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A liquids plugin for NCrystal

ICANS XXV

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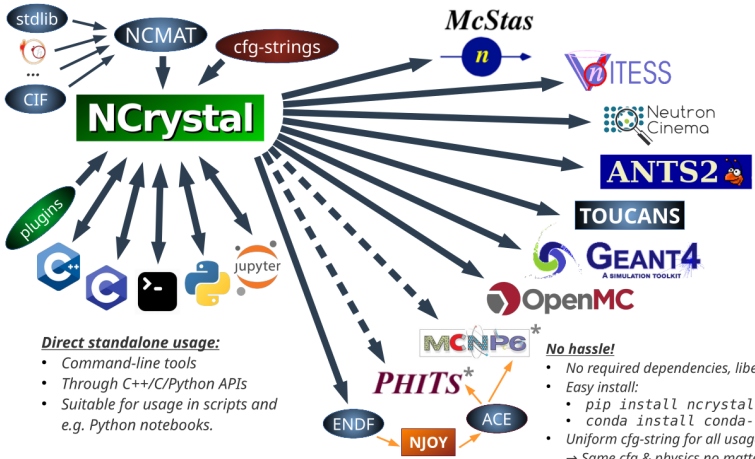
13-04-2026

Overview

- Brief NCrystal overview.
- Development of a liquids plugin for NCrystal.
- Some examples: water/heavy water, and liquid hydrogen and deuterium.

NCrystal



Direct standalone usage:

- *Command-line tools*
- *Through C++/C/Python APIs*
- *Suitable for usage in scripts and e.g. Python notebooks.*

No hassle!

- *No required dependencies, liberal license (Apache 2)*
- *Easy install:*
  - `pip install ncrystal`
  - `conda install conda-forge::ncrystal`
- *Uniform cfg-string for all usage*
  → Same cfg & physics no matter usage context
- *Multi-thread safe, support Linux/macOS/BSD/Windows*

***: Can not share bindings for projects that are not open-source**

Developed by Xiao Xiao Cai and Thomas Kittelmann at ESS.

NCrystal Materials

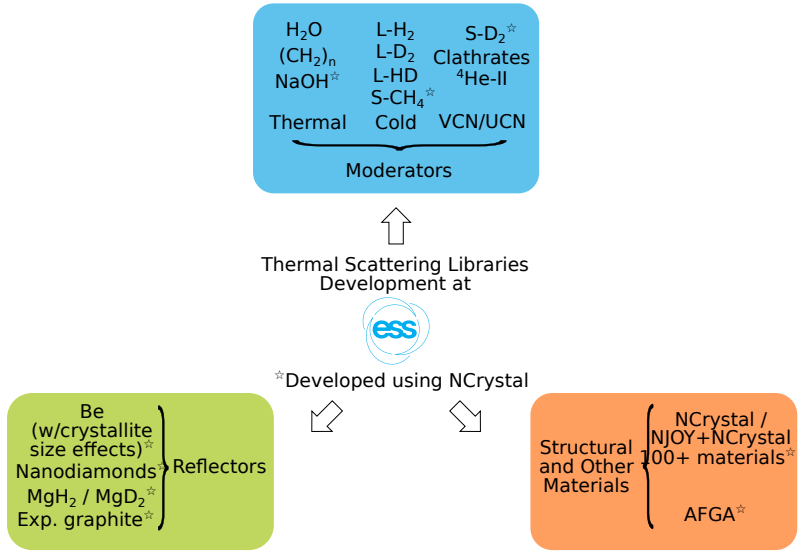
AcrylicGlass_C5O2H8.ncmat
AgBr_sg225_SilverBromide.ncmat
Ag_sg225.ncmat
Al2O3_sg167_Corundum.ncmat
Al4C3_sg166_AluminiumCarbide.ncmat
AlN_sg186_AluminiumNitride.ncmat
Al_sg225.ncmat
Ar_Gas_STP.ncmat
Au_sg225.ncmat
BaF2_sg225_BariumFluoride.ncmat
BaO_sg225_BariumOxide.ncmat
Ba_sg229.ncmat
Be3N2_sg206_BerylliumNitride.ncmat
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_C18H2003.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
LiN_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
Mg(OH)2_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_BetaQuartz.ncmat
Si_sg227.ncmat
Sn_sg141.ncmat
SrF2_sg225_StrontiumFluoride.ncmat
SrH2_sg62_StrontiumHydride.ncmat
Sr_sg225.ncmat
Th3N4_sg166_ThoriumNitride.ncmat
ThO2_sg225_ThoriumDioxide.ncmat
Th_sg225.ncmat
TiO2_sg136_Rutile.ncmat
TiO2_sg141_Anatase.ncmat
Ti_sg194.ncmat
TlBr_sg221_ThaliumBromide.ncmat
Tm2O3_sg206_ThuliumOxide.ncmat
UF6_sg62_UraniumHexaflouride.ncmat
UO2_sg225_UraniumDioxide.ncmat
void.ncmat
V_sg229.ncmat
W_sg229.ncmat
Xe_Gas_STP.ncmat
Y2O3_sg206_Yttrium_Oxide.ncmat
Y2SiO5_sg15_YSO.ncmat
Y3Al5O12_sg230_YAG.ncmat
Y_sg194.ncmat
ZnF2_sg136_ZincFlouride.ncmat
ZnO_sg186_ZincOxide.ncmat
Zn_sg194.ncmat
ZnS_sg216_Sphalerite.ncmat
ZrF4-beta_sg84.ncmat
ZrO2_sg137_Zirconia.ncmat
ZrO2_sg14_Zirconia.ncmat
Zr_sg194.ncmat

