NCrystal : a library for thermal neutron transport in crystals

Thomas KITTELMANN, Xiao Xiao CAI

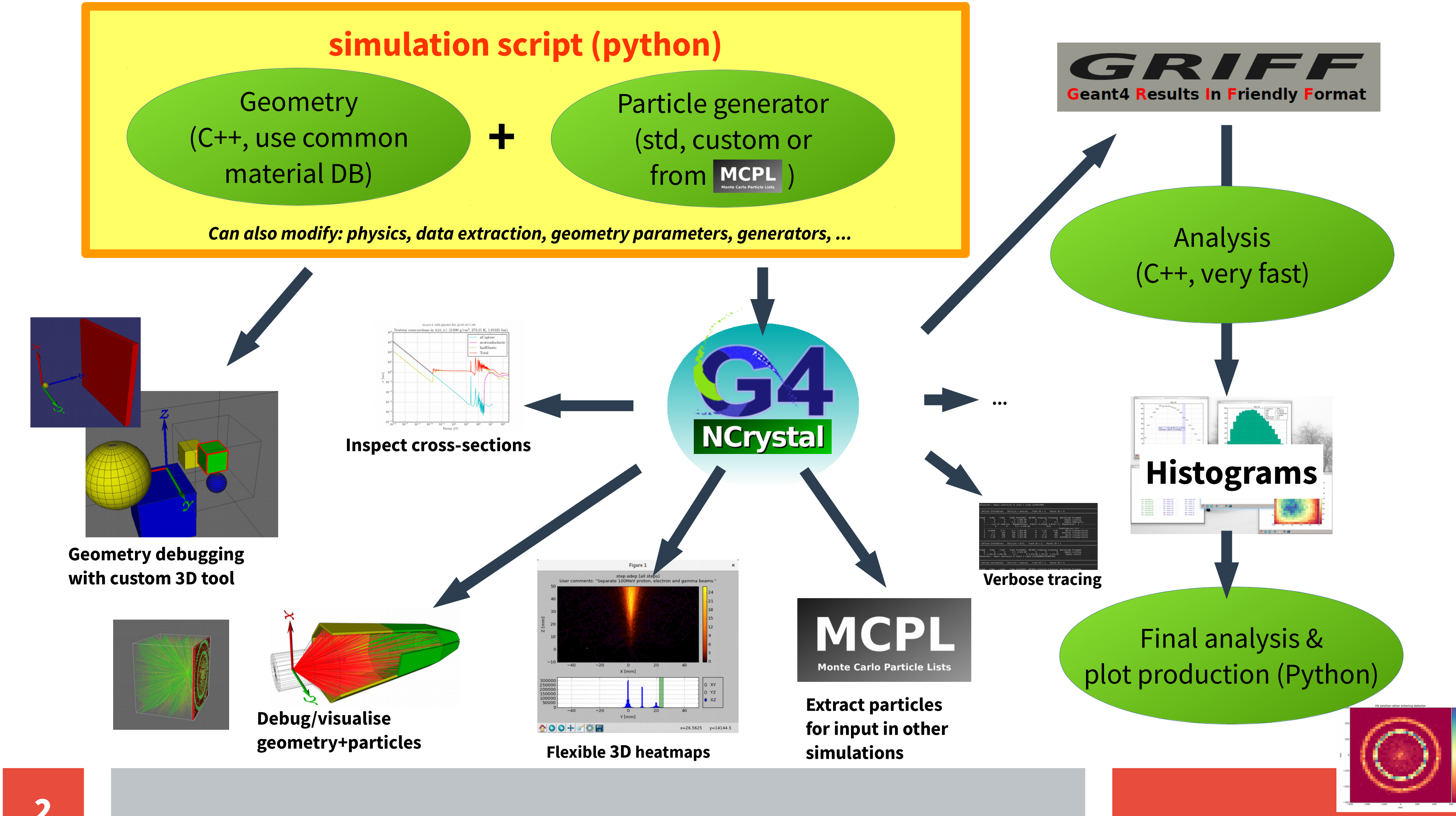
EUROPEAN SPALLATION SOURCE

DTU

brightness

