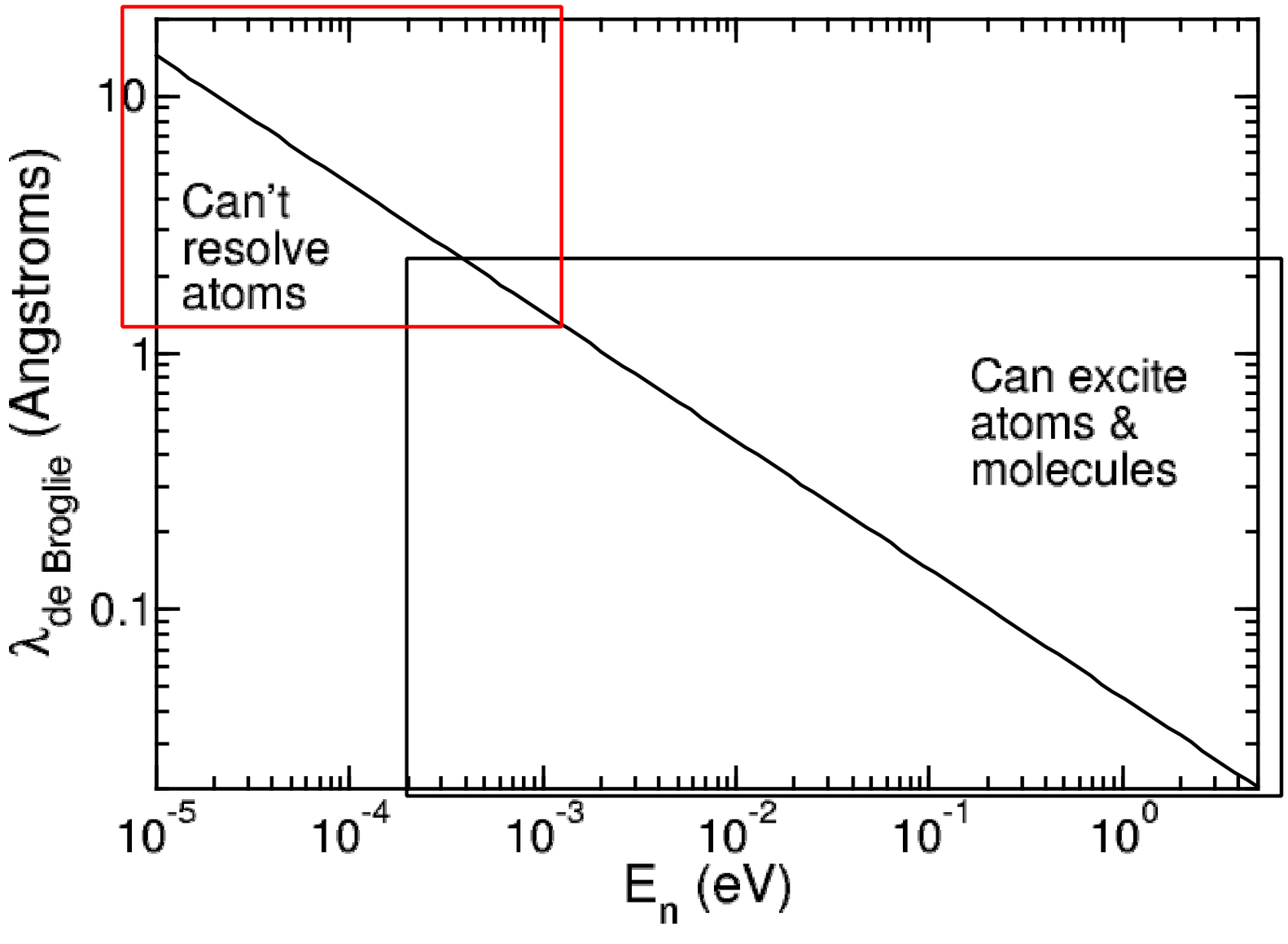
Now & future TSL formats

D. Brown (NNDC, BNL)
for SG-38 & EG-GNDS

TSL data covers range of energies, probes range of length scales

- At low energies, temperatures, need coherent elastic description of crystalline structure

