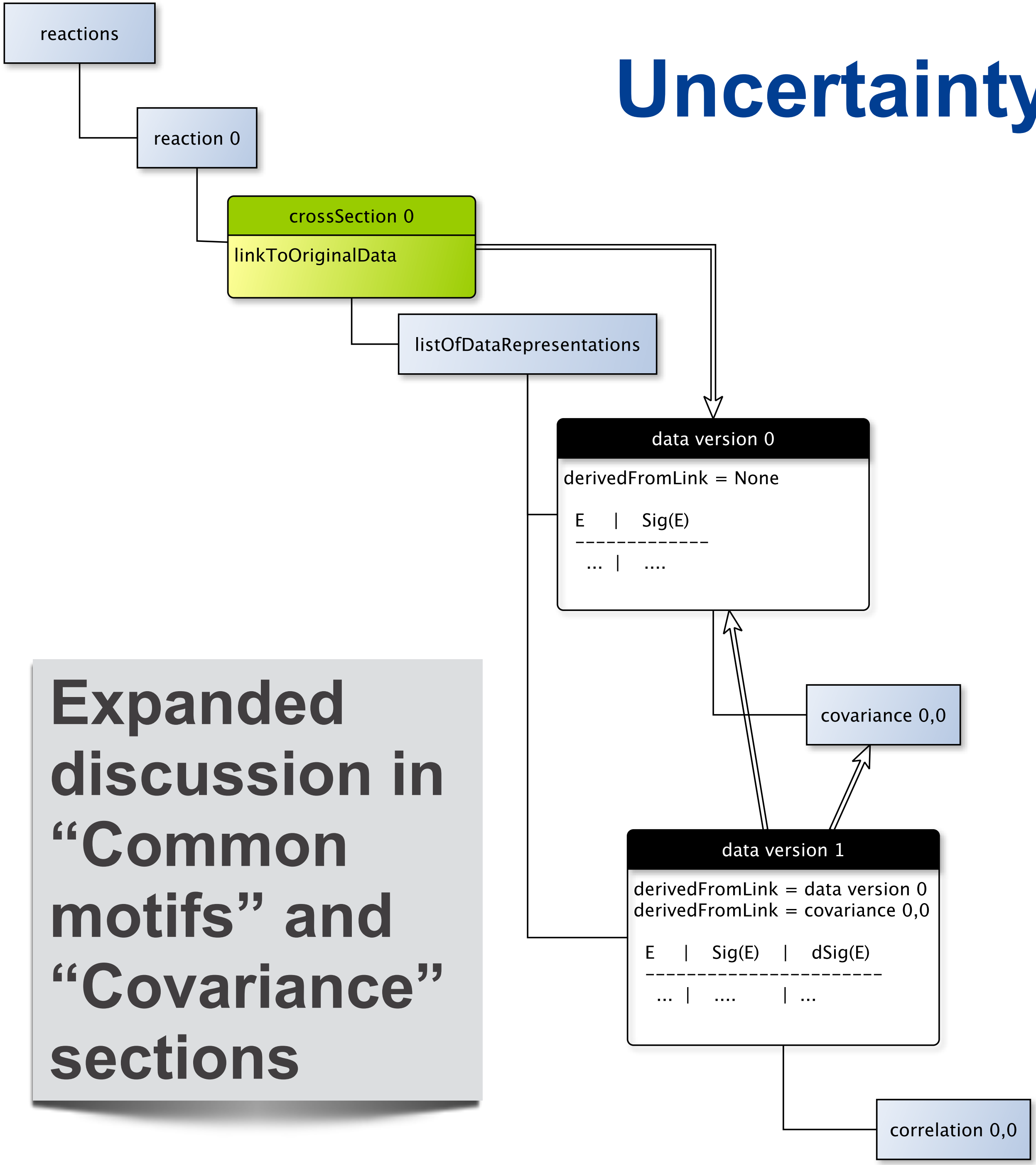
Self-covariance data and uncertainty data

- Should be as close to the data as possible
- Needs to be built into low-lying data structures

Cross-covariance/ correlation data

- Couples many different data
- Should be separate, but linked to all relevant data

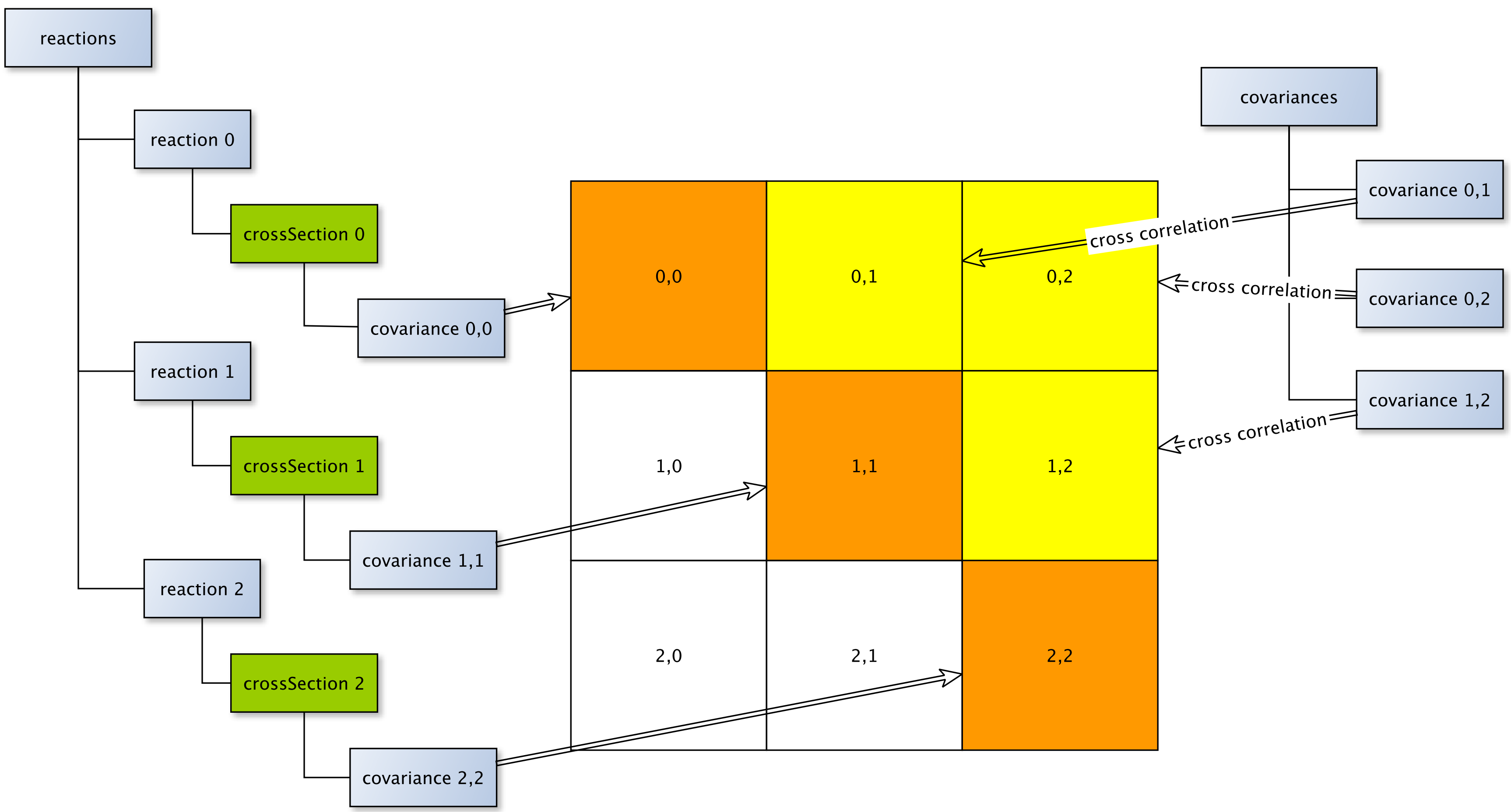
Uncertainty/covariance near data



- Most requested feature
- Can read uncertainty rather than grok MT=30-40
- Simplifies finding parts for plotting
- Revise low-level containers