Sep 11, 2018
IKON15, Lund

Since 2012ish, ESS-DG provides framework for detector modelling



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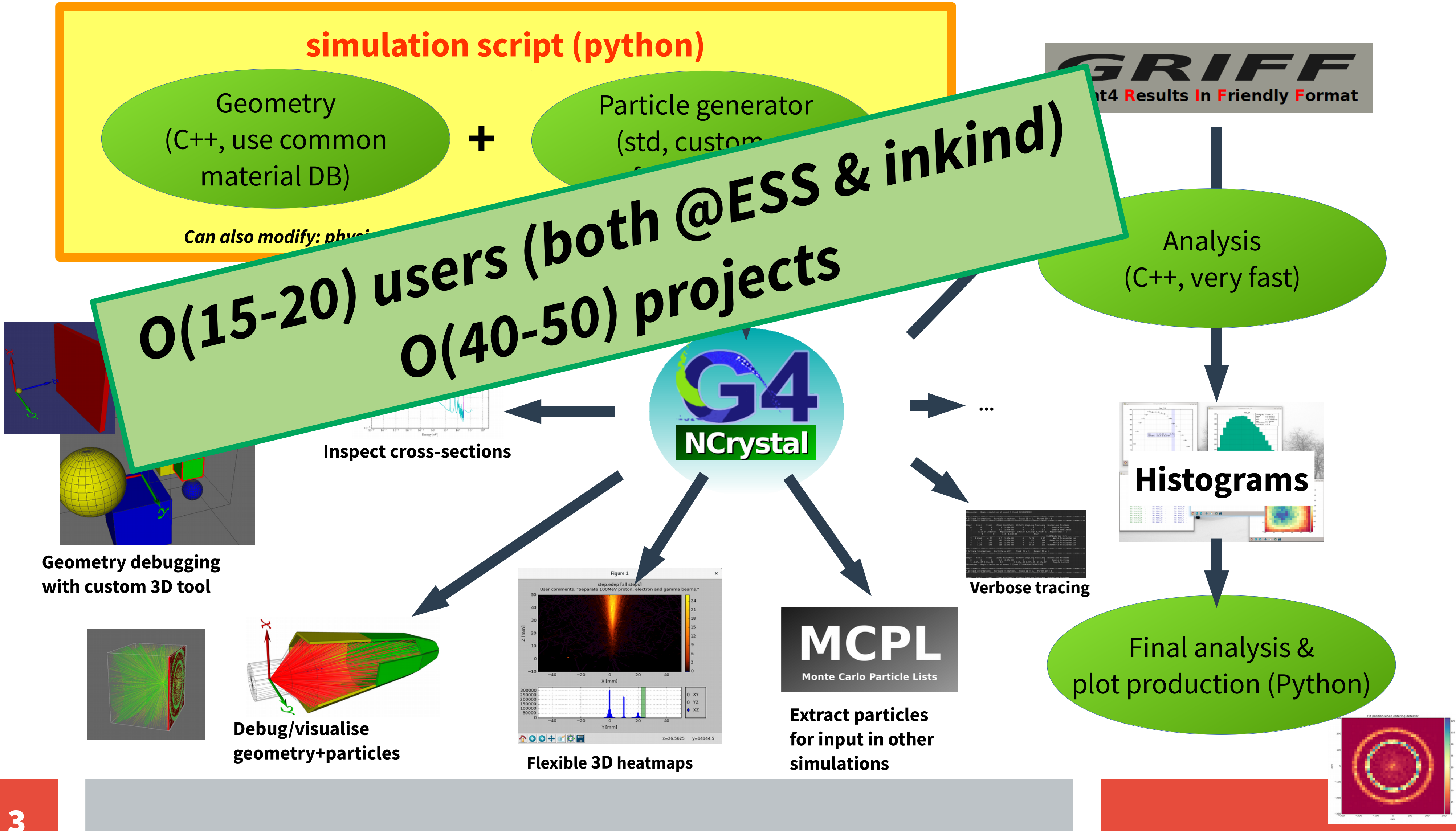