- At high temperatures, energies, need incoherent descriptions



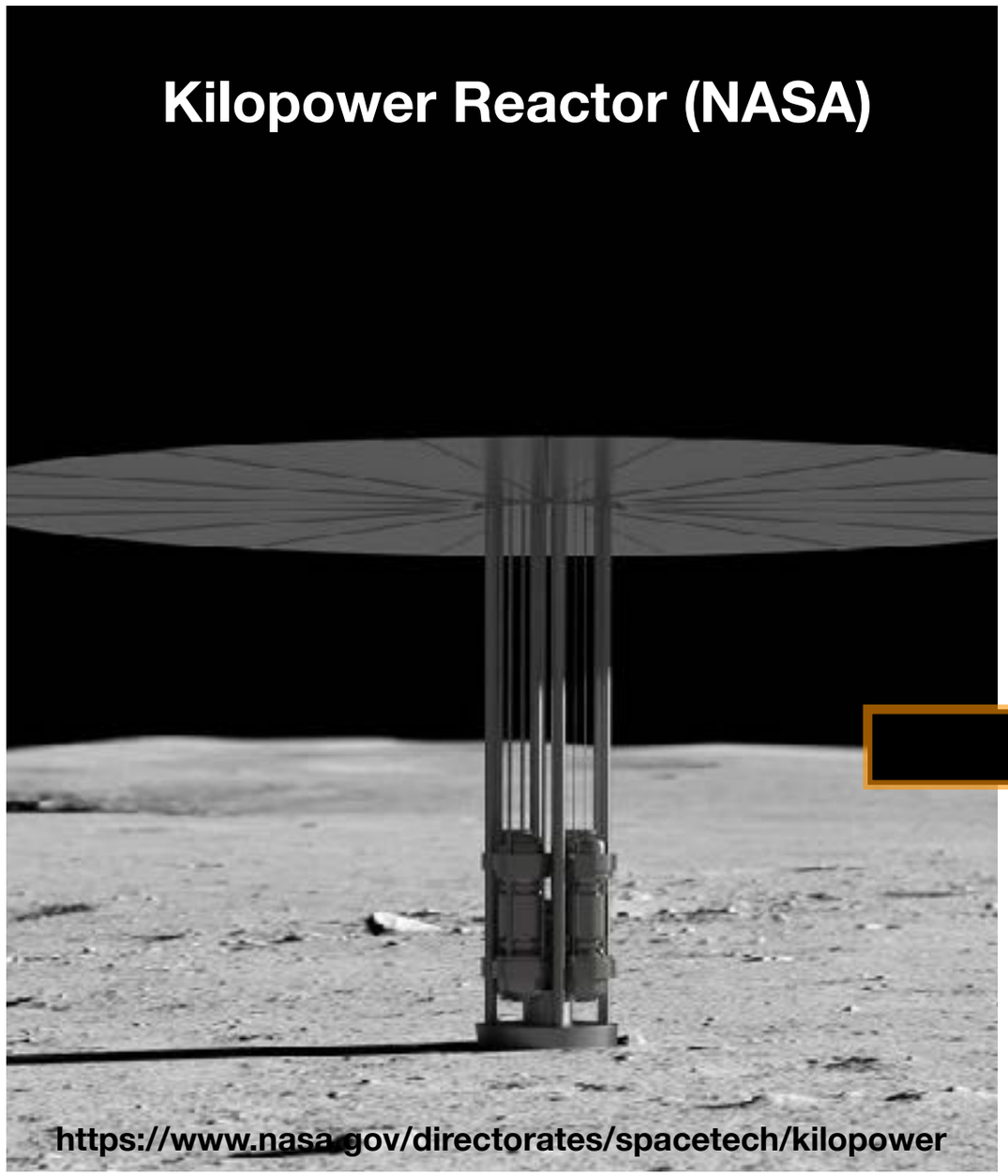
There are “two” TSL formats

- GNDS-1.9’s TSL format != planned TSL format
- Planned TSL format still under debate
- GNDS-1.9 TSL format is “simple” repackaging of ENDF-6 in a GNDS-like format
- No code “speaks” GNDS-1.9, yet

Future TSL format

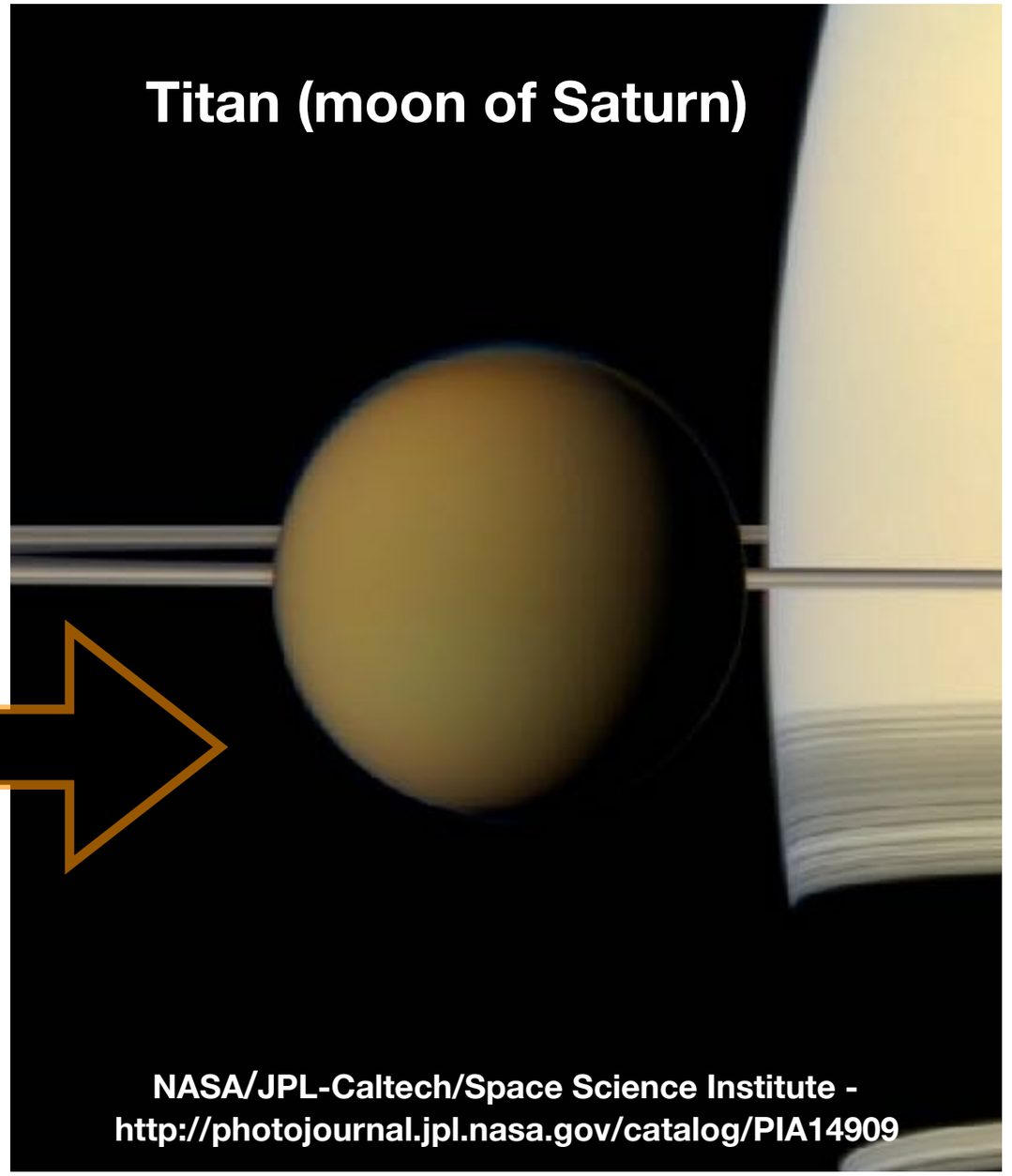
Hypothetical future problem

Kilopower Reactor (NASA)



https://www.nasa.gov/directorates/spacetech/kilopower

Titan (moon of Saturn)



