Requirements for TSL data in new format

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a passion for discovery

U.S. DEPARTMENT OF ENERGY | Office of Science

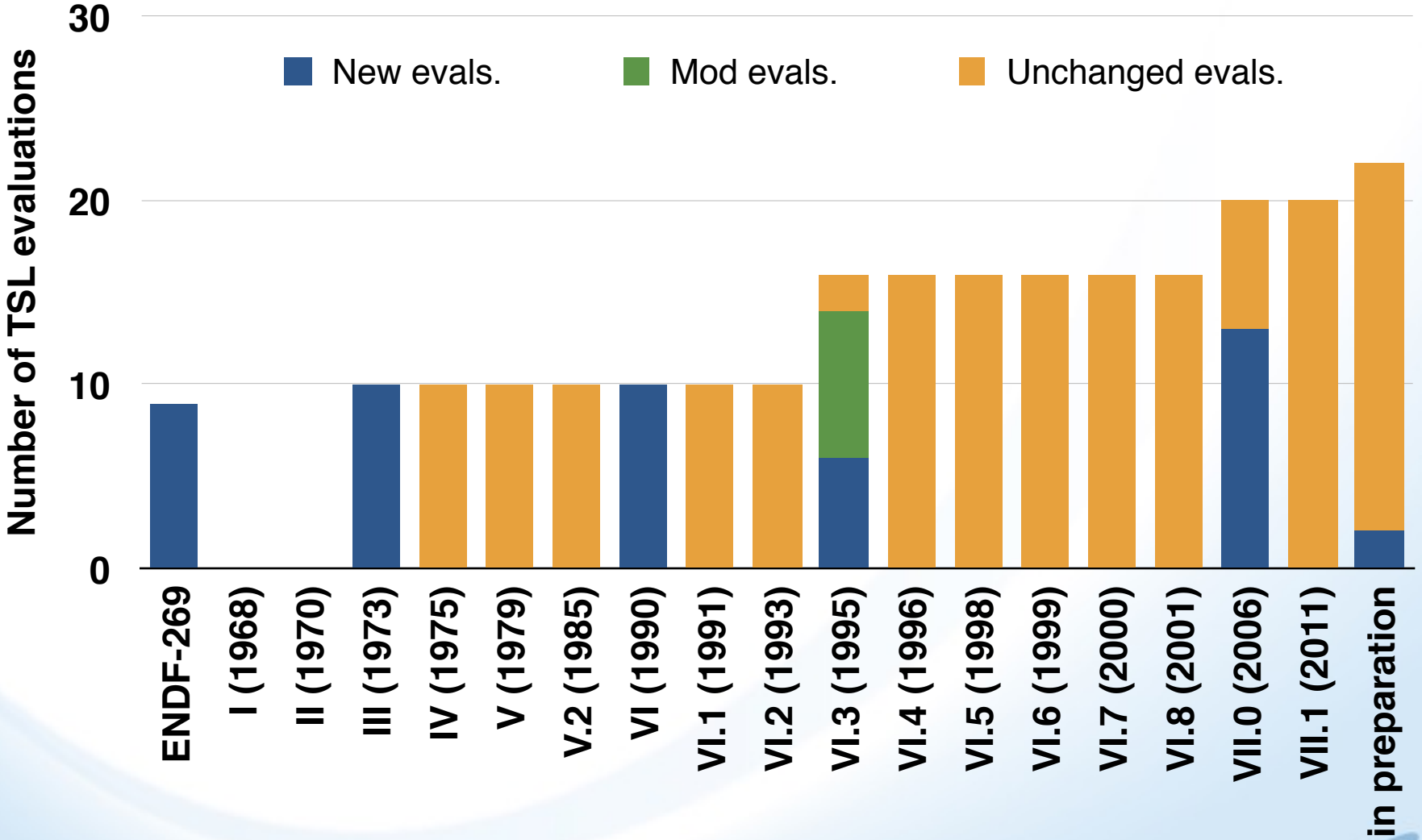
SG38: “Beyond the ENDF Format”