Expanded discussion in “Common motifs” and “Covariance” sections

Cross-covariance data should be collected together, but linked



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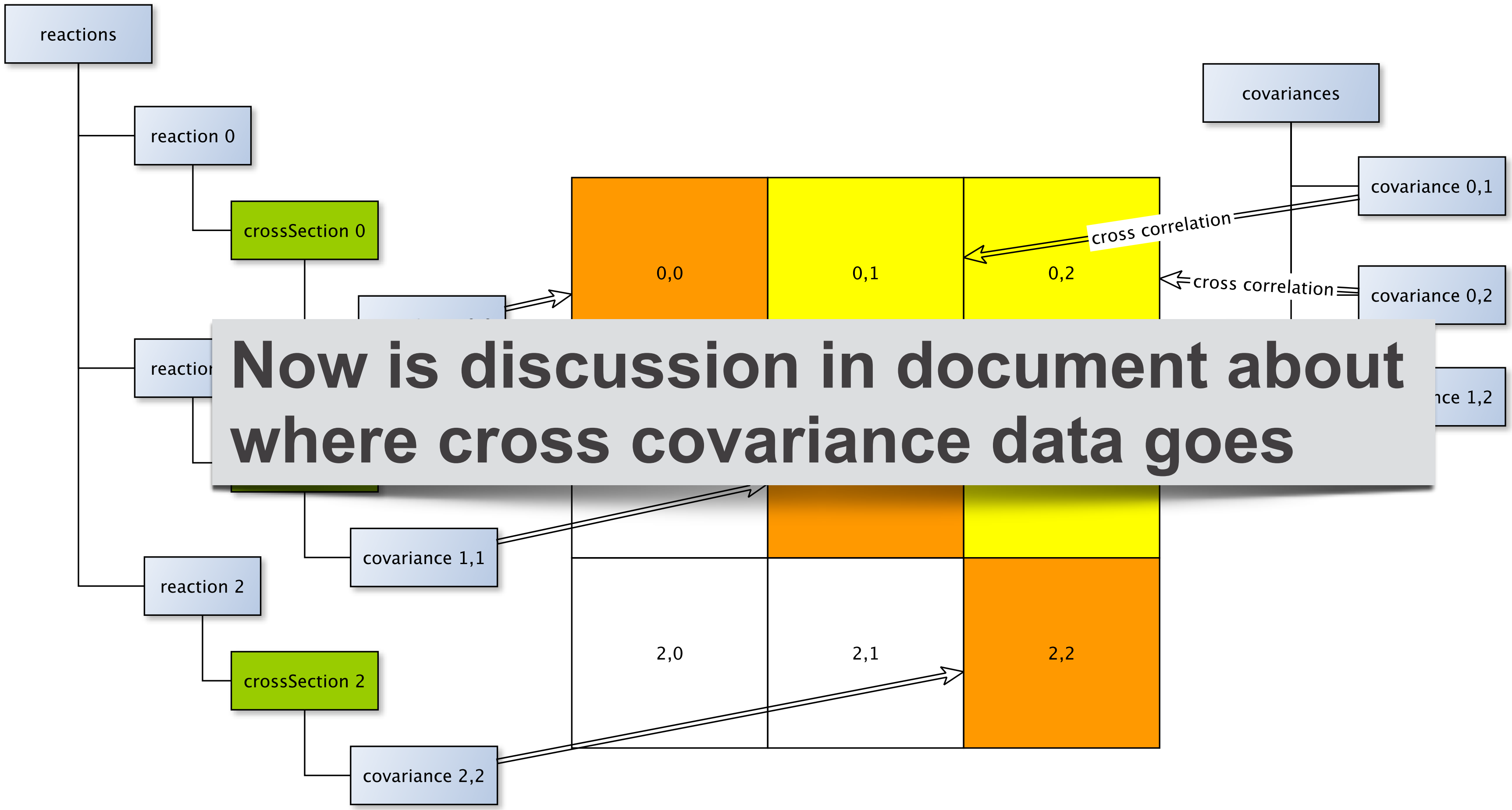

Now is discussion in document about where cross covariance data goes

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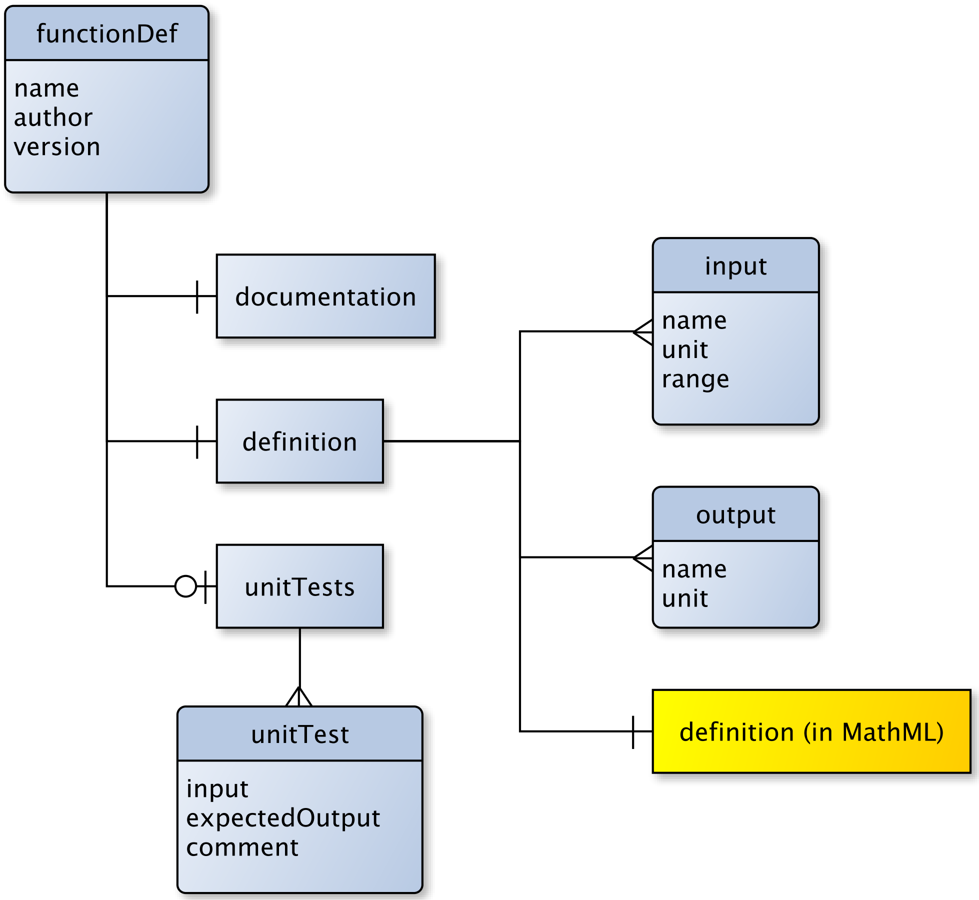
We wanted a way to prototype ideas

- Say you have a new parametric form for something…
- You create a format
- You know the parameters in your format have to be plugged into a function
- You've implemented it in your own code, but you want to share it
- Eventually, you hope it could be part of the standard format

How can you distribute your ideas to others in the nuclear data community?

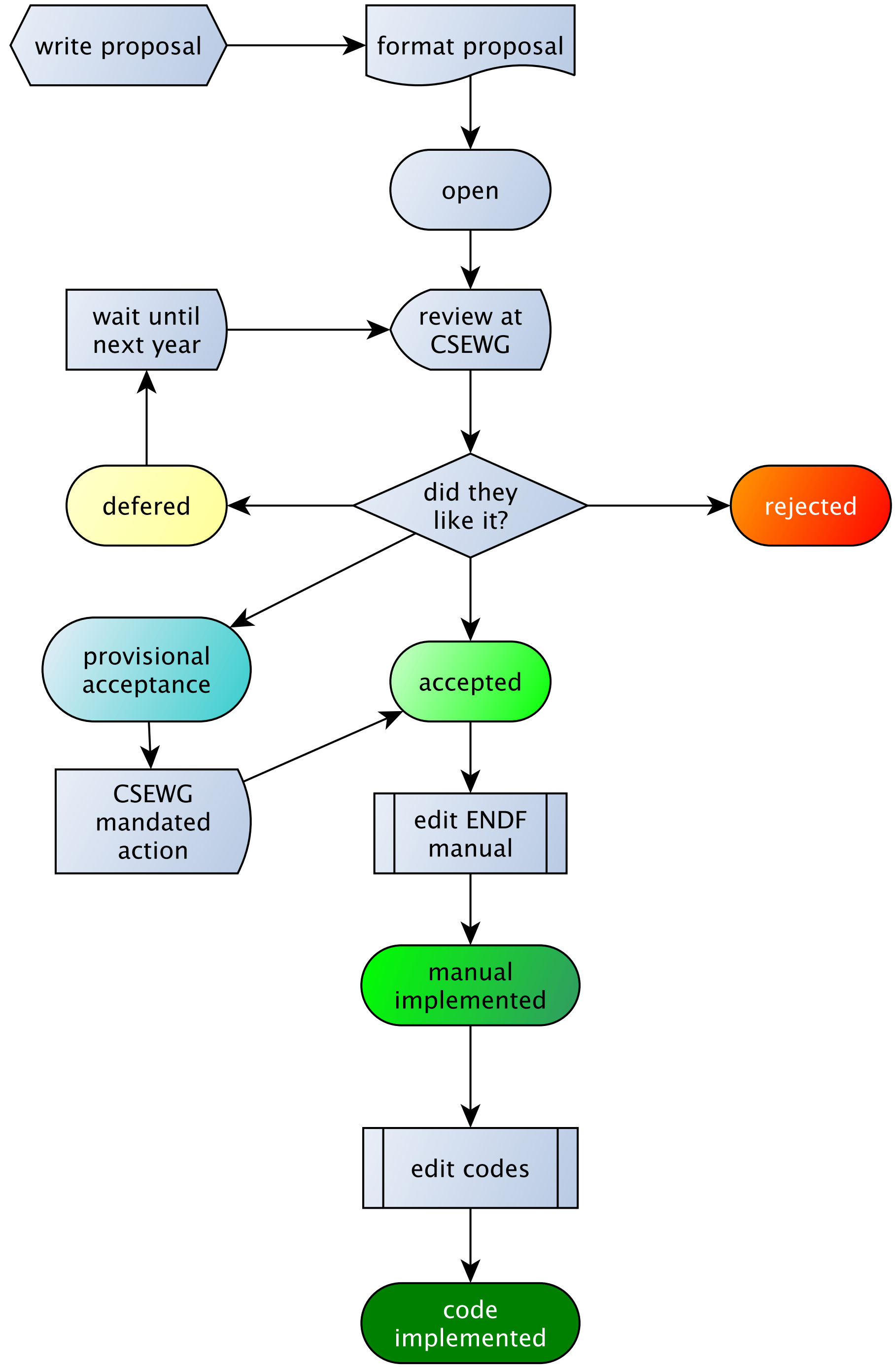
Behold, the <functionDef>



- **Not an implementation but a description of how to implement. Therefore we need**
  - inputs
  - output
  - documentation
  - unit tests
  - the actual definition
- **Very light weight, meant for simple ideas**
- **Defs collected in top of evaluation**
- **Is this what we want?**