NASA/JPL-Caltech/Space Science Institute -
http://photojournal.jpl.nasa.gov/catalog/PIA14909

Hypothetical future problem

Kilopower Reactor (NASA)

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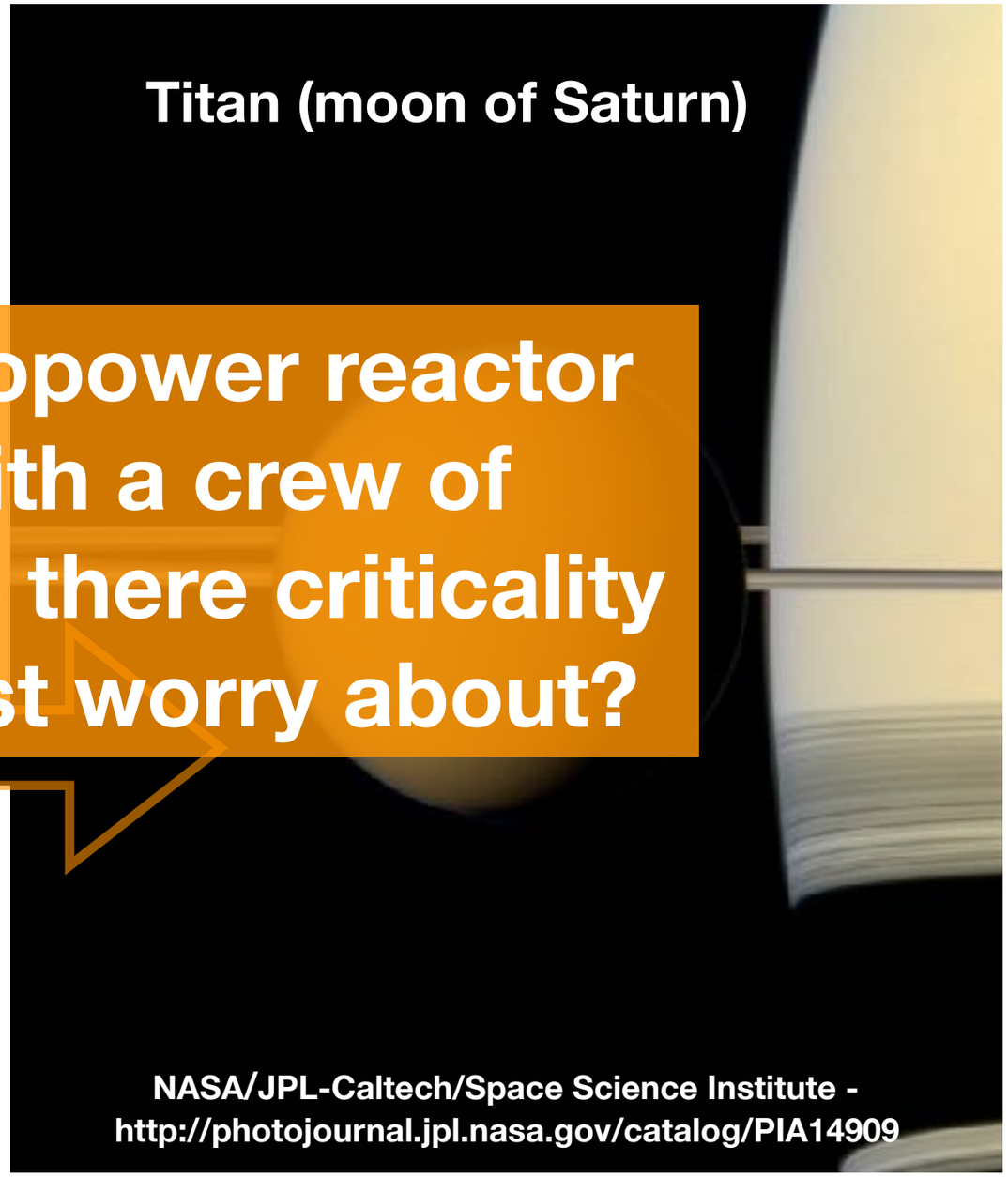
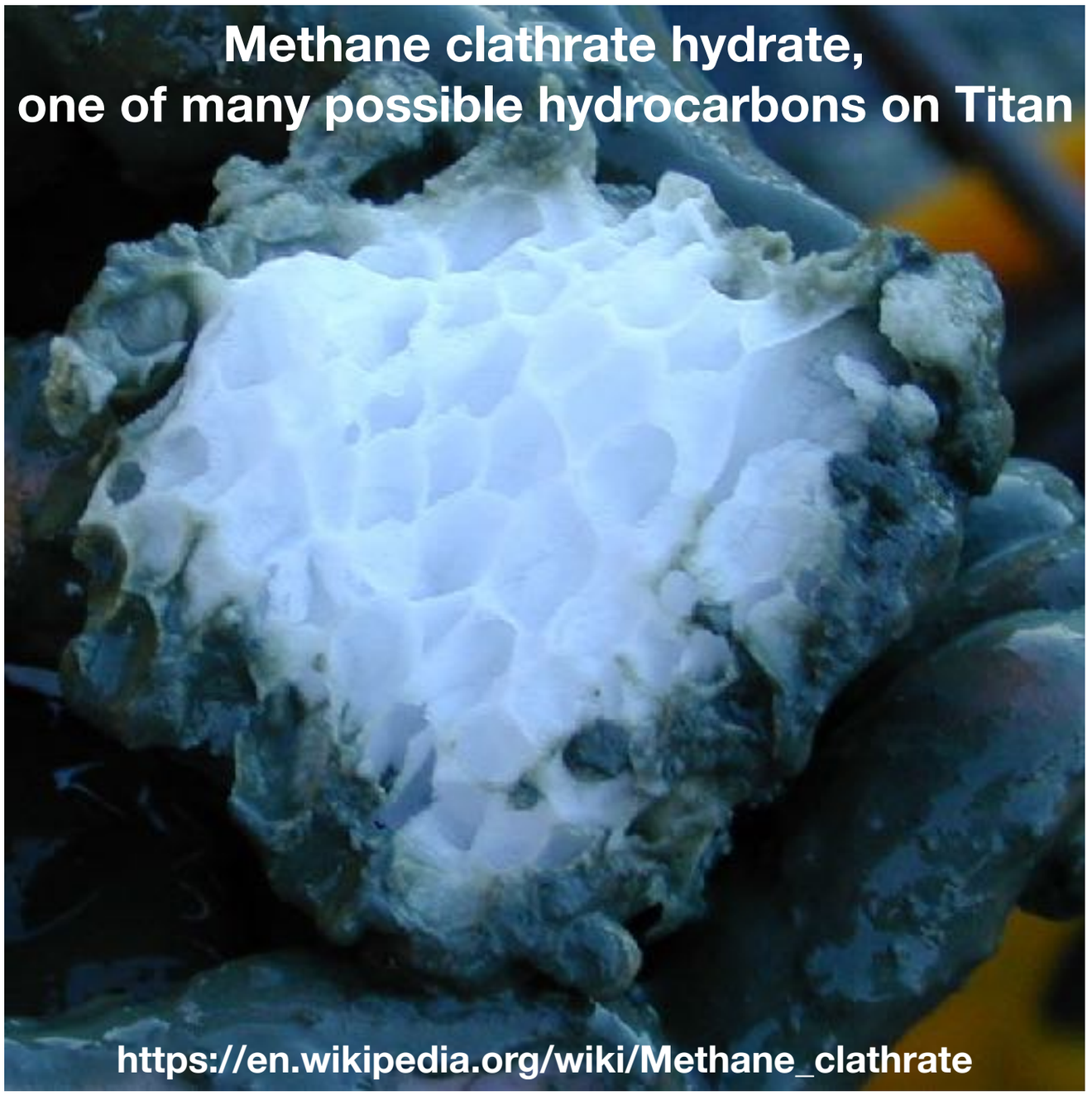