- **WPEC-SG38 approved in May 2012**
- **Develop new format to replace ENDF**
- **Requirements essentially developed** (*that’s why I’m here*)
- **Designing specifications**
- **Have working prototype of format (GND) and processing/translation code (Fudge)**

Special issues

- **In US (CSEWG), TSL data has lower profile, compared to say neutron sub library**
- **Want to revise overly complicated format**
  - Hierarchy of approximations unclear to uninitiated
  - Precision/dynamic range of $S_{\alpha\beta}$
  - Covariance data
- **Take advantage of improved methodology**
  - LEAPR
  - Split self & distinct
  - $d\sigma(E,T)/dE'd\Omega$ directly vs. $S_{\alpha\beta}(\alpha,\beta,T)$
- **How to group together evaluations**
  - TSL matching onto higher energies
  - How to resolve issues of stoichiometry and normalization
  - TSL is not just vs. T, but P and other parameters (EOS-related or not)

ENDF library has gradually evolved to current state



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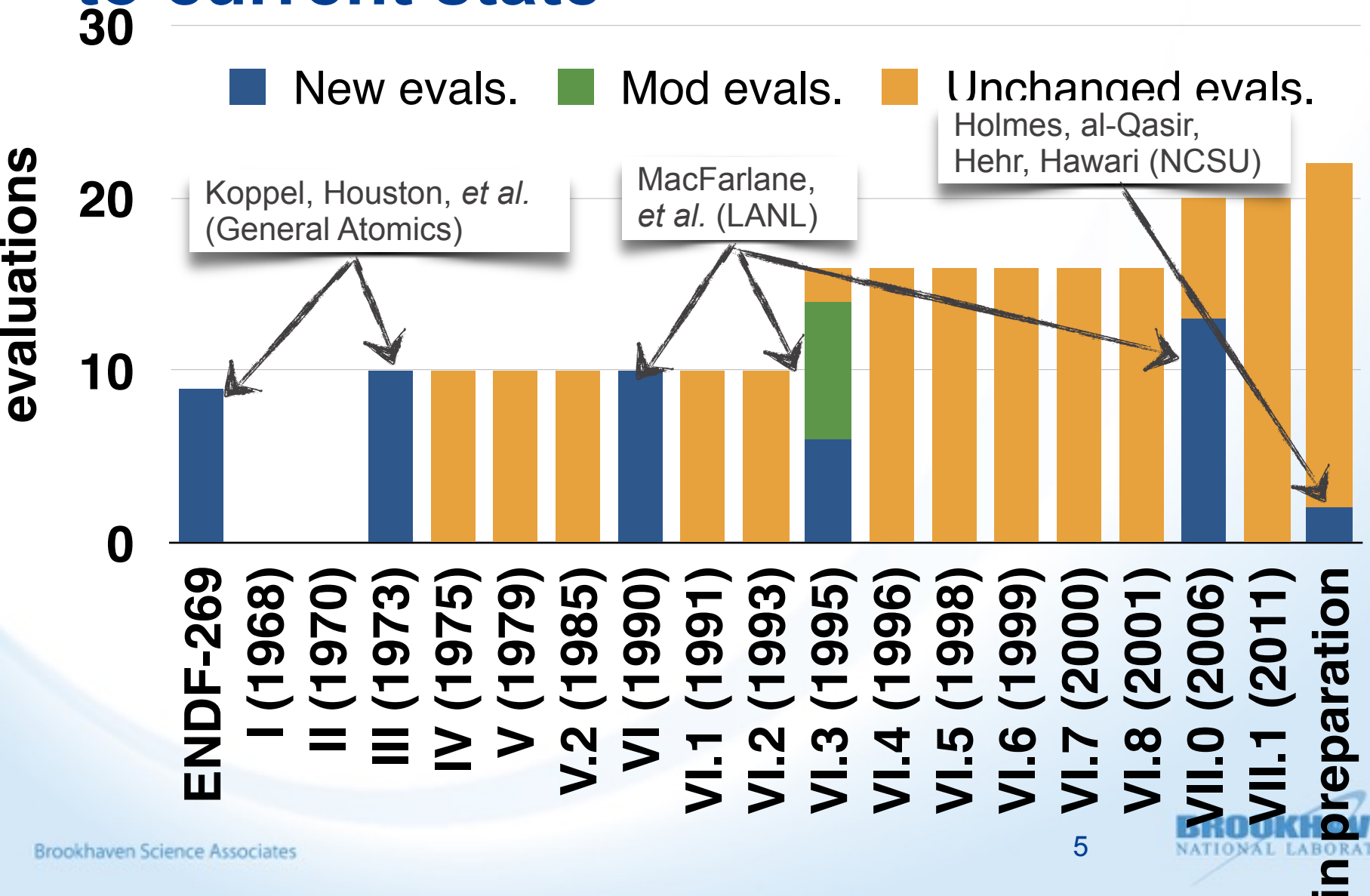