Things to consider with <functionDef>

- What are rules for promoting a <functionDef> to part of the formal format?
- How will we handle more complex format changes?
- At left is the *de facto* CSEWG workflow



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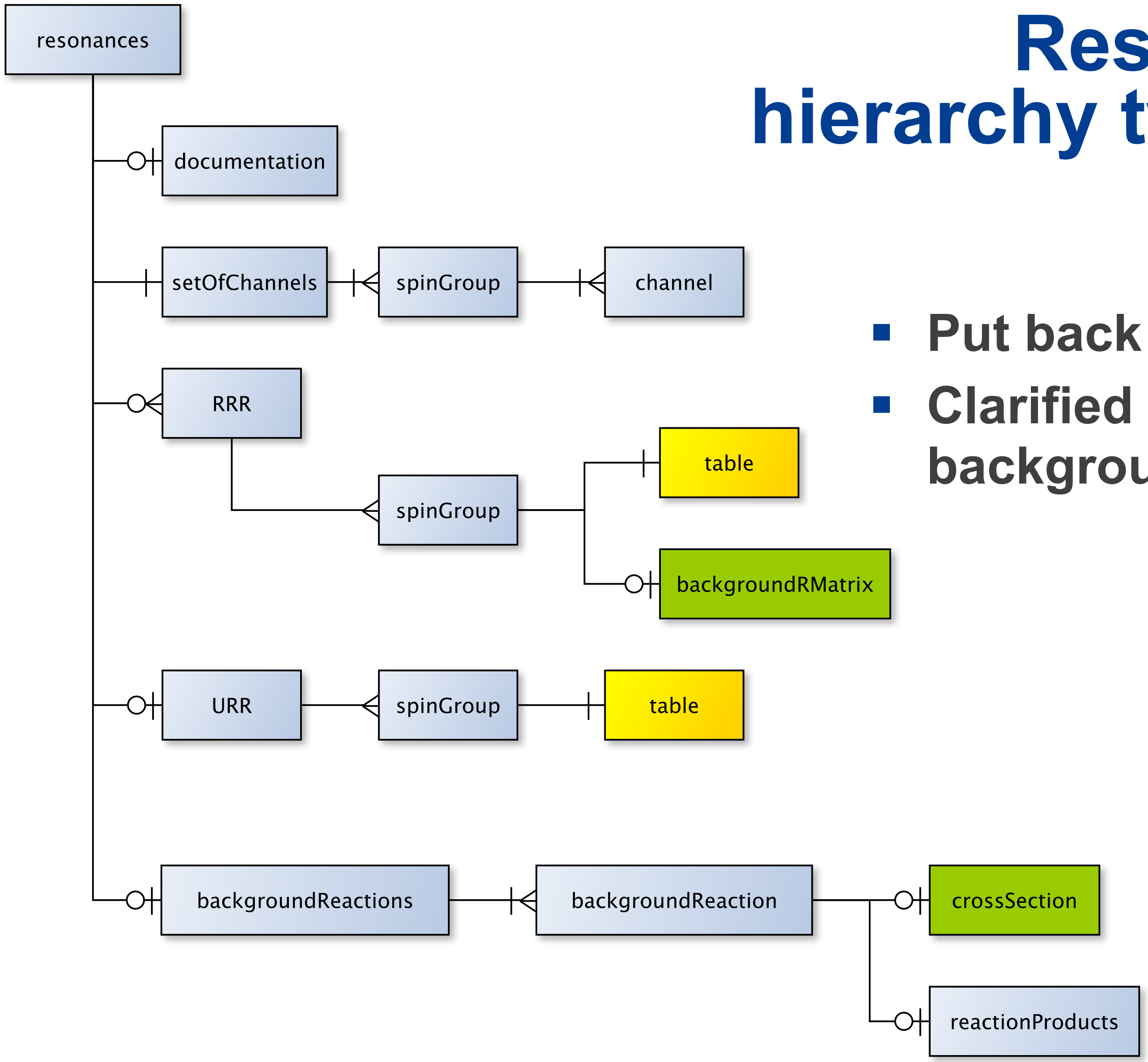
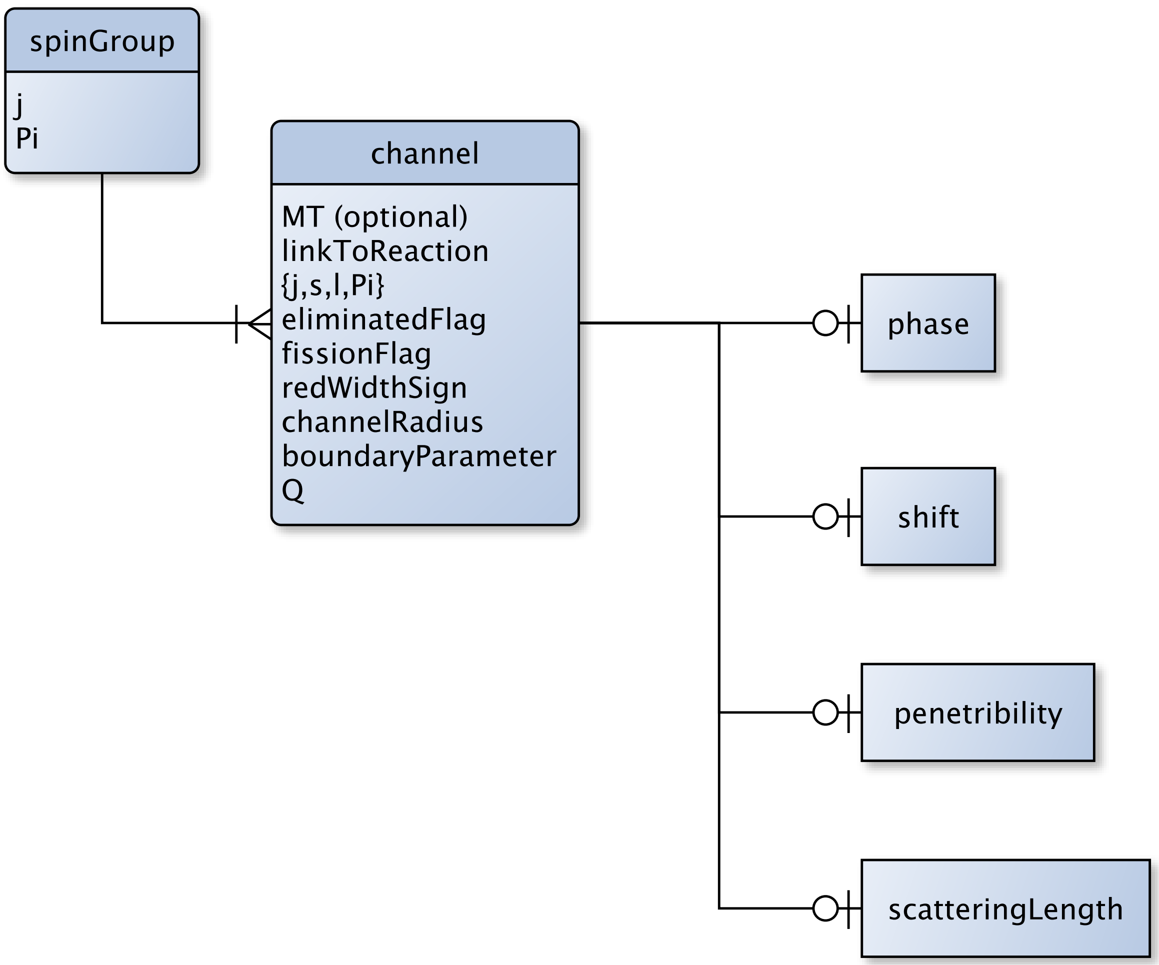
Resonance hierarchy tweaked