134 materials (v4.3.0):
Crystals (110), amorphous solids (16), liquids, gasses, ...

Small (few kB) file sizes:
- Entire collection normally embedded in NCrystal shared library.

Easy universal cfg:
"Al_sg225.ncmat;temp=250K"
"Rubber_C5H8.ncmat;comp=inelas"
- Same physics in all applications!

NCrystal supports many materials out of the box. Easy to create more.


H_2O
$(CH_2)_n$
NaOH☆
L-H_2
L-D_2
L-HD
S-CH_4☆
S-D_2☆
Clathrates
^{4}He-II
Thermal
Cold
VCN/UCN
Moderators
Thermal Scattering Libraries Development at
ess
☆Developed using NCrystal
Be (w/crystallite size effects)☆
Nanodiamonds☆
MgH_2 / MgD_2☆
Exp. graphite☆
Reflectors
Structural and Other Materials
NCrystal / NJOY+NCrystal
100+ materials☆
AFGA☆

NCrystal

[1]:
```
import numpy as np
import NCrystal as NC
import NCrystal.cifutils as nccif
```

Step 1: Create base `ncmat` model from `cif` information.

[2]:
```
cifsrc = nccif.CIFSource('ni.cif')
c_ni = NC.NCMATComposer.from_cif(cifsrc)
```

```
Loading data from file ni.cif
Attempting to load CIF data with gemmi
Self-consistency of structure was verified by spglib
```

Step 2: Replace dynamic information with VDOS.

[3]:
```
vdos_data = np.loadtxt('ni.dat')
c_ni.set_dyninfo_vdos(c_ni.find_label('Ni'), vdos_egrid=vdos_data[:,0], vdos=vdos_data[:,1])
```

Step 3: Export `ncmat` file and convert to `ENDF-6` format.

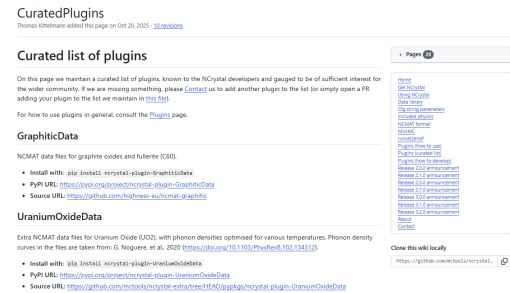
[4]:
```
a = c_ni.write('ni.ncmat')
!../ncrystal_ncmat2endf.py --name Ni ni.ncmat
```

```
Get nuclear data...
Prepare ENDF file tsl_Ni.endf...
Renumber lines...
Write ENDF file tsl_Ni.endf...
Files created:
  tsl_Ni.endf
```

NCrystal supports many materials out of the box. Easy to create more.

Plugins

- NCrystal physics can also be extended through development of plugins.
- List at of curated plugins at https://github.com/mctools/ncrystal/
- Magnetic scattering, texture, extinction, small-angle scattering to name a few.



CuratedPlugins

Thomas Kittelmann edited this page on Oct 20, 2025 · 10 revisions

Curated list of plugins

On this page we maintain a curated list of plugins, known to the NCrystal developers and gauged to be of sufficient interest for the wider community. If we are missing something, please Contact us to add another plugin to the list (or simply open a PR adding your plugin to the list we maintain in this file).

For how to use plugins in general, consult the Plugins page.

GraphiticData

NCMAT data files for graphite oxides and fullerite (C60).

- **Install with:** `pip install ncrystal-plugin-GraphiticData`
- **PyPI URL:** https://pypi.org/project/ncrystal-plugin-GraphiticData
- **Source URL:** https://github.com/highness-eu/ncmat-graphitic

UraniumOxideData

Extra NCMAT data files for Uranium Oxide (UO2), with phonon densities optimised for various temperatures. Phonon density curves in the files are taken from: G. Noguere, et al., 2020 (https://doi.org/10.1103/PhysRevB.102.134312).

