HighNESS International School on Thermal Neutron Scattering Kernel Generation

NCrystal : a library for thermal neutron transport

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Detector group & Data Management and Software Centre

BrightnESS is funded by the EU Framework Program for Research and Innovation Horizon 2020, under grant agreement 676548
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DISCLAIMER

Estimated time spent by me preparing for this school:

- **Adding new code in NCrystal needed for the school: 5 months.**
- **Preparing Jupyter notebooks for the school: 3 weeks.**
- **Meetings and discussion about the school: 1 week.**
- **Preparing these slides: 2 days.**
- **Rehearsing: 2 hours.**

Outline

NCrystal
Thermal Neutron Transport

- **Thermal neutron scattering theory (quick recap)**
- **The NCrystal project: Background, history, introduction**
  - Jupyter-lab Basic1 (1st half) 
- **NCrystal materials data**
  - Jupyter-lab Basic1 notebook (2nd half) 
- **NCrystal elastic physics algorithms**
  - Jupyter-lab Basic2 notebook 
- **NCrystal inelastic physics algorithms (high-level view)**
- **Miscellaneous subjects (atom defs, multiphase, SANS, amorph. materials, speed, ...)**
  - Jupyter-lab Advanced1, Advanced2, Advanced3 notebooks 
- **Anatomy of a scattering kernel**
- **VDOS to scattering kernel (the Sjolander method)**
  - Jupyter-lab Advanced4 notebook 

Jupyter tutorials for improved v3.6 API at:
https://github.com/mctools/ncrystal-notebooks/

Note: these slides available at:
https://indico.esss.lu.se/event/3096/

Thermal Neutron scattering theory

(recap for NCrystal)

Very brief, refer to Rolando Granada's lectures for much more detail!

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Thermal neutron scattering: Rich connection to material structure

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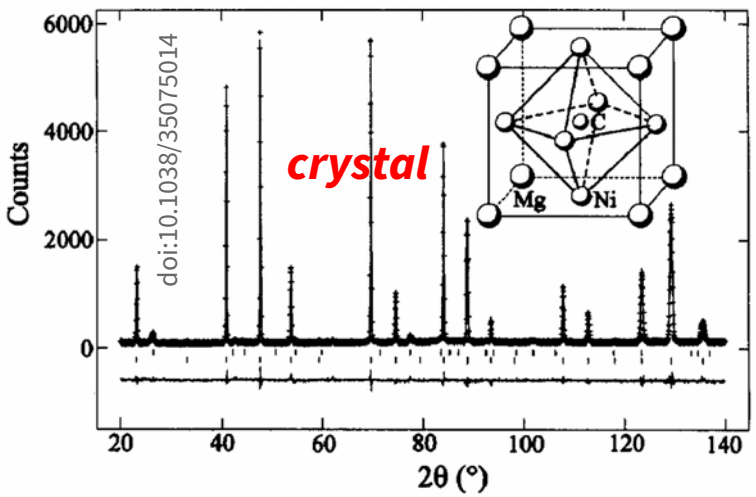
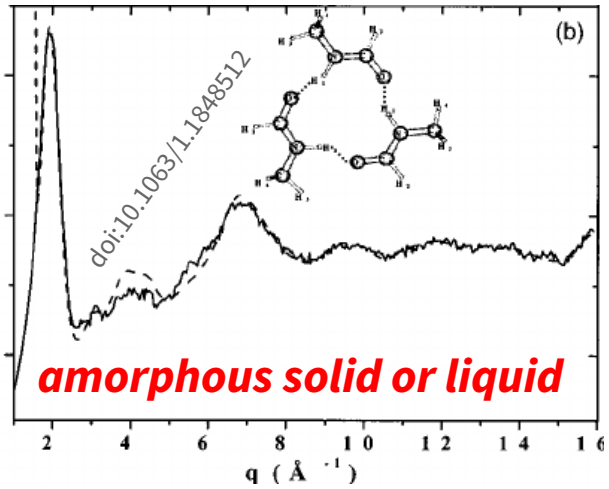
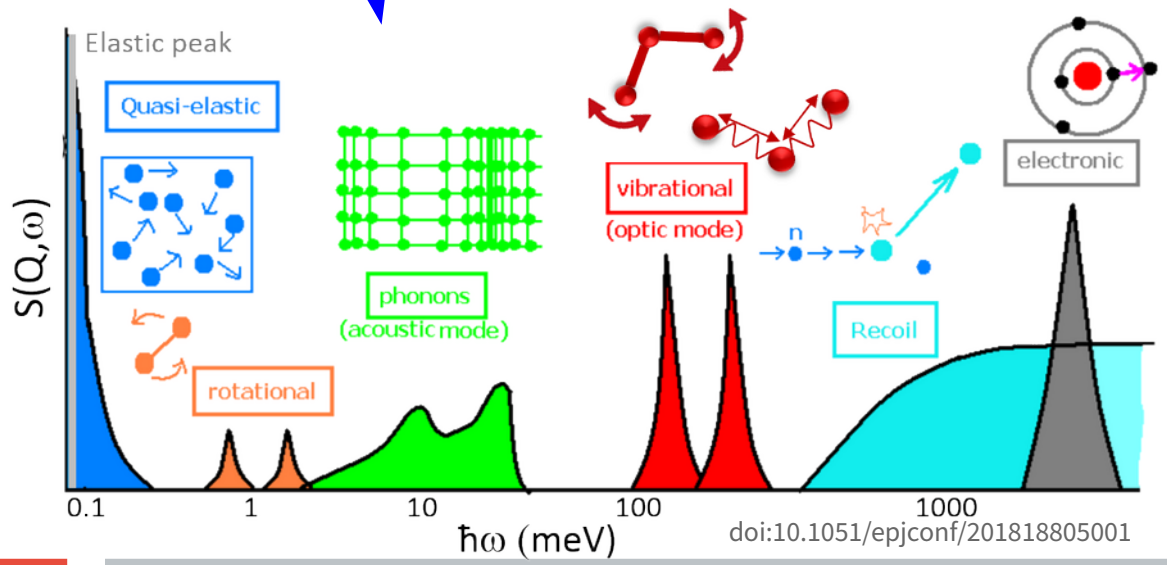
Thermal neutron wavelength
≈ interatomic distances.
⇒ **Sensitive to atomic positions**





Thermal neutron energy
≈ material energy levels
⇒ **sensitive to material dynamics**



Thermal neutron scattering a uniquely useful tool for understanding material structure

On the flipside it is impossible to ignore material structure in MC simulations!

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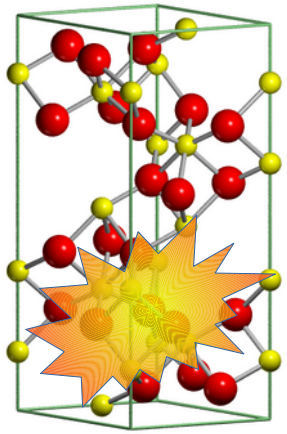
Thermal neutron scattering

$\bar{k}_i, E_i$



$\bar{k}_f, E_f$

Normally OK to assume neutrons travel as free waves between interactions ⇒ simplifies analysis and Monte Carlo simulations!

$$\vec{k} = \vec{p}/\hbar,\ \vec{q} \equiv \vec{k}_f - \vec{k}_i,\ \Delta E \equiv E_f - E_i \equiv -\hbar\omega$$
$$\lambda = 2\pi/k,\ 2E = m_n v^2 = p^2/m_n = \hbar^2 k^2/m_n$$

Probability to scatter to given $\bar{k}_f$ given by differential cross section:

$$\frac{d^2\sigma_{\vec{k}_i \Rightarrow \vec{k}_f}}{d\Omega_f dE_f} = \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{j,j'=1}^{N} b_j b_{j'} \int_{-\infty}^{\infty} dt \langle e^{-i\vec{q}\cdot\vec{\boldsymbol{R}}_{j'}(0)} e^{i\vec{q}\cdot\vec{\boldsymbol{R}}_j(t)} \rangle e^{-i\omega t}$$

N nuclei in target system

S(q̄,ω) — ***Scattering function*** **Depends on layout and dynamics of target particles. Does *not* depend on state of incident neutron.**

Scattering length of *j*th nucleus (depends on isotope & spin state)

Correlate position of nucleus *j* at time 0 with position of nucleus *j'* at time t. ⇒ Neutron X.S. depends on material structure!!

Scattering cross section depends on interference from scattering on different atoms, not just sum of 1-atom scatterings!!

Split in coherent / incoherent

NB: This is unique to neutrons, absent for x-ray scattering!

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Most target systems can be split into statistically equivalent subsystems (e.g. unit cells for crystals). Average contribution per sub-system:

Average

shorthand for $\langle e^{-i\vec{Q}\cdot\vec{\mathbf{R}}_{j'}(0)} e^{i\vec{Q}\cdot\vec{\mathbf{R}}_{j}(t)} \rangle$

$$S(\vec{Q},\omega) \equiv \frac{1}{2\pi\hbar} \sum_{j,j'=1}^{N} \overline{b_j b_{j'}} \int_{-\infty}^{\infty} dt \, \langle j', j \rangle e^{-i\omega t}$$

(only nuclear charge (Z) important for structure, not isotope/spin state)

Using $\overline{b_j b_{j'}} = \begin{cases} \overline{b_j} \cdot \overline{b_{j'}}, & \text{for } j \neq j' \\ \overline{b_j^2}, & \text{for } j = j' \end{cases}$ and reordering terms:

$$S(\vec{Q},\omega) = S_{\text{coh}}(\vec{Q},\omega) + S_{\text{inc}}(\vec{Q},\omega)$$

$$S_{\text{coh}}(\vec{Q},\omega) \equiv \frac{1}{2\pi\hbar} \sum_{j,j'=1}^{N} \overline{b_j} \cdot \overline{b_{j'}} \int_{-\infty}^{\infty} dt \, \langle j', j \rangle e^{-i\omega t}$$

$\overline{b_j} \cdot \overline{b_{j'}} \overset{\text{def}}{=} b_{\text{coh}}$

$$S_{\text{inc}}(\vec{Q},\omega) \equiv \frac{1}{2\pi\hbar} \sum_{j=1}^{N} \left(\overline{b_j^2} - \left(\overline{b_j}\right)^2 \right) \int_{-\infty}^{\infty} dt \, \langle j, j \rangle e^{-i\omega t}$$

$\left(\overline{b_j^2} - \left(\overline{b_j}\right)^2 \right) \overset{\text{def}}{=} (b_{\text{inc}})^2$

Always 0 in X-ray scattering!

Coherent:

- Keep pair-correlations as in full S(q,w)
- Plug in per-element scat. lengths, which are the *averages* of isotopic/spin scatlens

Incoherent:

- No pair-correlation, no interference! (but still *indirect* dep. on mat. structure!)
- Just sum up separate contributions.
- Plug in per-element scat. lengths which are the *variances* of isotopic/spin scatlens

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Coherent scat. len. (b_{coh}) for select elements

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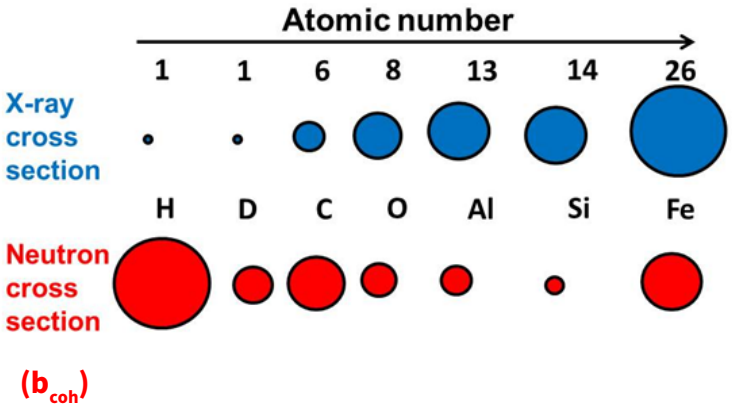
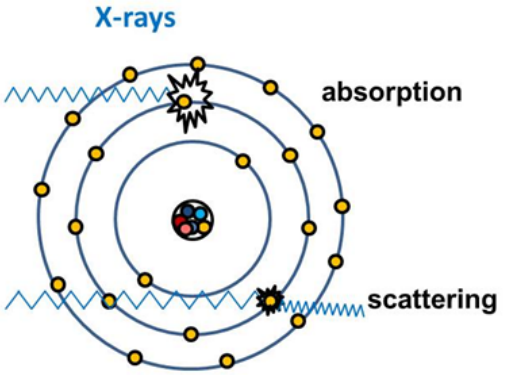
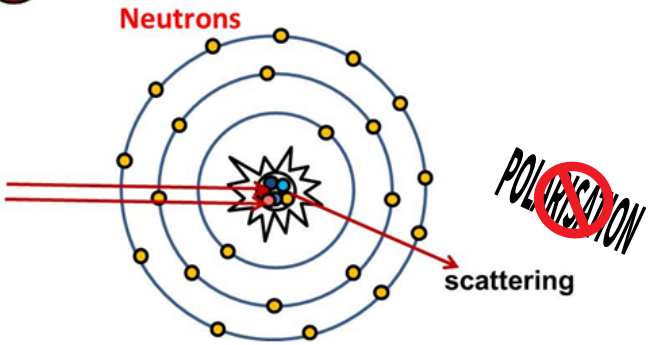
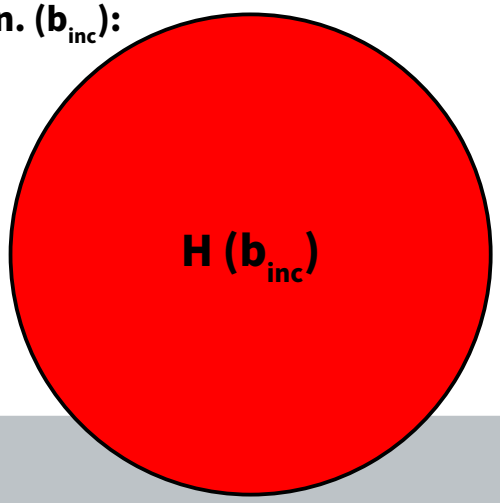
X-ray strength increases with Z, neutron strength various across isotopes:







Note: hydrogen has huge *incoherent* scat. len. (b_{inc}):



→ Neutron scattering sensitive to structure which is otherwise inaccessible to x-rays.
→ Sample deuteration (H→D) allows tuning hydrogen scattering strength

image from http://worldsciencereport.blogspot.com/2018/05/neutron-scattering.html

Elastic versus inelastic scatterings

(in the sense of ΔE=0 and ΔE≠0)

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- Mathematically speaking, elastic scattering means factors of delta-functions: δ(ΔE)
- δ(ΔE) appears as result of static (i.e. time-independent) correlations between atomic positions:

$$S(\vec{Q},\omega) \equiv \frac{1}{2\pi\hbar}\sum_{j,j'=1}^{N}\overline{b_j b_{j'}}\int_{-\infty}^{\infty} dt\,\langle j', j\rangle e^{-i\omega t}$$

$$\langle e^{-i\vec{Q}\cdot\vec{\boldsymbol{R}}_{j'}(0)} e^{i\vec{Q}\cdot\vec{\boldsymbol{R}}_{j}(t)}\rangle$$

(positional pair-correlations)

Fourier transform of static term gives δ-function in energy

$$\int_{-\infty}^{\infty} dt e^{-i\omega t} = 2\pi\hbar\delta(\hbar\omega) = 2\pi\hbar\delta(E_f - E_i)$$

Static correlations between atomic positions, and thus ΔE=0 scatterings is a feature of solid materials (crystalline or amorphous).

Does not strictly speaking occur in liquids or gasses, although correlations in such might give rise to "quasi-elastic" scatterings peaking around ΔE=0.

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In summary: four $S(\bar{q},\omega)$ components

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$$S(\bar{q},\omega) = S_{coh,inel}(\bar{q},\omega) + S_{inc,inel}(\bar{q},\omega) + S_{coh,el}(\bar{q},\omega) + S_{inc,el}(\bar{q},\omega)$$

solid systems only

Depending on material and neutron energy, any of these four components can dominate!

For isotropic materials: $S(\bar{q},\omega) \rightarrow S(q,\omega)$, allowing to treat scattering via 2D function (*scattering kernels*).

In practice, only inelastic scattering is modelled via 2D scattering kernels. Elastic scattering involves delta-functions and is best described by dedicated algorithms.

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NCrystal: Background, history, brief introduction.

The NCrystal project: Background

https://mctools.github.io/ncrystal/

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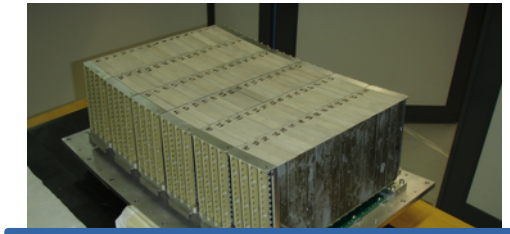
Original motivation back in ~2014 (X.X. Cai and T. Kittelmann):

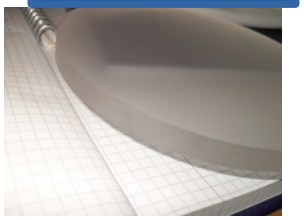
Augment Geant4 with proper modelling of thermalised neutrons in crystalline materials (and avoid the usual free-gas treatment)



Detector frames, vessels, supports (polycrystalline metals)

Crystalline samples

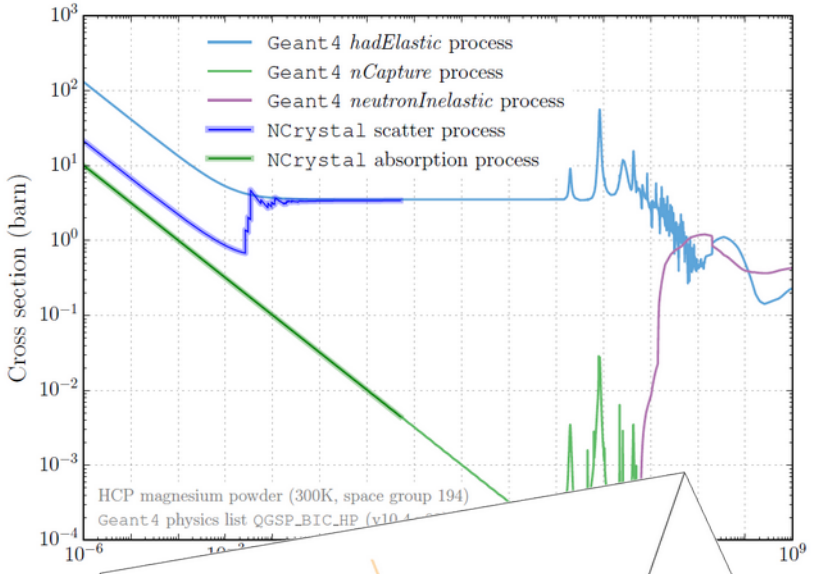
Filters (single- or poly-crystals)

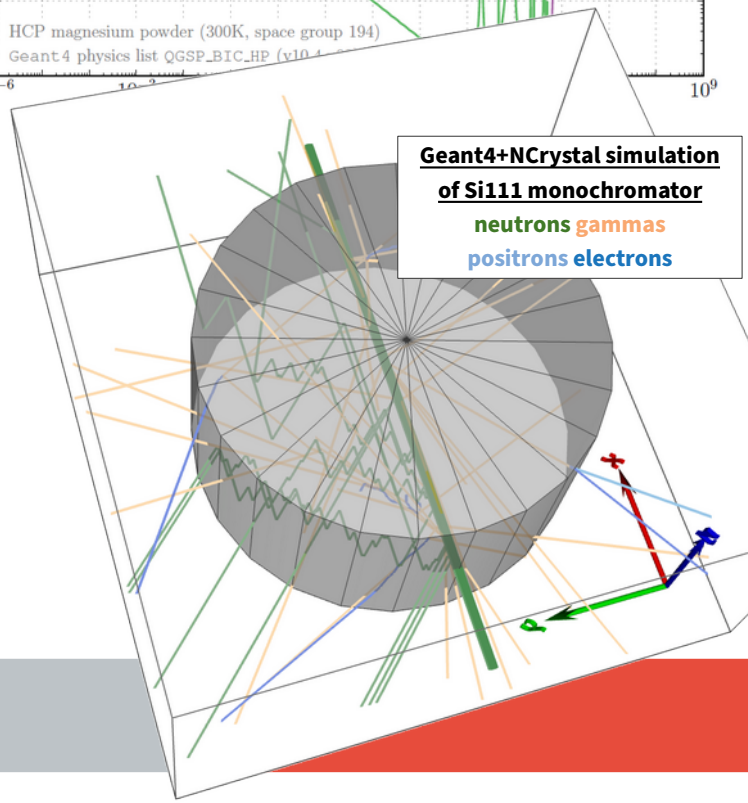


Monochromators, analysers (single crystals. layered crystals)

Advanced earlier efforts in older "NXSG4" plugin
- T. Kittelmann & M Boin 2015 *Comput. Phys. Commun.* **189**, 114-118
- Geant4-specific plugin for polycrystals, no inelastic, no tools/bindings – just a thin wrapper around nxslib by M. Boin.

Scope has since expanded beyond Geant4!
And the physics scope has extended beyond crystals and beyond Bragg diffraction!





Two regimes of neutron scattering

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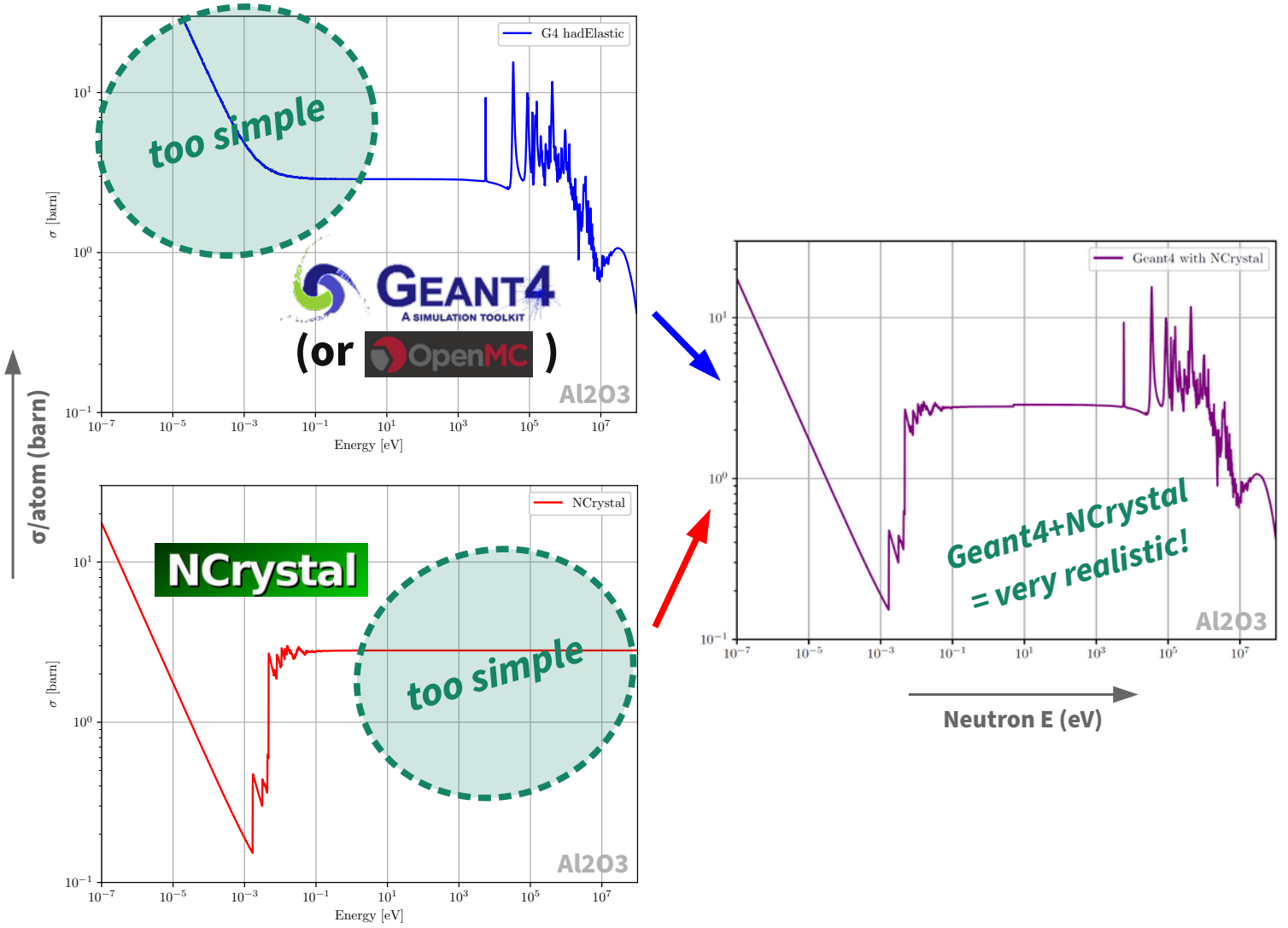
Higher energy (>>eV):

- Complex neutron-nuclei interactions with energy dependent strength.
- Not sensitive to material structure.

Low energy (<<eV):

- Simple (point-like) neutron-nuclei interactions with constant strength.
- Very sensitive to material structure.