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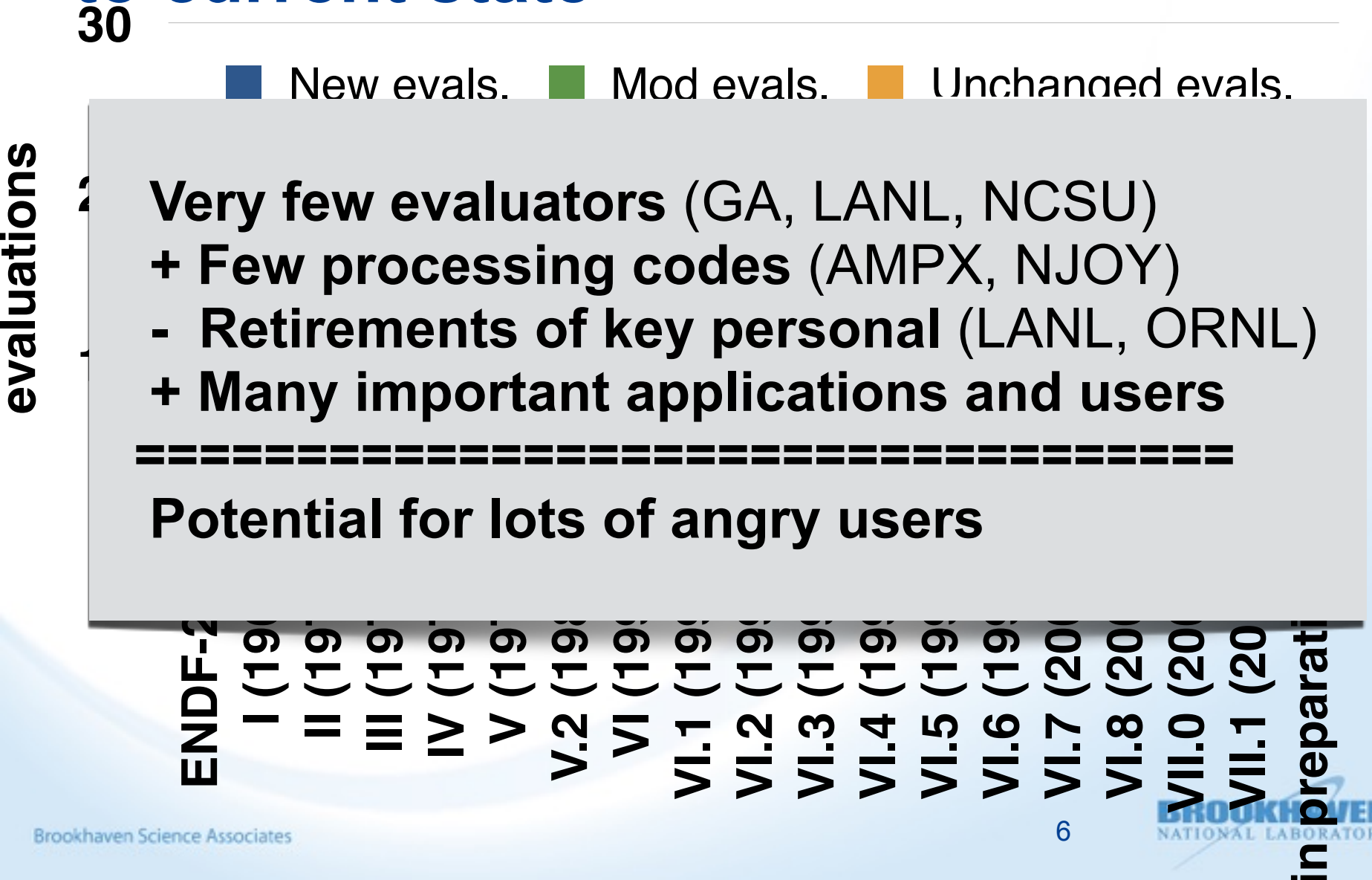