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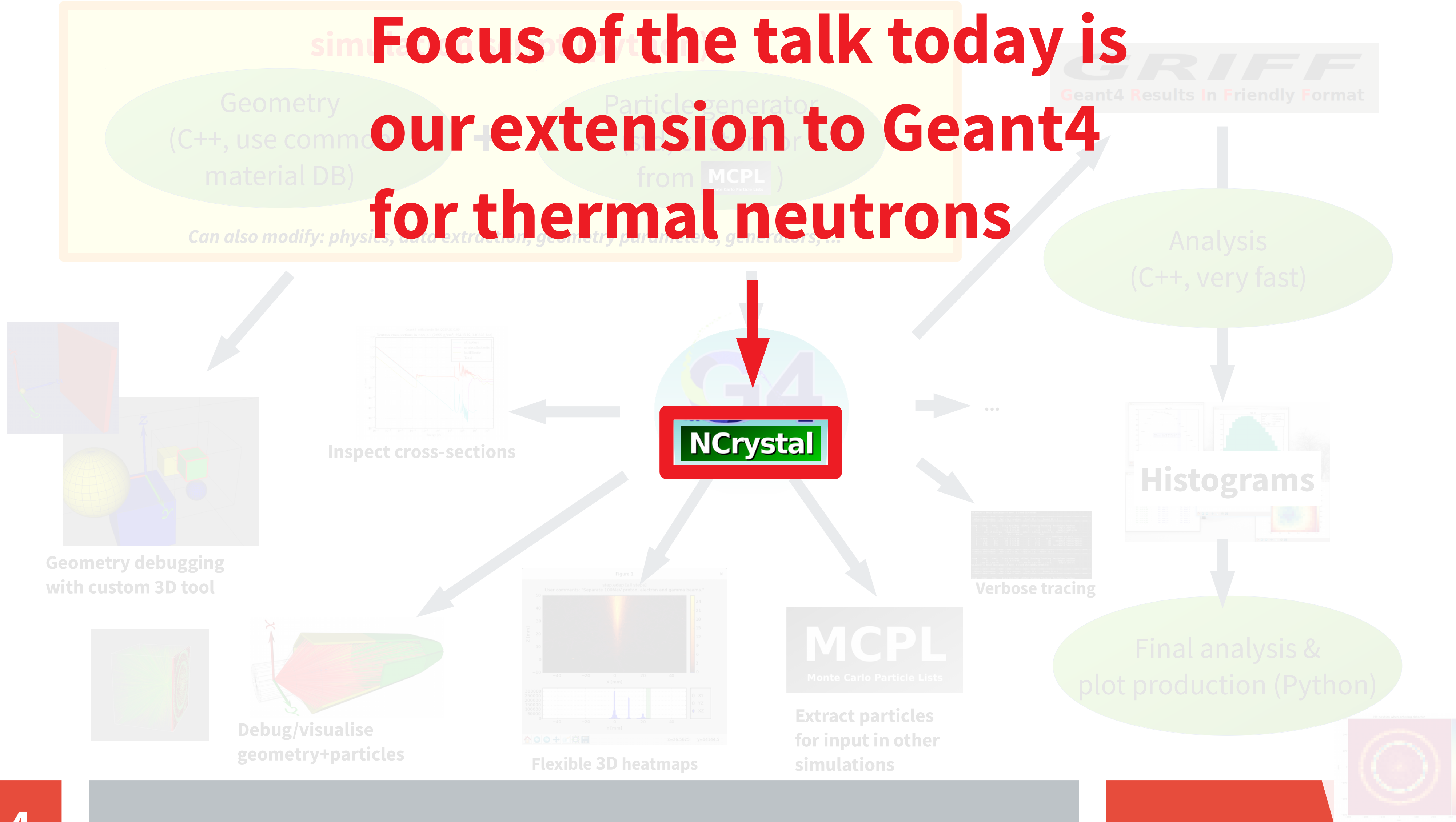
Focus of the talk today is our extension to Geant4 for thermal neutrons