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A brief history of NCrystal

(no, this will not be on the test)

NCrystal
Thermal Neutron Transport

- (prehistoric: NXSG4 in 2014 by T. Kittelmann + M. Boin)
- ~2015: T. Kittelmann + X. X. Cai of the ESS Detector Group and DTU NuTech join separate efforts aimed at adding thermal neutron physics to Geant4. Quickly decide to make it a standalone project and add support for McStas as well. Both join the Geant4 collaboration to get NCrystal integrated, and also work with P. Willendrup on McStas integration.
- 2019 (v1.0): After years of development and writing the first publication, release 1.0, focusing on Bragg diffraction and crystalline materials. HKL structure factors are calculated on the fly at startup. Contains minimal C++/C/Python API and hooks for Geant4 and McStas.
- 2020 (v2.0): with inelastic physics: scattering kernels and a unique capability to expand phonon spectra to scattering kernels on the fly.
- 2020 (fall) (v2.1-2.4): Support atomic/isotopic mixtures, virtual files, and a system for third-party plugins with specific new physics.
- March 2021 (v2.5): Major C++11 rewrite for safe modern C++. Becomes multi-thread safe and gets a flexible data-source structure.
- April 2021 (v2.6): K. Ramic, Ignacio Marquez Damian, and D.DiJulio join the efforts, and most files in the data library gets phonon DOS curves added. We also begin to estimate atomic displacements from such curves.
- May 2021 (v2.7): The data library grows enormously (now arguably world leading!) thanks again to collaboration with the same people. Add support for amorphous materials, add cmdline tools for adding new materials.
- April 2022 (v3.0): Large update with multi-phase materials, support for SANS physics, new cfg-parameters like “density”, “one-liner materials”, etc.
- June 2022 (v3.1): Focus on UCN (ultra cold neutron) production in inelastic collisions, ensuring artifact-free modelling and possibilities for biasing.
- August 2022 (v3.2): Support for easily configuring gas-mixtures.
- Aug-Dec 2022 (v3.3-3.5): Improve CMake layer and introduce ncrystal-config command. Improve integrations with McStas (with P. Willendrup and M. Bertelsen) and Geant4. Bindings for OpenMC in OpenMC 13.3 release. NCrystal appears on conda-forge. CI testing improves with help of M. Klausz.
- May 2023 (v3.6): Large improvement of python API, many utilities for creating new materials from a variety of sources. Publish Jupyter tutorials.
- Along the way, supported by: two EU projects, got physics in external plugins (Thanks N. Rizzi and S. Xu), and were supported in various fashions by many people not mentioned already, in particular (sorry for those I forgot): V. Santoro, R.H.Wilton, K.Kanaki, A. Morozov, E. Klinkby, E. Knudsen, ...
- Many ongoing ideas and developments at ESS (in various groups), and CSNS in particular.

Lots of stuff we want to do, that we simply have not got around to yet!

Not such an old project, but a lot of activity and many people contributing in many ways! Always looking for more contributions!

Standard physics in NCrystal
(crystals/liquids/amorphous solids)

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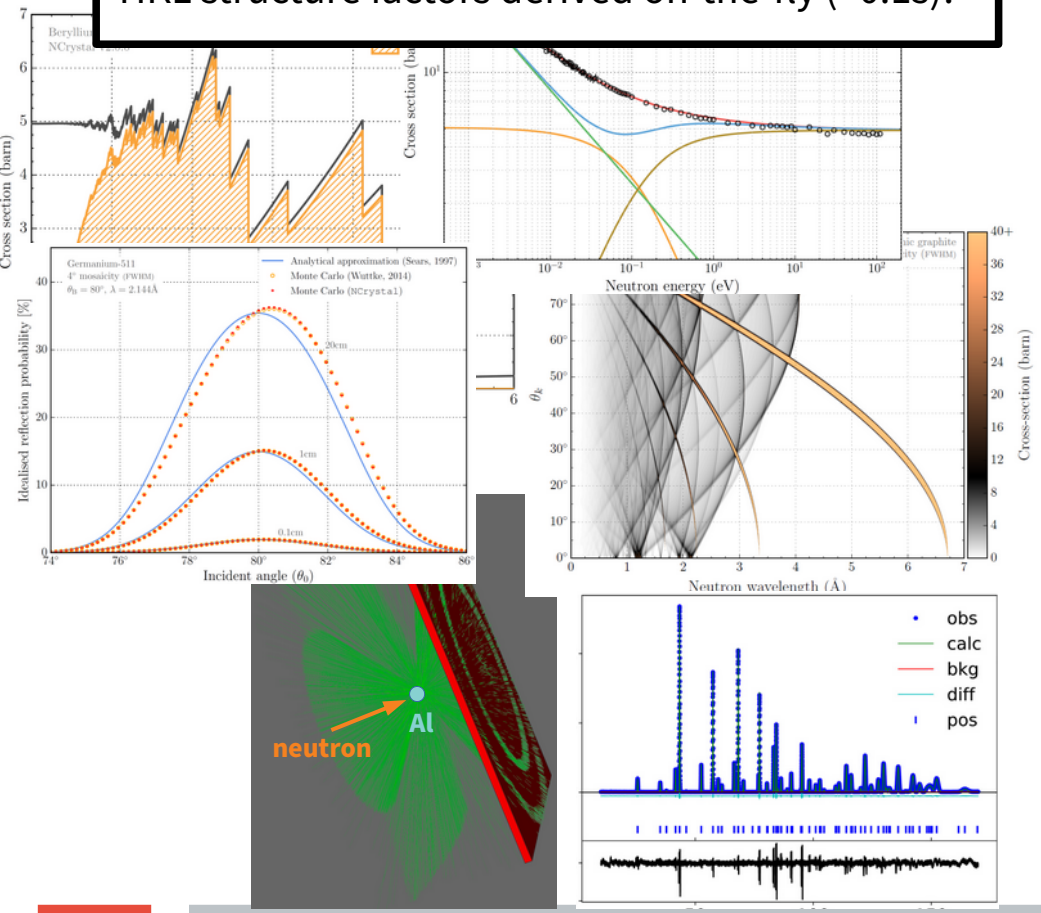
Elastic (ΔE=0) components

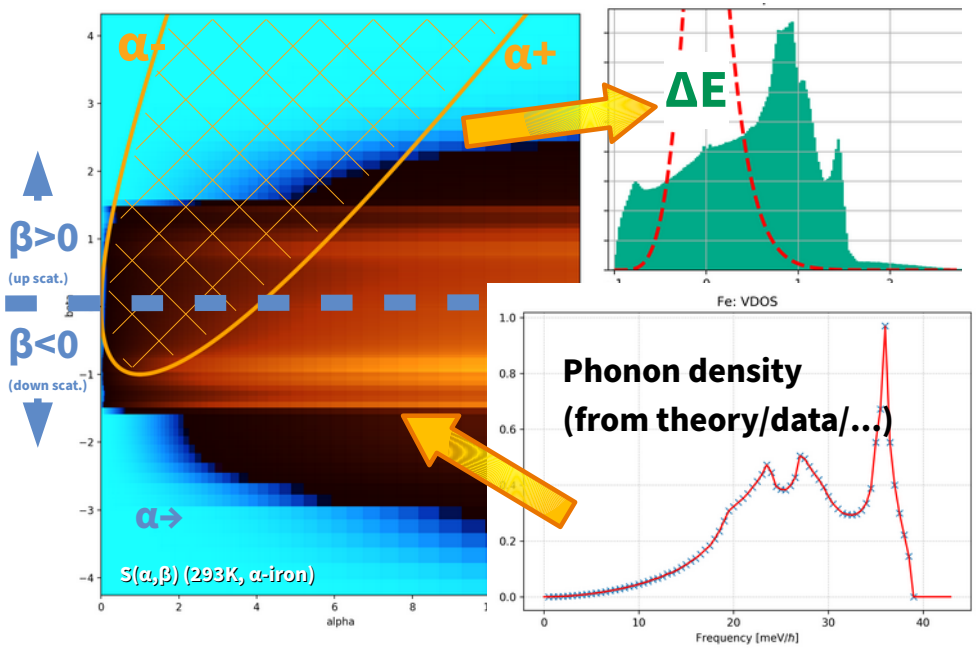
Bragg diffraction, incoherent, single crystals, isotropic materials (powders), HOPG.
HKL structure factors derived on-the-fly (<0.1s).



Inelastic (ΔE≠0) components

Scattering kernel based:

- Initialise from external kernel
- Or from phonon density curve (~0.1s).
- Using incoherent approx. (for now!)



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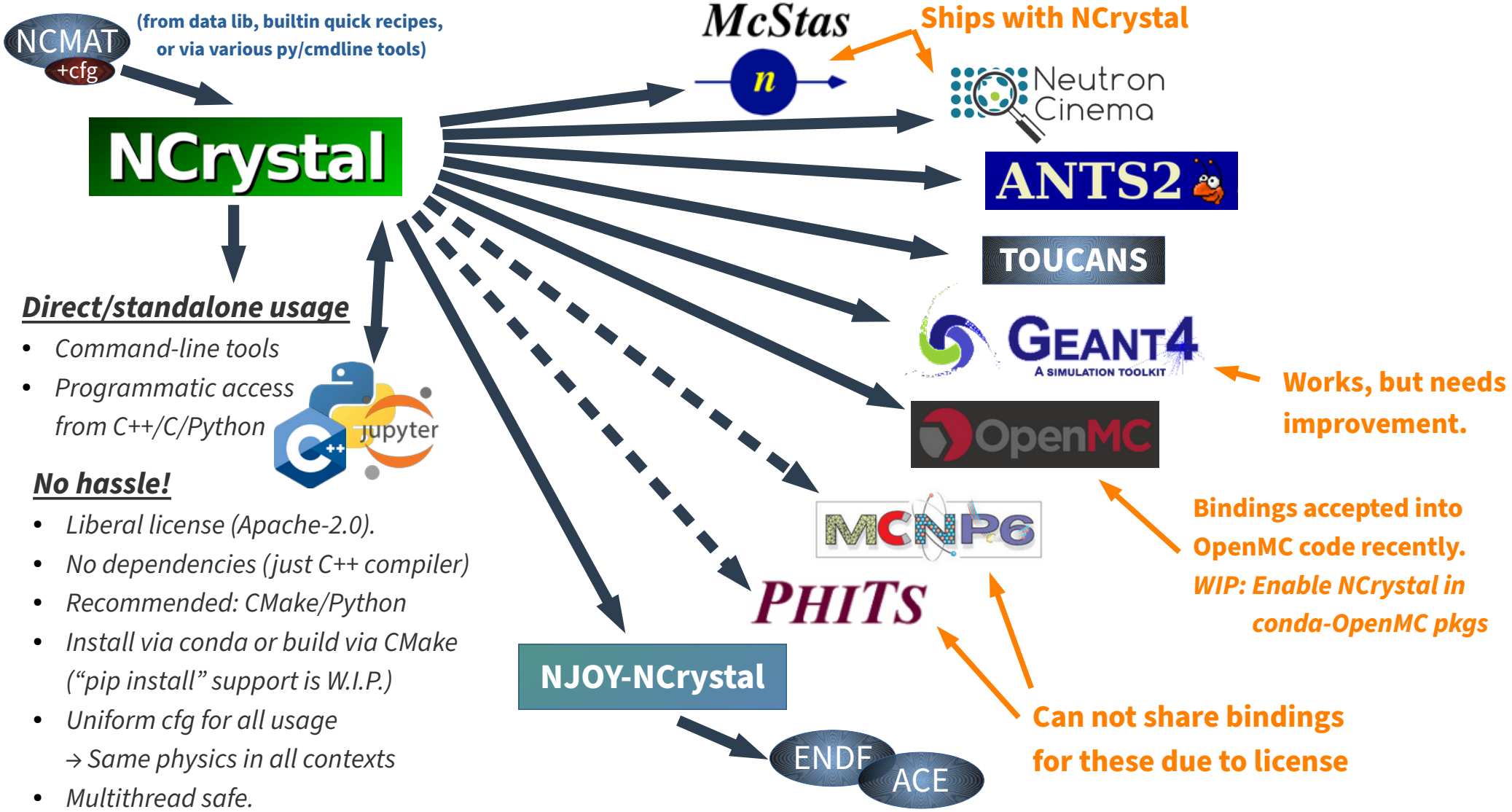
NCrystal: Open Source backend providing thermal neutron scattering to MC codes

NCrystal
Thermal Neutron Transport



Direct/standalone usage

- *Command-line tools*
- *Programmatic access from C++/C/Python*

No hassle!

- *Liberal license (Apache-2.0).*
- *No dependencies (just C++ compiler)*
- *Recommended: CMake/Python*
- *Install via conda or build via CMake ("pip install" support is W.I.P.)*
- *Uniform cfg for all usage → Same physics in all contexts*
- *Multithread safe.*

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More info about NCrystal

NCrystal
Thermal Neutron Transport

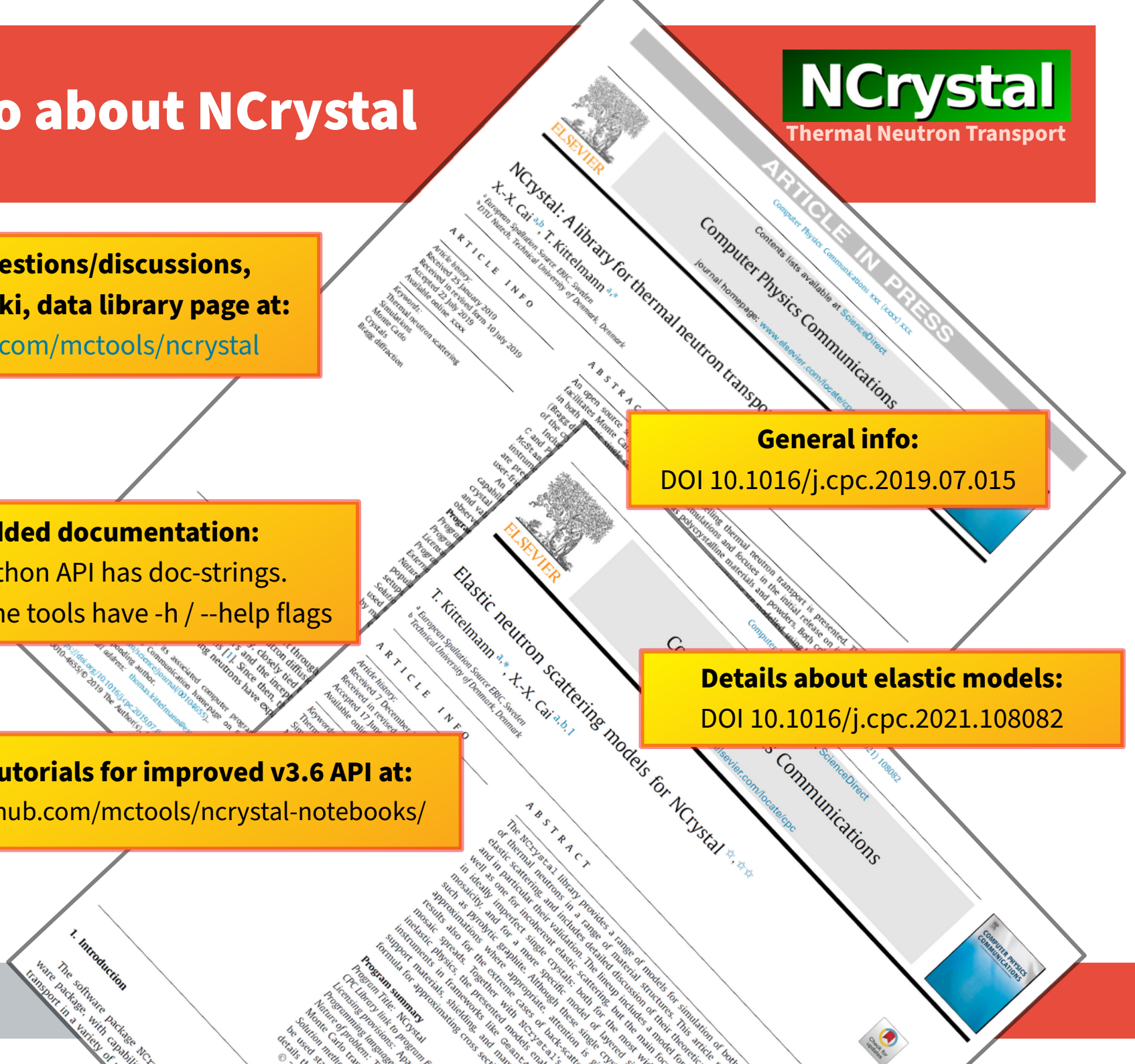
Forum for questions/discussions, issue tracker, wiki, data library page at:
https://github.com/mctools/ncrystal

General info:
DOI 10.1016/j.cpc.2019.07.015

Embedded documentation:
Entire Python API has doc-strings.
Command-line tools have -h / --help flags

Details about elastic models:
DOI 10.1016/j.cpc.2021.108082

Jupyter tutorials for improved v3.6 API at:
https://github.com/mctools/ncrystal-notebooks/



Example usage

(from standalone Python)

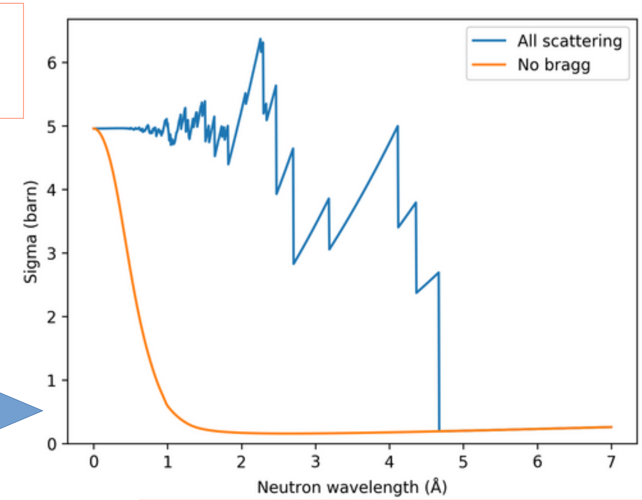
NCrystal
Thermal Neutron Transport

```
#Plot beryllium-oxide cross sections:
import NCrystal as NC
import matplotlib.pyplot as plt
import numpy
scBeO = NC.createScatter("BeO_sg186.ncmat")
scBeO_nobragg = NC.createScatter("BeO_sg186.ncmat;coh_elas=0")
wls = numpy.linspace(0.0,7.0,1000)
plt.plot( wls, scBeO.xsect(wl=wls), label='All scattering' )
plt.plot( wls, scBeO_nobragg.xsect(wl=wls), label='No bragg' )
plt.xlabel('Neutron wavelength (Å)')
plt.ylabel('Sigma (barn)')
plt.legend()
plt.show()

#Can also extract more detailed info:
info_BeO = NC.createInfo("BeO_sg186.ncmat")
info_BeO.dump()
print ('Density [g/cm3]: ',info_BeO.getDensity())
for fraction,atom in info_BeO.composition:
    print(f'Has {fraction*100}% {atom}')
for h,k,l,mult,dspacing,fsq in info_BeO.hklList():
    if 1.0 < dspacing < 1.2:
        print(f'd={dspacing:g}Aa, strength={mult*fsq:g}')
```

Universal cfg-strings
→ Same cfg in McStas, Geant4, …

Prints all info to terminal

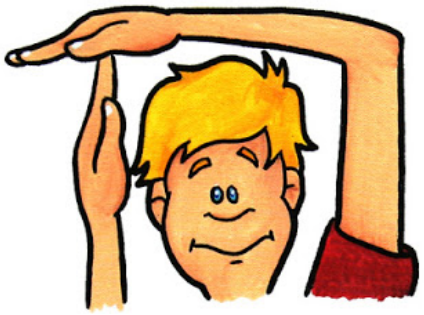


Additionally NCrystal can also perform Monte-Carlo sampling of scattering events

Jupyter tutorials for improved v3.6 API at:
https://github.com/mctools/ncrystal-notebooks/

```
Density [g/cm3]:  3.022865728266587
Has 50.0% Be=Be(cohSL=7.79fm cohXS=7.62579barn incXS=0.0018barn absXS=0.0076barn mass=9.01218amu Z=4)
Has 50.0% O=O(cohSL=5.805fm cohXS=4.23462barn incXS=0barn absXS=0.00019barn mass=15.9994amu Z=8)
1.16827Aa, strength=9.96888
Aa, strength=41.9296
Aa, strength=9.252
5Aa, strength=0.259484
7Aa, strength=10.2016
```

conda install -c conda-forge ncrystal
(“pip install ncrystal” is W.I.P.)



Time to look at the first notebook

(up to and including section 1.6)

Jupyter tutorials for improved v3.6 API at:
https://github.com/mctools/ncrystal-notebooks/

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NCrystal material data

Source of material definitions

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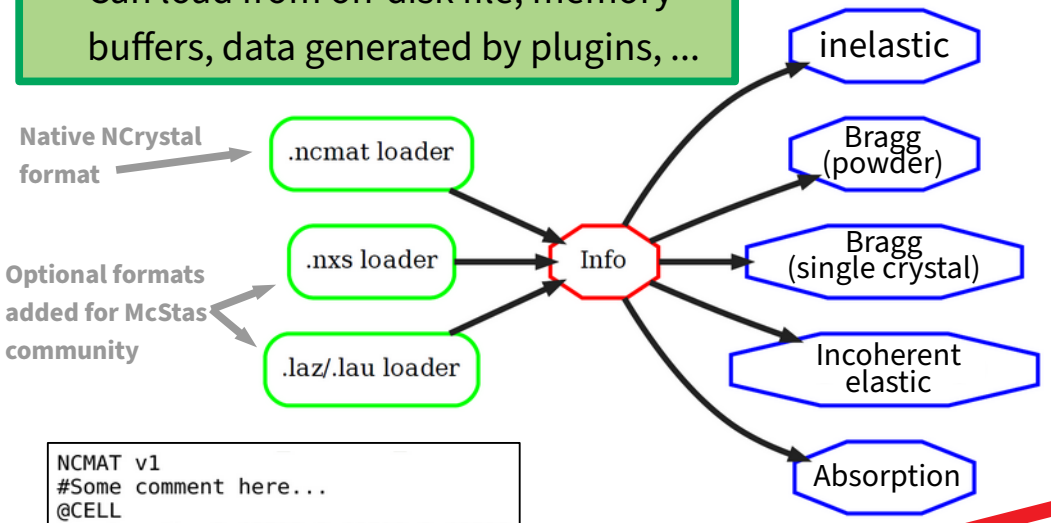
- Supports multiple input formats
- Can load from on-disk file, memory buffers, data generated by plugins, ...




```
NCMAT v1
#Some comment here...
@CELL
    lengths 5.65735 5.65735 5.65735
    angles 90. 90. 90.
@SPACEGROUP
    227
@ATOMPOSITIONS
    Ge 0.75 0.75 0.25
    Ge 0.5  0.5  0.
    Ge 0.75 0.25 0.75
    Ge 0.5  0.   0.5
    Ge 0.25 0.75 0.75
    Ge 0.   0.5  0.5
    Ge 0.25 0.25 0.25
    Ge 0.   0.   0.
@DEBYETEMPERATURE
    Ge 281.4
```

Ge_sg227.ncmat

NCMAT loader

Info

```
------------------------------------------------------------
Space group number       : 227
Lattice spacings   [Aa] : 5.65735 5.65735 5.65735
Lattice angles     [deg] : 90 90 90
Unit cell volume [Aa^3] : 181.067
Atoms / unit cell        : 8
------------------------------------------------------------
Atoms per unit cell (total 8):
     8 Ge atoms [T_Debye=281.437K, MSD=0.00760282Aa]
------------------------------------------------------------
Atomic coordinates:
      Ge            0            0            0
      Ge            0          0.5          0.5
      Ge         0.25         0.25         0.25
      Ge         0.25         0.75         0.75
      Ge          0.5            0          0.5
      Ge          0.5          0.5            0
      Ge         0.75         0.25         0.75
      Ge         0.75         0.75         0.25
------------------------------------------------------------
   Density : 5.32937 g/cm3
------------------------------------------------------------
   Temperature : 293.15 kelvin
------------------------------------------------------------
Neutron cross-sections:
   Absorption at 2200m/s : 2.2 barn
   Free scattering       : 8.36483 barn
------------------------------------------------------------
HKL planes (d_lower = 0.15 Aa, d_upper = inf Aa):
  H   K   L  d_hkl[Aa] Multiplicity FSquared[barn] Expanded-HKL-list
  1  -1  -1    3.26627            8         20.8434 1,-1,-1 | -1,1,1 | 1,
  0   2  -2    2.00018           12         39.7773 0,2,-2 | 0,-2,2 | 0,2
  1  -3  -1    1.70576           24         19.3369 1,-3,-1 | -1,3,1 | 1,
  0   0   4    1.41434            6         36.9022 0,0,4 | 0,0,-4 | 0,4,(
  1  -3  -3    1.29789           24         17.9392 1,-3,-3 | -1,3,3 | 1,
  2  -4  -2     1.1548           24          34.235 2,-4,-2 | -2,4,2 | 2,
  1  -5  -1    1.08876           32         16.6426 1,-5,-1 | -1,5,1 | 1,
  0   4  -4    1.00009           12         31.7605 0,4,-4 | 0,-4,4 | 0,4
  1  -5  -3   0.956267           48         15.4397 1,-5,-3 | -1,5,3 | 1,
  0   2  -6   0.894506           24         29.4649 0,2,-6 | 0,-2,6 | 0,2
  3  -5  -3   0.862738           24         14.3238 3,-5,-3 | -3,5,3 | 3,
  4  -4  -4   0.816568            8         27.3353 4,-4,-4 | -4,4,4 | 4,
                                                                      1,
                                                                      2
```

- Native NCMAT format: https://github.com/mctools/ncrystal/wiki/NCMAT-format
- Well defined and versioned

New in v3.6.0: Python utilities for more easily composing NCMAT data.