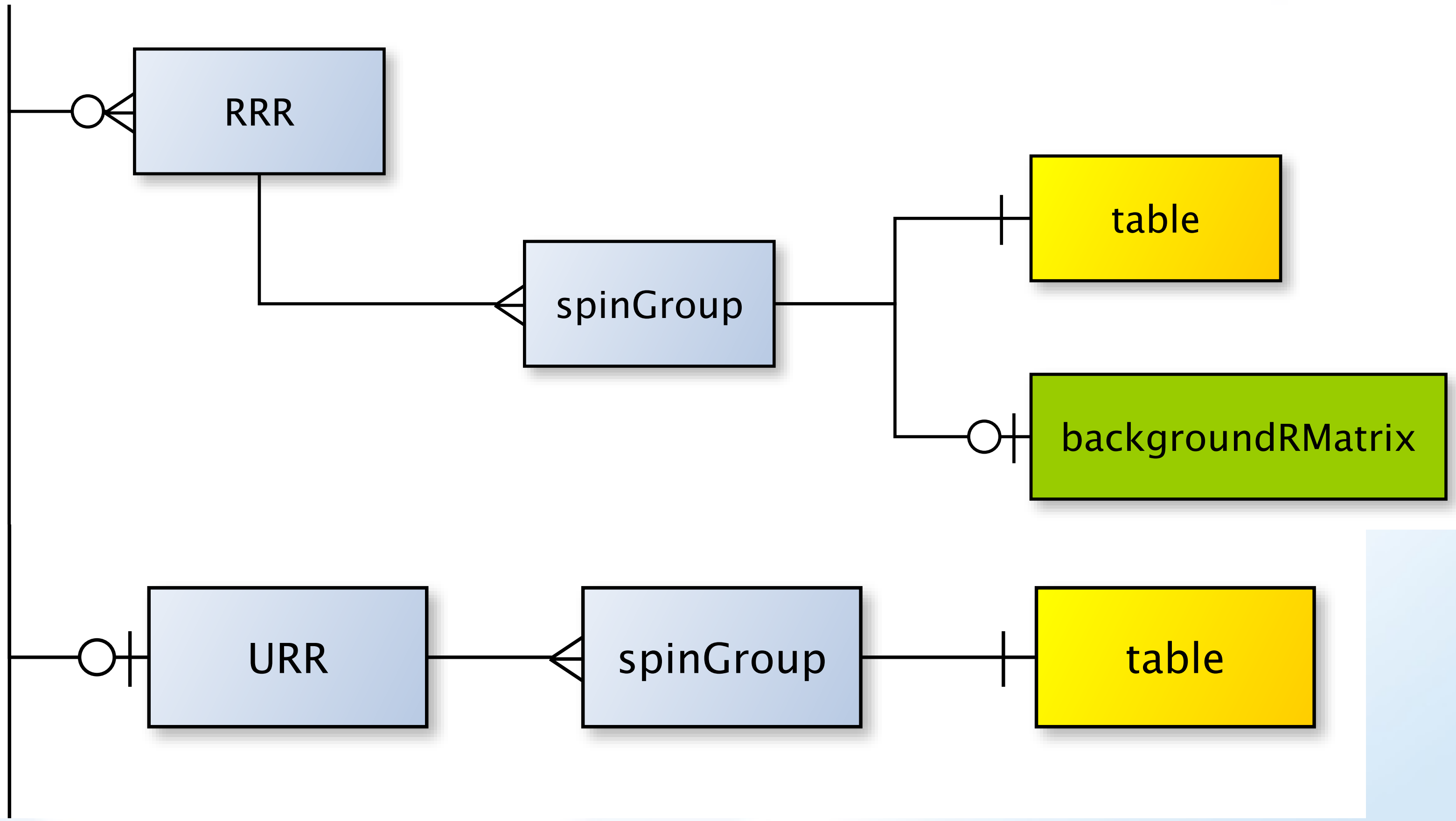
- Put back spinGroup
- Clarified backgroundReactions

ENDF's spinGroup collects channels with same channel JPi

- Denser (more efficient packing) RR parameter tables
- Basically improved version of LRF=7

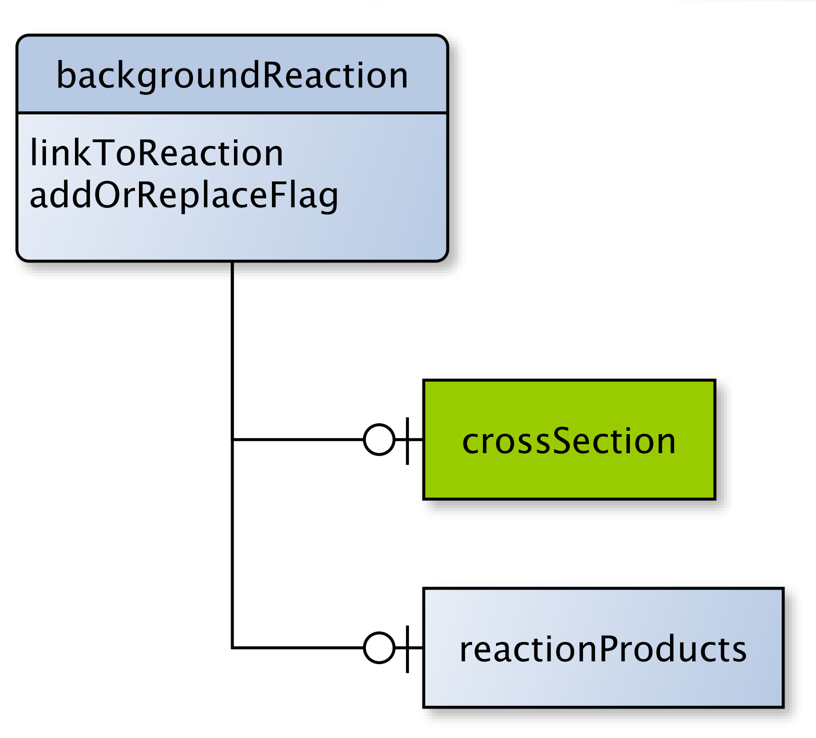


Leads to obvious change in RRR's and URR's hierarchies



backgroundReaction used to collect all the extra stuff needed to make transport ready data from RR

- **background crossSection to add to reconstructed resonance data**
- **extra reaction product distributions** (e.g. angular distributions of neutrons)
  - especially useful if don't trust output from reconstruction of angular distributions or want smoothed version
  - best way to do capture gammas in RR



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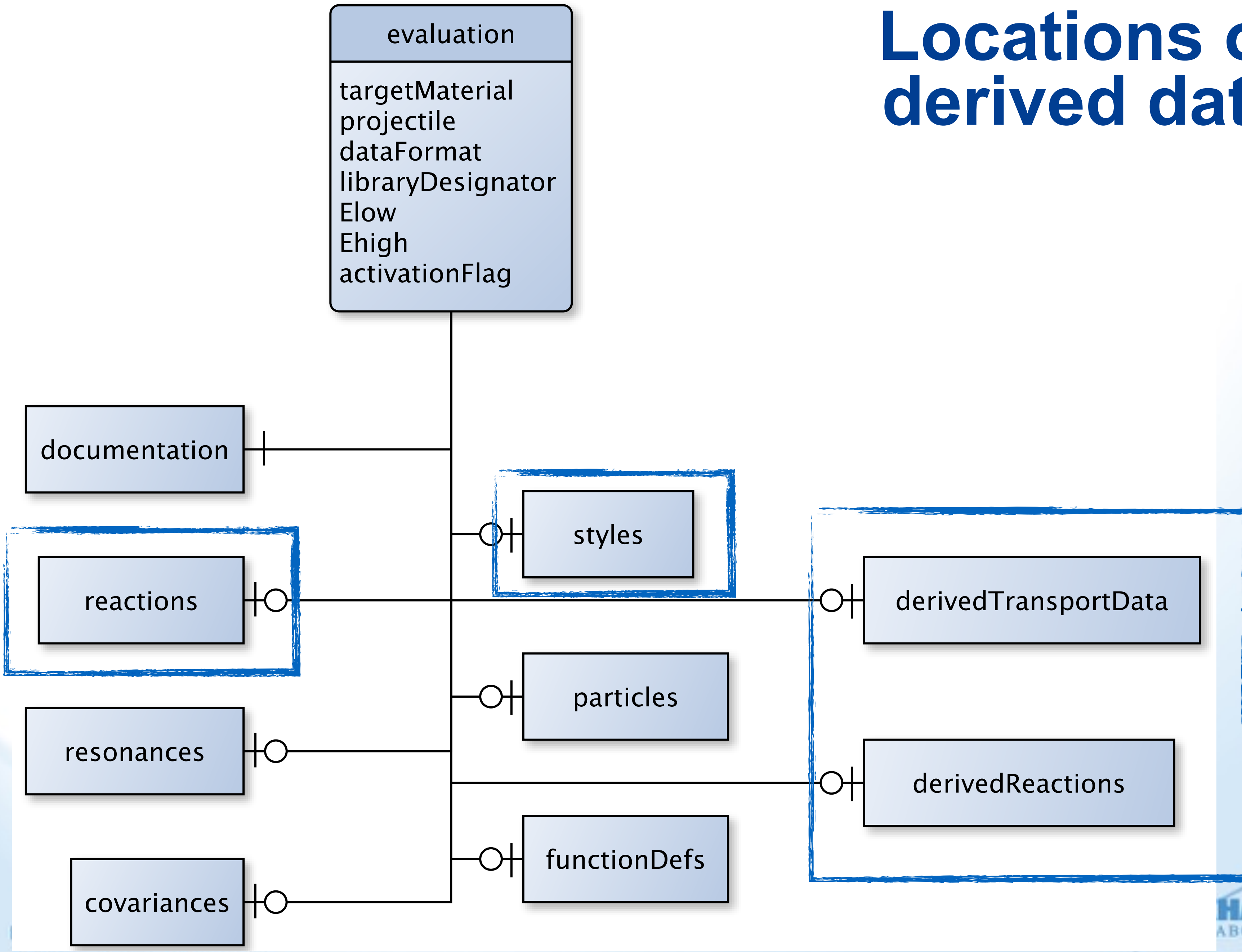
Derived data is data that can be derived from other data in an evaluation