Very few evaluators (GA, LANL, NCSU)
+ Few processing codes (AMPX, NJOY)
- Retirements of key personal (LANL, ORNL)
+ Many important applications and users

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Potential for lots of angry users

These are the requirements that we've gathered from you, the nuclear data community

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.

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This is (or will be anyway) your format

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- We've been listening to you and others, but…
- Did we get it right?
- What are we still missing?
- What is wrong?

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Main goals/requirements

1. The hierarchy should ***reflect our understanding of nuclear reactions and decays***, clearly and uniquely specifying all such data.
2. It should ***support storing multiple representations of these quantities simultaneously***, for example evaluated and derived data.
3. It should ***support both inclusive and exclusive reaction data***, that is discrete reaction channels as well as sums over multiple channels.
4. It should use ***general-purpose data containers*** suitable for reuse across several application spaces.
5. It should ***eliminate redundancy where possible***.
6. As a corollary to requirements 1 and 2, ***multiple representations of the same data should be stored as closely together*** in the hierarchy as feasible.

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Main approximations in TSL treatments

- First Born approximation
- Lots of scatterers
- Orientation average
- Gaussian approximation
  - coherent elastic
  - incoherent
    - elastic
    - inelastic
      - short collision time approximation

Always have to do these in practice

ENDF always assumes these, but it could be done better

Supporting ENDF's Thermal Scattering Law would be easy…

- **3 cases supported by ENDF**:
  - coherent elastic (off ordered substances)
  - incoherent elastic (hydrogenous solids)
  - incoherent inelastic (famous Sαβ data)
- **All cases are parameterized forms of dσ/dΩdE'**, so use
  - **`<dcrossSection_dOmega>`** (elastic) or **`<dcrossSection_dOmega_dE>`** (inelastic)
  - Parameterizations for elastic cases given in ENDF manual
  - Parameterization for inelastic case implied in ENDF manual

In general case, can break scattering kernel up to some extent, but not enough to help

$$S(\vec{\kappa},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-\omega t} I(\vec{\kappa},t) \qquad I(\vec{\kappa},t) = \frac{1}{N}\sum_{j,j'}\left\langle e^{-\vec{\kappa}\cdot\vec{R}_{j'}(0)} e^{-\vec{\kappa}\cdot\vec{R}_{j}(t)}\right\rangle$$