NASA/JPL-Caltech/Space Science Institute -
http://photojournal.jpl.nasa.gov/catalog/PIA14909

If we put a Kilopower reactor on Titan, with a crew of astronauts, are there criticality issues we must worry about?

TSL

Hypothetical future problem



Common structure of all GNDS transport files

```
<reactionSuite
    projectile="n"
    target="(CH4)4(H2O)23"
    evaluation="ENDF/B-8.14"
    format="10.9" projectileFrame="lab">
  <styles>…
  <documentations>…
  <PoPs name="protare_internal" version="1.0" format="0.1">…
  <reactions>…
  <sums>…
</reactionSuite>
```

Styles defines different forms of evaluated and/or processed data

```
<styles>
    <!--
      Information relevant for detailing the processed version(s) of the
      data in this evaluation.
    -->
    <evaluated label="eval" date="1959-01-01" library="endfb" version="8.0">
      <targetTemperatureDomain min="4" max="373.15" unit="K"/>
      <projectileEnergyDomain min="1e-5" max="5.0" unit="eV"/></evaluated>
    <integratedCrossSections derivedFrom="eval" date="2018-04-11"/>
</styles>
```

One evaluated style

One processed style

Evaluated style declares energy and temperature ranges of the evaluation

Plain old documentation

```
<documentations>
  <documentation style="endfDoc">
      <documentation name="endfDoc"><![CDATA[
          Methane clathrate hydrate

          Eval-Dec35
          A. Hawari

          -----ENDF/B-VIII.14
          ------TSL DATA
          -------GNDS FORMAT

          We're sending KRUSTY to Titan!
          ]]>
  </documentation>
</documentations>
```

GNDS eventually will allow more expressive documentation, but that is another talk

Define all particles in evaluation (in future, want to shift to central database)

```
<PoPs name="protare_internal" version="1.0" format="0.1">
  <!--
      Database of particle properties here.  Specifically, the properties
      of the chemical elements that make up the current target material as
      well as the incident neutron information (for now included until have
      central database of default particle properties).
  -->
  <baryons>
    <baryon id="n">…
  </baryons>
  <chemicalElements>
    <chemicalElement symbol="H" Z="1" name="Hydrogen"></chemicalElement>
    <chemicalElement symbol="C" Z="6" name="Carbon"></chemicalElement>
    <chemicalElement symbol="O" Z="8" name="Oxygen"></chemicalElement>
  </chemicalElements>
</PoPs>
```

List of reactions give possible event outcomes

```
<reactions>
  <reaction label="tsl_coherent_elastic">⋯
  <reaction label="tsl_incoherent_elastic">⋯
  <reaction label="tsl_inelastic">⋯
  <reaction label="tsl_gaussian_approximation">⋯
  <reaction label="tsl_short_collision_time_approximation">⋯
</reactions>
```

Labels are just labels, nothing more

In real life, would never have all these at once in the same file as several are the same thing at a different level of approximation

An aside on Monte Carlo transport

- Decide we're going to have a reaction based on path length, x:

$$P(x) = \exp(-x/l_{mfp})$$

Here $l_{mfp}=\sum_i \sigma_i \rho_i$ and σ_i is the total cross section for the i^{th} particle species