NCrystal data library

Browse with performance plots at: https://github.com/mctools/ncrystal/wiki/Data-library

NCrystal
Thermal Neutron Transport

AcrylicGlass_C5O2H8.ncmat
AgBr_sg225_SilverBromide.ncmat
Ag_sg225.ncmat
Al2O3_sg167_Corundum.ncmat
Al4C3_sg166_AluminiumCarbide.ncmat
AlN_sg186_AluminumNitride.ncmat
Al_sg225.ncmat
Ar_Gas_STP.ncmat
Au_sg225.ncmat
BaF2_sg225_BariumFluoride.ncmat
BaO_sg225_BariumOxide.ncmat
Ba_sg229.ncmat
Be3N2_sg206_BerylliumNitride.ncmat
BeF2_sg152_Beryllium_Fluoride.ncmat
BeO_sg186.ncmat
Be_sg194.ncmat
Bi_sg166.ncmat
CaCO3_sg62_Aragonite.ncmat
CaF2_sg225_CalciumFlouride.ncmat
CaH2_sg62_CalciumHydride.ncmat
CaO2H2_sg164_CalciumHydroxide.ncmat
CaO_sg225_CalciumOxide.ncmat
Ca_sg225.ncmat
Ca_sg229_Calcium-gamma.ncmat
CaSiO3_sg2_Wollastonite.ncmat
CeO2_sg225_CeriumOxide.ncmat
Cr_sg229.ncmat
C_sg194_pyrolytic_graphite.ncmat
C_sg227_Diamond.ncmat
Cu2O_sg224_Cuprite.ncmat
Cu_sg225.ncmat
Dy2O3_sg206_DysprosiumOxide.ncmat
Epoxy_Araldite506_C18H20O3.ncmat
Fe_sg225_Iron-gamma.ncmat
Fe_sg229_Iron-alpha.ncmat
GaN_sg186_GalliumNitride.ncmat
GaSe_sg194_GalliumSelenide.ncmat
Ge3Bi4O12_sg220_BismuthGermanate.ncmat
Ge_sg227.ncmat
He_Gas_STP.ncmat
HfO2_sg14_HafniumOxide.ncmat
Ho2O3_sg206_HolmiumOxide.ncmat
Kapton_C22H10N2O5.ncmat
KBr_sg225_PotassiumBromide.ncmat
KF_sg225_PotassiumFlouride.ncmat
KOH_sg4_PotassiumHydroxide.ncmat
Kr_Gas_STP.ncmat
K_sg229.ncmat
LaBr3_sg176_LanthanumBromide.ncmat
Li2O_sg225_LithiumOxide.ncmat
Li3N_sg191_LithiumNitride.ncmat
LiF_sg225_LithiumFlouride.ncmat
LiH_sg225_LithiumHydride.ncmat
LiquidHeavyWaterD2O_T293.6K.ncmat
LiquidWaterH2O_T293.6K.ncmat
Lu2O3_sg206_LutetiumOxide.ncmat
Lu2SiO5_sg15.ncmat
Mg2SiO4_sg62_MagnesiumSilicate.ncmat
MgAl2O4_sg227_MAS.ncmat
MgCO3_sg167_MagnesiumCarbonate.ncmat
MgD2_sg136_MagnesiumDeuteride.ncmat
MgF2_sg136_MagnesiumFlouride.ncmat
MgH2_sg136_MagnesiumHydride.ncmat
MgO2H2_sg164_MagnesiumHydroxide.ncmat
MgO_sg225_Periclase.ncmat
Mg_sg194.ncmat
Mo_sg229.ncmat
Na4Si3Al3O12Cl_sg218_Sodalite.ncmat
NaBr_sg225_SodiumBromide.ncmat
NaCl_sg225_SodiumChloride.ncmat
NaF_sg225_SodiumFlouride.ncmat
NaI_sg225_SodiumIodide.ncmat
Na_sg229.ncmat
Nb_sg229.ncmat
Ne_Gas_STP.ncmat
Ni_sg225.ncmat
Nylon11_C11H21NO.ncmat
Nylon12_C12H23NO.ncmat
Nylon610_C16H30N2O2.ncmat
Nylon66or6_C12H22N2O2.ncmat
PbF2-beta_sg225_BetaLeadFlouride.ncmat
PbO-alpha_sg129_Litharge.ncmat
PbO-beta_sg57_Massicot.ncmat
Pb_sg225.ncmat
PbS_sg225_LeadSulfide.ncmat
Pd_sg225.ncmat
PEEK_C19H12O3.ncmat
Polycarbonate_C16O3H14.ncmat
Polyester_C10H8O4.ncmat
Polyethylene_CH2.ncmat
Polylactide_C3H4O2.ncmat
Polypropylene_C3H6.ncmat
Polystyrene_C8H8.ncmat
Pt_sg225.ncmat
PVC_C2H3Cl.ncmat
Rb_sg229.ncmat
Rubber_C5H8.ncmat
Sc_sg194.ncmat
SiC-beta_sg216_BetaSiliconCarbide.ncmat
SiO2-alpha_sg154_AlphaQuartz.ncmat
SiO2-beta_sg180_BetaQua
Si_sg227.ncmat
Sn_sg141.ncmat
SrF2_sg225_StrontiumFlu
SrH2_sg62_StrontiumHydr
Sr_sg225.ncmat
Th3N4_sg166_ThoriumNitr
ThO2_sg225_ThoriumDioxi
Th_sg225.ncmat
TiO2_sg136_Rutile.ncmat
TiO2_sg141_Anatase.nc
Ti_sg194.ncmat
TlBr_sg221_ThaliumBro
Tm2O3_sg206_ThuliumOx
UF6_sg62_UraniumHexaf
UO2_sg225_UraniumDiox
void.ncmat
V_sg229.ncmat
W_sg229.ncmat
Xe_Gas_STP.ncmat
Y2O3_sg206_Yttrium_Ox
Y2SiO5_sg15_YSO.ncmat
Y3Al5O12_sg230_YAG.nc
Y_sg194.ncmat
ZnF2_sg136_ZincFlouride.ncmat
ZnO_sg186_ZincOxide.n
Zn_sg194.ncmat
ZnS_sg216_Sphalerite.
ZrF4-beta_sg84.ncmat
ZrO2_sg137_Zirconia.n
ZrO2_sg14_Zirconia.nc
Zr_sg194.ncmat

132 materials (v3.0.0):

Crystals (108), amorphous solids (16), liquids, gasses, …

Easy universal cfg:

"Al_sg225.ncmat;temp=250K"
"Rubber_C5H8.ncmat;comp=inelas"

- Same physics in all applications!
- Cfg variables documented at:
  github.com/mctools/ncrystal/wiki/CfgRefDoc

Small (few kB) file sizes:

- Optionally embed in binary and avoid need for actual files.

Easy to create more:

- Hand-write NCMAT file (human readable ASCII, format well-defined & versioned) or use new NCMATComposer.
- Convert from ENDF, CIF, online crystal DB carbohydrate chemical formula, Quantum Espresso output, …
- Request help on GitHub/ncrystal.

Can be converted to other formats:

- To .laz/.lau for McStas
- To ENDF via the NJOY-NCrystal project
- But limited by target format physics capabilities!

NCrystal data library wiki page

https://mctools.github.io/ncrystal/ → wiki → Data-library

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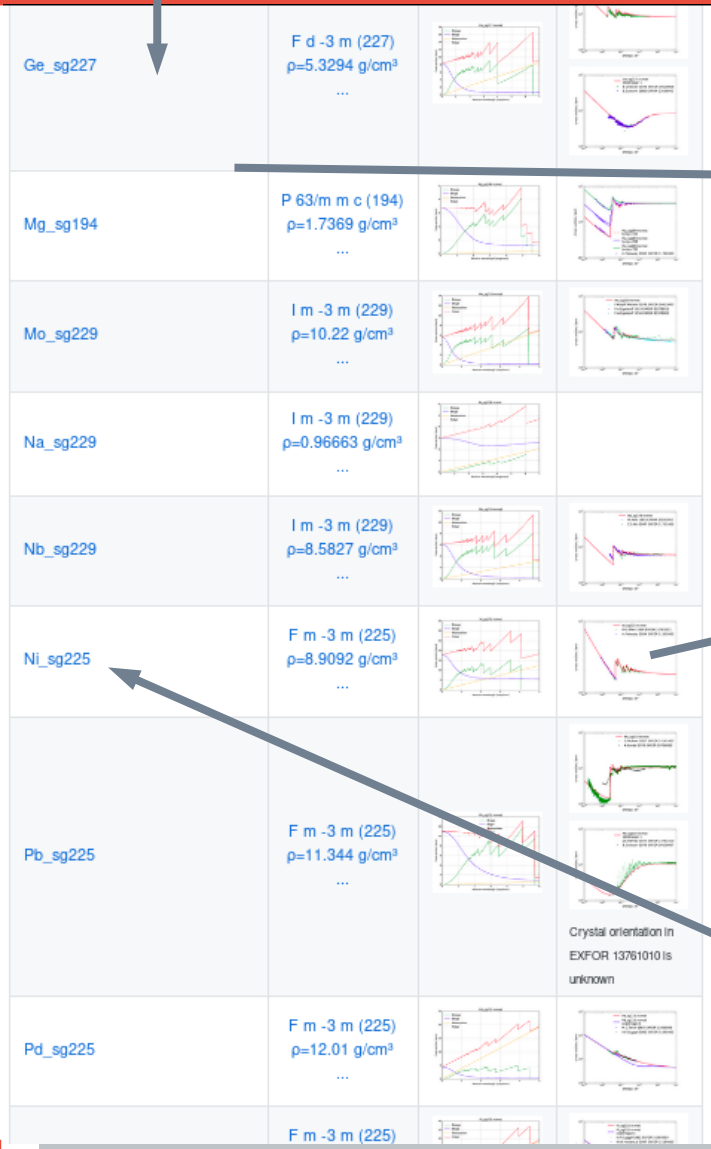
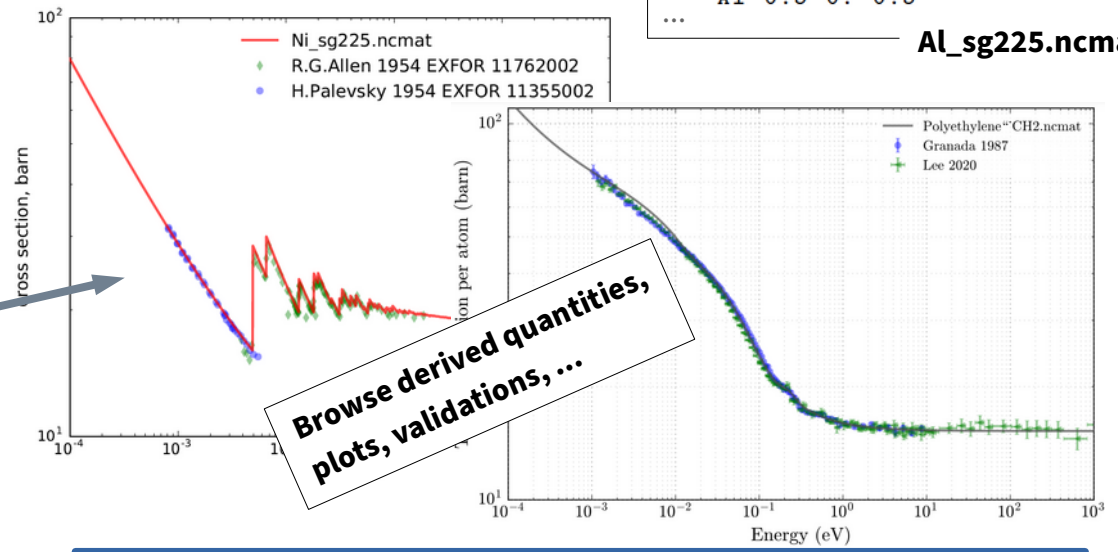



```
NCMAT v1
#Some comment here...
@CELL
    lengths 4.04958 4.04958 4.04958
    angles 90. 90. 90.
@SPACEGROUP
    225
@ATOMPOSITIONS
    Al 0. 0.5 0.5
    Al 0. 0. 0.
    Al 0.5 0.5 0.
    Al 0.5 0. 0.5
...
```

Al_sg225.ncmat



Browse derived quantities, plots, validations, …

To use in Geant4/ McStas/OpenMC/..., simply supply name of material file, along with relevant parameters like temperature, orientation of single crystal, etc.

In-memory data files

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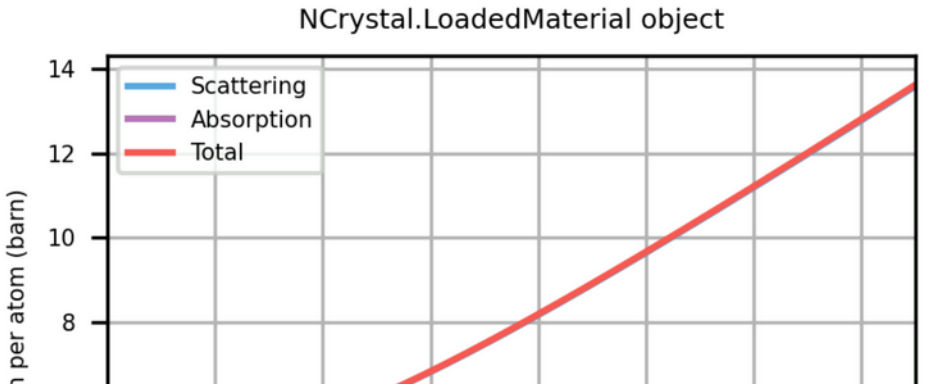
Register as virtual file with filename:

```
import NCrystal as NC
content="""NCMAT v3
@CELL
 lengths 4.04958 4.04958 4.04958
 angles 90 90 90
@SPACEGROUP
  225
@ATOMPOSITIONS
  Al 0   1/2 1/2
  Al 0     0   0
  Al 1/2 1/2   0
  Al 1/2   0 1/2
@DEBYETEMPERATURE
  Al   410.4
"""

NC.registerInMemoryFileData( "MyAl.ncmat",content)
sc = NC.createScatter("MyAl.ncmat")
```

Load NCMAT data directly:

```
a_string_with_ncmat_data="""NCMAT v7
#Don't use this material for anything
@DENSITY
  1.2345 g_per_cm3
@DYNINFO
  element  C
  fraction 1
  type     freegas
"""
NC.load(a_string_with_ncmat_data).plot()
```



Avoid physical files for standard data library:

Simply use the CMake option:

`-DNCRYSTAL_ENABLE_DATA=EMBED`

Quick one-liner materials

- NCrystal's flexible data infrastructure allows plugins to provide one-liner materials.
- The one-liner goes in the "filename" part of a cfg-string.
- Dedicated plugins (currently "freegas", "solid", "gasmix") analyse the "filename" and produces corresponding NCMAT data on-the-fly (run "nctool --browse" for examples).
- Examples:

```
"freegas::He/0.17kgm3/7bar/He_is_He3"
"solid::B4C/2.52gcm3/B_is_0.95_B10_0.05_B11"
"gasmix::0.72xCO2+0.28xAr/massfractions/1.5atm/250K"
"gasmix::0.7xCO2+0.3xAr/0.001relhumidity"
"gasmix::0.7xCO2+0.3xAr/1.5atm/250K"
"gasmix::BF3/2atm/25C/B_is_0.95_B10_0.05_B11"
"gasmix::CO2"
"gasmix::He/1.64kgm3"
"gasmix::He/10bar"
"gasmix::air"
"gasmix::air/-10C/0.8atm/0.30relhumidity"
```

Quick data for hydrogen-rich amorphous solids

New feature in NCrystal v2.7.0

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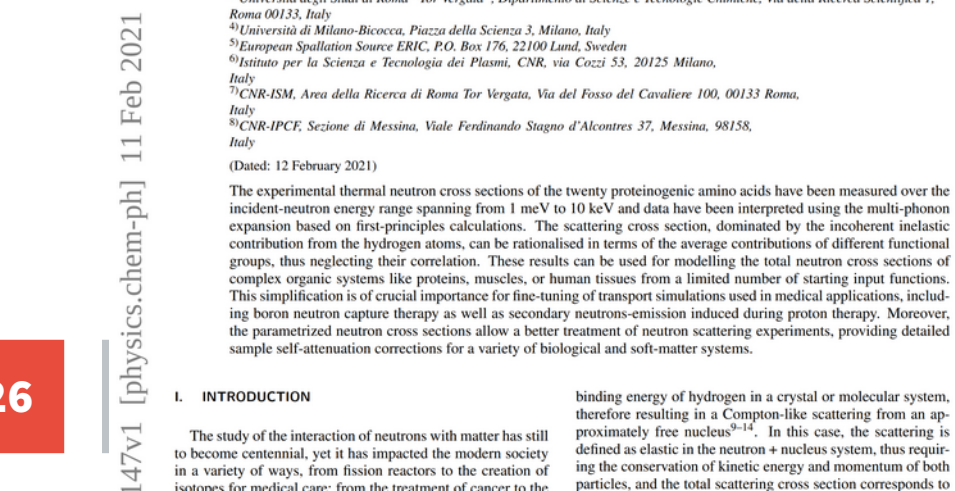
- **DFT/MD modelling of amorphous materials can be difficult and time consuming.**
- **Recent paper (Romanelli et. al., arxiv 2102.06147) provides trustworthy and cheap alternative for hydrogen-rich materials.**
- **Relies on universality of hydrogen vibrations in different materials: Overall hydrogen VDOS can be composed from list of hydrogen bindings.**
- **We provide script for setting up NCMAT files with this.**



Thermal neutron cross sections of amino acids from average contributions of functional groups

Giovanni Romanelli,[1] Dalila Onorati,[2,a)] Pierfrancesco Ulpiani,[3] Stephanie Cancelli,[4] Enrico Perelli-Cippo,[4] José Ignacio Márquez Damián,[5] Silvia C. Capelli,[1] Gabriele Croci,[4,6] Andrea Muraro,[6] Marco Tardocchi,[6] Giuseppe Gorini,[4] Carla Andreani,[2,7] and Roberto Senesi[2,8]
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[2)]*Università degli Studi di Roma "Tor Vergata", Dipartimento di Fisica and NAST Centre, Via della Ricerca Scientifica 1, Roma 00133, Italy*
[3)]*Università degli Studi di Roma "Tor Vergata", Dipartimento di Scienze e Tecnologie Chimiche, Via della Ricerca Scientifica 1, Roma 00133, Italy*
[4)]*Università di Milano-Bicocca, Piazza della Scienza 3, Milano, Italy*
[5)]*European Spallation Source ERIC, P.O. Box 176, 22100 Lund, Sweden*
[6)]*Istituto per la Scienza e Tecnologia dei Plasmi, CNR, via Cozzi 53, 20125 Milano, Italy*
[7)]*CNR-ISM, Area della Ricerca di Roma Tor Vergata, Via del Fosso del Cavaliere 100, 00133 Roma, Italy*
[8)]*CNR-IPCF, Sezione di Messina, Viale Ferdinando Stagno d'Alcontres 37, Messina, 98158, Italy*

(Dated: 12 February 2021)

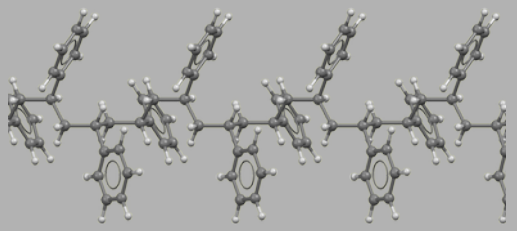
The experimental thermal neutron cross sections of the twenty proteinogenic amino acids have been measured over the incident-neutron energy range spanning from 1 meV to 10 keV and data have been interpreted using the multi-phonon expansion based on first-principles calculations. The scattering cross section, dominated by the incoherent inelastic contribution from the hydrogen atoms, can be rationalised in terms of the average contributions of different functional groups, thus neglecting their correlation. These results can be used for modelling the total neutron cross sections of complex organic systems like proteins, muscles, or human tissues from a limited number of starting input functions. This simplification is of crucial importance for fine-tuning of transport simulations used in medical applications, including boron neutron capture therapy as well as secondary neutrons-emission induced during proton therapy. Moreover, the parametrized neutron cross sections allow a better treatment of neutron scattering experiments, providing detailed sample self-attenuation corrections for a variety of biological and soft-matter systems.

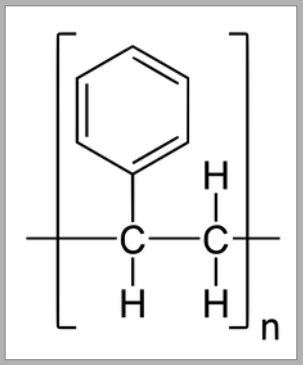
I. INTRODUCTION

The study of the interaction of neutrons with matter has still to become centennial, yet it has impacted the modern society in a variety of ways, from fission reactors to the creation of isotopes for medical care: from the treatment of cancer to the binding energy of hydrogen in a crystal or molecular system, therefore resulting in a Compton-like scattering from an approximately free nucleus[9–14]. In this case, the scattering is defined as elastic in the neutron + nucleus system, thus requiring the conservation of kinetic energy and momentum of both particles, and the total scattering cross section corresponds to

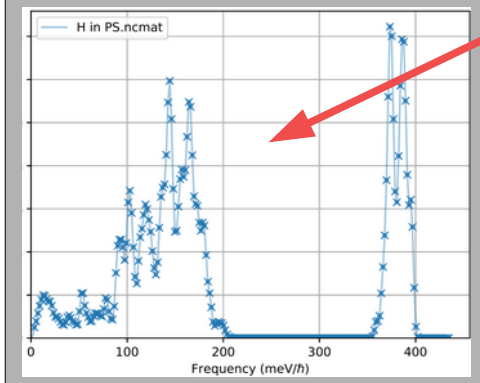
Example (polystyrene):

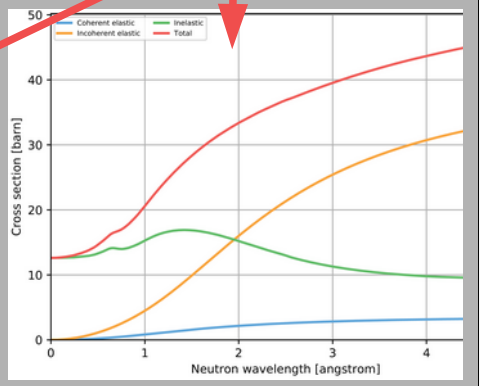
- 1 aromatic ring with 5 H
- 1 CH2 group
- 1 aliphatic CH binding






```
$> ncrystal_hfg2ncmat --formula C8H8 \
                       --spec 5xCHaro+1xCHali+1xCH2 \
                       --density 0.99 -o PS.ncmat
```

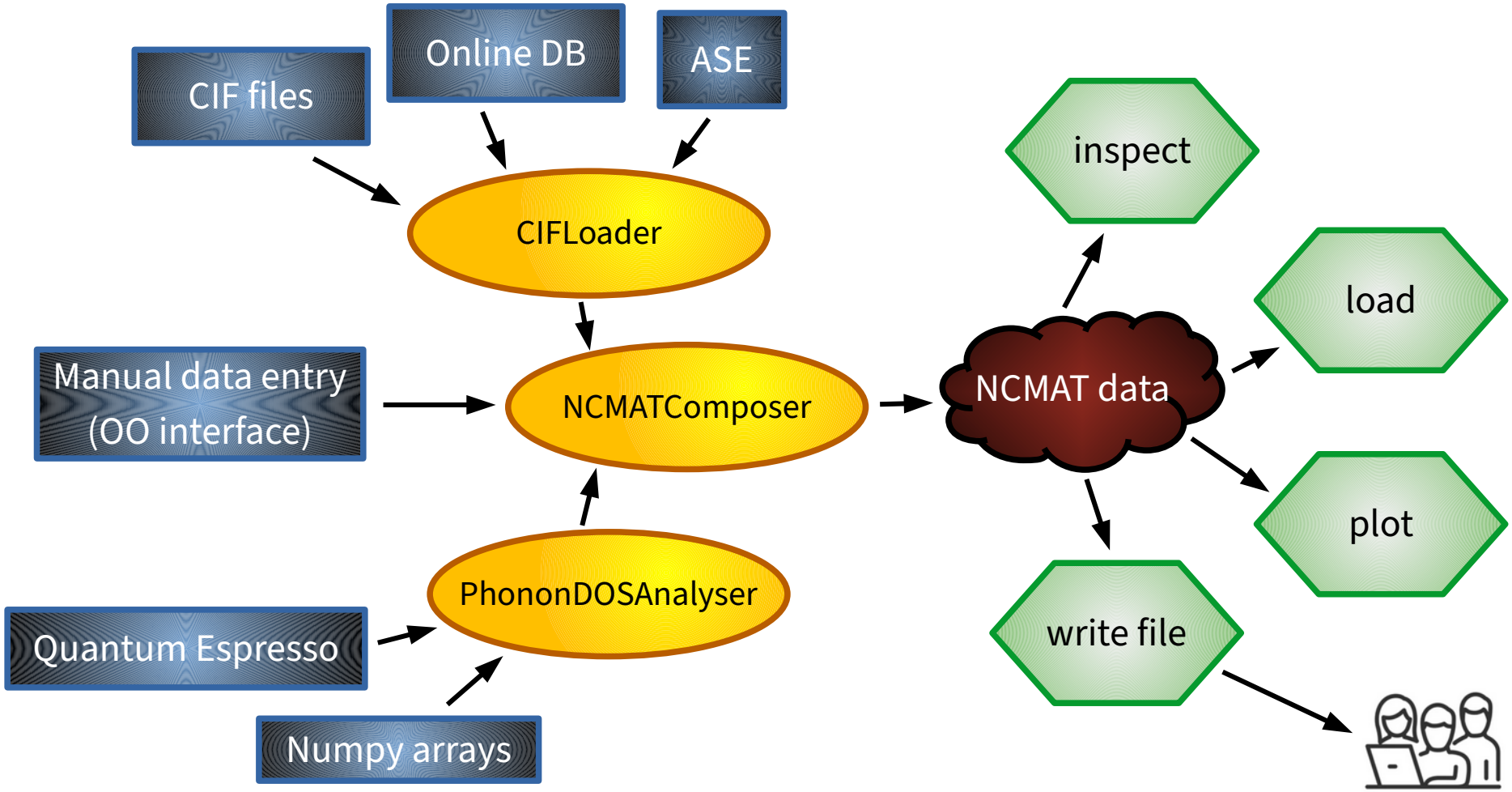


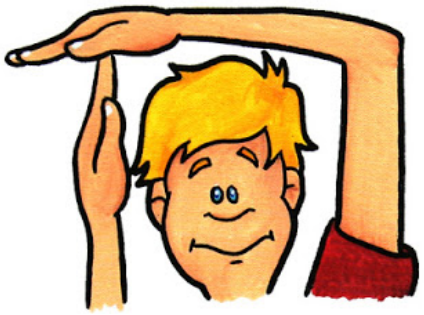


New Python tools for material compositon

The subject of 3 Jupyter notebooks in this school!

- NCrystal v3.6 brings new Python tools for creating new materials.





Notebook time: finish first notebook

Jupyter tutorials for improved v3.6 API at:
https://github.com/mctools/ncrystal-notebooks/

BrightnESS is funded by the European Union Framework Program for Research and Innovation Horizon 2020, under grant agreement 676548
HighNESS is funded by the European Union Framework Program for Research and Innovation Horizon 2020, under grant agreement 951782

NCrystal elastic physics algorithms

BrightnESS is funded by the European Union Framework Program for Research and Innovation Horizon 2020, under grant agreement 676548
HighNESS is funded by the European Union Framework Program for Research and Innovation Horizon 2020, under grant agreement 951782

$S_{coh,el}(\bar{q},\omega)$ in crystals: Bragg diffraction!