Write

$$\frac{d^2\sigma(E)}{d\Omega dE'} = \frac{k'}{k}\left[\sigma_{coh} S(\vec{\kappa},\omega) + \sigma_{inc} S_s(\vec{\kappa},\omega)\right]$$

where

$$S(\vec{\kappa},\omega) = S_s(\vec{\kappa},\omega) + S_d(\vec{\kappa},\omega)$$

$$\sigma_{coh} = 4\pi \left\langle b\right\rangle^2$$

$$\sigma_{inc} = 4\pi(\left\langle b^2\right\rangle - \left\langle b\right\rangle^2)$$

Just store these? Note S(κ,ω) is rewritten Sαβ so this is still huge

In the incoherent Gaussian approximation, the scattering kernel is computed by LEAPR as follows

$$\mathcal{S}_s(\alpha,\beta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, e^{i\beta t} e^{-\gamma(t)}$$

where

$$\gamma(t) = \alpha \int_{-\infty}^{\infty} d\omega \rho(\omega) \left(1 - e^{-i\omega t}\right) \frac{e^{-\omega/2}}{2\omega \sinh(\omega/2)}$$

In this approximation, only store ρ(ω) & its covariance

Phonon spectrum is sole input, rest is math, including the structure factor in ω→0 limit

However, we were asked to support much more in the new format

- **Requested to support covariance data in TSL**
- **Requested to store stuff to generate $S_{\alpha\beta}$ using photon spectrum ρ(ω) of material and structure factor S(q) in NJOY's LEAPR module**
  - Both ρ(ω) and S(q) are 2d tables that can have covariance
  - Would need to "encode" LEAPR somehow
  - Could put covariance on these very easily but uncertainty propagation through LEAPR tough
- **New measurements and theory produce Sαβ directly, without ENDF's approximations**
  - Can we store this? It is a 4d data set (S x α x β x T)!
  - What about covariance?