- Sample reaction: $P_{ic} = \sigma_{c,i} / \sigma_i$

- Cross section for c^{th} reaction of i^{th} particle in a <reaction>

Each reaction has a cross section element of some sort that can be used to sample

```
<reaction label="tsl_coherent_elastic">
  <dCrossSection_dE_dOmega label="eval">
    <tslCoherentElastic>…
  </dCrossSection_dE_dOmega>
  <crossSection label="integratedCrossSections">...</crossSection>
</reaction>
```

This declares the stuff inside to be $d^2\sigma(E)/dE'd\Omega$

Styles defines different forms of evaluated and/or processed data

```
<styles>
    <!--
      Information relevant for detailing the processed version(s) of the
      data in this evaluation.
    -->
    <evaluated label="eval" date="1959-01-01" library="endfb" version="8.0">
      <targetTemperatureDomain min="4" max="373.15" unit="K"/>
      <projectileEnergyDomain min="1e-5" max="5.0" unit="eV"/></evaluated>
    <integratedCrossSections derivedFrom="eval" date="2018-04-11"/>
</styles>
```

One evaluated style

One processed style

Evaluated style declares energy and temperature ranges of the evaluation

For cross checking against higher energy data, need total cross section

```
<reaction label="tsl_coherent_elastic">
  <dCrossSection_dE_dOmega label="eval">
    <tslCoherentElastic>…
  </dCrossSection_dE_dOmega>
  <crossSection label="integratedCrossSections">...</crossSection>
</reaction>
```

Style above explains this connection

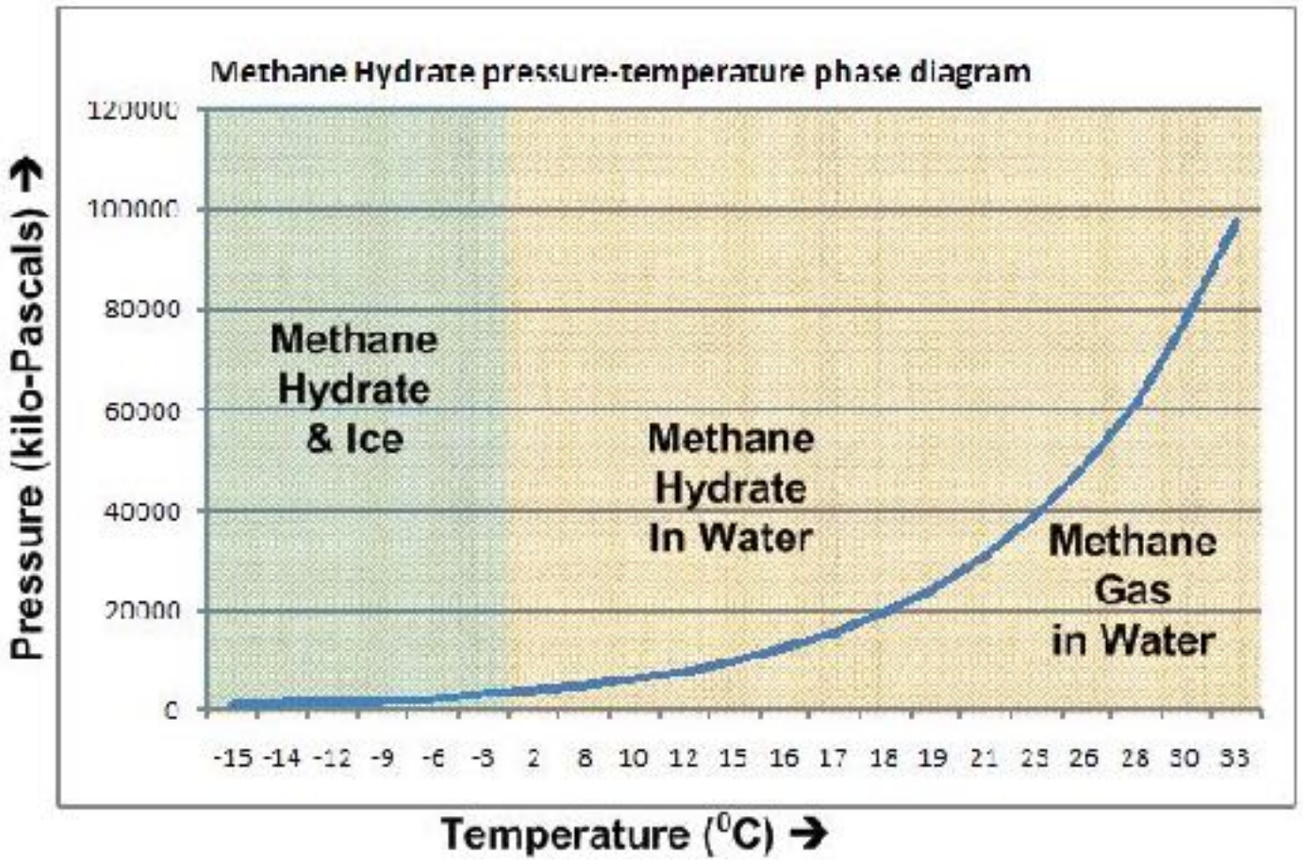
The summands element explains this connection

```
<sums>
  <crossSections>
    <crossSectionSum label="total_tsl_scattering">
      <summands>
        <add href="/reactionSuite/reactions/reaction[@label='tsl_inelastic']/crossSection"/>
        <!-- instead of "total_tsl_scattering" I could used "total" and put hyperlinks to
        capture cross sections here too -->
      </summands>
      <Q>...</Q>
      <crossSection>...</crossSection>
    </crossSectionSum>
  </crossSections>
</sums>
```