Microscopic scatter function:

sum over "crystal planes"

$$S^{el}_{coh}(\vec{Q},\omega) = \frac{(2\pi)^3\delta(\hbar\omega)}{V_{uc}} \sum_{hkl} \delta(\vec{Q}-\vec{\tau}_{hkl})\,|F(\vec{\tau}_{hkl})|^2$$

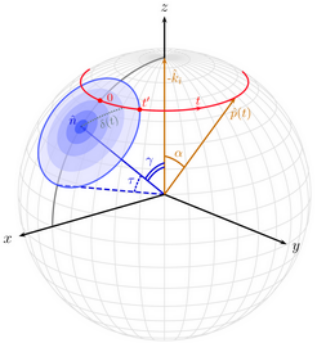
unit cell volume

plane normal with magnitude $2\pi/d_{hkl}$

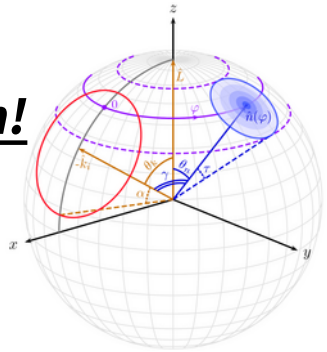
unit cell structure factor, depends on layout of atoms in unit cell

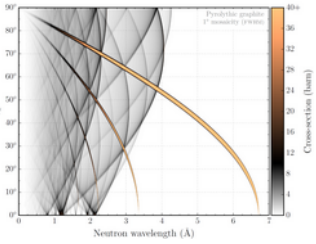
$$F(\vec{Q}) \equiv \sum_i \overline{b_i} e^{-W_i(\vec{Q})} e^{i\vec{Q}\cdot\vec{p}_i}$$

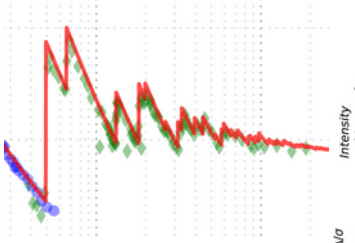
$2W=\delta^2q^2$, δ=atomic displacement

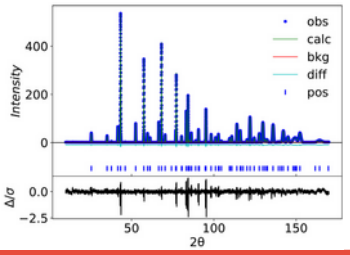


Macroscopic** values are found from convoluting microscopic values with crystal grain distributions → **geometrical problem!









Supported geometries in NCrystal:

- *Completely disoriented layout ("powder approximation")*
- *Gaussian deviations from completely oriented ("Mosaic single crystals")*
- *Layered crystals ("rotated mosaic single crystals", pyrolythic graphite)*

Not supported yet:

- *Bent/deformed crystals, corrections for very small grain sizes.*
- *Textured crystals (as in most metals/polycrystals). But powder approximation OK for many use-cases!!*

BrightnESS is funded by the European Union Framework Program for Research and Innovation Horizon 2020, under grant agreement 676548
HighNESS is funded by the European Union Framework Program for Research and Innovation Horizon 2020, under grant agreement 951782

Bragg diffraction in powders (and texture-free polycrystals)

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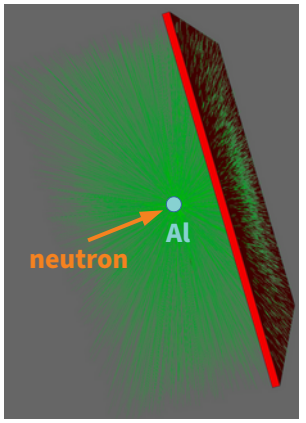
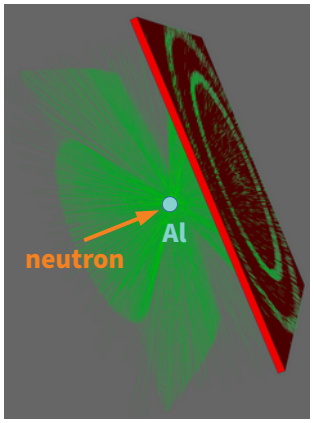
Based on provided HKL planes with d-spacings and structure factors, the implementation is straight-forward.

Care is taken to be extremely fast O(10ns/call), even in case of huge number of planes.

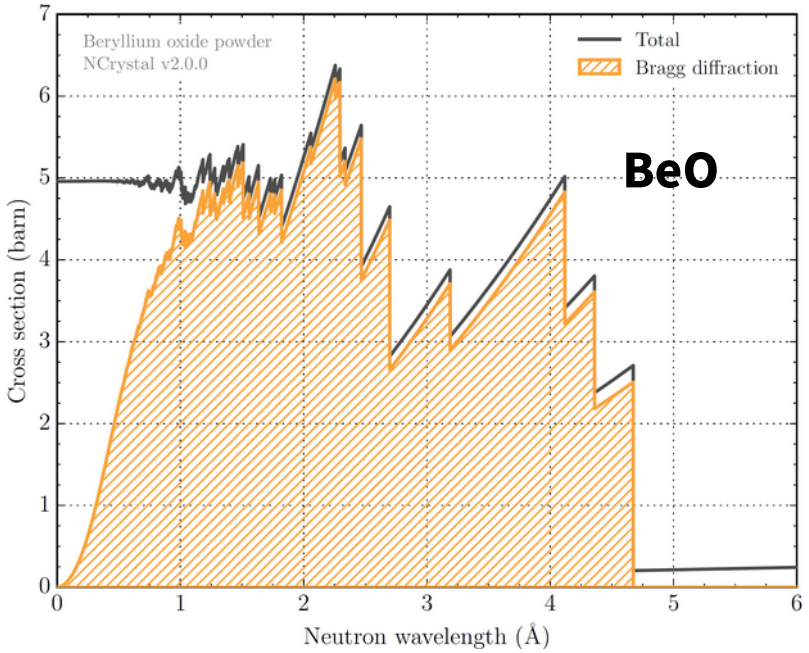
Currently no texture/grain-size effects.

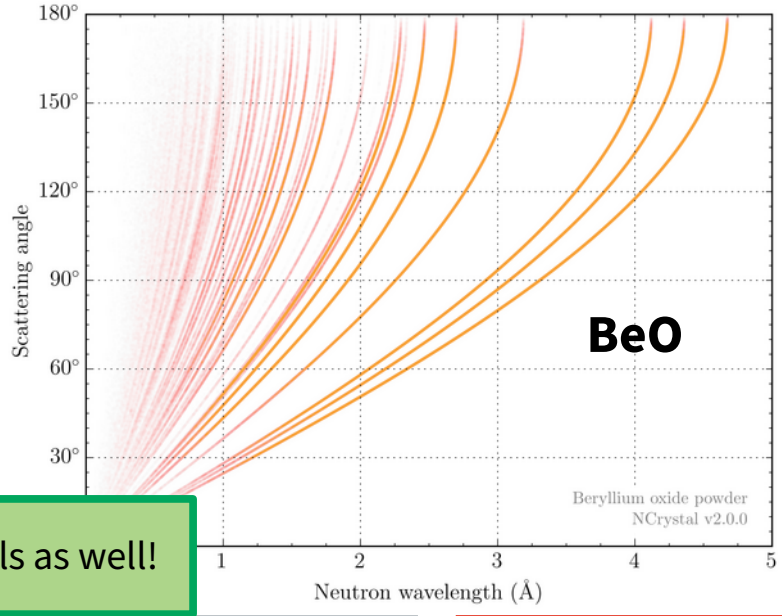


Geant4 free-gas model
(wrong MFP, wrong scatter)



Geant4 with NCrystal
⇒Debye-Scherrer cones





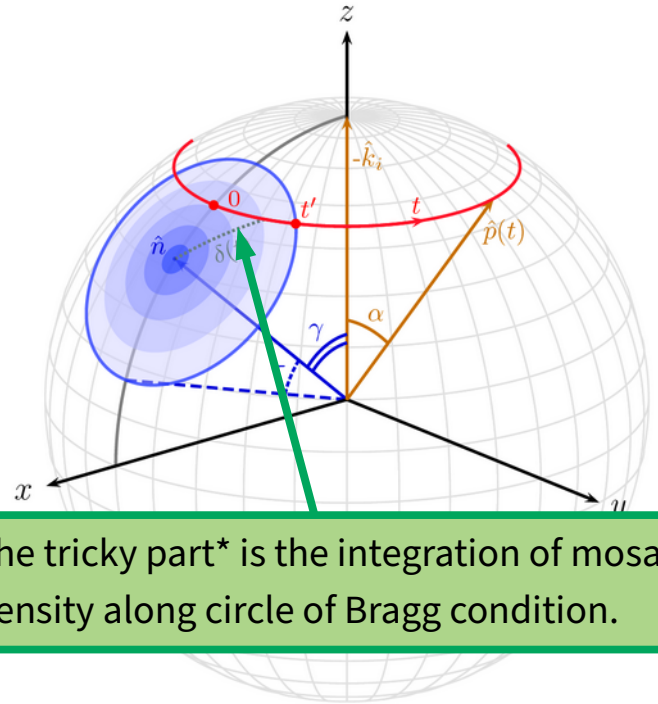
There is interest in extending this to textured materials as well!

Single Crystals with Gaussian mosaicity

Can model monochromators, analysers, filters, samples

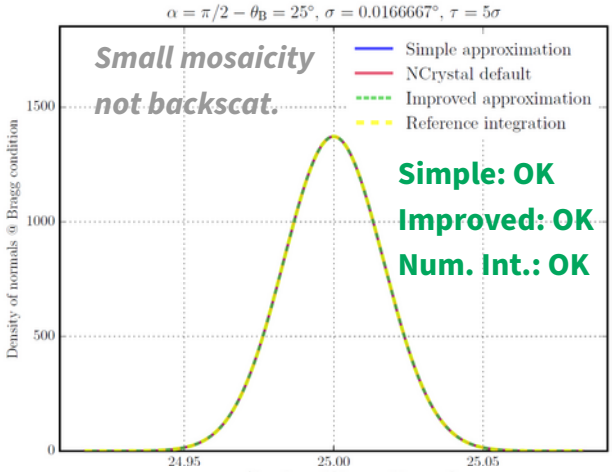
Handles also large mosaicities and backscattering!

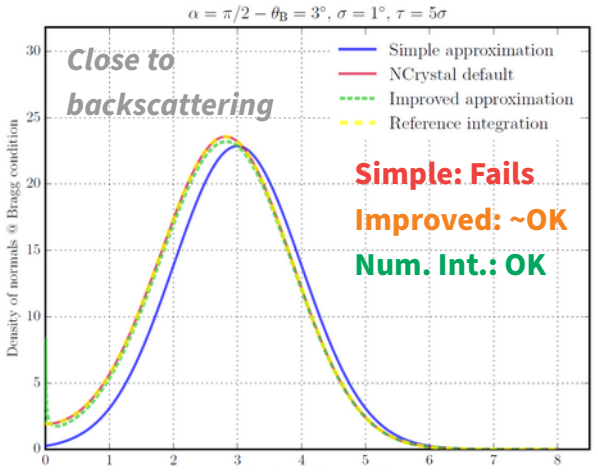
NCrystal
Thermal Neutron Transport

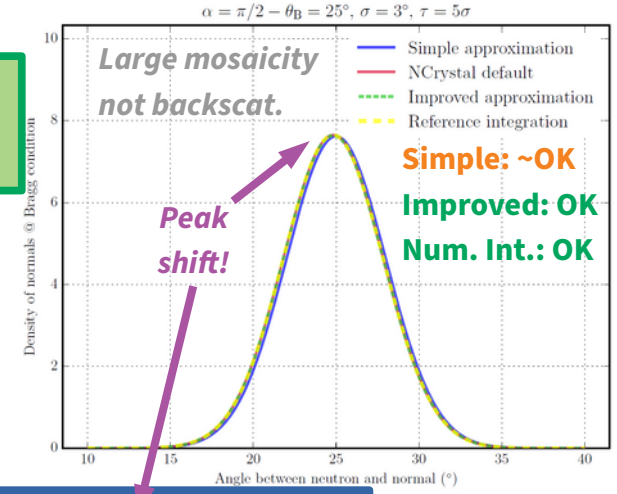


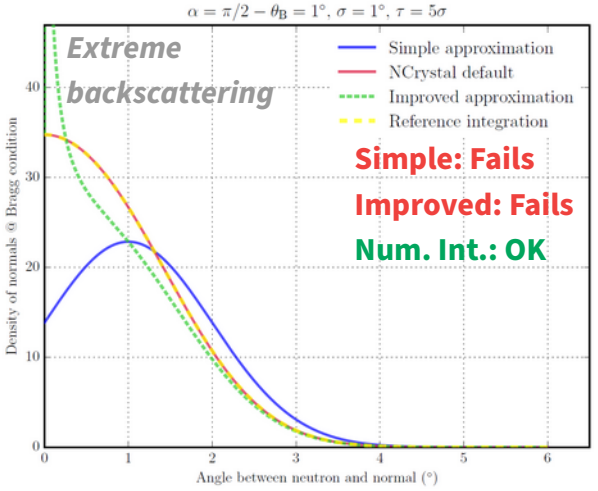
The tricky part* is the integration of mosaic density along circle of Bragg condition.

*: Once contributing normals Have been identified.









Simple closed-form approx. valid for small mosaicity (and not backscattering):

$$\sigma_{\text{Bragg}}(\alpha,\gamma) = Q \times \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\tfrac{1}{2}\delta_0^2/\sigma^2\right] \times \operatorname{erf}\left[\sqrt{\frac{\tau^2-\delta_0^2}{2\sigma^2}}\right] \times \sqrt{\frac{\sin\alpha}{\sin\gamma}} \times \frac{N}{1/(2\pi\sigma^2)}$$

$$\delta_0 = |\alpha - \gamma|$$

Our improved form extends validity to much larger mosaicities

Code picks best method from:

- Our closed form approximation
- Full numerical integration

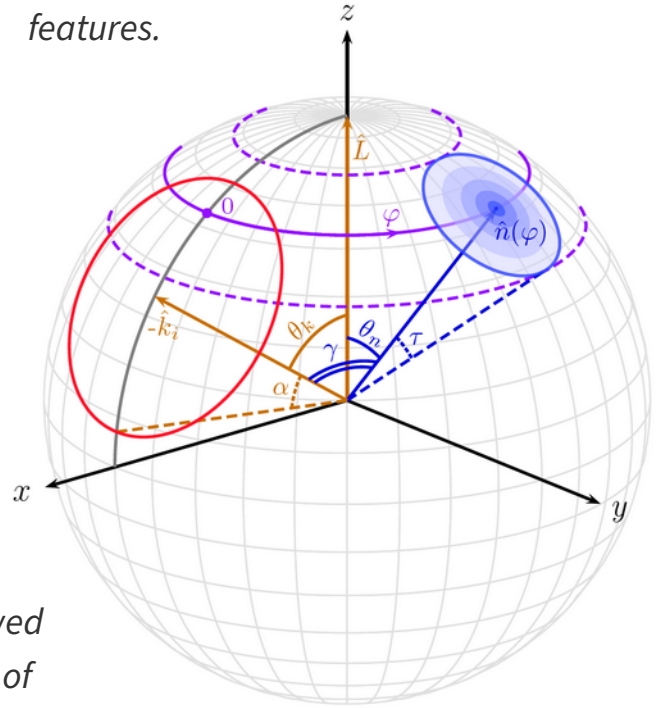
Special anisotropic model for Pyrolytic Graphite

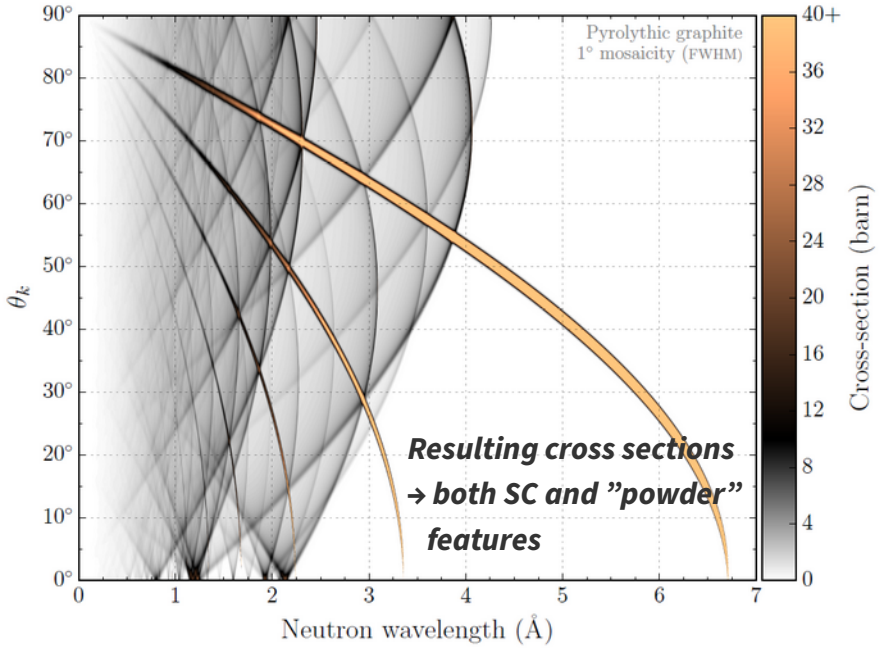
PG often used as filters, monochromator, analyser

NCrystal
Thermal Neutron Transport

Layered crystal model:

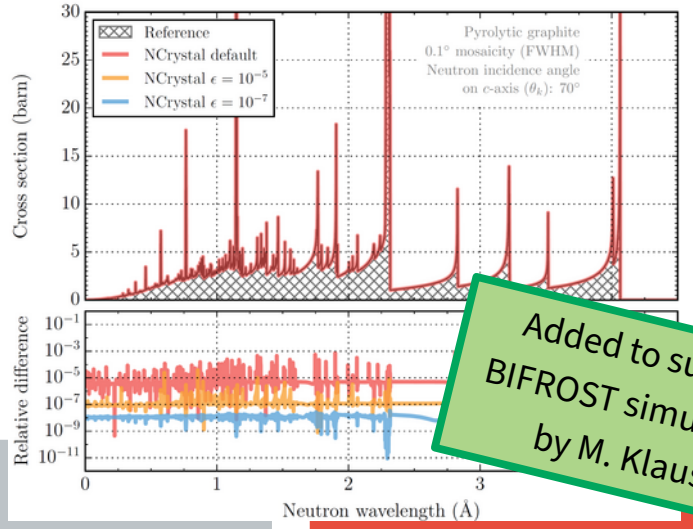
- *Usual Gaussian mosaic distribution is "smeared out" by rotation*
- *Exhibits both single-crystal and powder features.*





Features:

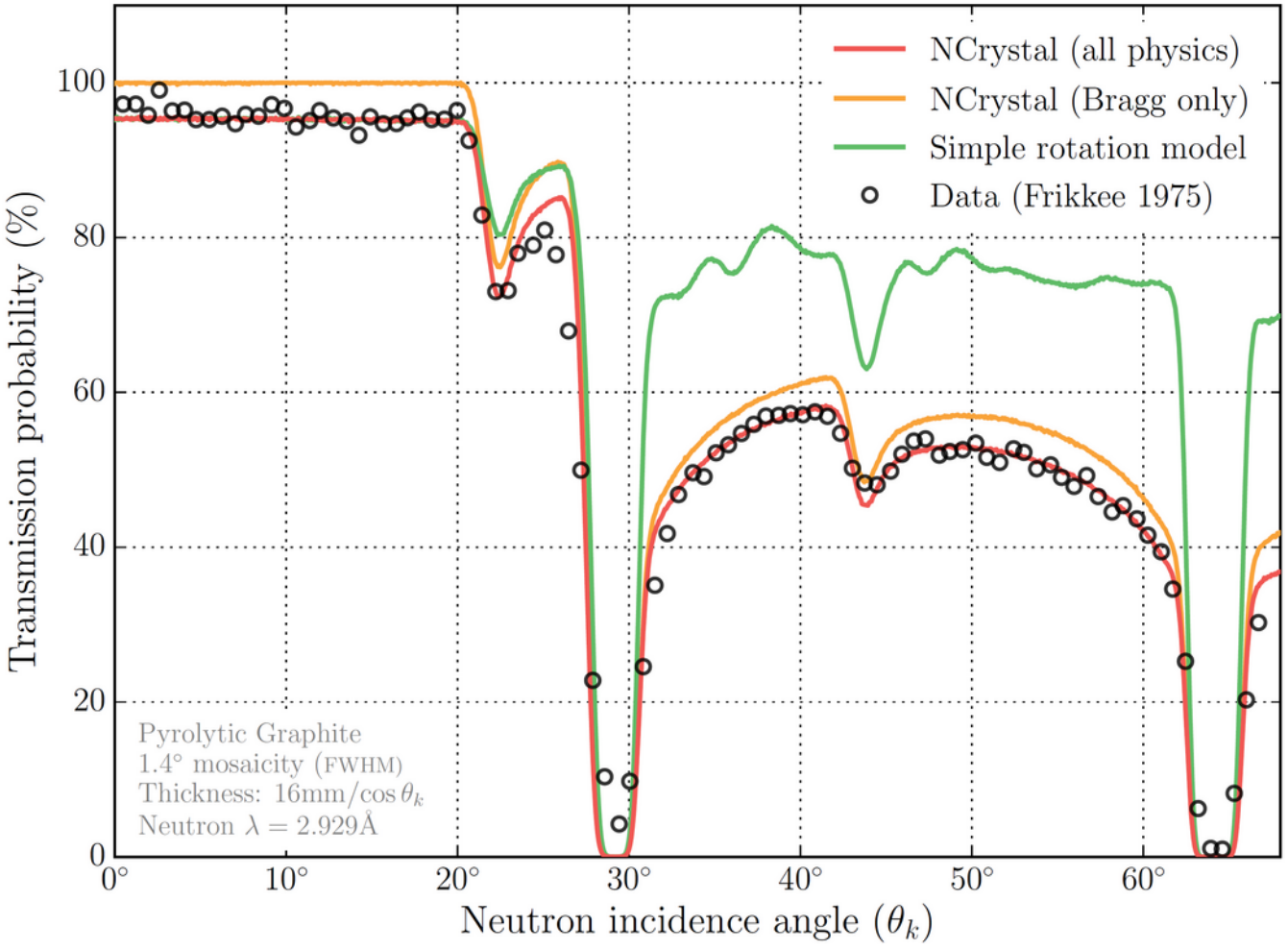
- *Cross-sections determined by efficient pre-search followed by fast Romberg integration of non-layered single crystal code.*
- *Features realistic transmission probabilities and multiple-scattering effects (incl. "zig-zag walk")*



Added to support BIFROST simulations by M. Klausz.

Can reproduce PG transmission spectra!

NCrystal
Thermal Neutron Transport



Validation also includes:

- Comparison against (very very) slow but simple+precise implementation.
- Verification that cross section maxima structure matches predictions (Frikkee1975).
- Technical validations (zig-zag, “powdered”).