- A "virgin" evaluation, created by an evaluator and distributed by a library maintainer usually won't have any
- Processing codes will insert what is needed for certain applications
  - particle transport vs. activation vs. production
- Some derived data will need to be generated for visualization (e.g. reconstructed cross sections in the resonance range)
- Data placed where it is most needed

Locations of derived data



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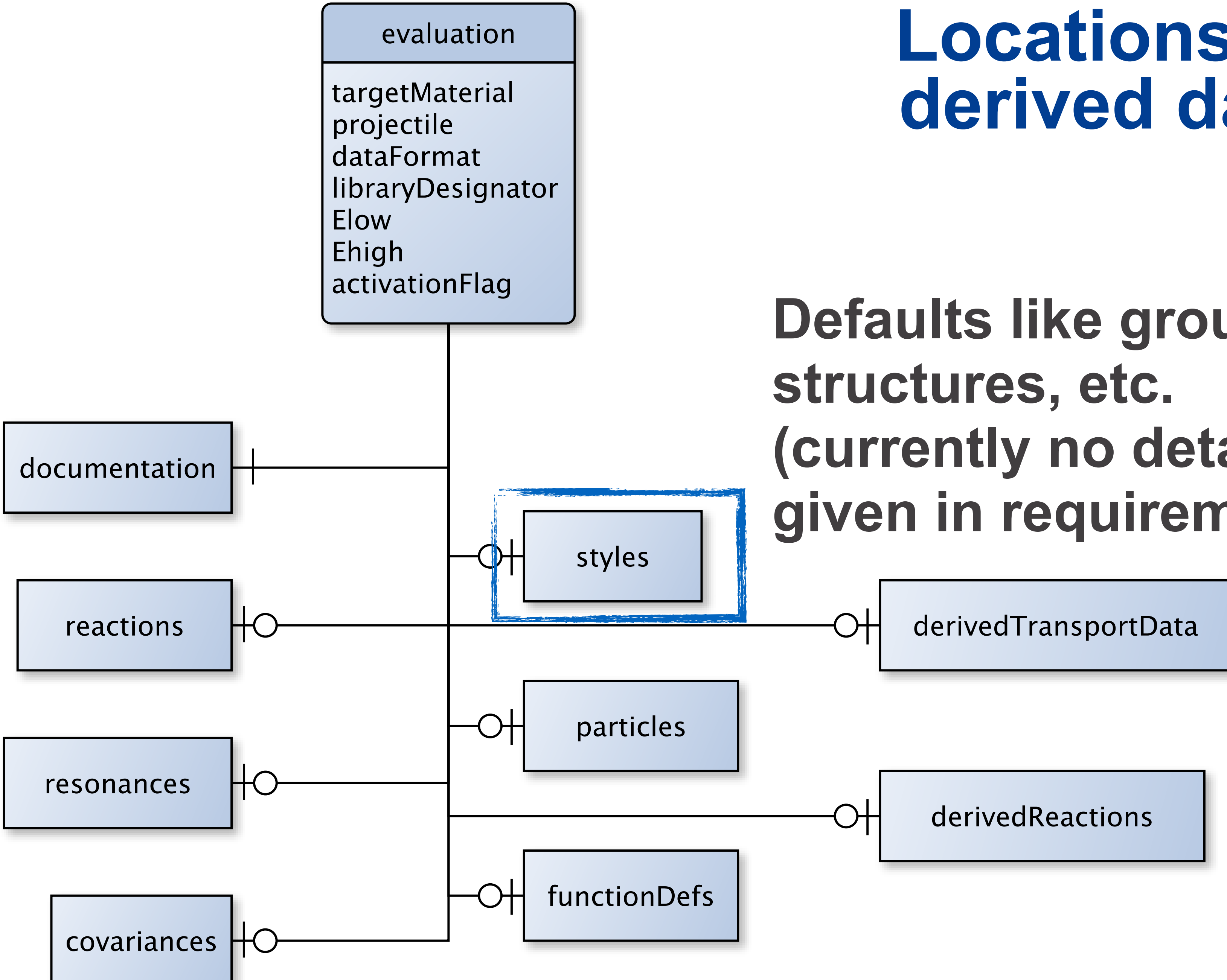
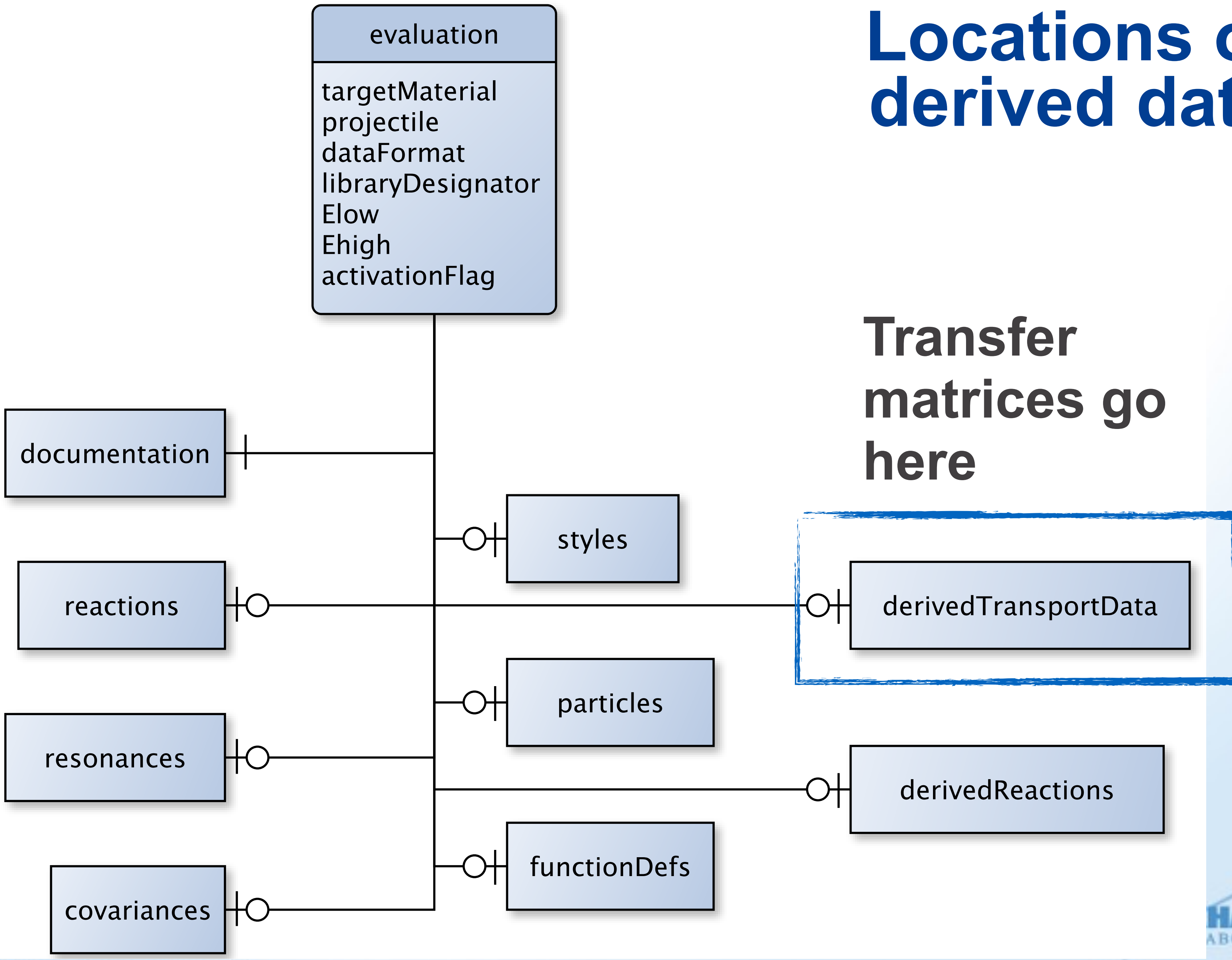