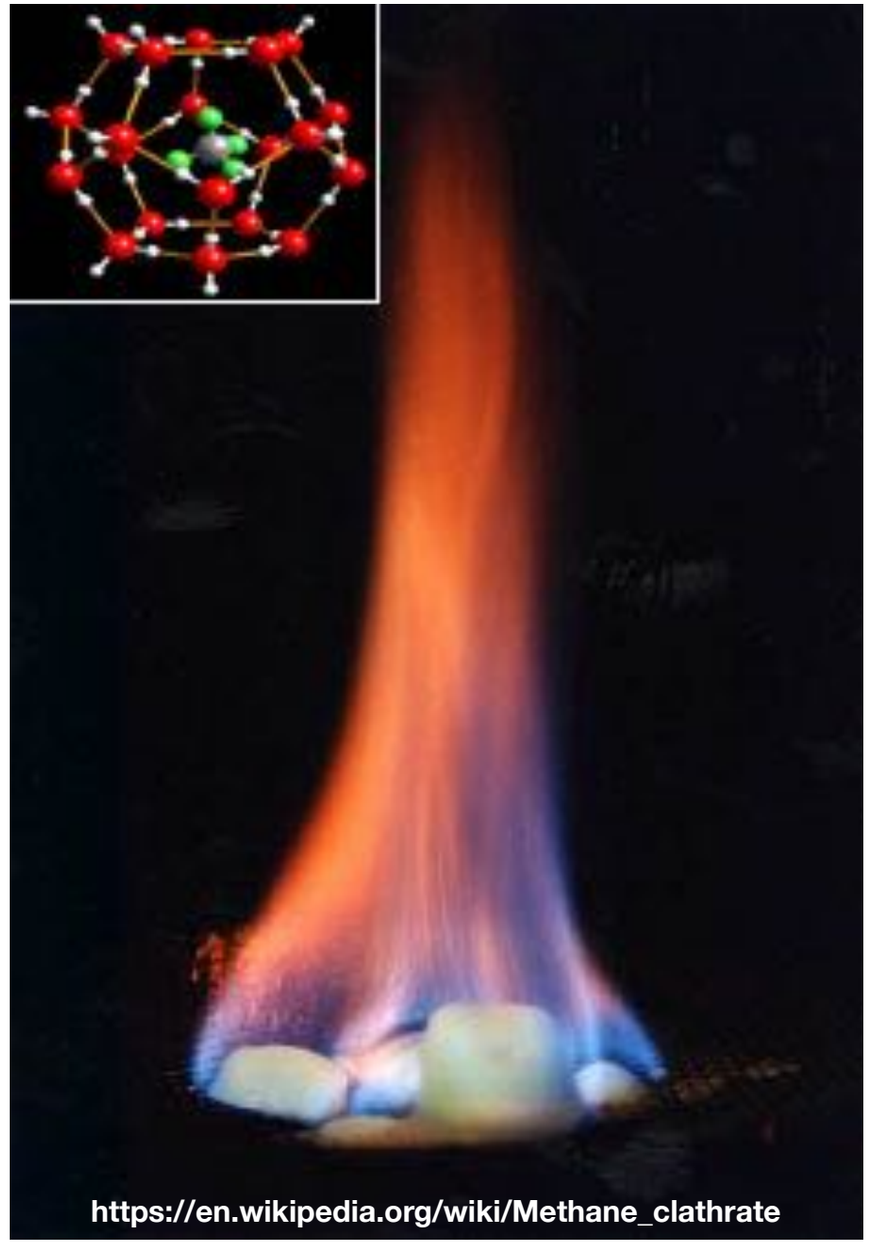
Evaluated total can go here

Methane clathrate hydrate

https://en.wikipedia.org/wiki/Methane_clathrate



- “Crystal”, but can melt and is flammable
- Common on Earth in undersea deposits



