TNSL support in GNDS 2.0 and beyond

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TNSL format options went through a major overhaul in GNDS-2.0

- Changes in 2.0:
  - TNSL has been integrated into the reactionSuite. Coherent elastic, incoherent elastic and incoherent inelastic scattering terms are all listed as unique reactions, with terms like Debye-Waller and S(α,β) stored as double-differential cross sections
    - Elastic term can be split into two reactions if both coherent and incoherent are present
  - For incoherent inelastic, GNDS adds support for storing the phonon spectrum instead of S(a,b)
    - no evaluations so far use that option
  - Adds 'distinctScatteringKernel' as an allowed child of each scatteringAtom, to support lifting the incoherent approximation
    - no evaluations so far using this option

… but some further changes should be considered

- First issue: need some guidance on what to expect when we start getting evaluations with **coherent inelastic**

$$\frac{d^2\sigma_i(E \to E', \mu, T)}{dE' d\Omega} = \frac{M_i}{4\pi k_B T}\sqrt{\frac{E'}{E}}\left[\sigma_{\text{bound},i}\mathcal{S}_{\text{self},i}(\alpha,\beta,T) + \sigma_{\text{coh},i}\mathcal{S}_{\text{dis},i}(\alpha,\beta,T)\right]$$

  - Equation suggests that coherent and incoherent terms are separable. Should they be stored as a single reaction, or broken up into two separate reactions?

  - If separate, need to modify GNDS specifications to allow for a scatteringAtom with only a distinct scattering kernel, and add ‘thermalNeutronScattering_coherentInelastic’ double-differential form

Issues with target stoichiometry

- Second issue: GNDS-2.0 does not provide a way to clearly specify in the evaluation how to switch to 'standard' incident neutron evaluations for energies or temperatures outside the TNSL domain
  - For 'whole molecule' evaluations like benzene, CH4, and SiO2, if an application involves a mixture of thermal and fast neutrons the user must take care to switch to the right mix of isotopes outside the thermal region
  - Even if TNSL is only for one atom (e.g. Zr in ZrH), it may need to be replaced by multiple isotopic evaluations (Zr90, Zr91, etc.) outside thermal region
    - Additional complication: isotopic abundance may be function of time due to burnup, e.g. for UinUN
- This could be left up to the user, but explicit instructions would be valuable

Current status (GNDS-2.0)

- Scattering atoms are stored inside incoherent inelastic section
  - May not include all atoms in the molecule! Example is missing O from C5O2H8
  - No indication of whether evaluation is for individual atom or whole molecule

```
<scatteringAtoms>
  <scatteringAtom pid="H1" numberPerMolecule="8" primaryScatterer="true">
    <mass value="1.00782500046" unit="amu"/>
    <e_critical value="197.6285" unit="eV"/>
    <e_max value="5.000001" unit="eV"/>
    <boundAtomCrossSection value="40.5722288111" unit="b"/>
    <selfScatteringKernel symmetric="true">
      <gridded3d>...</gridded3d>
    </selfScatteringKernel>
    <T_effective>
      <XYs1d>...</XYs1d></T_effective></scatteringAtom>
  <scatteringAtom pid="C12" numberPerMolecule="5">
    <mass value="12.0010951675" unit="amu"/>
    <e_max value="0" unit="eV"/>
    <boundAtomCrossSection value="0.42808571156" unit="b"/>
    <selfScatteringKernel symmetric="true">
      <freeGasApproximation/></selfScatteringKernel></scatteringAtom>
</scatteringAtoms>
```

Tentative proposal: move the definition of scattering atoms up to become child of ‘reactionSuite’

For example, if benzene should be replaced primarily with C12 but sometimes with C13:

```
<reactionSuite projectile="n" target="benzene" interaction="TNSL" ...>
  ...
  <thermalScatteringAtoms>
    <scatteringAtom pid="H1" numberPerMolecule="6">
      <aboveTNSLFraction pid="H1" value="1.0"/>
    </scatteringAtom>
    <scatteringAtom pid="C" numberPerMolecule="6">
      <aboveTNSLFraction pid="C12" value="0.9893"/>
      <aboveTNSLFraction pid="C13" value="0.0107"/>
    </scatteringAtom>
  </scatteringAtoms>
  ...
</reactionSuite>
```

Provides guidance to user codes for how to replace molecule above thermal region.

TBD: burnup-dependent rule? That may still need to be left to user.

Interpolation issues for S(α,β) / S(α,β,T)

- Third issue: when designing GNDS-2.0, we assumed that S(α,β) would always be given on a uniform interpolation grid

- ENDF-6 format supports using a different S(α) / S(T) interpolation rules for each value of β, but until recently all ENDF evaluations consistently used log-lin interpolation for S along α, β and T. GNDS-2.0 tried to simplify things by storing S(α,β,T) in a 'gridded' container that only supports one interpolation rule along each axis

New JENDL-5 TNSL evaluations have some complications

—D in D20, O in D2O: different values of β claim different interpolation rules for S with respect to T
  - *Should users interpolate S with with temperature?*

—Ortho-H / Para-H / Ortho-D / Para-D: use LLN=1 (indicates that ln(S) is stored instead of S) but also claims log-lin interpolation. Unclear how we should handle this: interpolate ln(ln(S)) linearly with $\alpha/\beta/T$?

All issues are open for discussion on the GNDS specifications repository on NEA gitlab

- https://git.oecd-nea.org/science/wpec/gnds/formats/-/issues/80
- https://git.oecd-nea.org/science/wpec/gnds/formats/-/issues/124

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