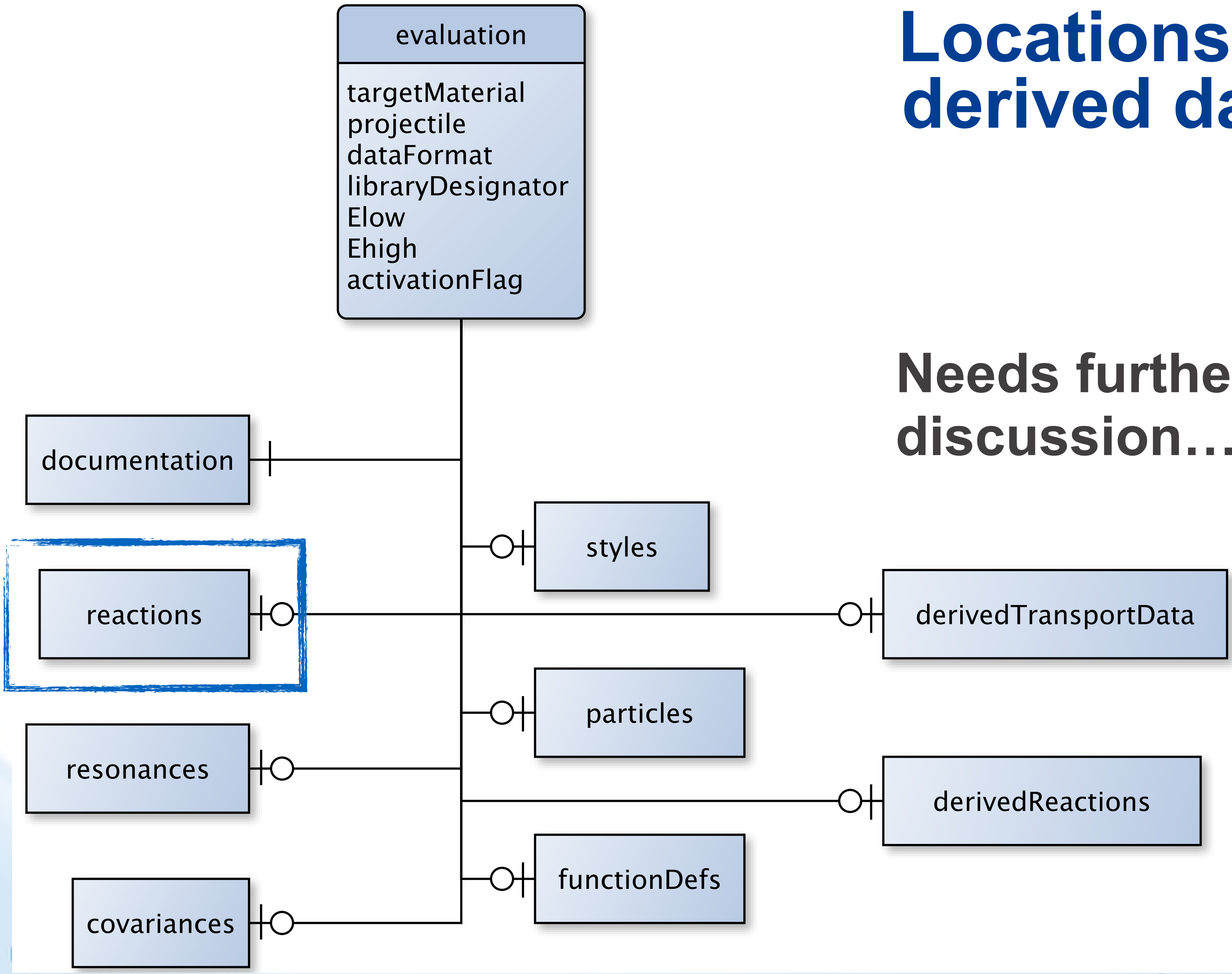
Defaults like group structures, etc. (currently no detail given in requirements)

Locations of derived data



Transfer matrices go here

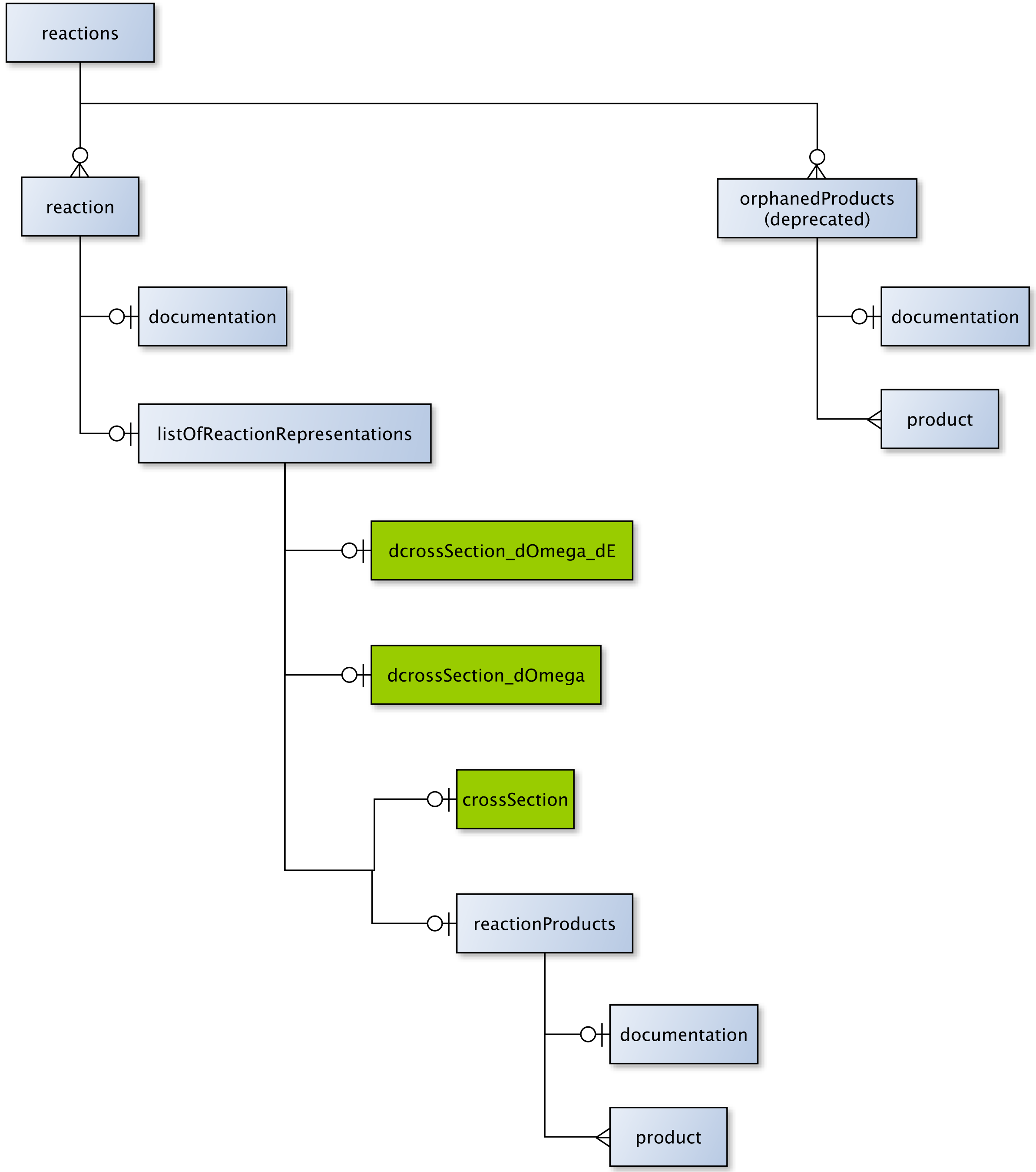
Locations of derived data



Needs further discussion…

Derived data can be anywhere

- Dictated by nature of derived data
- Should be linked to original data
- Should be as near to original as possible