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Methane clathrate hydrate

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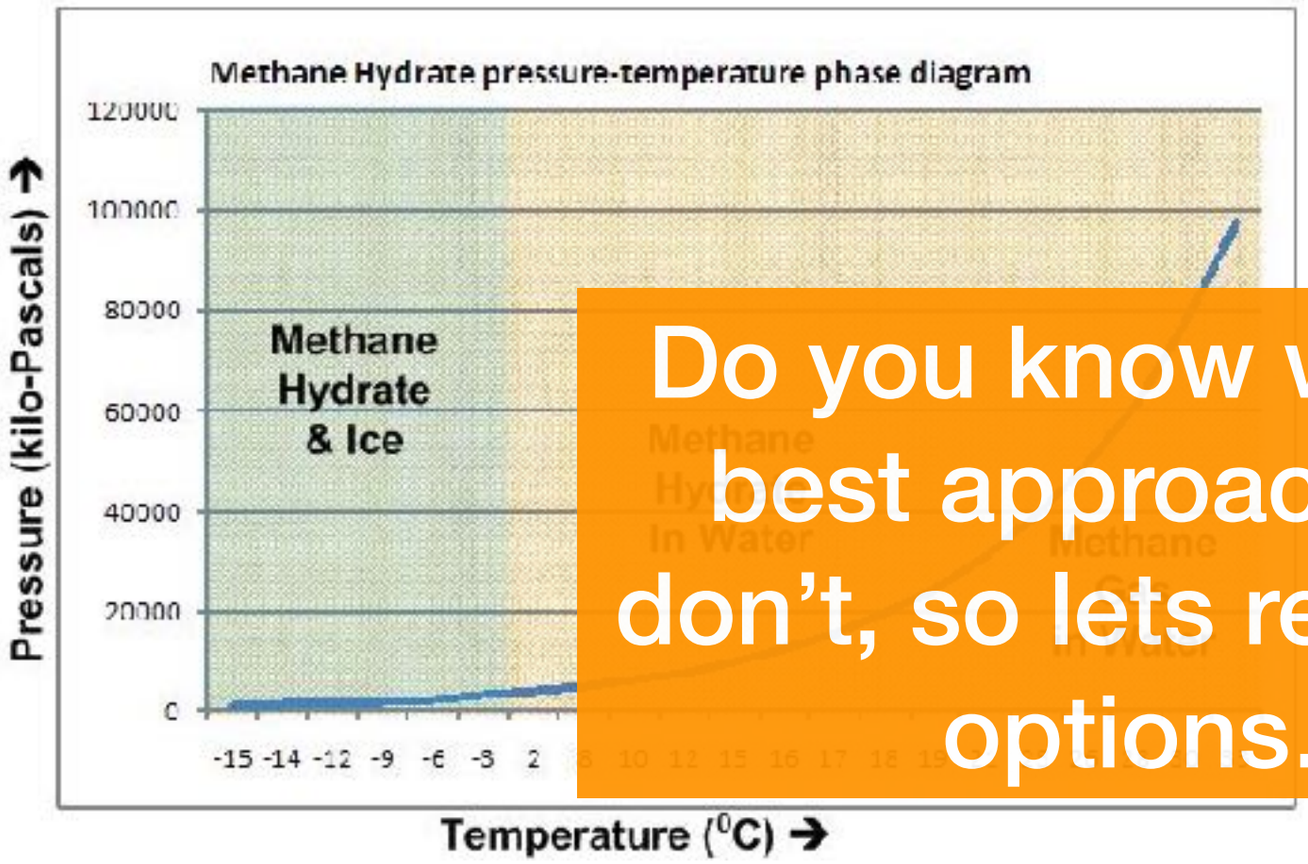
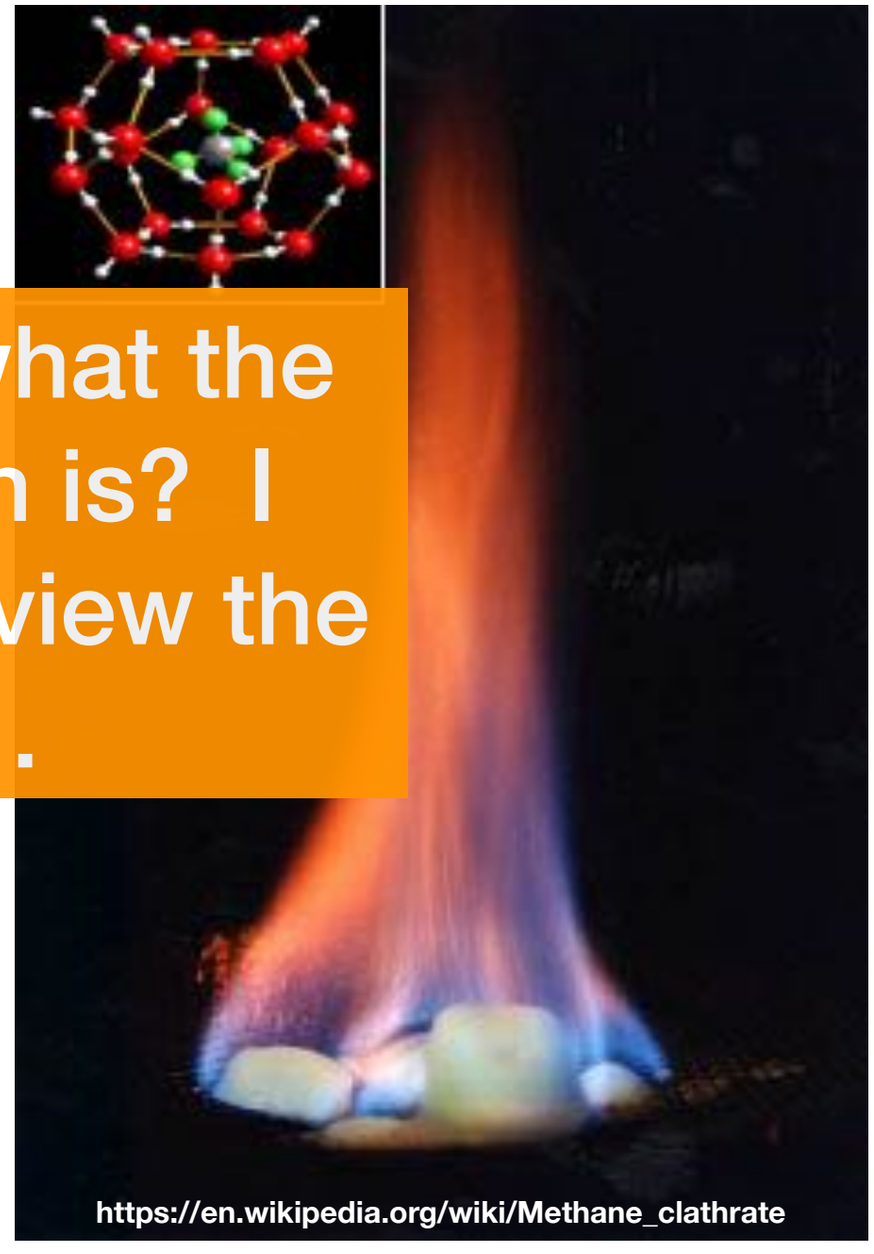