Incoherent-elastic scattering

NCrystal
Thermal Neutron Transport

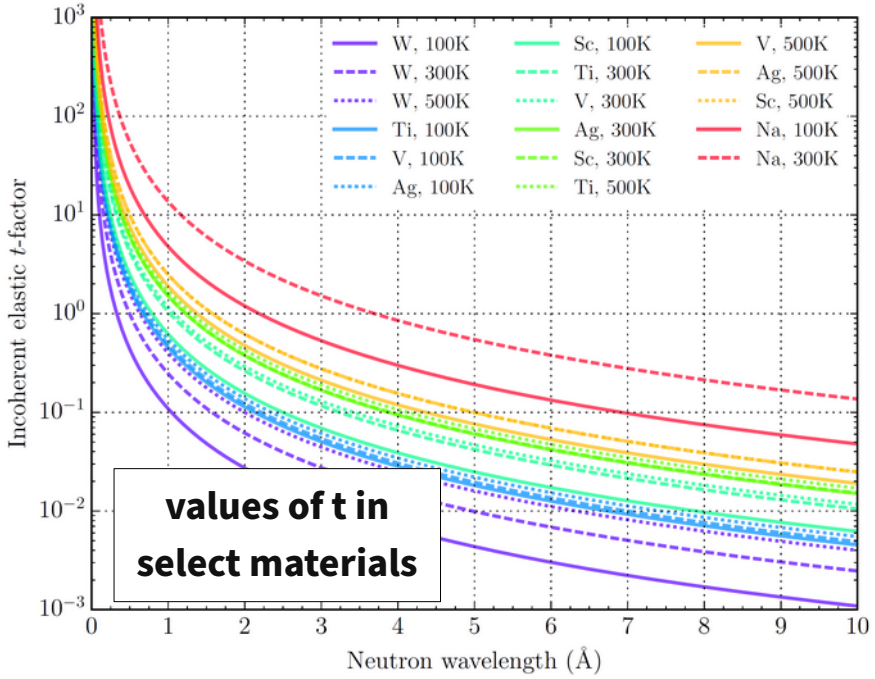
$$\frac{d\sigma^{\mathrm{inc,el}}_{\vec{k}_i\to\vec{k}_f}}{d\Omega_f} = \frac{1}{N}\sum_{j=1}^{N}\frac{\sigma_j^{\mathrm{inc}}}{4\pi}e^{-2W_j(\vec{Q})}$$

$$\sigma^{\mathrm{inc,el}}(k) = \sigma_{\mathrm{inc}}\frac{1-\exp(-t)}{t}$$

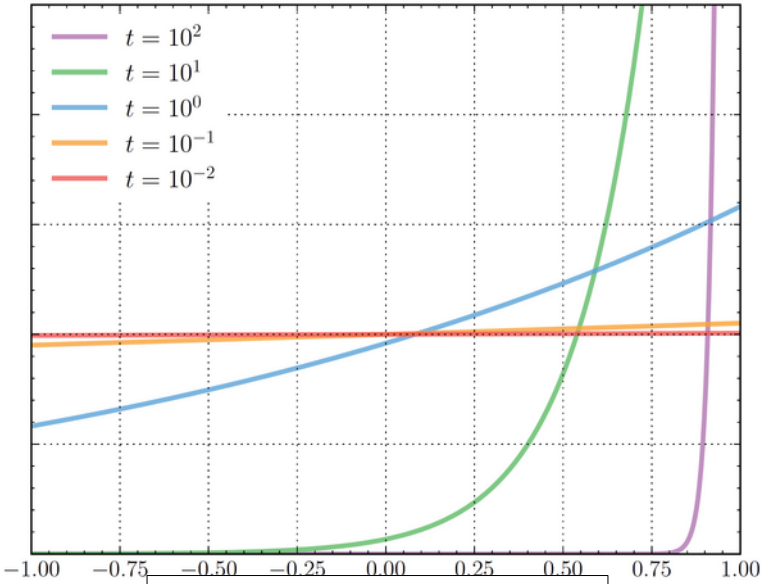
$$P(\mu) = N_t \exp\left(\frac{t\mu}{2}\right)$$

$$t \equiv (2k\delta)^2 = \left(\frac{4\pi\delta}{\lambda}\right)^2$$

Get Debye-Waller factors (or δ^2) from phonon DOS (or Debye temp.).



values of t in select materials



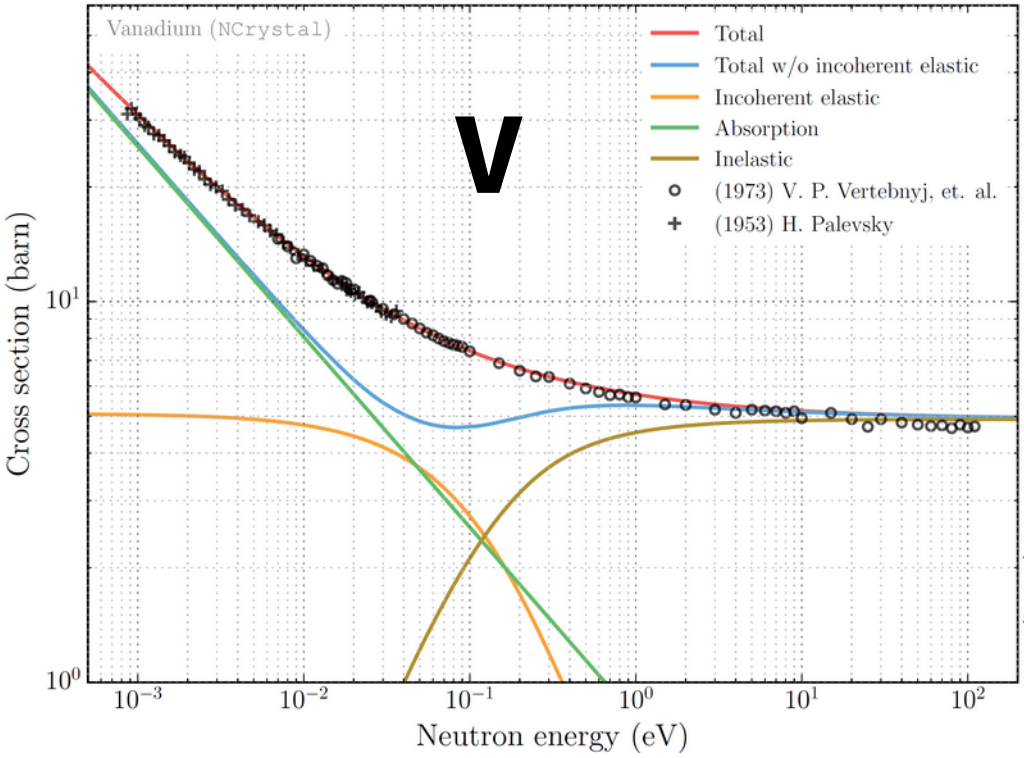
cos(θ)=μ distribution (isotropic=flat)

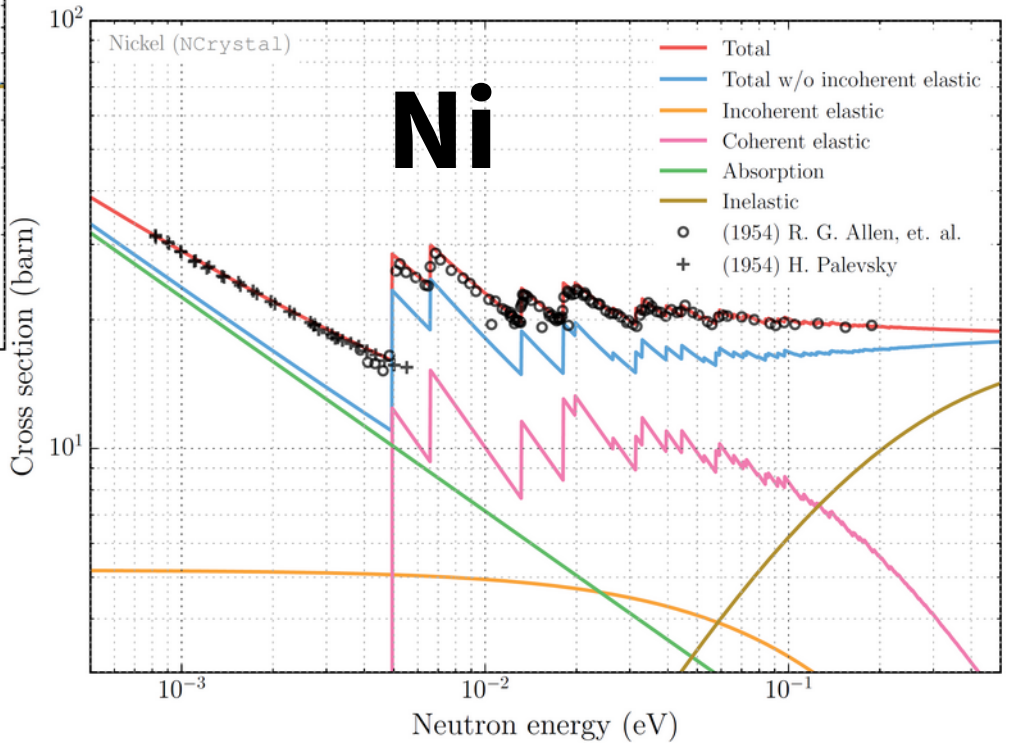
→ Not always completely isotropic!!

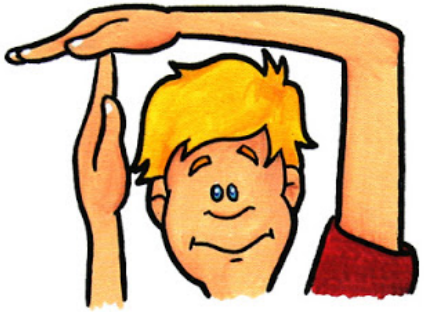
Incoherent-elastic model validations

→ so far only with total cross sections

NCrystal
Thermal Neutron Transport







Notebook time: second basic notebook.

This NB covers a few optional topics, skim through it, focus on what you want, read it in detail later if you wish.

Jupyter tutorials for improved v3.6 API at:
https://github.com/mctools/ncrystal-notebooks/

BrightnESS is funded by the European Union Framework Program for Research and Innovation Horizon 2020, under grant agreement 676548
HighNESS is funded by the European Union Framework Program for Research and Innovation Horizon 2020, under grant agreement 951782

NCrystal inelastic physics algorithms (high-level view)

BrightnESS is funded by the European Union Framework Program for Research and Innovation Horizon 2020, under grant agreement 676548
HighNESS is funded by the European Union Framework Program for Research and Innovation Horizon 2020, under grant agreement 951782

Inelastic physics : Scattering kernels

NCrystal
Thermal Neutron Transport

$$\frac{d^2\sigma_{\vec{k}_i \Rightarrow \vec{k}_f}}{d\Omega_f dE_f} = \frac{k_f}{k_i} S(\vec{Q}, \omega)$$

$$S(\vec{Q}, \omega) = S_{\mathrm{coh}}(\vec{Q}, \omega) + S_{\mathrm{inc}}(\vec{Q}, \omega)$$

$$S_{\mathrm{coh}}(\vec{Q}, \omega) \equiv \frac{1}{2\pi\hbar} \sum_{j,j'=1}^{N} \overline{b_j} \cdot \overline{b_{j'}} \int_{-\infty}^{\infty} dt \langle j', j \rangle e^{-i\omega t}$$

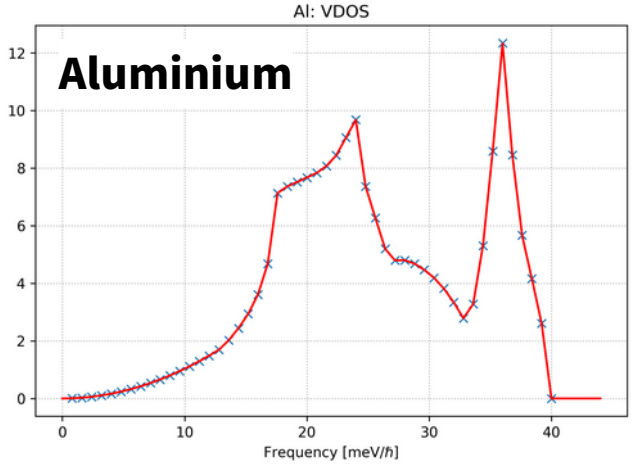
$$S_{\mathrm{inc}}(\vec{Q}, \omega) \equiv \frac{1}{2\pi\hbar} \sum_{j=1}^{N} \left(\overline{b_j^2} - \left(\overline{b_j}\right)^2 \right) \int_{-\infty}^{\infty} dt \langle j, j \rangle e^{-i\omega t}$$

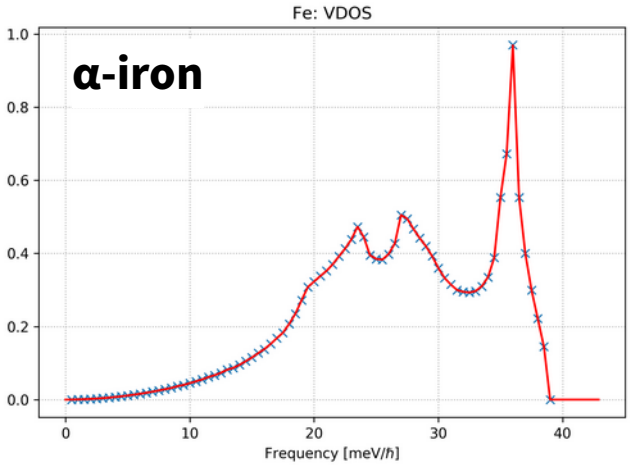
Under some assumptions S(Q,w) can be described with a single “smooth” 2D function (one per atom type):

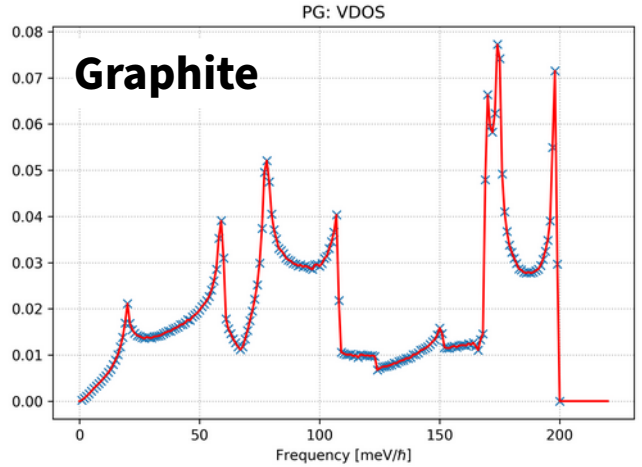
- Elastic scattering is dealt with separately (as it is in NCrystal).
- *Isotropic material* (Q dependency becomes scalar)
- *Incoherent approximation*: Off-diagonal entries in S_{coh} wash out when integrating over isotropic grain distribution, so shape(S_{coh}) ≈shape(S_{inc}).

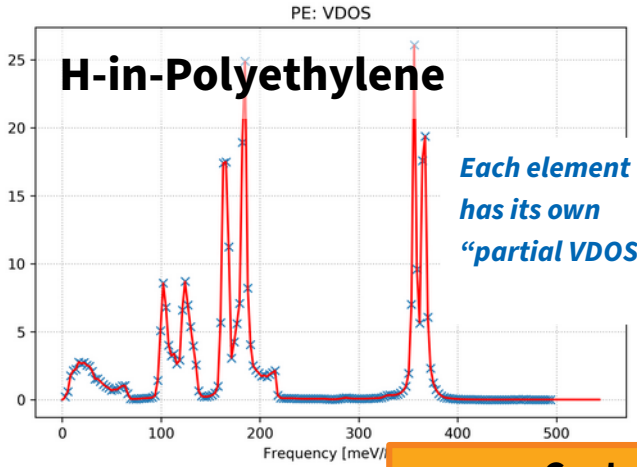
Tabulate this function on a grid → **scattering kernel**.

Solids: Scattering kernels are connected to phonon frequency spectrums (aka Vibrational Density Of States, VDOS)

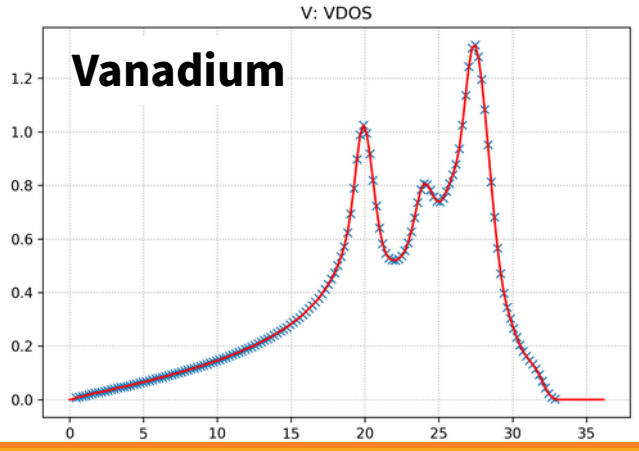




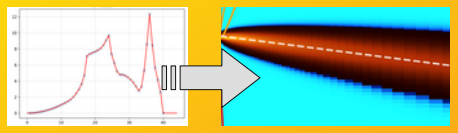




Each element has its own "partial VDOS"



NCrystal can expand VDOS to scattering kernels on-the-fly in O(100ms).



Captures material structure info relevant for *inelastic* neutron scatterings (isotropic materials, incoherent approximation) + gives displacements (Debye-Waller factors) needed for *elastic* scatterings.

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HighNESS is funded by the European Union Framework Program for Research and Innovation Horizon 2020, under grant agreement 951782

Phonon spectrum (VDOS) sources

NCrystal
Thermal Neutron Transport

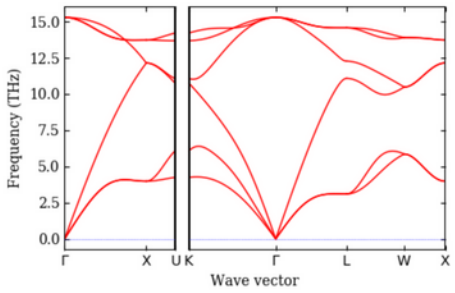
VDOS is not specific to neutrons!

→ Many resources exists

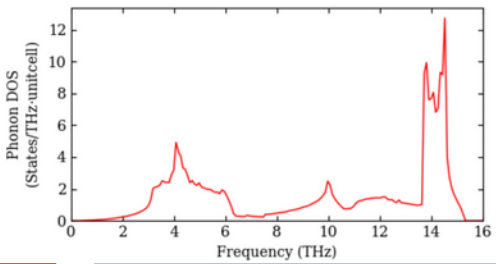
Materials id 149 / Si / Fd-3m (227)

- Date page updated: 2018-4-17
- Space group type: Fd-3m (227) / F 4d 2 3 -1d
- Number of formula units (Z): 8
- Phonon raw data: `mp-149-20180417.tar.lzma`
- Link to Materials Project: https://www.materialsproject.org/materials/mp-149/

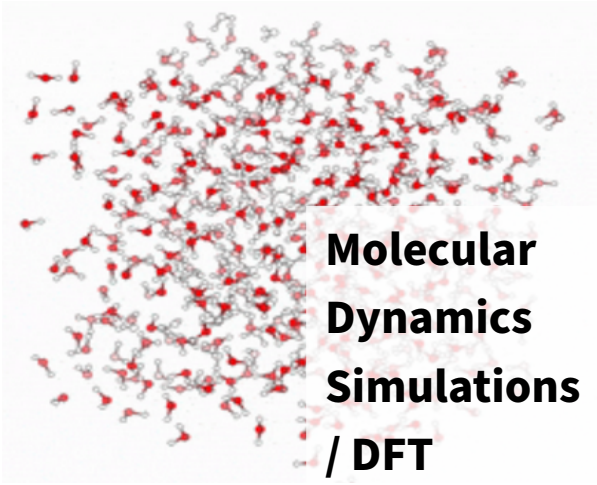
Phonon band structure



Phonon DOS



http://phonondb.mtl.kyoto-u.ac.jp/



Molecular Dynamics Simulations / DFT

VDOS can also be measured experimentally...

... or dug out from old research papers!

Or a combination, potentially using other SW (QuantumEspresso / VASP / phononpy / Oclimax / ...)

Refer to Davide Campi's lectures for a much more thorough discussion!

QUANTUMESPRESSO

Many VDOS curves need a bit of processing and cleanup to be used.

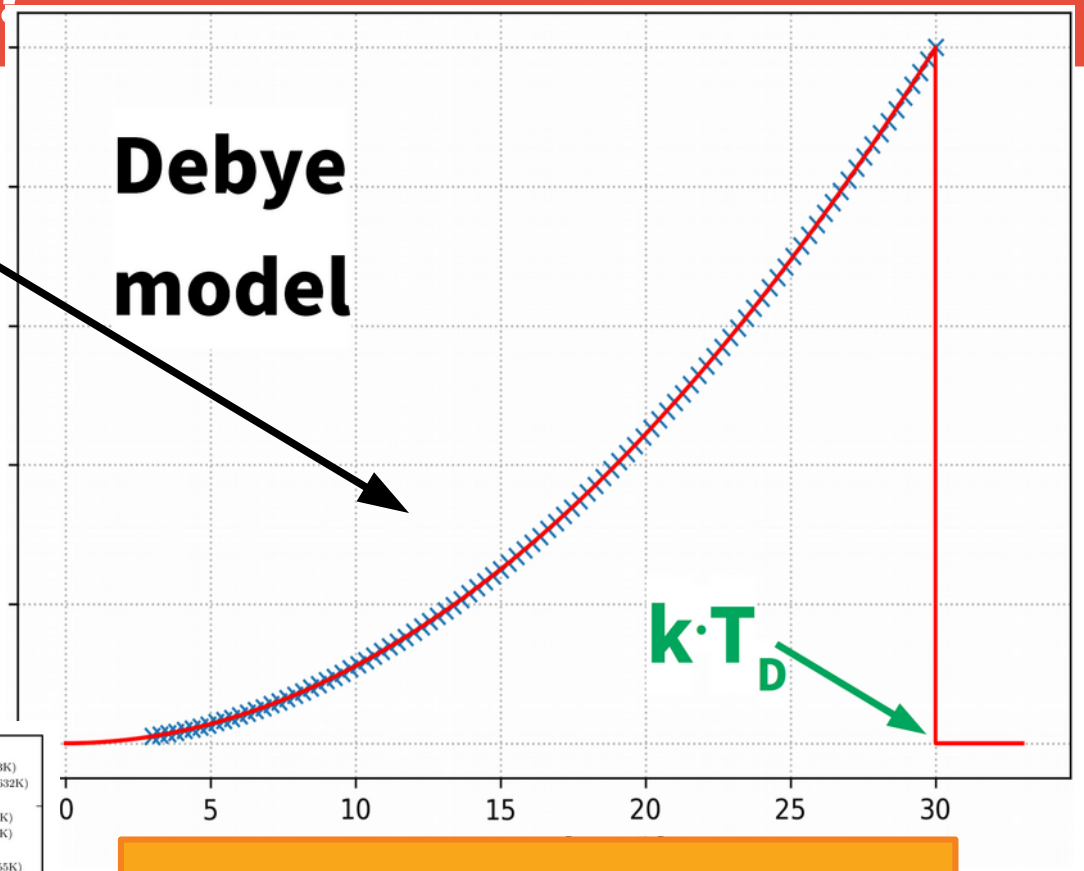
This can be done in Python using the PhononDOSAnalyser class provided with NCrystal.

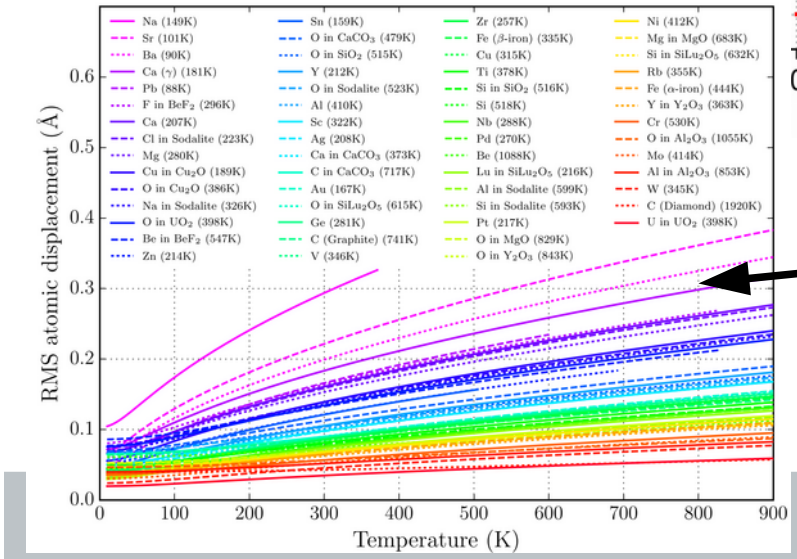
How we handle materials with no phonon DOS specified?

NCrystal
Thermal Neutron Transport

Idealised DOS (Debye Model) is constructed and fed into same infrastructure as any other DOS.

Lacks details of course, but gives consistent kinematics and handles multi-phonon physics ~OK.

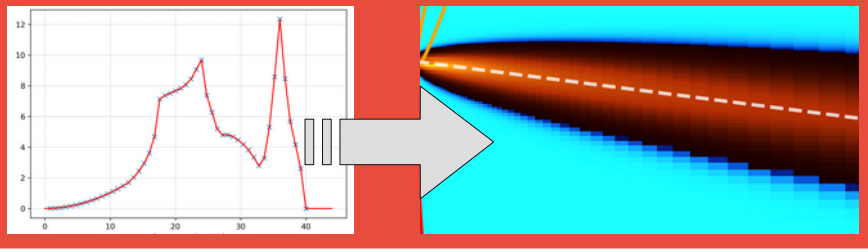




T-dependent atomic displacements (δ), from Debye temperature (T_D)

Of course, a real DOS gives more realistic δ.

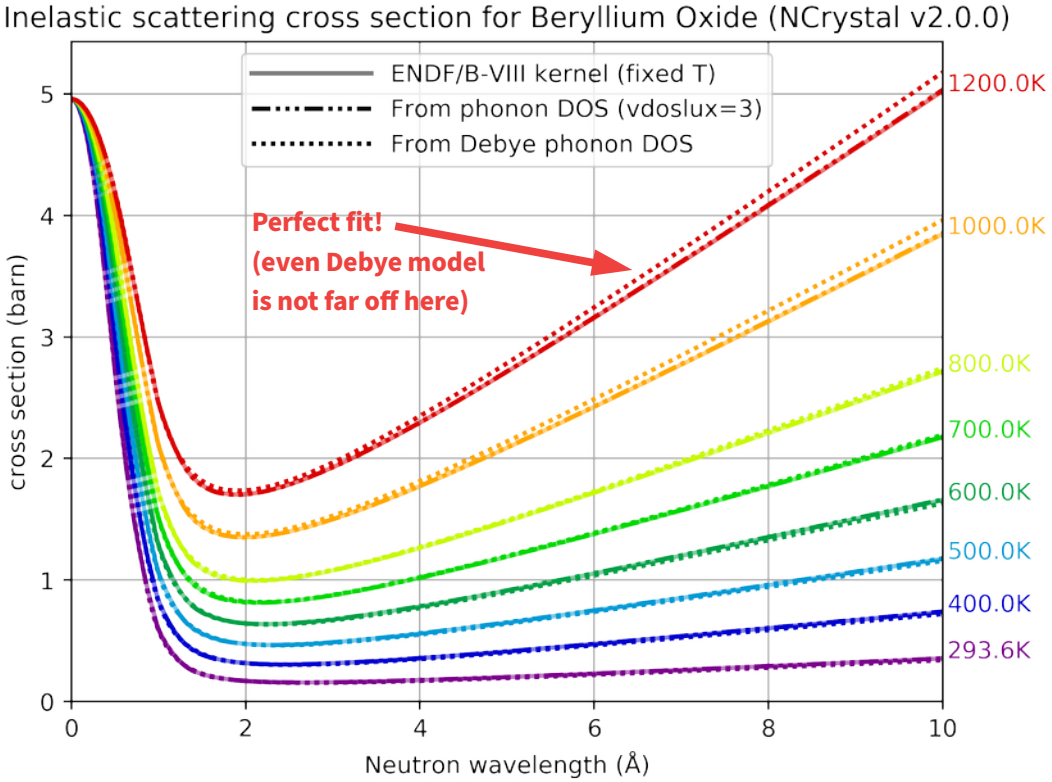
VDOS → S(α,β) [solids]

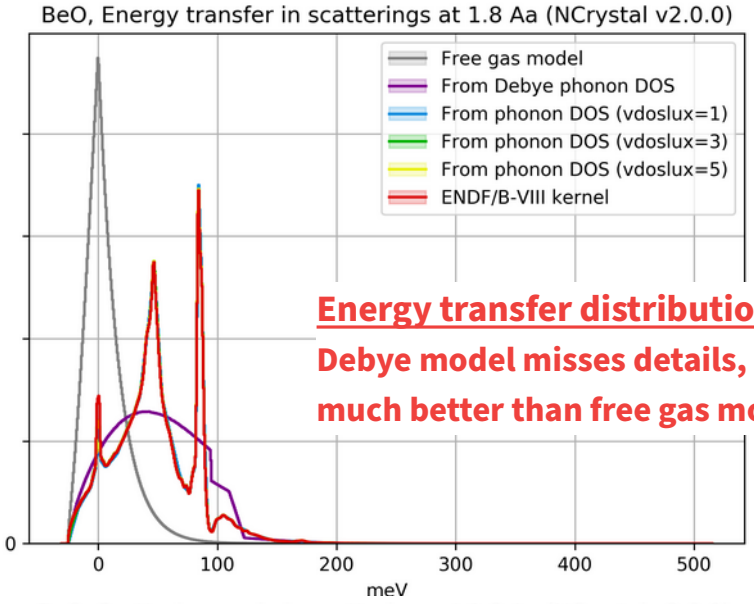


NCrystal
Thermal Neutron Transport

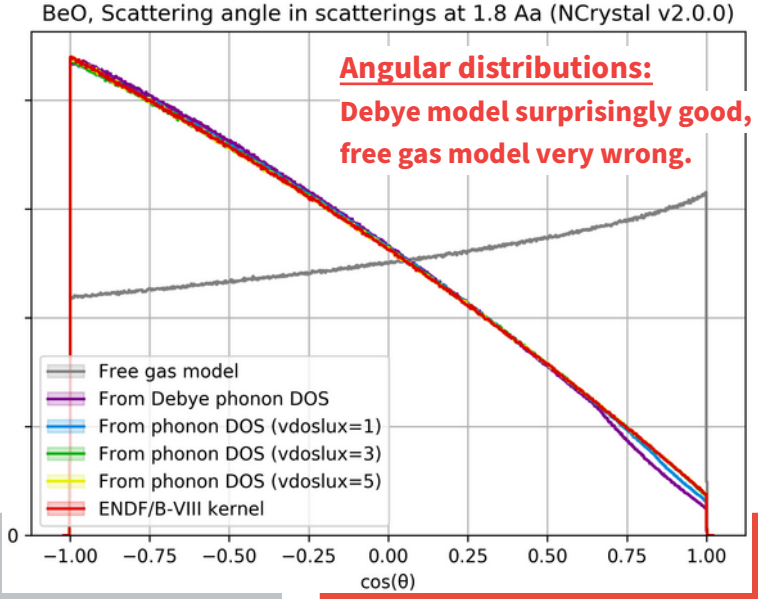
Identical results as when using LEAPR/ENDF kernels:

- Comparing at fixed temperature values from ENDF/B-VIII, using the same VDOS curve.
- NCrystal "luxury" level (cfg param "vdoslux", default value 3) mostly affects scattering kernel grid size+granularity.