- **Install with:** `pip install ncrystal-plugin-UraniumOxideData`
- **PyPI URL:** https://pypi.org/project/ncrystal-plugin-UraniumOxideData
- **Source URL:** https://github.com/mctools/ncrystal-extra/tree/HEAD/pypkgs/ncrystal-plugin-UraniumOxideData

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https://github.com/mctools/ncrystal.

Development of a liquids plugin

- Currently NCrystal only supports liquids through pre-computed scattering law tables.
- To model liquids of interest to neutron sources, several new physics need to be included.
- Diffusive motion: Model of Egelstaff-Schofield.
- Coherent scattering: Vineyard and Sköld approximations.
- Quantum treatment of the rotations: Young-Koppel model.

Liquid: Incoherent scatterer

- To model incoherent scattering in a liquid, the convolution approach is used.

$$S(Q,\omega) = S_{\text{solid}}(Q,\omega) \otimes S_{\text{diff}}(Q,\omega)$$

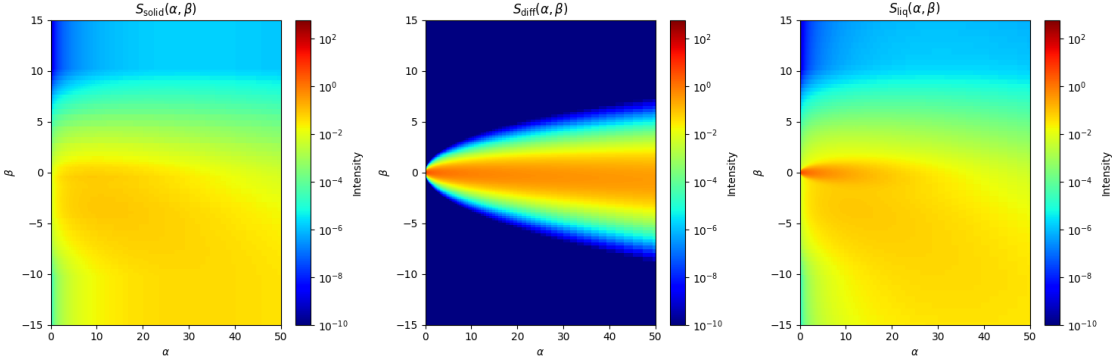
- Where $S_{\text{solid}}(Q,\omega)$ is the scattering law from NCrystal for a solid and $S_{\text{diff}}(Q,\omega)$ is the diffusive scatteirng law, given by the model of Egelstaff and Schofield.

$$S_{\text{diff}}(Q,\omega) = \frac{\hbar}{k_B T}\frac{DQ^2}{\pi} e^{\frac{MD^2Q^2}{w_t k_B T} - \frac{\hbar\omega}{2k_B T}} \times \frac{c^2 + 0.25}{\omega^2 + (DQ^2)^2} K_1\left[\frac{\hbar}{k_B T}\sqrt{c^2+0.25}\sqrt{\omega^2 + (DQ^2)^2}\right],$$

User provided parameters:

- $c = \frac{MD}{w_t \hbar}$ where D is the self-diffusion coefficient
- w_t is the effective diffusion weight in the system

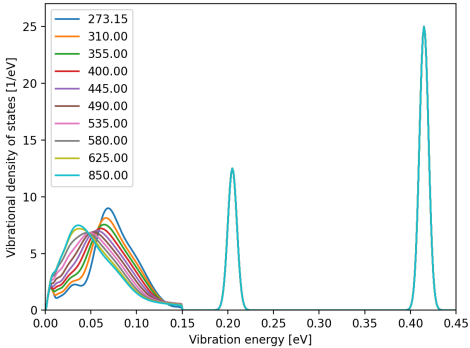
Liquid: Incoherent scatterer



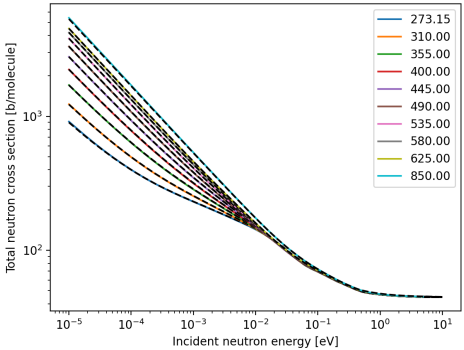
Liquid: Incoherent scatterer

Liquid water

Input data



Calculated cross-section compared to ENDF/B-VIII.1



The cross section for each temperature is computed in 1 second compared with 2.5 minutes when computed with NJOY.