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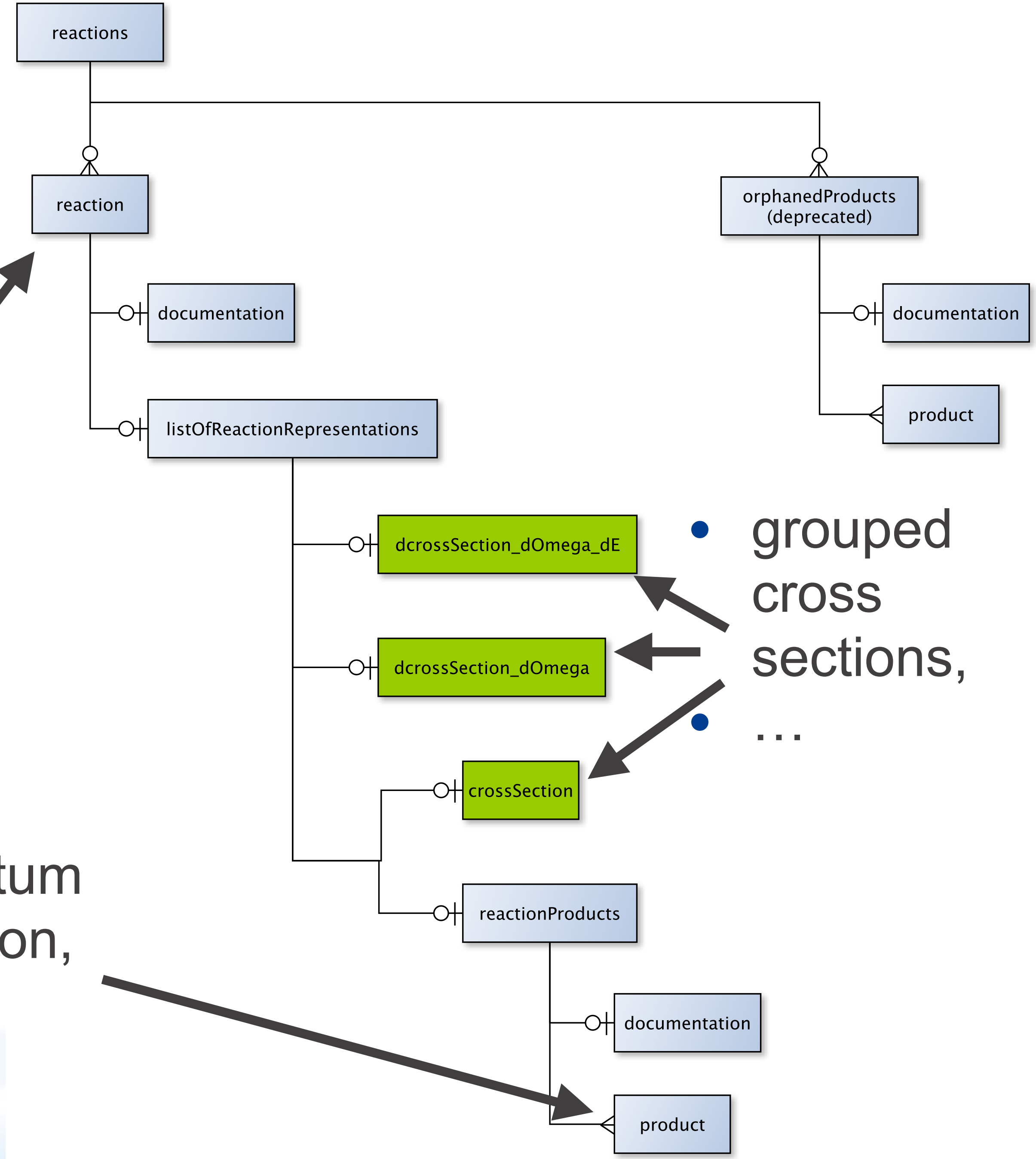
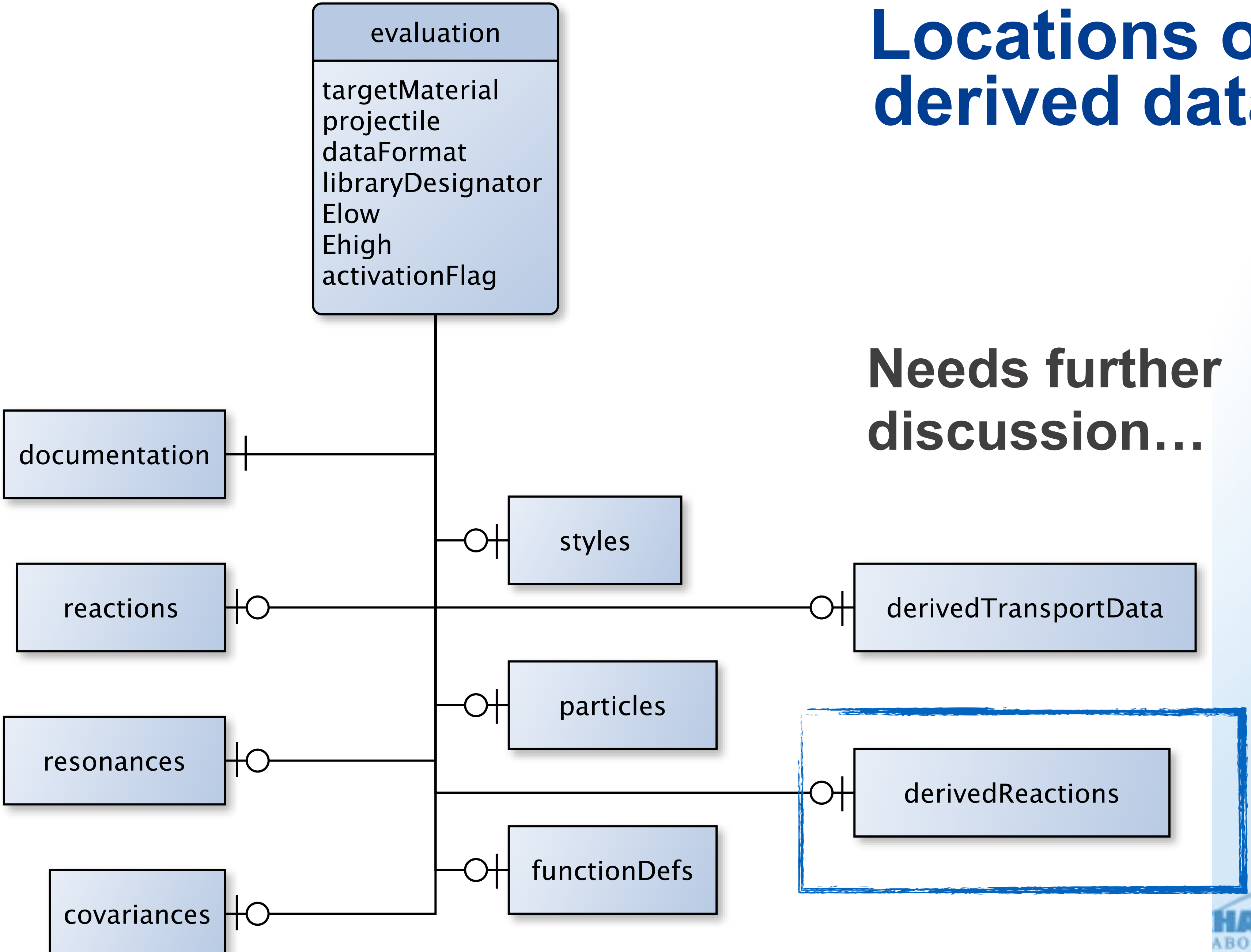


- KERMA,
- DPA,
- …

- grouped cross sections,
- …

- energy/ momentum deposition,
- CDF's,
- mubar,
- …

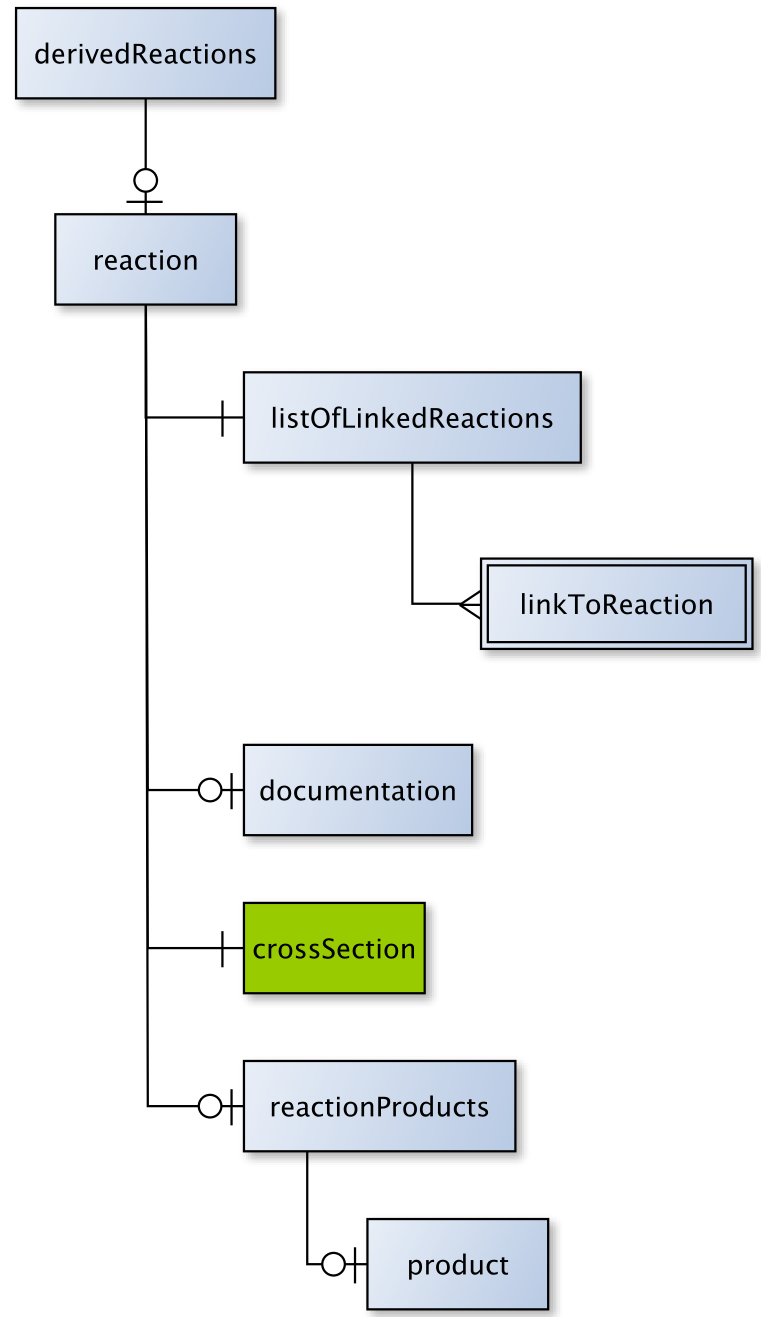
Locations of derived data



Needs further discussion…

derivedReactions are like regular reactions

- **Things defined by sumrules**
  - total
  - absorption
  - …
- **Production data**
- **Reconstructed data from resonances** (URR tables or cross sections)
- **Should be able to reconstruct derivedReaction data from rest of evaluation**
- **Should be linked to original data**



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Through our SG38 discussions, it became clear that we don't all speak the same language

- physicist vs. engineer
- experimentalist vs. theorist vs. computational scientist
- ***We need common definitions to avoid confusion***

Appendix C: Terminology

A: The total number of protons and neutrons in a given nucleus.

abundance: For isotopes that occur naturally, the abundance values are proportional to the probability of finding these isotopes and normalized so that the sum of the abundances for all the isotopes of a given chemical element is equal to 100. The source is (Holden, 2004).