Energy transfer distributions:
Debye model misses details, but much better than free gas model.



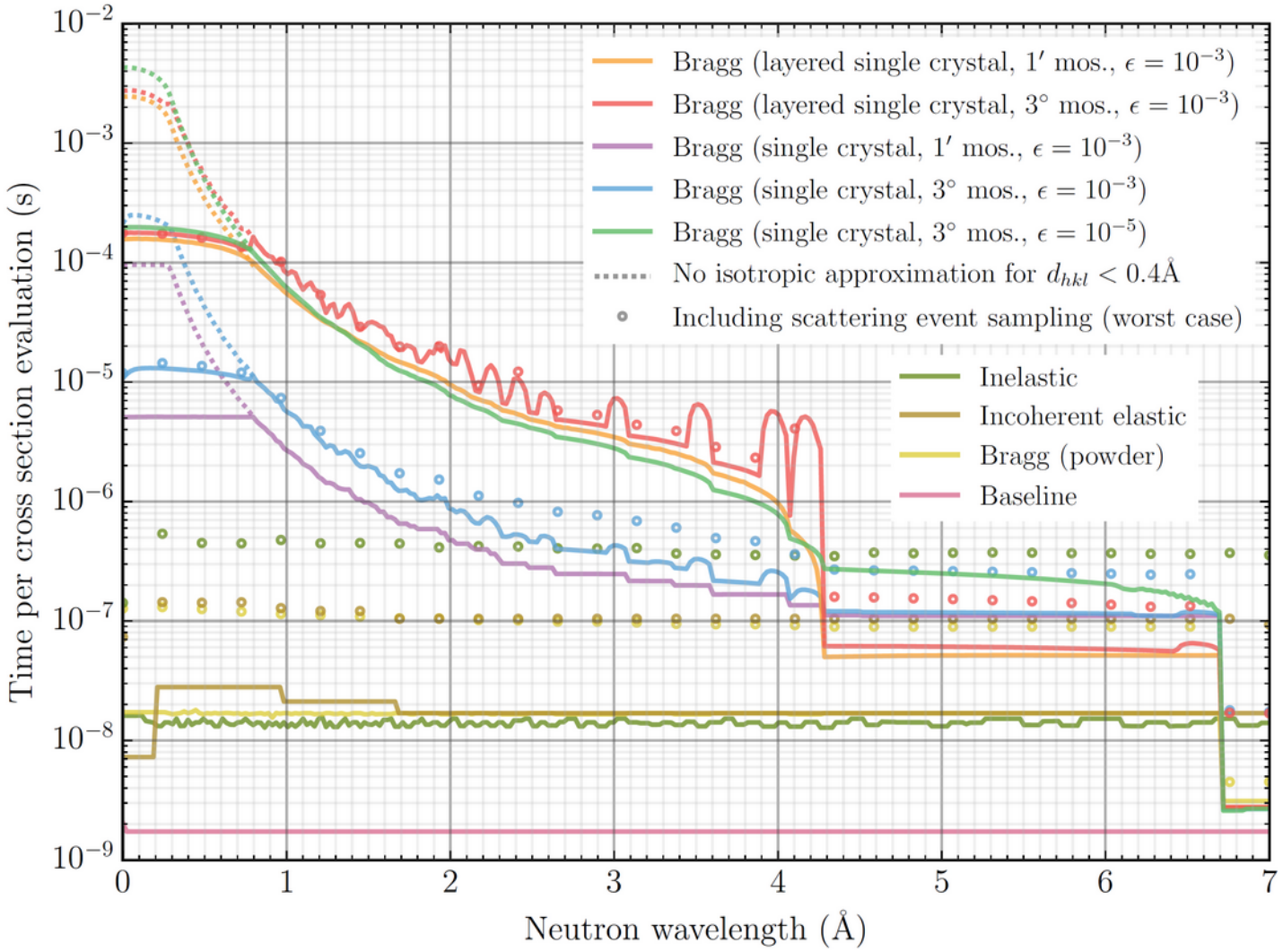
Angular distributions:
Debye model surprisingly good, free gas model very wrong.

Miscellaneous subjects:

- Computational speed
- Treatment of amorphous materials
- Flexible atomic definitions
- Multiphase materials + SANS
- Externally developed plugins

Strong focus on computational speed

NCrystal
Thermal Neutron Transport



Rough conclusions for MC simulations with thin samples:

- **O(1-100MHz) neutrons in powder**
- **O(0.1-10MHz) neutrons in single crystal (depends on λ)**

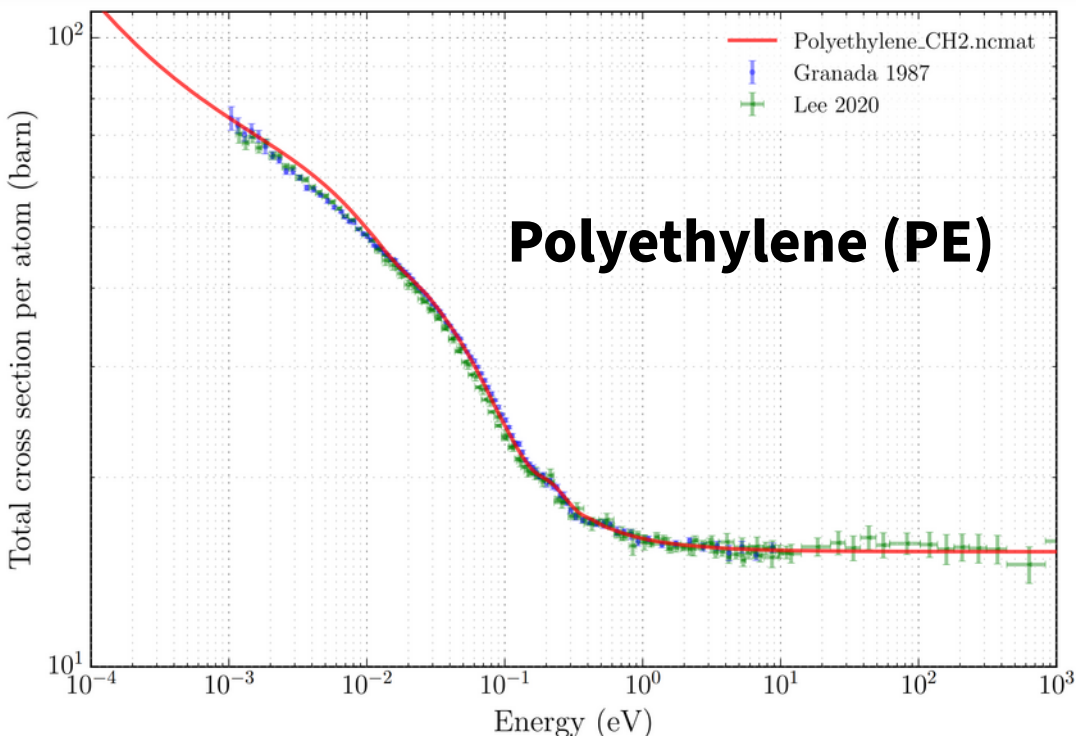
Have several ideas for additional speedups. (just needs time to implement...)

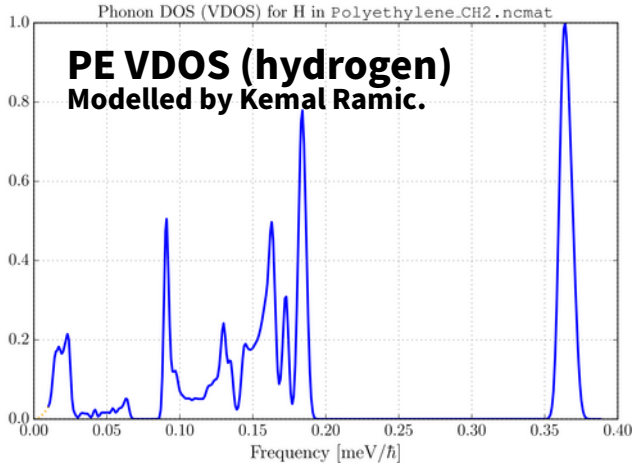
Amorphous solids

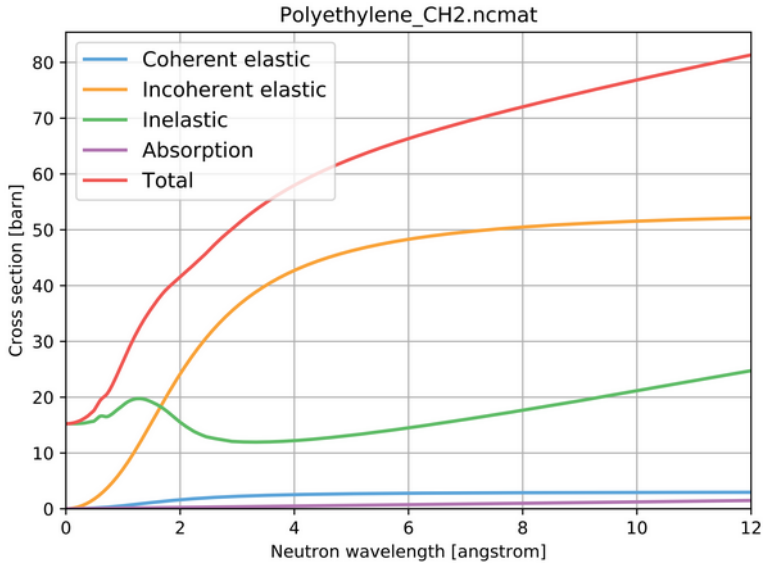
Since NCrystal v2.7.0

NCrystal
Thermal Neutron Transport

- **Uses same inelastic and incoherent-elastic approach as for crystalline solids.**
- **Coherent-elastic scattering via incoherent approximation. Hope to add proper support for static structure factor at some point.**



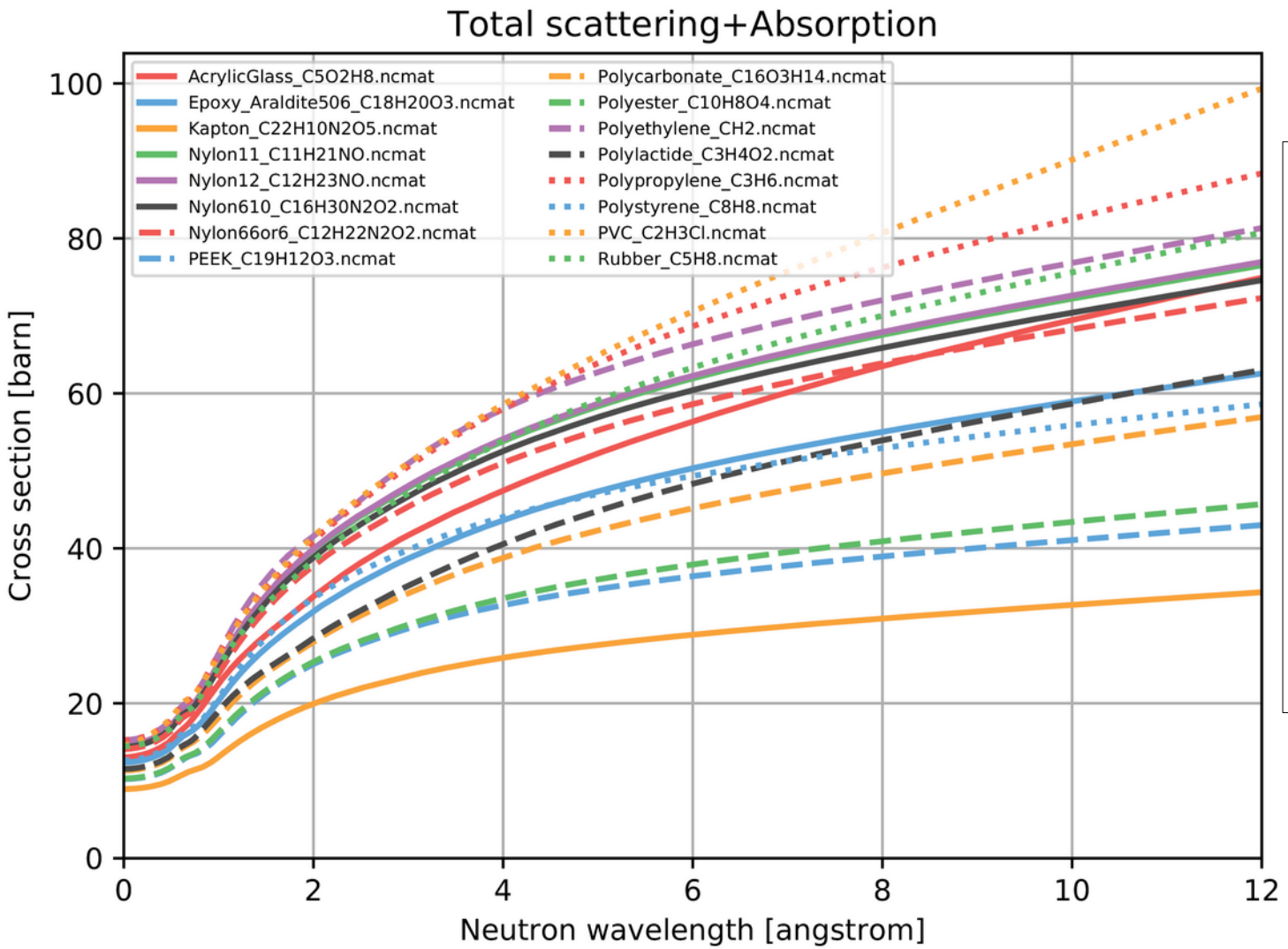




Amorphous materials in data library

New feature in NCrystal v2.7.0

NCrystal
Thermal Neutron Transport

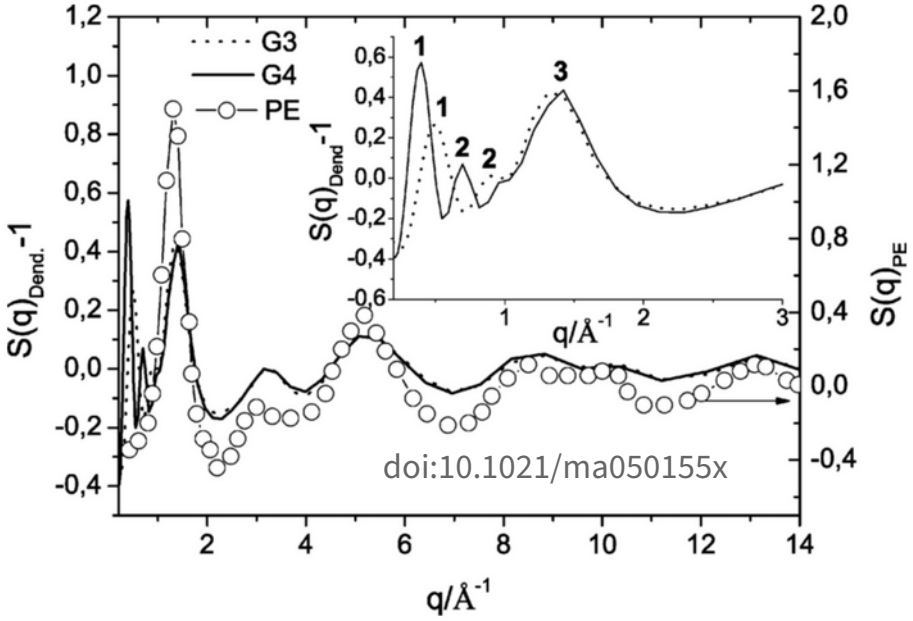


- **Adding ~16 such materials in v2.7.0.**
- **Polyethylene and AcrylicGlass (a.k.a. Plexiglass/Lucite) based on VDOS from other sources.**
- **14 others based on ncrystal_hfg2ncmat script.**
- **Let us know if we are missing something useful!**

Amorphous materials & Static structure factors

NCrystal
Thermal Neutron Transport

- We plan to eventually also optionally include static structure factors S(q) in our treatment of amorphous solids, but for now they are modelled under the *incoherent approximation.*
- The *incoherent approximation* is very good for esp. hydrogen-rich materials, but amorphous materials without strong incoherent cross sections might suffer in realism currently.



Flexible atomic (re)definitions

NCrystal
Thermal Neutron Transport

NCrystal supports atoms which are not just natural elements!

- **Ships with database of 80+ natural elements and 261+ isotopes.**
- **Possibility to customise:**
  - **In NCMAT data**
  - **In cfg-string parameter**
  - **With the NCMATComposer**

```
NCMAT v3
@ATOMDB
  #Override data for whatever reason:
  H 1.008u -3.7fm 80.3b 0.3b
  #Provide absent data:
  Rn222 222.017u 123fm 0.456b 789b
  #Enrich Boron:
  B mix 0.95 B10 0.05 B11
  #Add dopants on Al positions:
  Al mix 0.99 Al 0.01 Cr
  #Alternatively use "variable names"
  #(for usage elsewhere in the file):
  X mix 0.2 Al 0.4 Cr 0.4 Th
  #Or simply assign:
  B is B10
```

```
auto sc = NCrystal::createScatter("Al2O3_sg167_Corundum.ncmat;atomdb=Al:mix:0.99:Al:0.01:Cr");
```

Multiphase materials

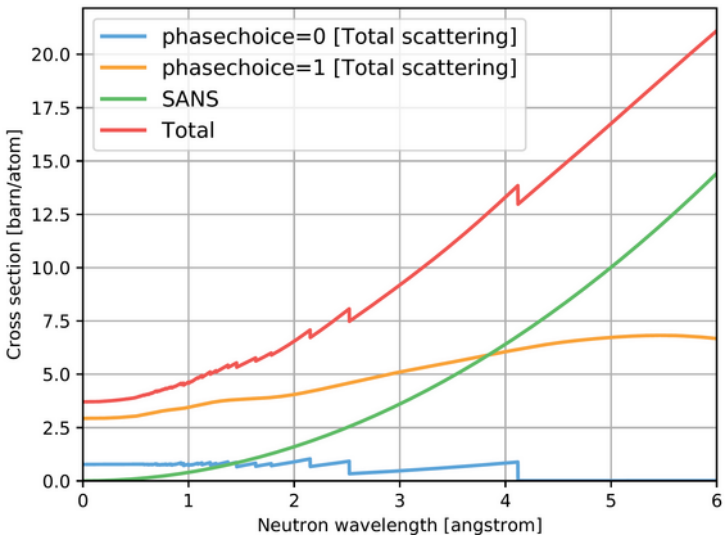
NCrystal
Thermal Neutron Transport

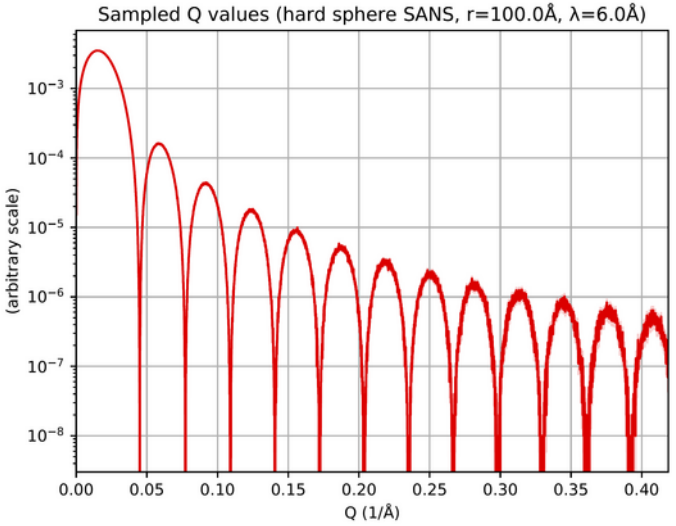
- Multiphase materials can be defined inside NCMAT data (i.e. with the NCMATComposer), or in a cfg-string:
  - `“phases<FRAC1*CFGSTR1&...&FRACN*CFGSTRN>;COMMONCFG”`
- Example (enriched B4C pellets in epoxy):
  - `“phases<0.01*solid::B4C/2.52gcm3/B_is_0.95_B10_0.05_B11`
    `&0.99*Epoxy_Araldite506_C18H20O3.ncmat>;temp=250K”`
- NB: Using volume fractions, not mass fractions (for now).
- NB: Syntax designed so you can always append e.g. “;temp=250K” to a cfg-string, and have it work.

SANS

NCrystal
Thermal Neutron Transport

- Closely connected to multiphase support, NCrystal now contains a framework for SANS physics (= phase interference).
- For now, only a basic hard-sphere SANS model can be enabled, as proof of concept.
- Colleagues at CSNS working on adding support for more SANS models.





Extend NCrystal with 3rd-party plugins

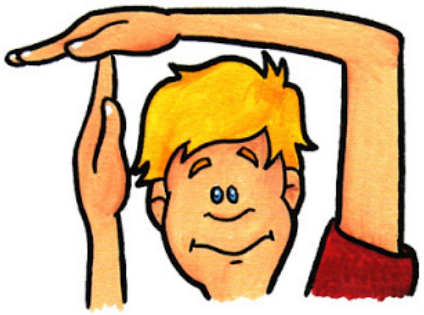
NCrystal
Thermal Neutron Transport

NCrystal v2.x made it easier to add custom physics models to NCrystal

- This can help people with their specific simulation use-case, and (in an ideal world) high quality models can eventually be adopted into the main NCrystal code.
- Extending NCrystal will naturally require C++ knowledge.
- Such plugins can be developed in separate github repos, with standard mechanism for how to include them in a given NCrystal setup.
- More details on: https://github.com/mctools/ncrystal/wiki/Plugins

Dedicated session about plugins on Friday!

With presentations about:
nanodiamond plugin (N. Rizzi, DTU)
magnetic scattering plugin (S. Xu, ESS)



Notebook time: “Advanced1”, “Advanced2”, “Advanced3”.

These multi-hour tutorials show how to compose realistic material data for NCrystal, using CIF/QuantumEspresso/... as input.

Jupyter tutorials for improved v3.6 API at:
https://github.com/mctools/ncrystal-notebooks/

BrightnESS is funded by the European Union Framework Program for Research and Innovation Horizon 2020, under grant agreement 676548
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Anatomy of scattering kernels

(optional)

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Formulation in dimensionless variables: α,β

(q,ω) preferred in neutron scattering community, (α,β) preferred in nuclear industry (incl. MCNP, ENDF, ...)