Liquid: Coherent scatterer

For a liquid that scatterings coherently, we have adopted either the Vineyard or Sköld approximation. The total scattering law is given by:

$$S(Q,\omega) = c_{\mathrm{frac}} \cdot S_d(Q,\omega) + (1 - c_{\mathrm{frac}}) \cdot S_{\mathrm{self}}(Q,\omega)$$

Vineyard:

$$S_d(Q,\omega) = S(Q) \cdot S_{\mathrm{self}}(Q,\omega)$$

Sköld:

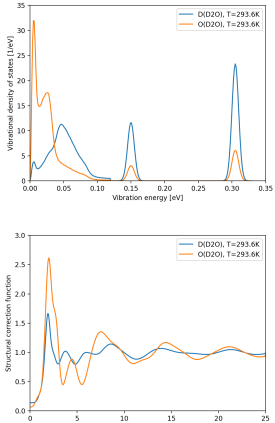
$$S_d(Q,\omega) = S(Q) \cdot S_{\mathrm{self}}\left(\frac{Q}{\sqrt{S(Q)}},\omega\right)$$

where $S(Q)$ is the structure factor and c_{frac} is the coherent fraction. $S_{\mathrm{self}}(Q,\omega)$ is the result of the solid part convolved with the diffusion part.

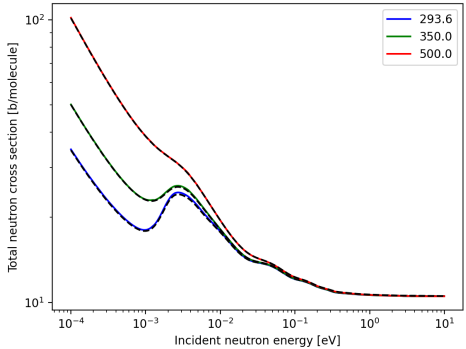
Liquid: Coherent scatterer

Heavy Water

Input data



Calculated cross-section compared to ENDF/B-VIII.1



Liquid Hydrogen and Deuterium

- To model liquid hydrogen deuterium, the Young-Koppel model for quatum rotations is used in addition to the Sköld approximation.

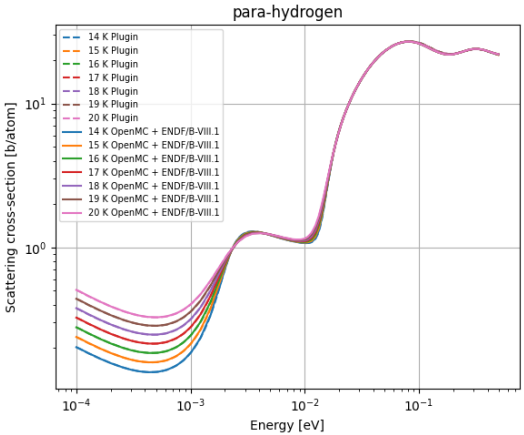
$$S(Q,\omega) = u(Q)\, S_d(Q,\omega) + \frac{1}{b_c^2 + b_i^2} \sum_J P_J \sum_{J'=0}^{J_{\max}} G(J,J',Q)\, S_{\mathrm{Self}}(Q,\, \omega + \omega_{JJ'})$$

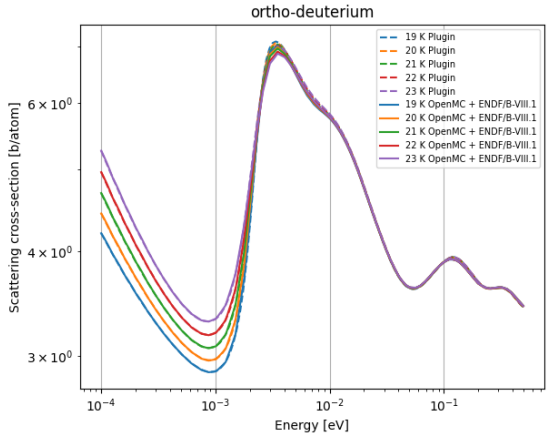
with

$$S_d(Q,\omega) = S(Q)\, S_{\mathrm{Self}}\left(\frac{Q}{\sqrt{S(Q)}}, \omega\right) - S_{\mathrm{Self}}(Q,\omega)$$

- $u(Q)$: coherent prefactor.
- P_J: statistical weight of rotational state J.
- $G(J, J', Q)$: rotational transition factor.
- $S(Q)$: structure factor.

Liquid Hydrogen and Deuterium





Concluding Remarks

- We have developed a liquids plugin for NCrystal.
- Tested on various moderator materials relevant for neutron source design, i.e. liquid hydrogen and deuterium and water/heavy water.
- Work on expanding materials, models and introducing improvements in the algorithms.
- This work was co-funded by the European Union under grant agreement 101164596 - APRENDE Project. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Atomic Energy Community (’EC-Euratom’).