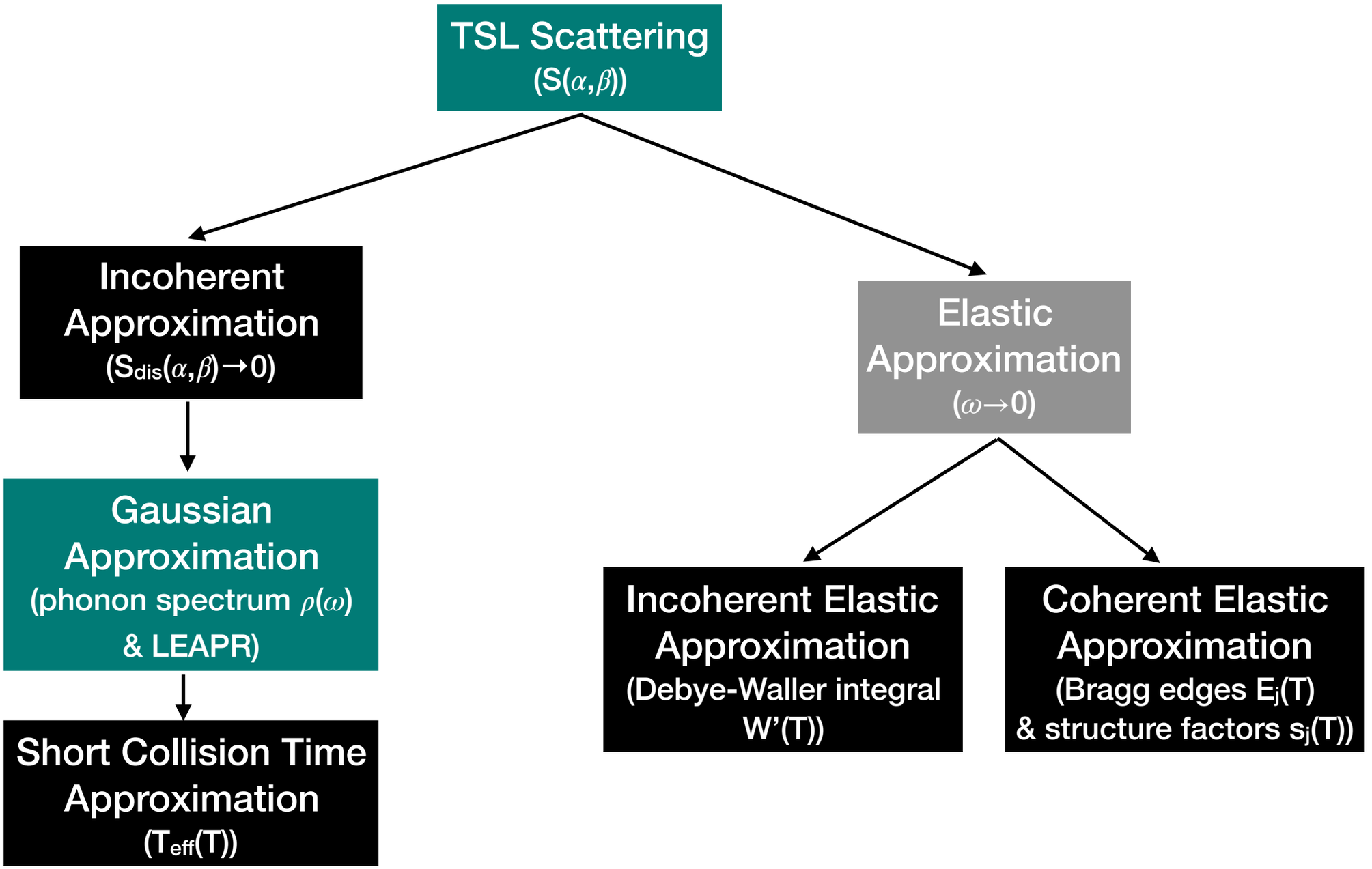
Do you know what the best approach is? I don't, so lets review the options…

- "Crystal", but can melt and is flammable
- Common on Earth in undersea deposits



https://en.wikipedia.org/wiki/Methane_clathrate

Taxonomy of TSL approximations



Elastic scattering options are very similar to ENDF-6 options

```
<tslIncoherentElastic>
  <DebyeWallerIntegral>...</DebyeWallerIntegral>
  <boundAtomCrossSection>...</boundAtomCrossSection>
</tslIncoherentElastic>
```

```
<tslCoherentElastic>
  <BraggEdges>
    <BraggEdge label="0">
      <BraggEnergy>...</BraggEnergy>
      <structureFactor>...</structureFactor>
    </BraggEdge>
    <BraggEdge label="1">...</BraggEdge>
  </BraggEdges>
</tslCoherentElastic>
```

$E_j(T)$, $s_j(T)$ allowed
Both given as interpolation table

Un-approximated S(α,β) data supported

```
<tslIncoherentInelastic realTempUsed="true" incoherentApproximation="false">
  <cutOffEnergy><!-- 5 eV as a physical quantity --></cutOffEnergy>
  <scatterers>
    <scatterer pid="C" numberPerMolecule="2">
      <Teff><!-- effective temp. data goes here --></Teff>
      <freeAtomCrossSection>...</freeAtomCrossSection>
      <boundAtomCrossSection>...</boundAtomCrossSection>
      <coherentAtomCrossSection>...</coherentAtomCrossSection>
      <incoherentAtomCrossSection>...</incoherentAtomCrossSection>
      <selfScatteringKernel symmetric="true">
        <!-- S(alpha,beta) data goes here -->
      </selfScatteringKernel>
      <distinctScatteringKernel>
        <!-- S(alpha,beta) data goes here -->
      </distinctScatteringKernel>
    </scatterer>
  </scatterers>
</tslIncoherentInelastic>
```

In incoherent approximation, don't include this term (argues for ditching incoherentApproximation flag)

“New” options: SCT, Gaussian approximation?

```
<tslGaussianApproximation>
  <phononSpectrum>...</phononSpectrum>
</tslGaussianApproximation>
```

This is ρ(ω)

Not shown: new documentation format would allow direct storage of LEAPR input in file

```
<reaction label="tsl_short_collision_time_approximation">
  <dCrossSection_dE_dOmega label="eval">
    <tslSCTApproximation/>
  </dCrossSection_dE_dOmega>
</reaction>
```

I think this requires a $T_{eff}(T)$ sub-element

GNDS 1.9 vs. Planned GNDS

- More possible ways to express TSL data
- Logical arrangement consistent with other transport data
- Checking against total/elastic cross section fully supported
- No format abuse (e.g. coherent elastic)
- “infinite precision”
- Covariance *everywhere*