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α: dimensionless q^2

β: dimensionless ΔE

$$\beta = \frac{E_f - E}{kT} = -\frac{\hbar\omega}{kT}$$

$$\begin{aligned}\alpha &= \frac{\hbar^2}{2m_n kT} q^2 \\ &= \frac{E + E_f - 2\mu\sqrt{EE_f}}{kT} \qquad \mu = \cos\theta_{\mathrm{scat}} \\ &= \frac{2E}{kT} + \beta - 2\mu\sqrt{\frac{E}{kT}\left(\frac{E}{kT} + \beta\right)}\end{aligned}$$

Scattering lengths taken outside definition of S:

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}E_f \mathrm{d}\Omega} = \sqrt{\frac{E_f}{E}} \frac{\sigma_b}{4\pi} \frac{S(\alpha,\beta)}{k_b T}$$

Total cross section, with explicit kinematic limits:

μ=-1, complete backwards scattering

$$\sigma(E) = \frac{\sigma_b kT}{4E} \int_{-E/kT}^{\infty} \int_{\alpha_-(E,\beta)}^{\alpha_+(E,\beta)} S(\alpha,\beta) d\alpha d\beta$$

constant affects σ(E), but not (α,β)-sampling

neutron lose all its energy

μ=+1, complete forward scattering

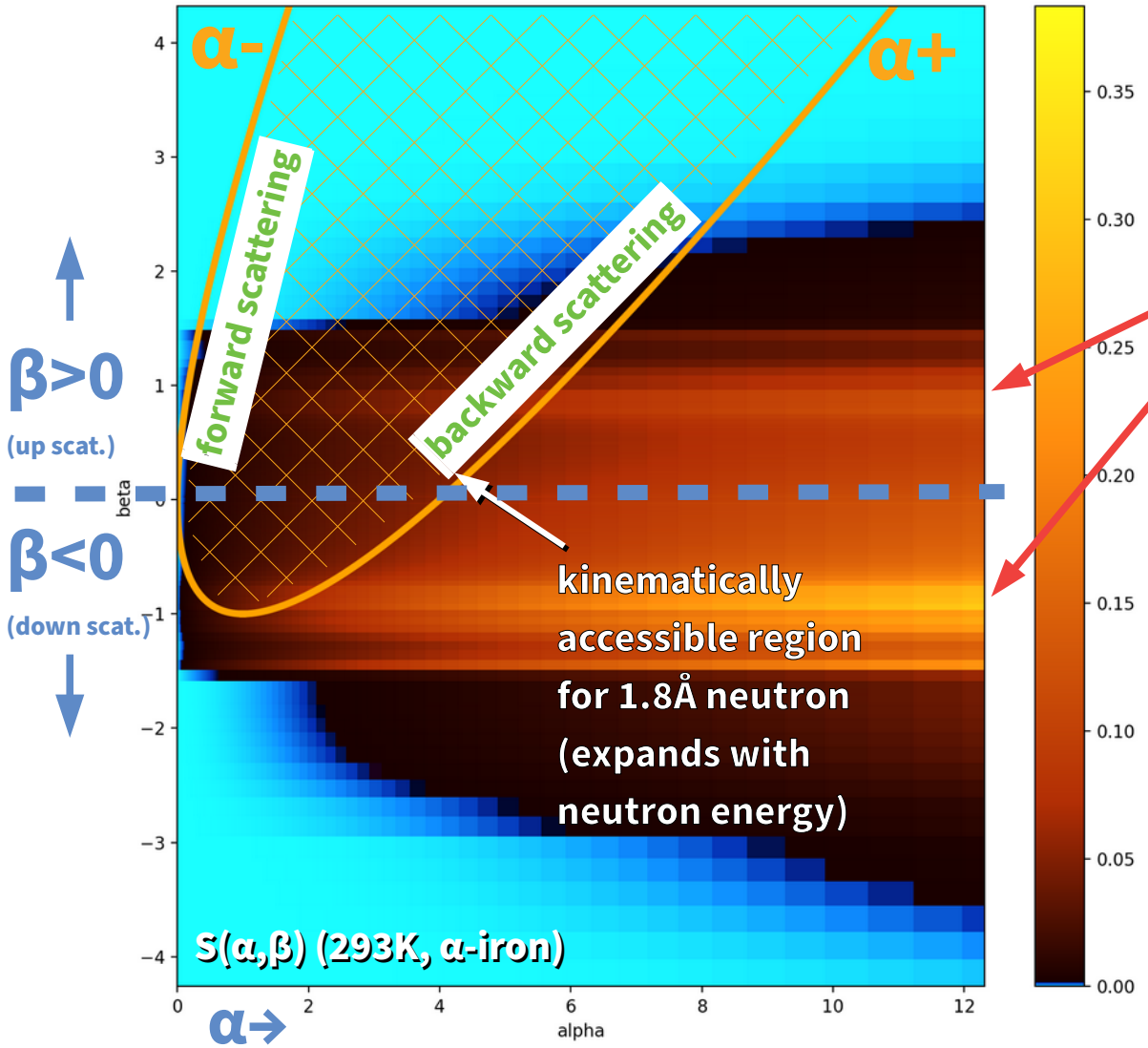
$$\alpha_\pm(E,\beta) = \frac{2E}{kT} + \beta \pm 2\sqrt{\frac{E}{kT}\left(\frac{E}{kT} + \beta\right)}$$

kinematically accessible region is a parabola in the (α,β)-plane

Scattering kernel and connection to neutron

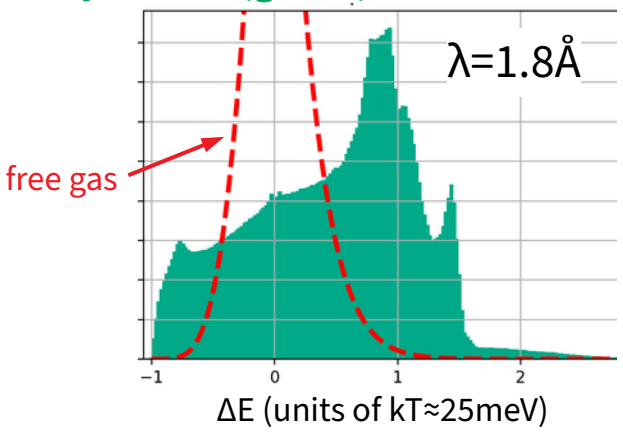
S(q,ω) ~ S(α,β); α: dimensionless q², β: dimensionless ω (~ΔE)

NCrystal
Thermal Neutron Transport



"Detailed balance":
Boltzmann factor + identical strength of phonon absorption & emission → Symmetry around β=0, given by $S(\alpha,-\beta)=\exp(\beta)\cdot S(\alpha,\beta)$

β-projection of kinematically accessible region → energy transfer spectrum (green):



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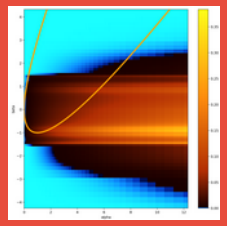
NCrystal has unique features for *using* scattering kernels



NCrystal
Thermal Neutron Transport

- Given S(α,β) values on a grid (α_i,β_i) and a neutron with energy, E, we must define suitable interpolation scheme to provide S(α,β) for any (α,β) value, and be able to:

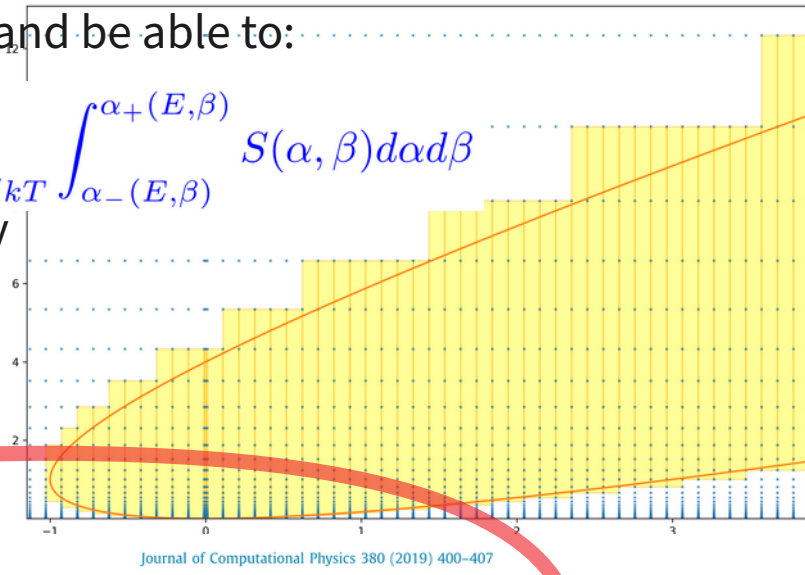
  1) Estimate scattering cross section: $\sigma(E) = \frac{\sigma_b kT}{4E} \int_{-E/kT}^{\infty} \int_{\alpha_-(E,\beta)}^{\alpha_+(E,\beta)} S(\alpha,\beta) d\alpha d\beta$

  2) Sample (α,β) values randomly within the kinematically accessible region, with density proportional to S(α,β).

- This must be done accurately and with reasonable computing resources! **Tricky part is sampling.**

- NCrystal has novel method for accurate+fast sampling, without ACE-like discretisation, with attention to near-endpoint sampling (crucial for ultra-cold neutron moderator studies).

- **We have ideas to further improve this** (make it faster, remove unwanted artifacts).



Journal of Computational Physics 380 (2019) 400–407

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

ELSEVIER

Rejection-based sampling of inelastic neutron scattering

X.-X. Cai [a,b,*], T. Kittelmann [b], E. Klinkby [a,b], J.I. Márquez Damián [c]

[a] Technical University of Denmark, Denmark
[b] European Spallation Source ERIC, Sweden
[c] Nuclear Data Group, Neutron Physics Department, Centro Atómico Bariloche, CNEA, Argentina

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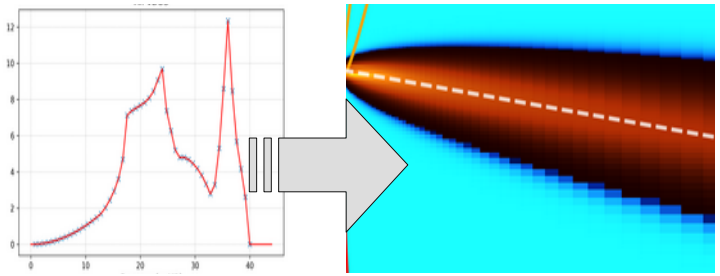
NCrystal
Thermal Neutron Transport

VDOS → Scattering kernel

(the Sjölander method)



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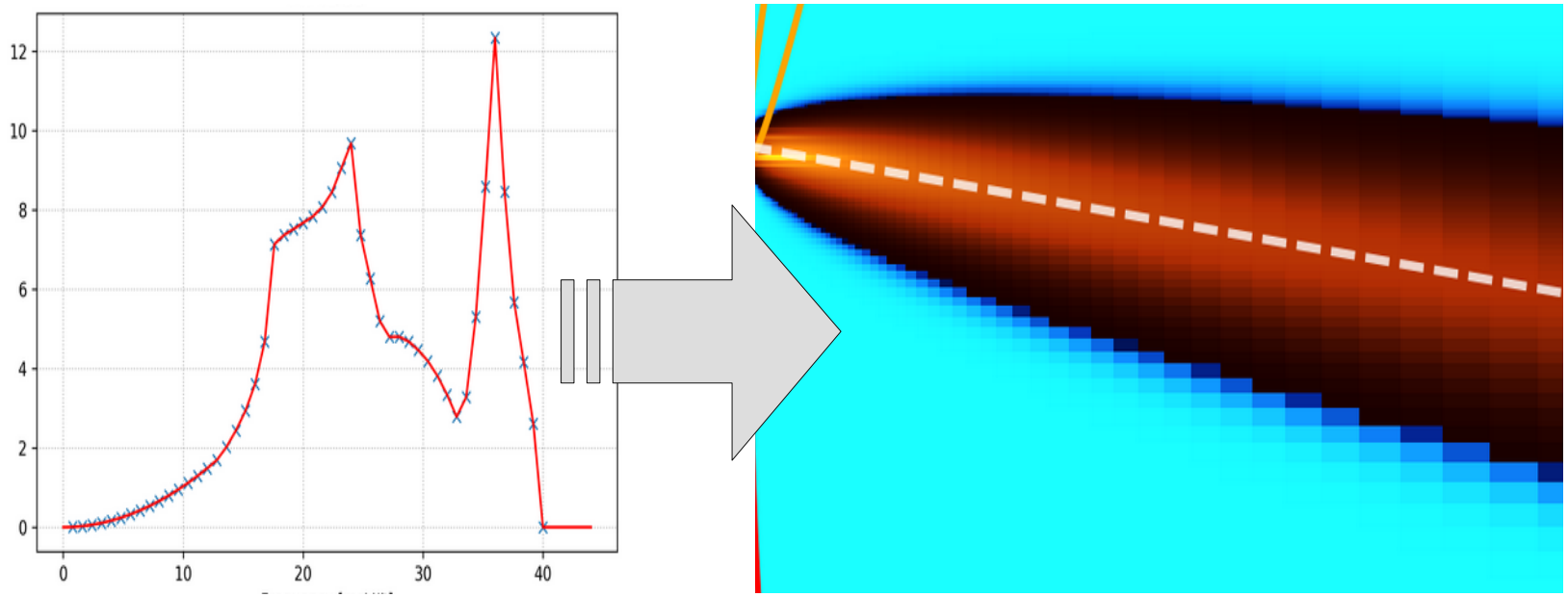
Connecting scattering kernels to phonons

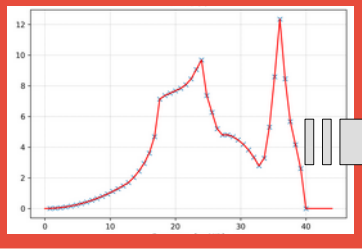
Unlike scat. kernels, phonon spectra widely available

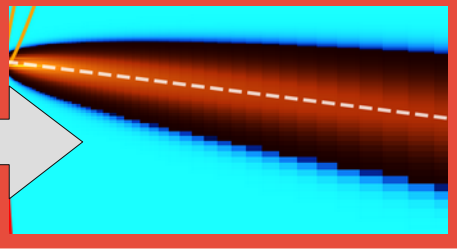
NCrystal
Thermal Neutron Transport



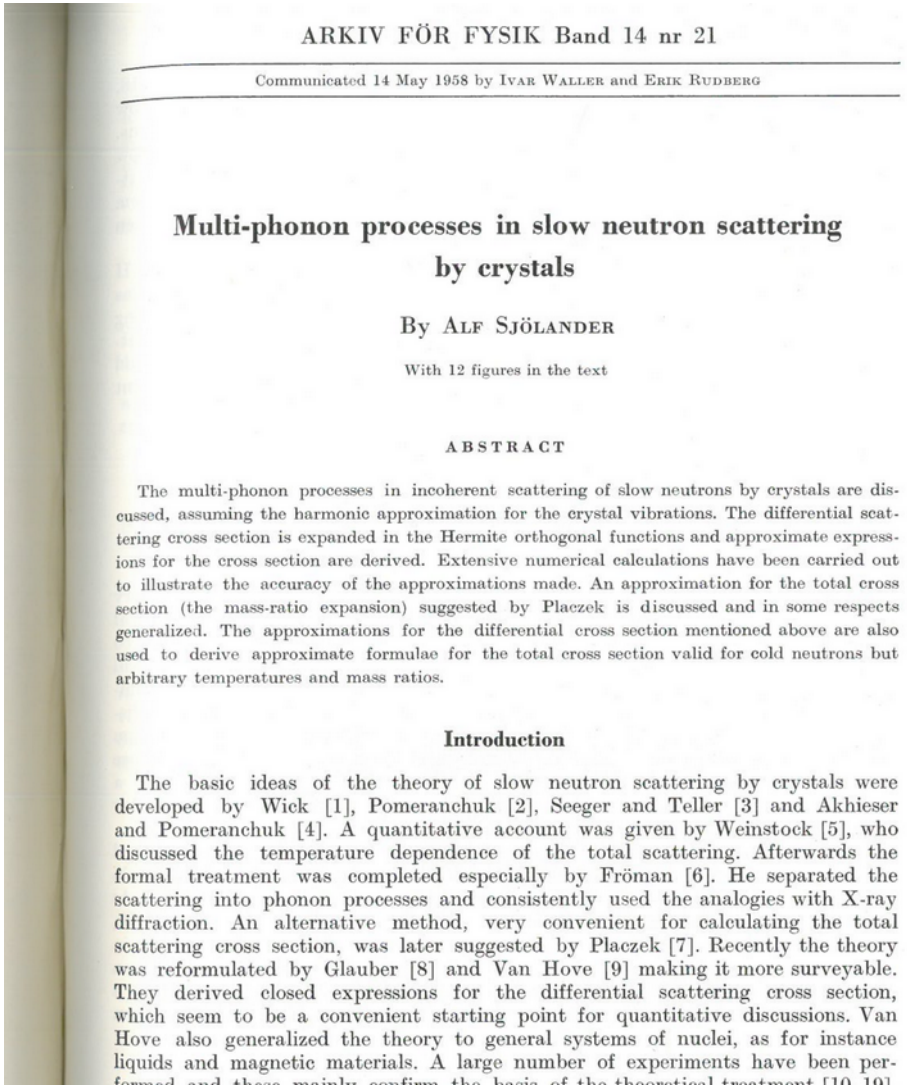
Captures material structure info relevant for inelastic neutron scatterings (isotropic materials, incoherent approximation)

VDOS → S(α,β)





NCrystal
Thermal Neutron Transport



ARKIV FÖR FYSIK Band 14 nr 21

Communicated 14 May 1958 by IVAR WALLER and ERIK RUDBERG

Multi-phonon processes in slow neutron scattering by crystals

By ALF SJÖLANDER

With 12 figures in the text

ABSTRACT

The multi-phonon processes in incoherent scattering of slow neutrons by crystals are discussed, assuming the harmonic approximation for the crystal vibrations. The differential scattering cross section is expanded in the Hermite orthogonal functions and approximate expressions for the cross section are derived. Extensive numerical calculations have been carried out to illustrate the accuracy of the approximations made. An approximation for the total cross section (the mass-ratio expansion) suggested by Placzek is discussed and in some respects generalized. The approximations for the differential cross section mentioned above are also used to derive approximate formulae for the total cross section valid for cold neutrons but arbitrary temperatures and mass ratios.

Introduction

The basic ideas of the theory of slow neutron scattering by crystals were developed by Wick [1], Pomeranchuk [2], Seeger and Teller [3] and Akhieser and Pomeranchuk [4]. A quantitative account was given by Weinstock [5], who discussed the temperature dependence of the total scattering. Afterwards the formal treatment was completed especially by Fröman [6]. He separated the scattering into phonon processes and consistently used the analogies with X-ray diffraction. An alternative method, very convenient for calculating the total scattering cross section, was later suggested by Placzek [7]. Recently the theory was reformulated by Glauber [8] and Van Hove [9] making it more surveyable. They derived closed expressions for the differential scattering cross section, which seem to be a convenient starting point for quantitative discussions. Van Hove also generalized the theory to general systems of nuclei, as for instance liquids and magnetic materials. A large number of experiments have been per-

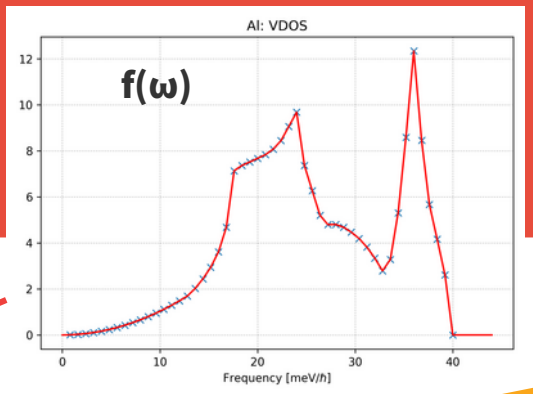
Well-established method!
Used in NJOY/LEAPR. Most ENDF S(α,β) kernels were created this way.

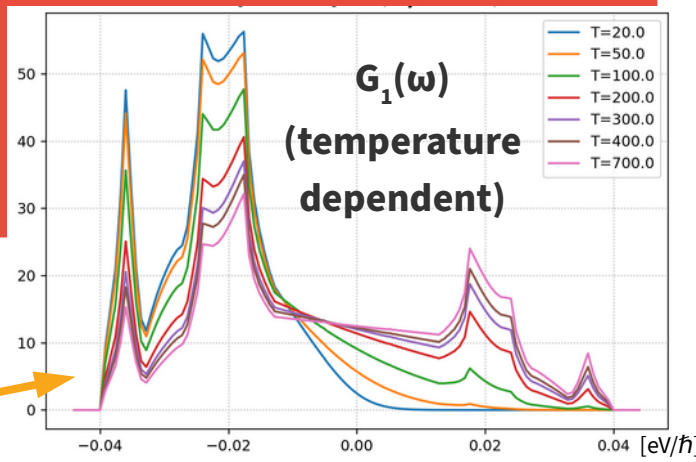
Idea: Build this capability into NCrystal and make it fast (<1s) so can invoke on-the-fly.

Gives us:

- **Flexibility.** Work directly from VDOS input, avoid usage of non-trivial third-party SW.
- **More materials.** VDOS are much more easily obtained than full kernels.
- **Small data files!**
  Can easily include everywhere.
- **Temperature dependency built in:**
  Static S(α,β) is only valid for specific T.

VDOS→S(α,β) Sjölander's recipe



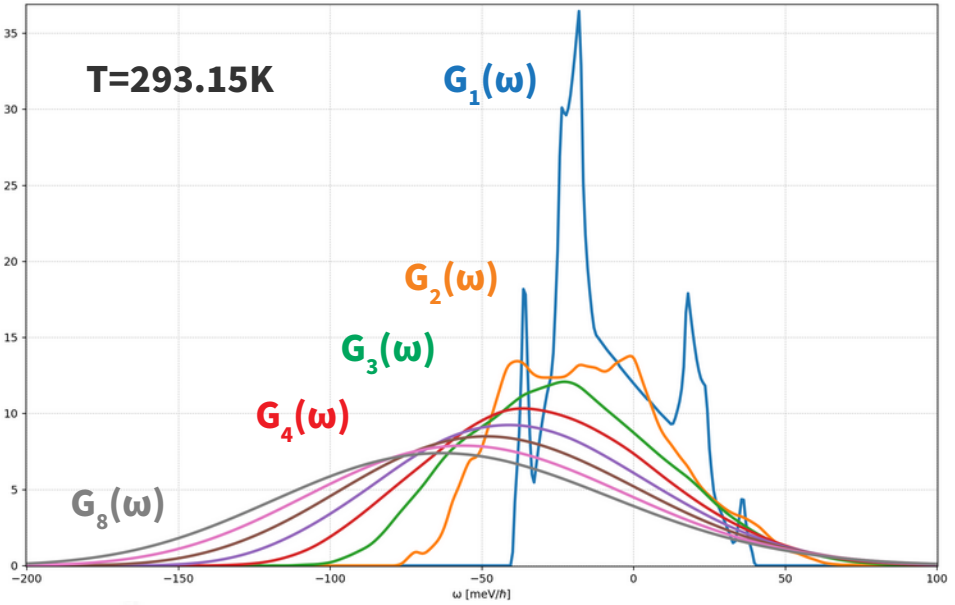


$$G_1(\omega) = g(\omega) = \frac{f(\omega)}{\omega\,\gamma(0)}\,\frac{\coth\left(\frac{\hbar\omega}{2kT}\right)-1}{2},$$

$$G_2(\omega) = \int_{-\infty}^{\infty} g(\omega-\omega')\,G_1(\omega')\,d\omega',$$

. . . . . .

$$G_{n+1}(\omega) = \int_{-\infty}^{\infty} g(\omega-\omega')\,G_n(\omega')\,d\omega'.$$



σ_b

2W=δ²q², δ=atomic displacement

$$\frac{d^2\sigma_{\text{incoh}}^{\text{inel}}}{d\Omega\,d\omega} = A\,\frac{k}{k_0}\,e^{-2W}\sum_{n=1}^{\infty}\frac{(2W)^n}{n!}\,G_n(\omega-\omega_0).$$

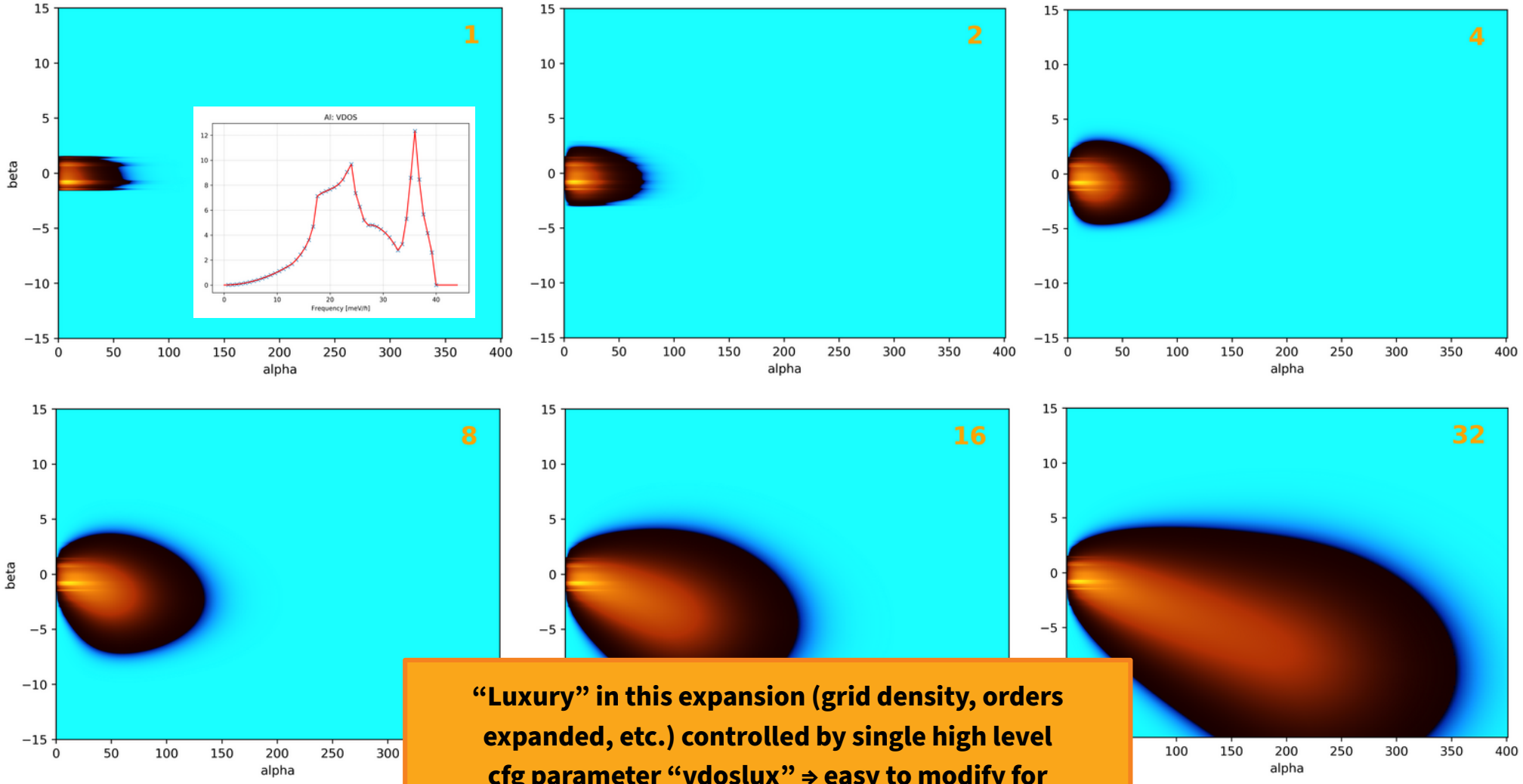
$$= \sqrt{\frac{E_f}{E}}\,\frac{\sigma_b}{4\pi}\,\frac{S(\alpha,\beta)}{k_bT}$$

$-\hbar(\omega-\omega_0)/kT=\Delta E/kT=\beta$

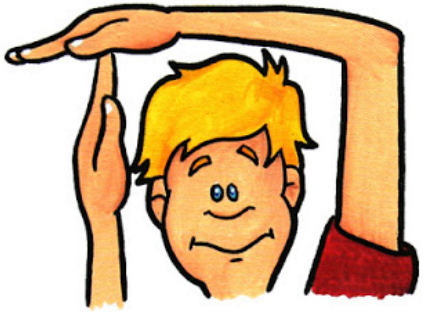
VDOS→S(α,β): → Aluminium

http://cern.ch/tkittel/vdosanim

NCrystal
Thermal Neutron Transport



"Luxury" in this expansion (grid density, orders expanded, etc.) controlled by single high level cfg parameter "vdoslux" ⇒ easy to modify for any user (see backup slide for details). Default value is of course sensible.