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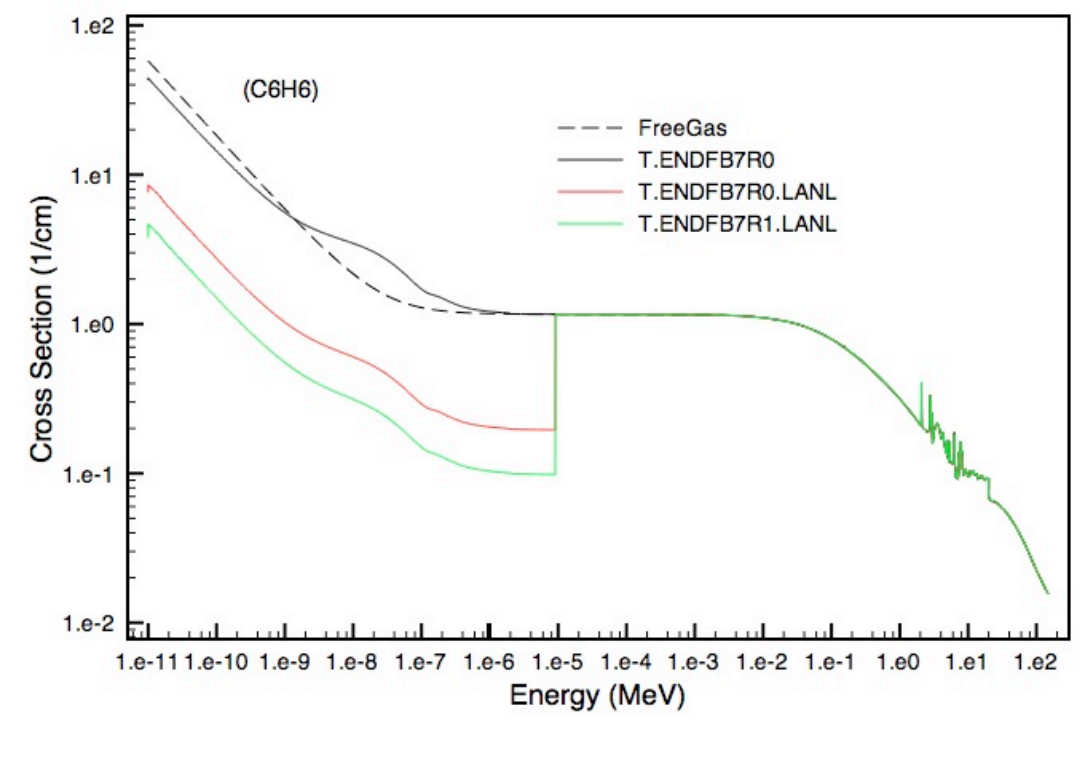
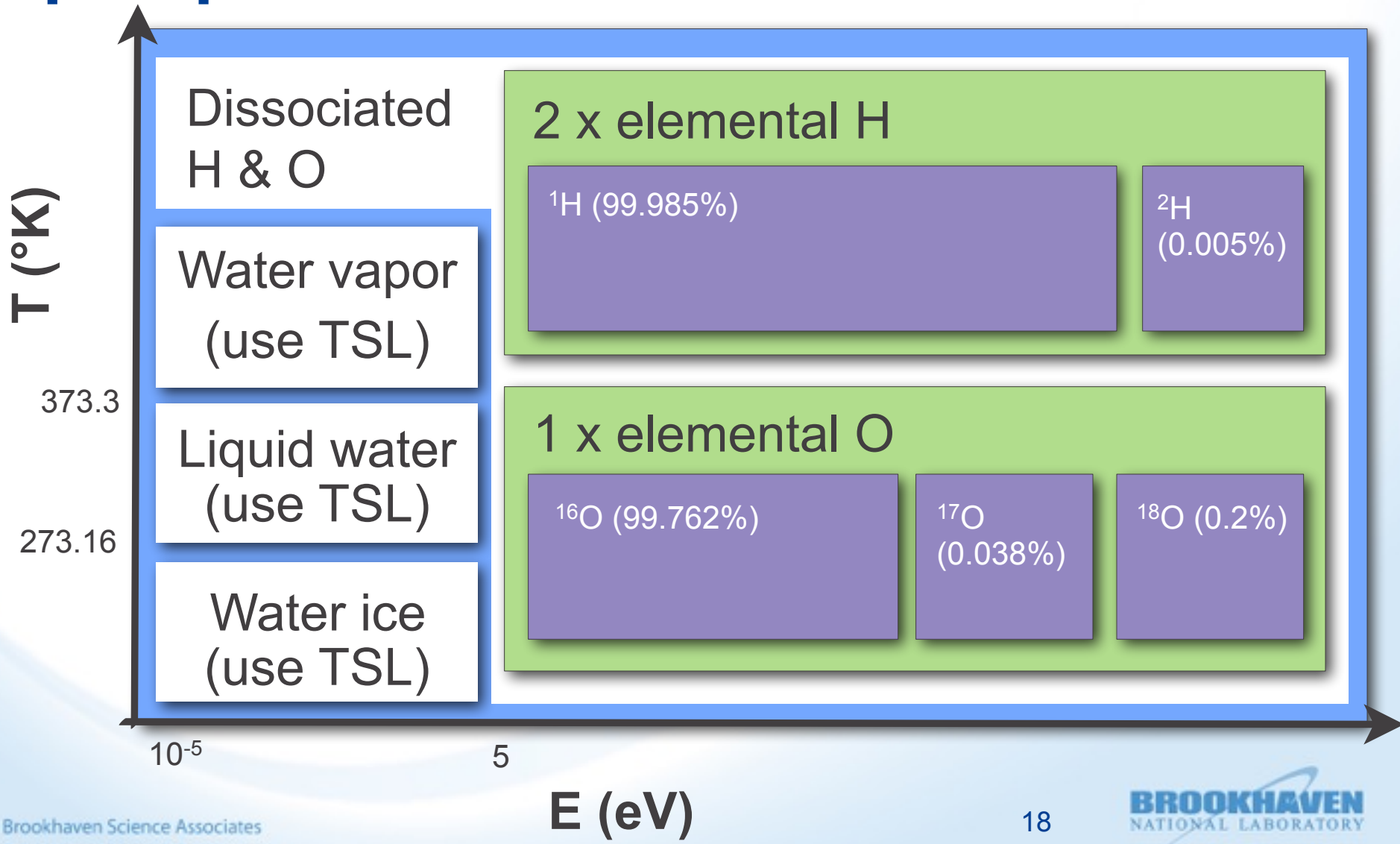
Normalization inconsistencies

