Designing a high-level hierarchy for nuclear reaction data

David Brown

NNDC, Brookhaven National Laboratory

BROOKHAVEN NATIONAL LABORATORY

a passion for discovery

U.S. DEPARTMENT OF ENERGY | Office of Science

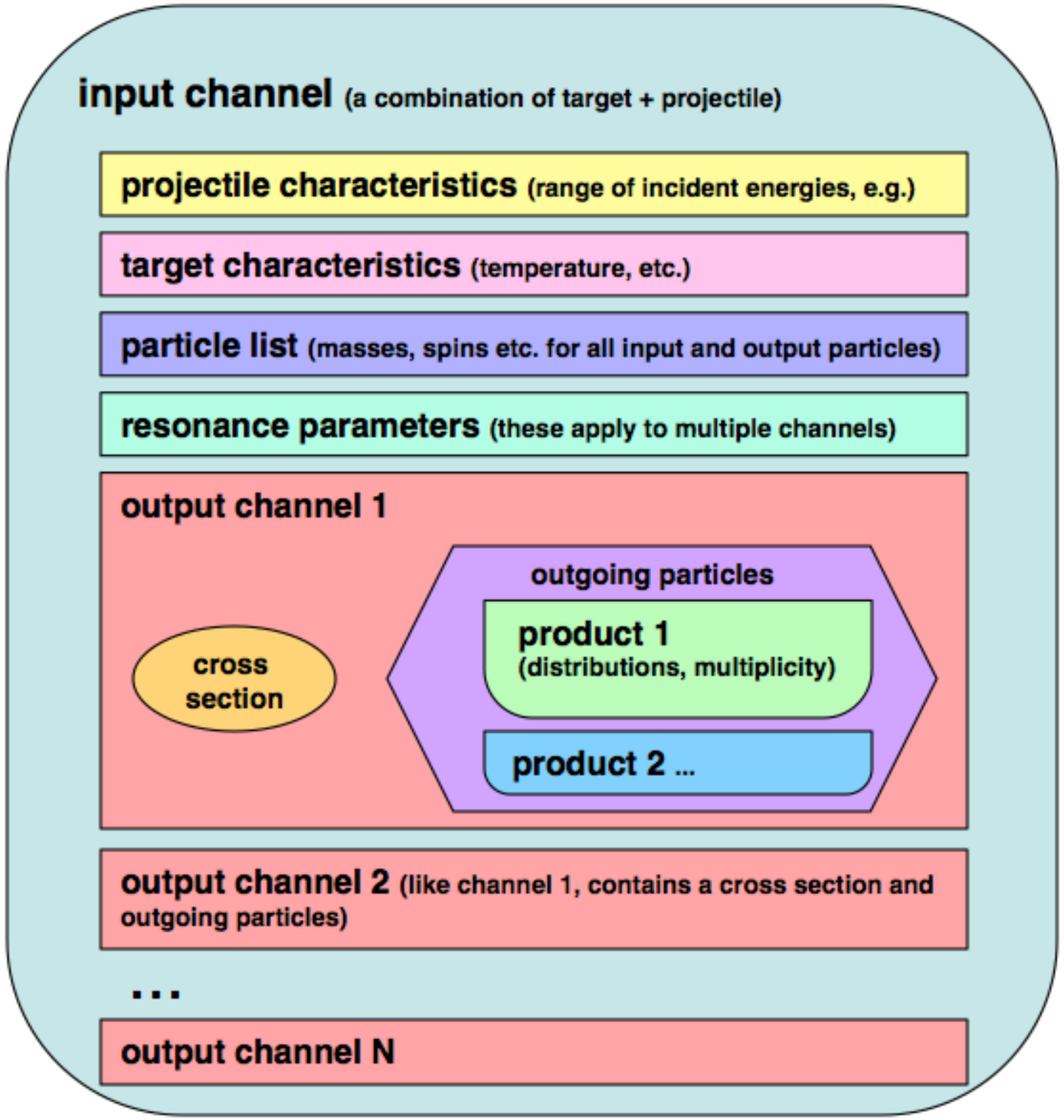
Goals

- *Use a hierarchy that reflects our understanding of nuclear reactions and decays, and that clearly and uniquely specifies all data.*

- *Support storing multiple representations of the same quantity simultaneously (e.g. evaluated and processed).*

- *Support any particle and any combination of reaction products (and subsequent decay products).*