α **decay:** The emission of a ^{4}He nucleus (α particle).

α **particle:** A ^{4}He nucleus, that is, a nucleus made up of 2 neutrons and 2 protons.

AMPX: AMPX (Dunn, 2002) is a modular system of computer programs developed at ORNL with pri-

β^- **decay:** The transformation of one neutron inside a nucleus into a proton plus an electron and an antineutrino: $n \rightarrow p + \bar{\nu}_e$

β^+ **decay:** The transformation of one proton inside a nucleus into a neutron plus a positron and a neutrino: $p \rightarrow n + \nu_e$

β**–delayed particle emission:** The emission of a nucleon, nucleons or a nucleus following β-decay. For proton rich nuclei, the emission of a proton following β^+ decay and electron capture has been observed. For neutron rich nuclei, the release of one or two neutrons following β^- decay is possible. The emission of α particles has been observed for some nuclei in all types of β decay. Also, for a few nu-

The terminology section is unfinished

- I didn't write some yet (especially variations of cross section)
- Others I need to figure out (multi-band treatment & Bondarenko factors)
- There are many others I didn't even think to add

I can really use more help here

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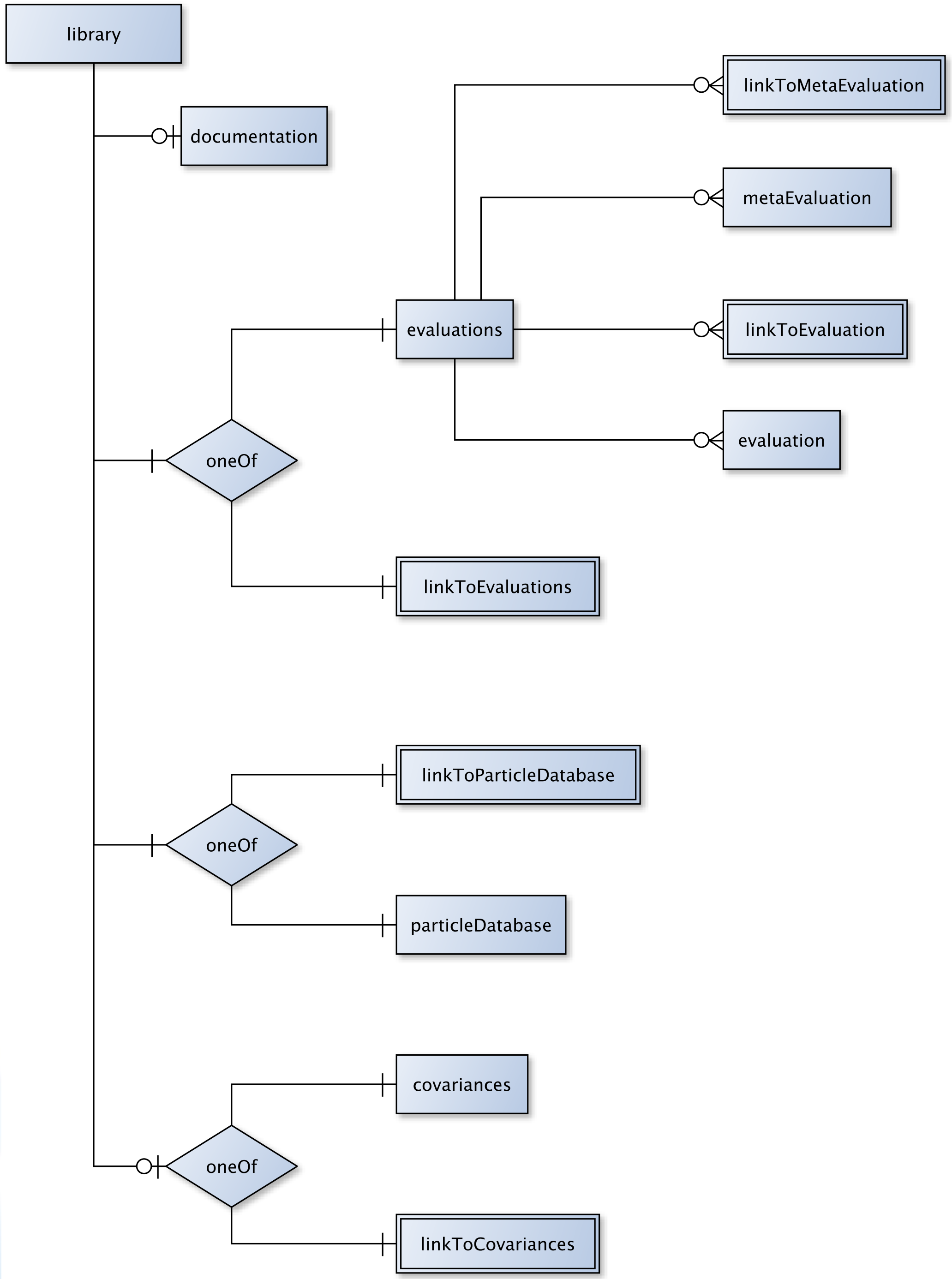
Request for scheme to group together evaluations

- Define a (sub) library
- Collect evaluations for batch web retrieval
- Essentially a directory of files/ evaluations
- Deliberately light weight



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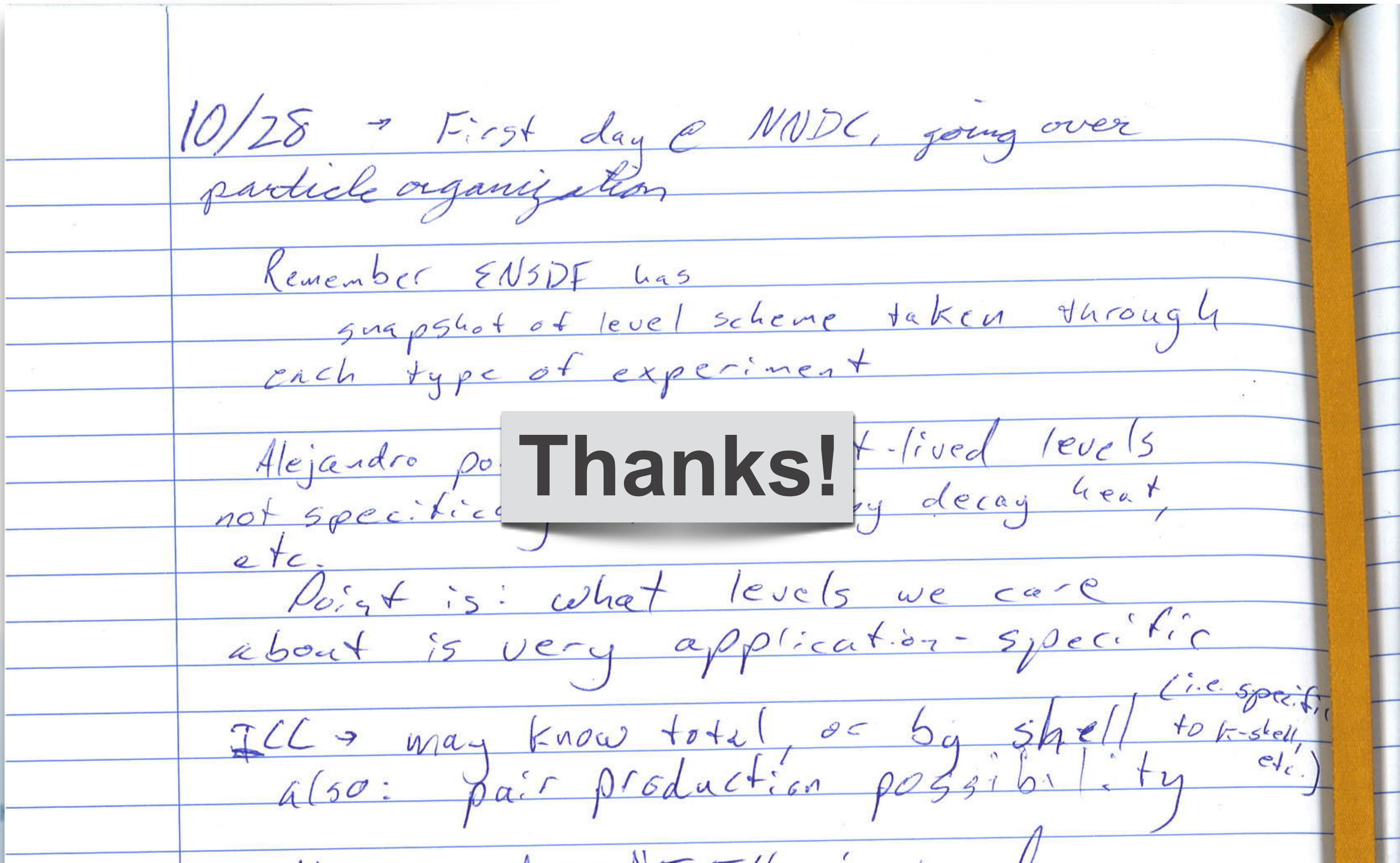
Notes like these from Caleb and Bret and edits from Morgan were essential. Also, a special thanks to Jeremy for LaTeX help



Thanks!

What's left to do

- The occasional FIXME
- Update affiliations
- Update acknowledgements
- Update GND info in appendix
- Integrate responses from review(s)
- Integrate feedback from SG42

What else?