- For benzene (C6H6):
  - T.ENDFB7R0 transitions smoothly across the thermal boundary
  - T.ENDFB7R0.LANL is off by a factor of 6
  - T.ENDFB7R1.LANL is off by a factor of 12



From Dave Heinrichs

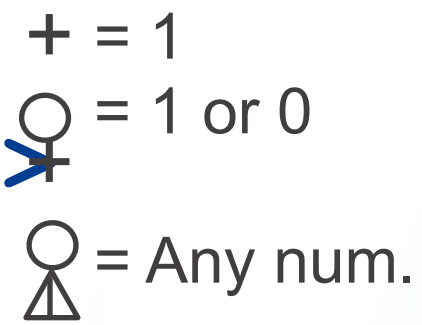
Think about water from a neutron's perspective



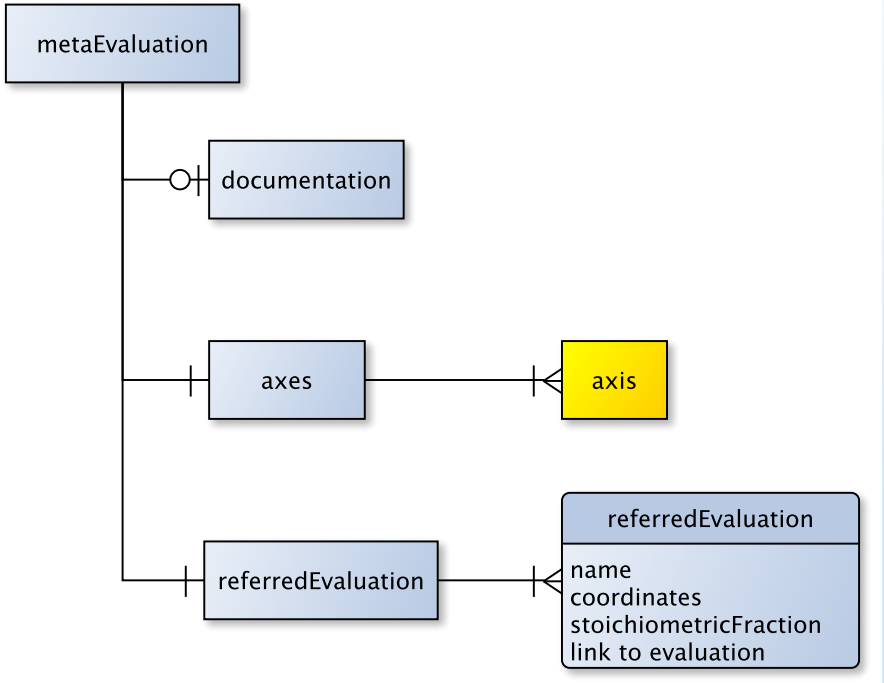
Gluing together evaluations: <metaEvaluation>

- **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 w/ weighted average of fission fragment evals.
  - Putting together the parts of a TSL evaluation at fixed temperature, but including all the scatterers.

Defining a <metaEvaluation>



- **<axis> elements define grid on which we will use evaluations.** Could be:
  - incident neutron energy
  - material temperature
- **<referredEvaluation> actual evaluation**
  - define stoichiometry
  - define location in grid defined by axis



Notes on `metaEvaluation` concept

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

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

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