Current GND hierarchy for reaction data is very ENDF-like



Where I am coming from as ENDF library manager

- **ENDF/B-VII.1 has 14 sublibraries**
  - neutron incident
  - charged particle incident: p, d, t, 3He
  - photonuclear
  - decay
  - atomic: atomic relaxation, photoatomic, electron
  - NFY
  - SFY
  - neutron standards
  - thermal neutron scattering
- **I can easily envision more**
  - More charged particles: all Z<=6
  - A structure-lite library
  - muons, pi0 (cosmic rays)
  - GFY, PFY
  - heavy-ion projectiles
  - activation

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Pending a review, I would say GND supports all these already

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I am even OK with covariance implementation in GND currently

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With the addition of FY markup to fission channels, these can be handled

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Tomorrow's discussion will deal with this

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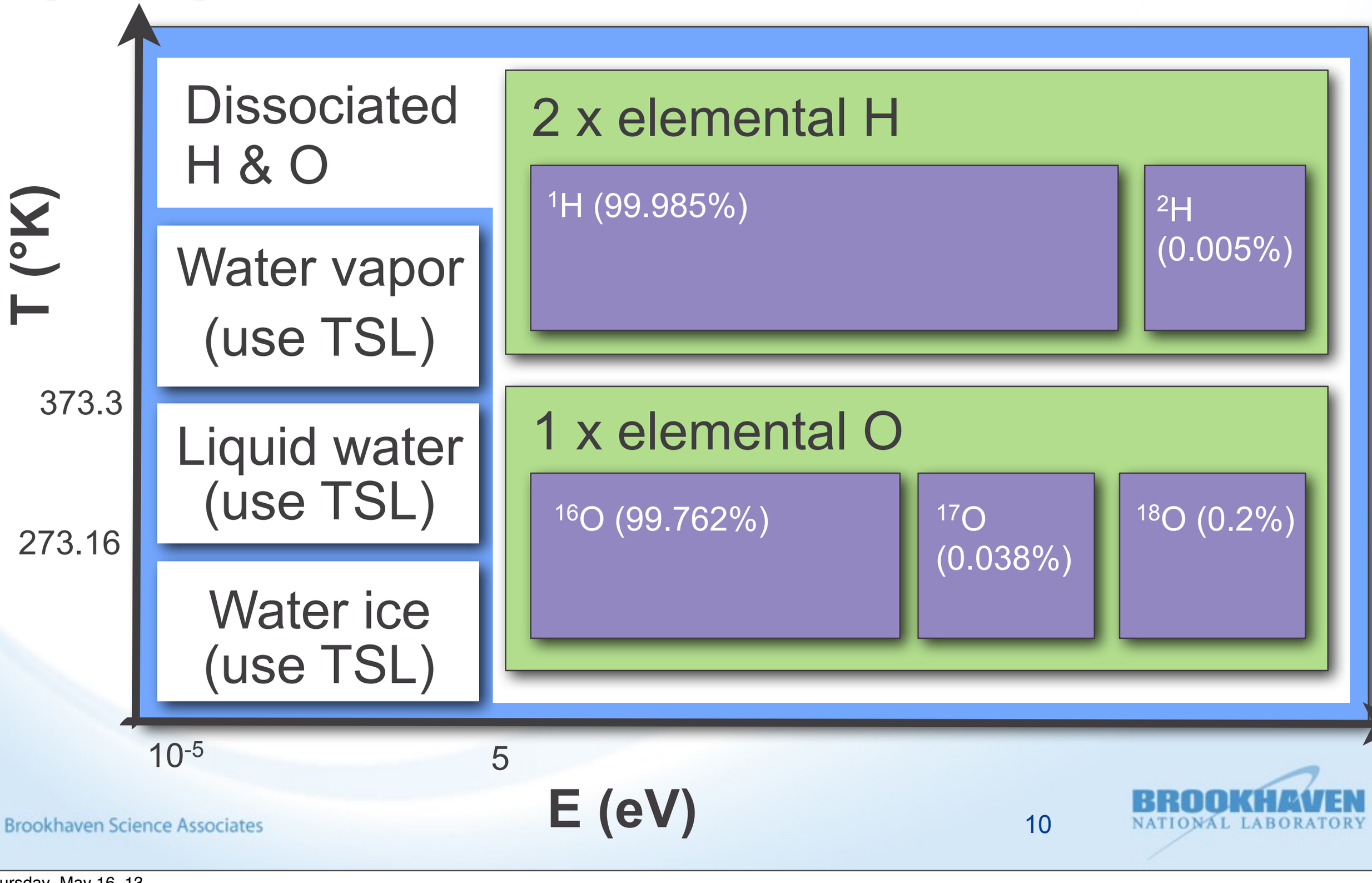
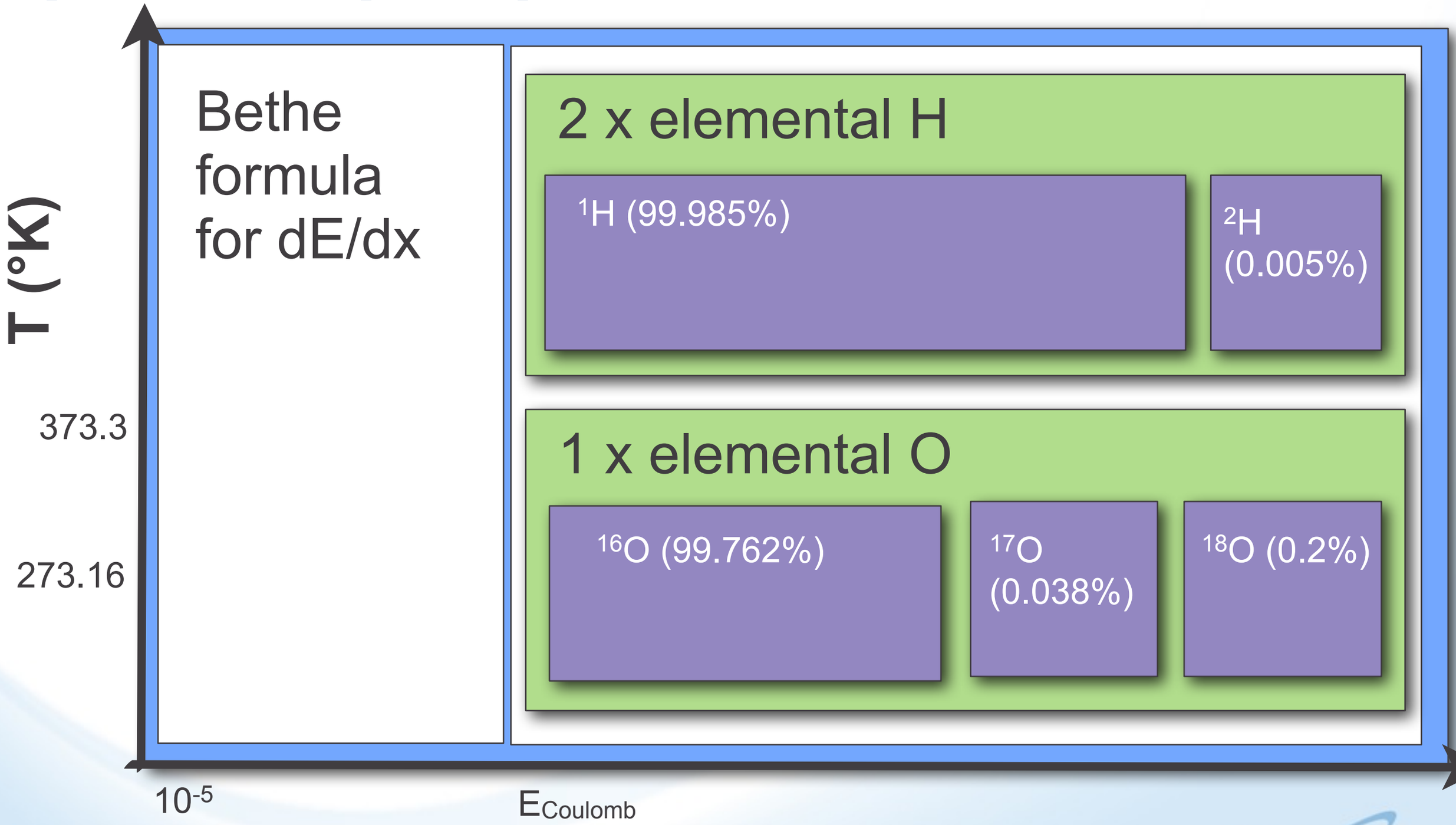
The rest require us to think harder about what we mean by a "target"