Notebook time: “Advanced4”.

Study the Sjolander expansion in practice.

Consider this optional, if time allows.

Alternatively, at least watch the movies at

http://cern.ch/tkittel/vdosanim

Jupyter tutorials for improved v3.6 API at:
https://github.com/mctools/ncrystal-notebooks/

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(of these slides)

Backup slides

Control DOS→scat. kernel expansion through cfg parameter "vdoslux"

NCrystal
Thermal Neutron Transport

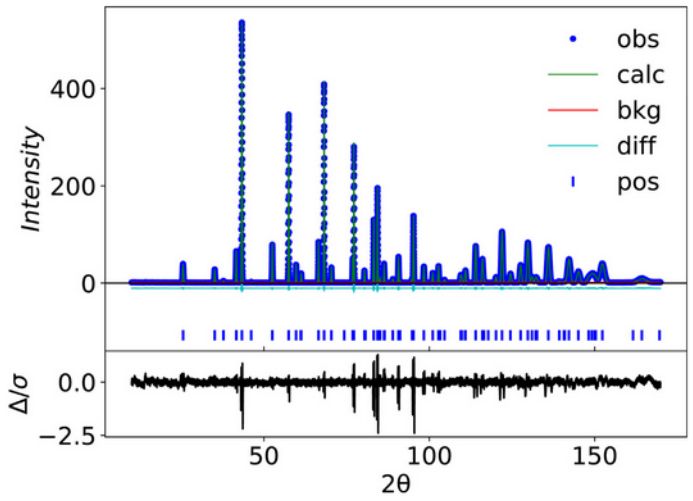
- Controls all aspects of DOS→kernel expansion with only one high level user-accessible parameter.
  - Exposing the underlying multitude of parameters to end-users would do no good in practice since no-one would understand how to change them in a self-consistent way.

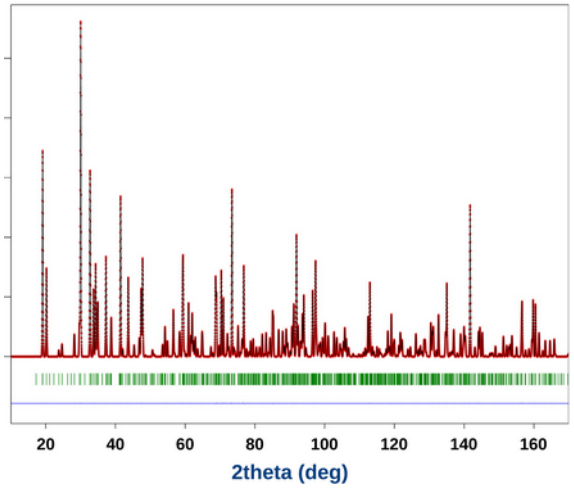
- **vdoslux=0**: Extremely crude, 100x50 grid, Emax=0.5eV (costs 0.1MB mem, 0.02s init time) ← The default if using Debye model instead of actual input data (vdoslux gets reduced by 3 for these mats.)
- **vdoslux=1**: Crude, 200x100 grid, Emax=1eV (costs 0.5MB mem, 0.04s init time)
- **vdoslux=2**: Decent, 400x200 grid, Emax=3eV (costs 2MB mem, 0.08s init time) ← ~level of premade ENDF kernels
- **vdoslux=3** : Good, 800x400 grid, Emax=5eV (costs 8MB mem, 0.2s init time) ← The default!
- **vdoslux=4**: Very good, 1600x800 grid, Emax=8eV (costs 30MB mem, 0.8s init time)
- **vdoslux=5**: Extremely good, 3200x1600 grid, Emax=12eV (costs 125MB mem, 5s init time) ← Overkill, exists for validation purpose

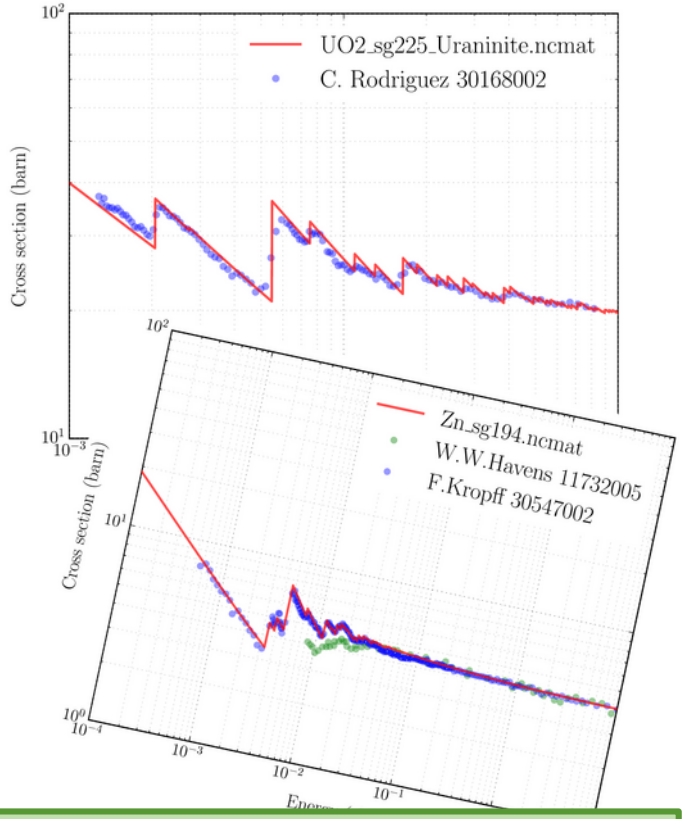
Users adviced to leave at default (3), or change with ±1 to 2 or 4.

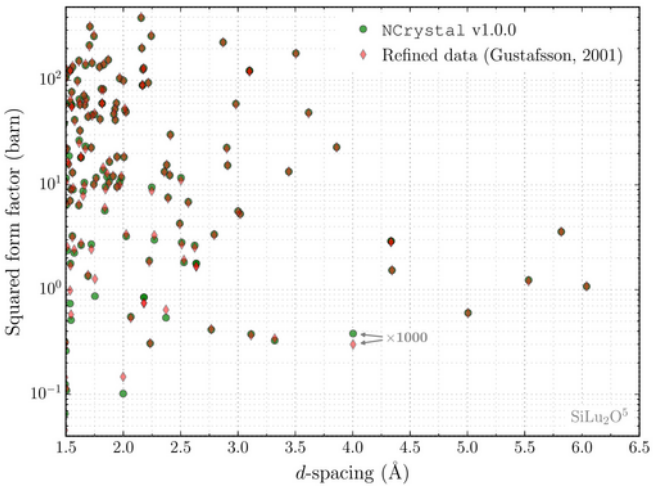
HKL structure factors initialised on-the-fly (validated thoroughly)

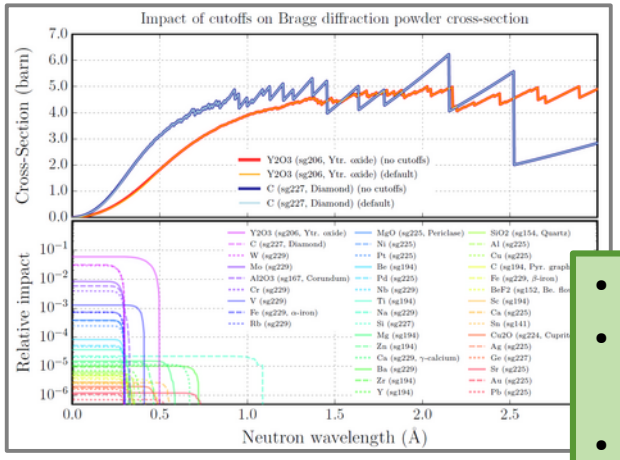
NCrystal
Thermal Neutron Transport











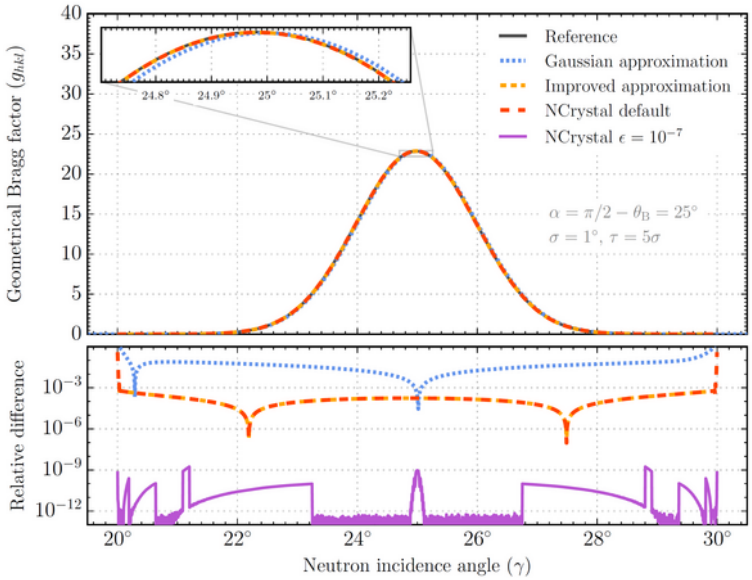
- Fast (few ms) init. of **all** relevant planes.
- Comparisons to measured structure factors and total cross sections.
- NCrystal+McStas simulated scattering patterns analysed with GSAS-II/Fullprof (recovering input crystal parameters).
- Comparison with NXS library predictions.

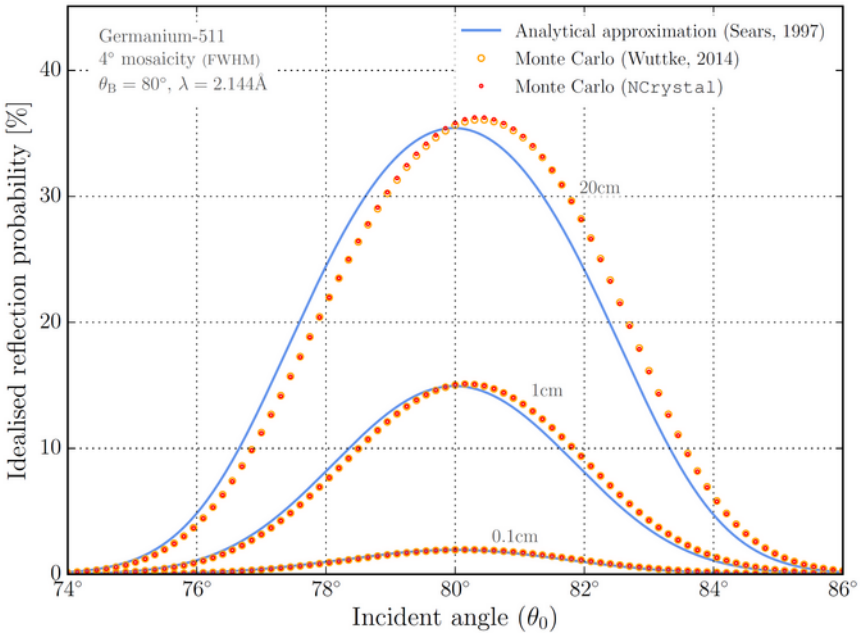
Single crystal model validated

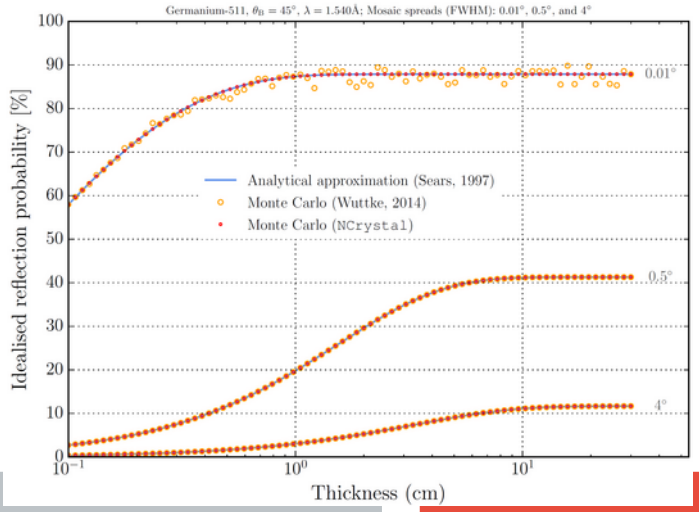
NCrystal
Thermal Neutron Transport

Validation includes:

- Against existing codes (Wuttke2014) or analytical results (Sears1997) in their domains of validity.
- Against (very) slow but simple+precise implementation (using mpmath high-precision math module)
- Technical validations (zig-zag, “powdered”)



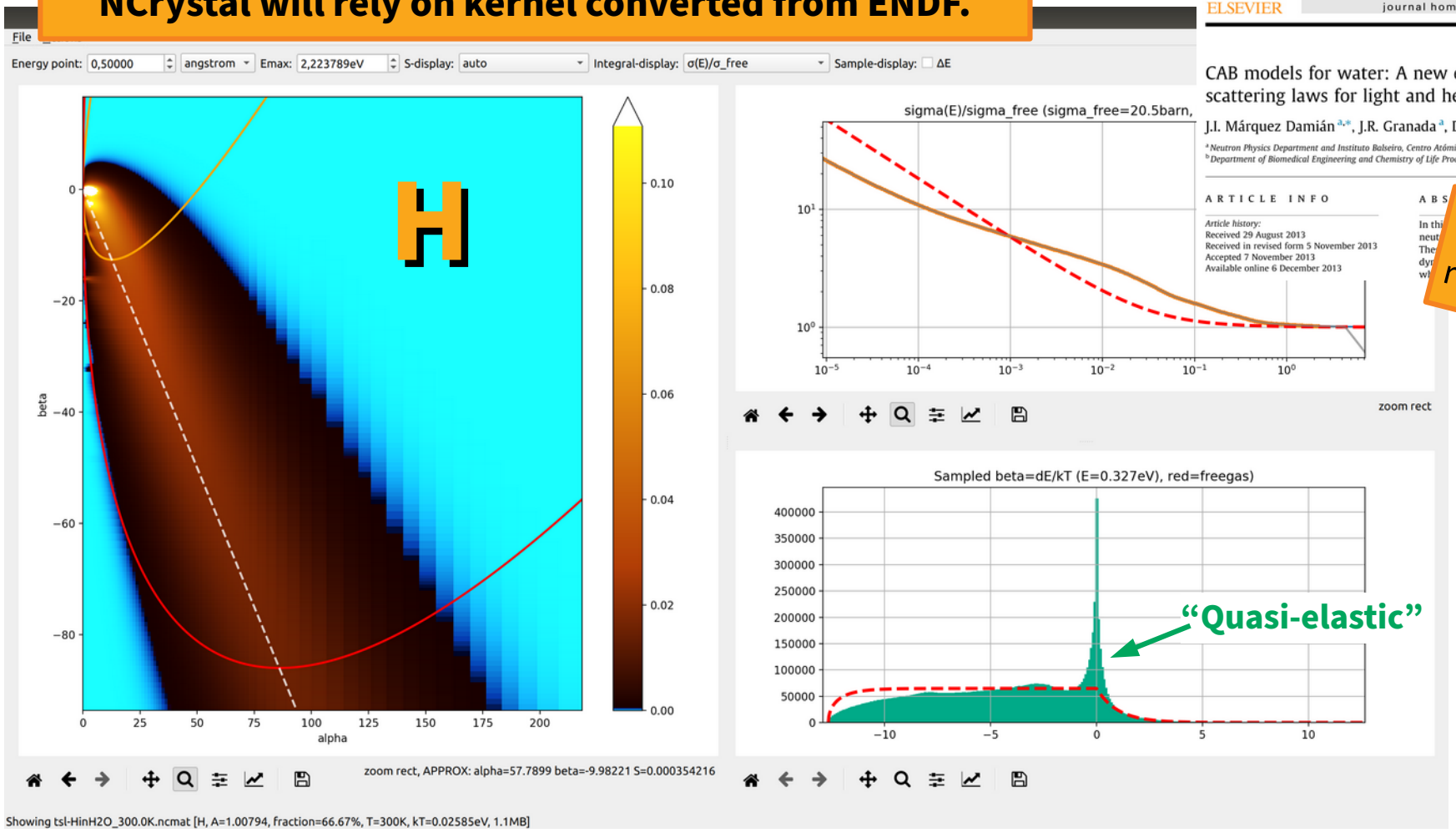


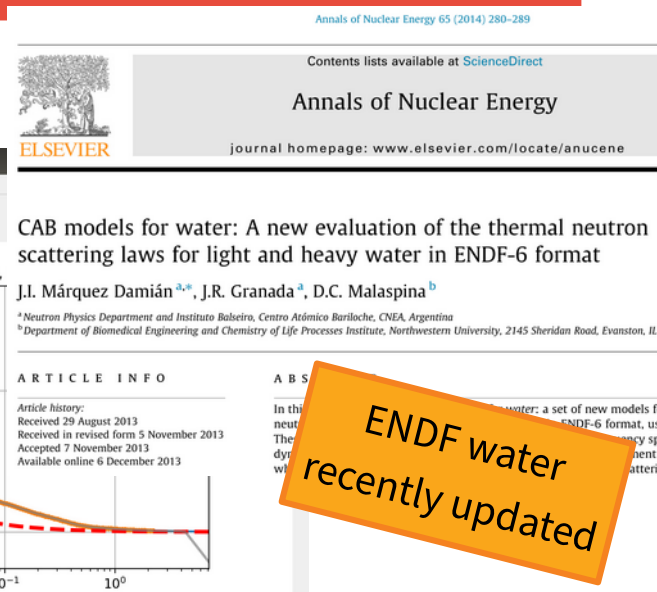


Support for liquids rely on externally provided kernels, here water (converted from ENDF8)

NCrystal
Thermal Neutron Transport

VDOS→S(α,β) does not work directly for liquids!
NCrystal will rely on kernel converted from ENDF.




Annals of Nuclear Energy 65 (2014) 280–289

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Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

ELSEVIER

CAB models for water: A new evaluation of the thermal neutron scattering laws for light and heavy water in ENDF-6 format

J.I. Márquez Damián [a,*], J.R. Granada [a], D.C. Malaspina [b]

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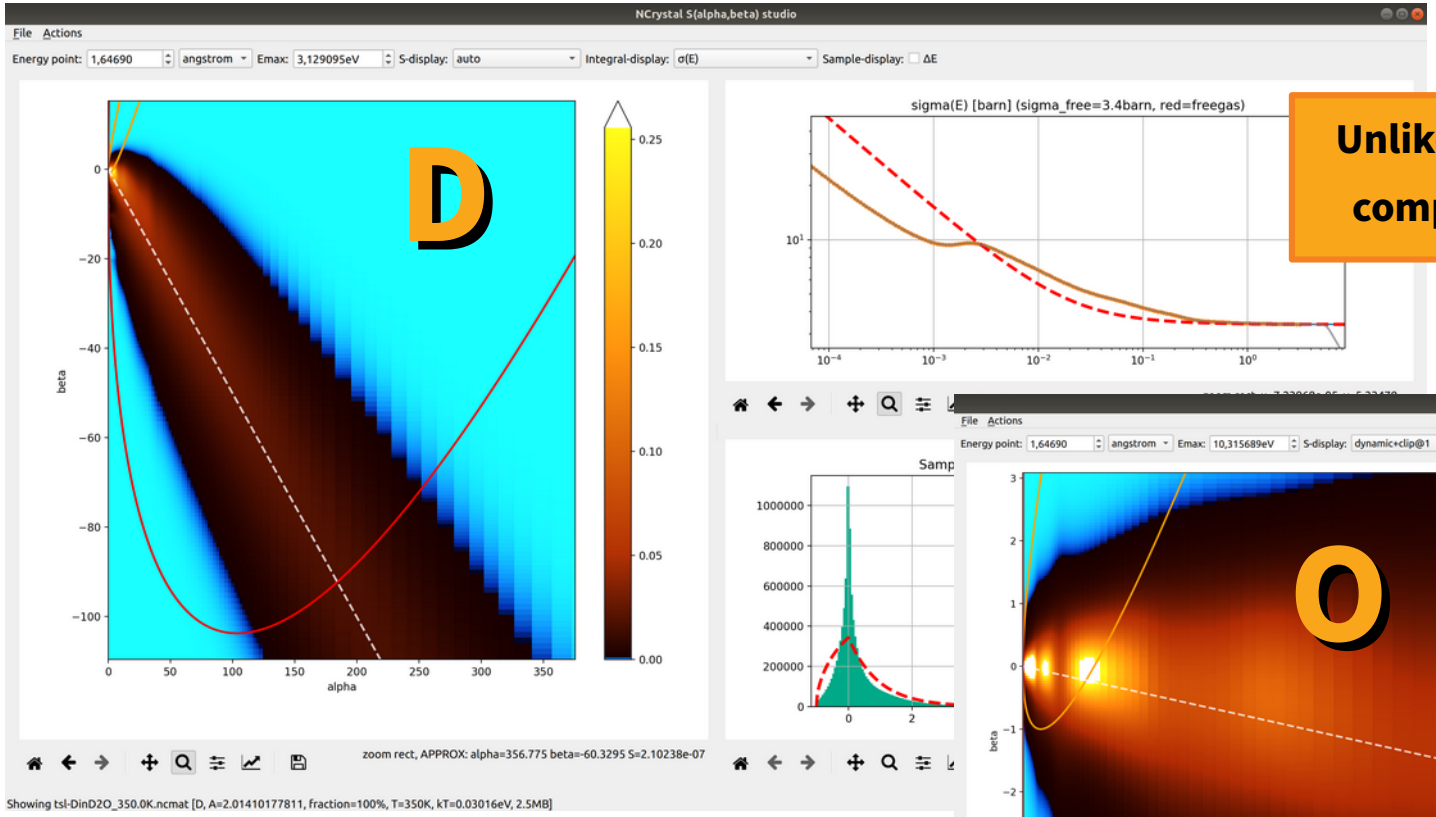
ENDF water recently updated

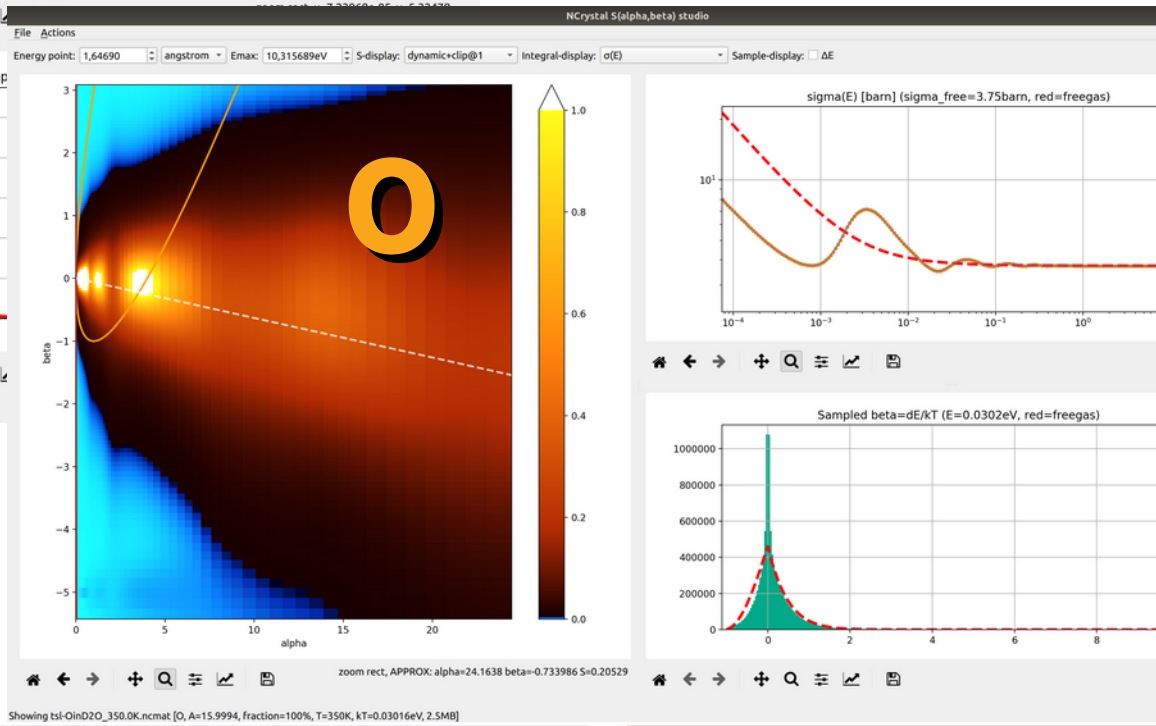
Oxygen is modelled as free gas

… and heavy water
(also converted from ENDF8)

NCrystal
Thermal Neutron Transport



Unlike liquid H_2O (where H dominates completely), D_2O needs two kernels



NCrystal supports non-natural elements since v2.1.0 (isotope D=H2 since v2.0.0)