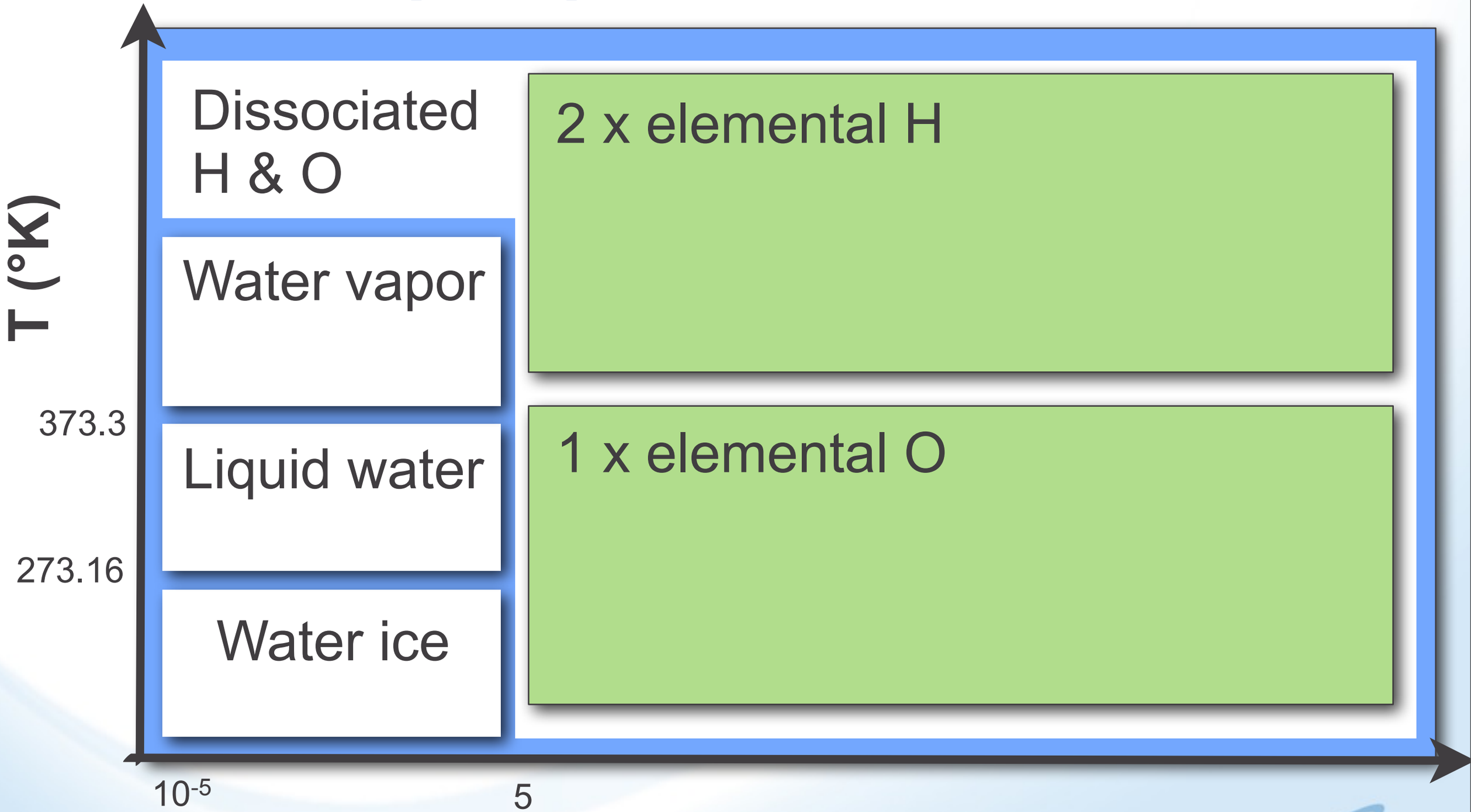
Think about water from a neutron's perspective



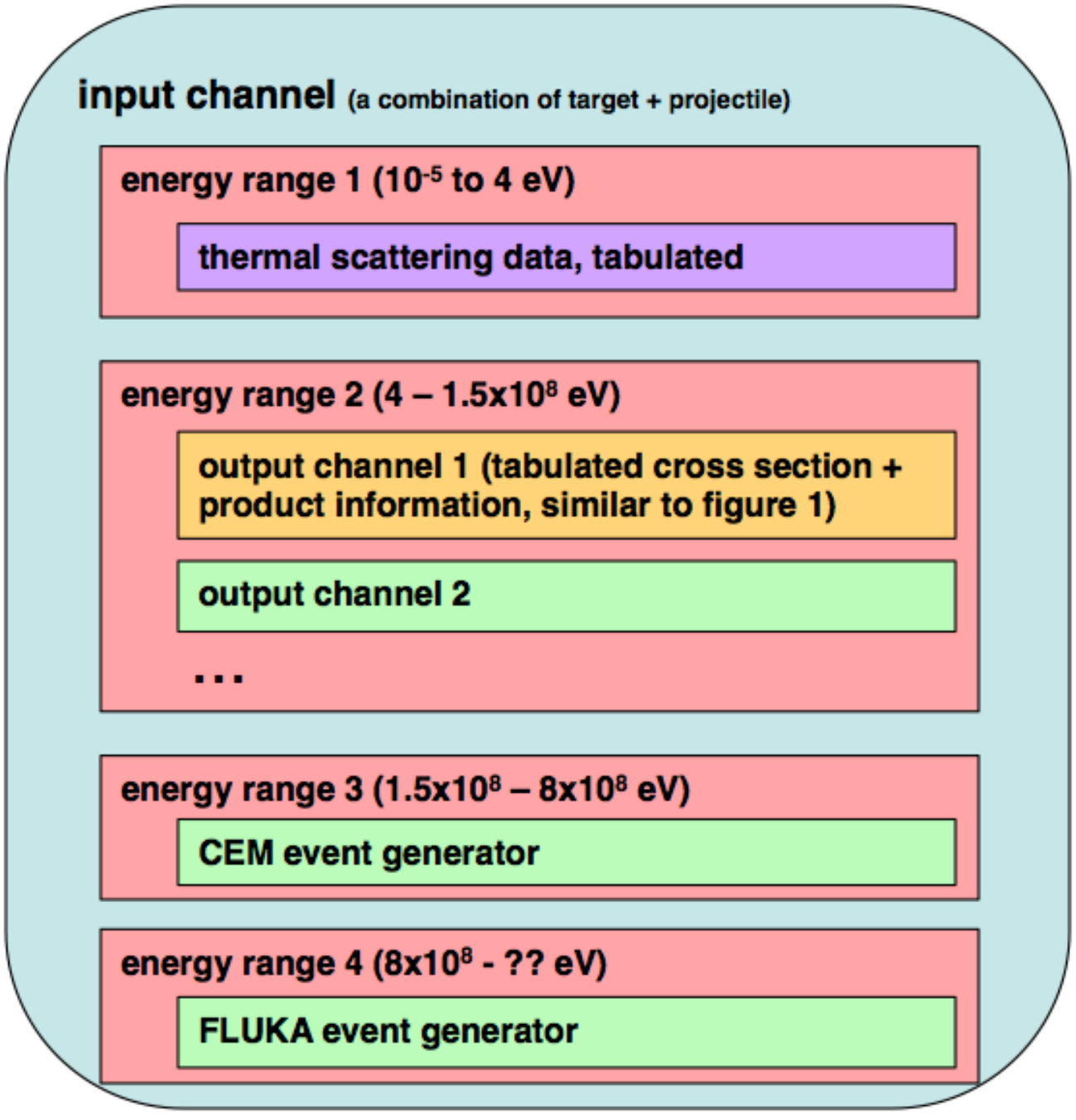
Now, think about water from a proton's perspective



And finally, think about water from an electron's perspective



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



There are actually many other instances where we want a broader notion of a “target”

- Elemental evaluations
- Grouping data on same target, but heated to different temperatures
- Ion stopping in complex material
- Generic Fission Fragments
- ...

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="..."
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Defining a metaTarget

names it and defines the valid projectile

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gotta say where we got it from

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Defining a metaTarget

defines regions of validity of `metaTarget` parts

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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 **`referredTarget`**s 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`**
- **`metaTarget`**s are often reusable across different libraries

Tasks

- Re-review GND reaction hierarchy, just to be sure
- Re-review GND resonance hierarchy, just to be sure
- Re-review GND covariance hierarchy, just to be sure
- Add FY markup (cumulative & independent)
- Structure + decay formats (see tomorrow)
- Refine metatargets markup, provide fudge coding
- Markup for atomic processes
- Review newly added markup for thermal neutron scattering data

Resources needed

- IUPAC maintains abundance tables, we'll need someone to maintain ours
- Need someone familiar with thermal neutron scattering to aid in markup
- Need someone familiar with R matrix theory to review RR markup
- Need someone familiar with atomic physics to aid in atomic physics markup (see next page for further comment)

Potential problems?

- Don’t want to have to specify equation of state, and we don’t want to get deep into molecular and atomic scattering issues. We need to draw some clear physics-coverage lines.
- What about non-terrestrial abundances?
- Should we be interacting with VAMDC project on atomic physics issues? (http://www.vamdc.eu/)