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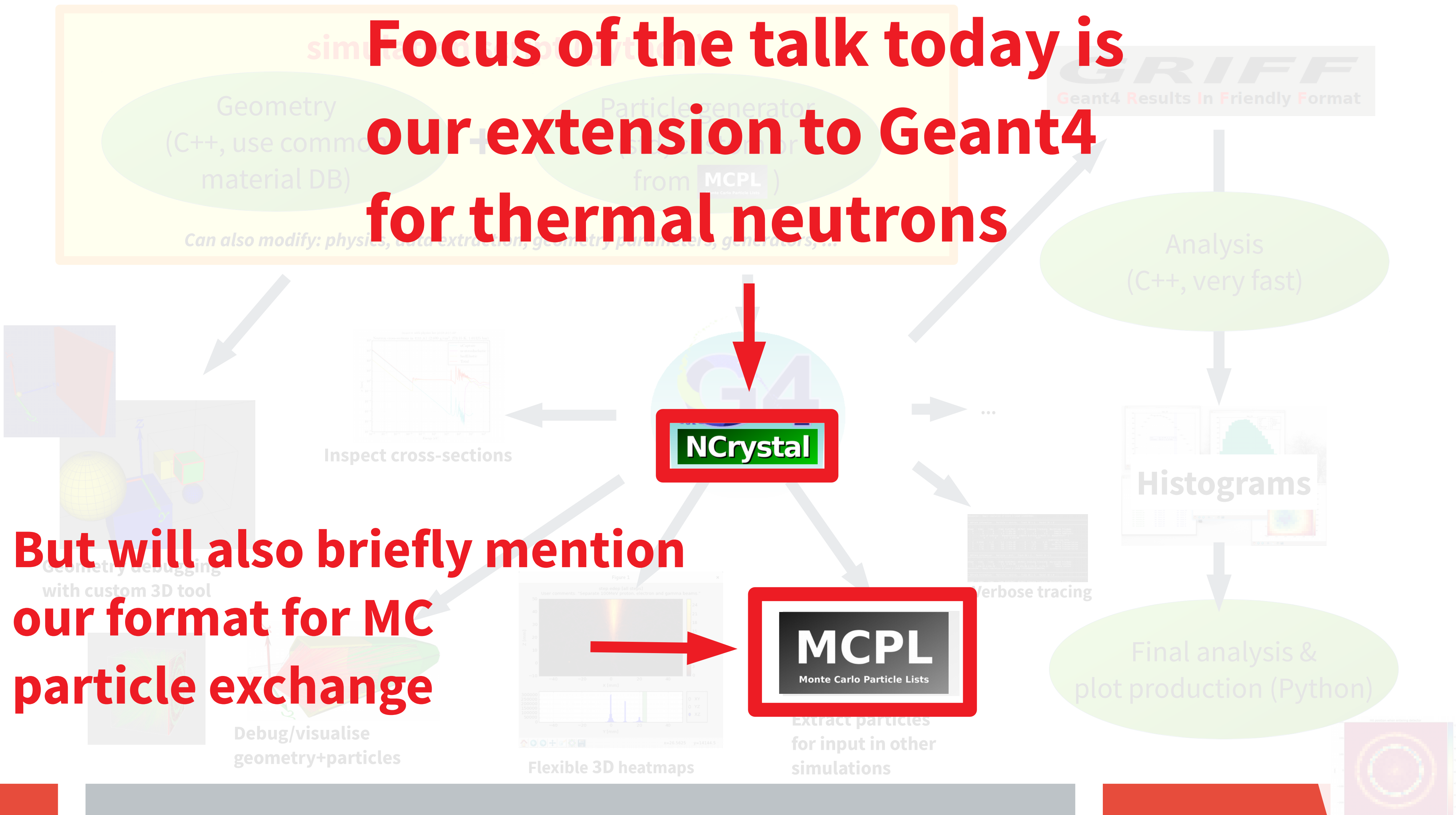
But will also briefly mention our format for MC particle exchange



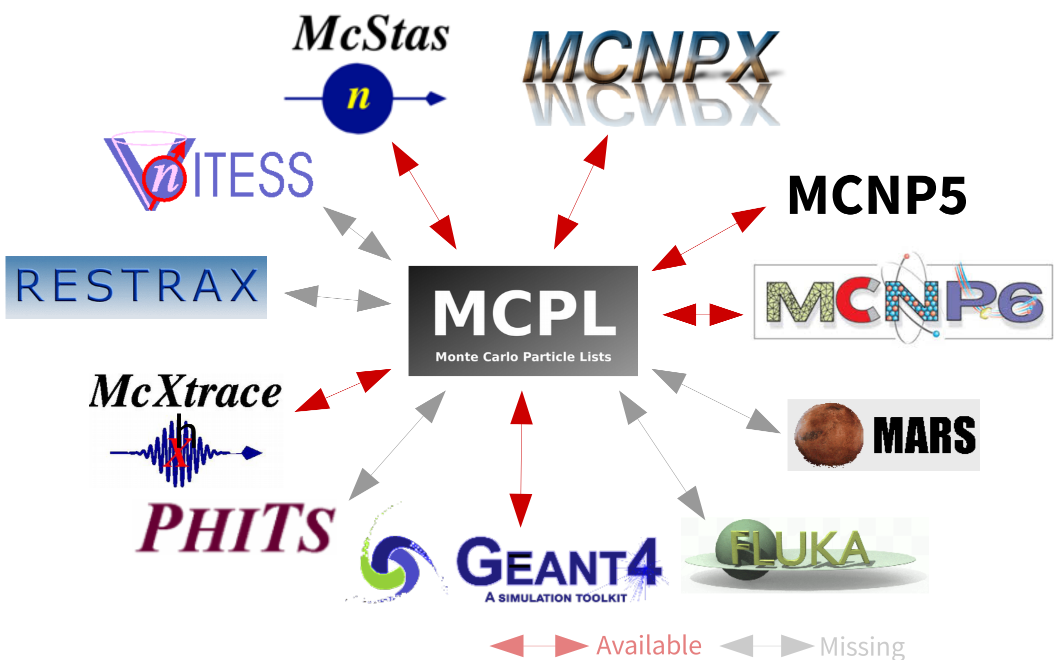
The MCPL project

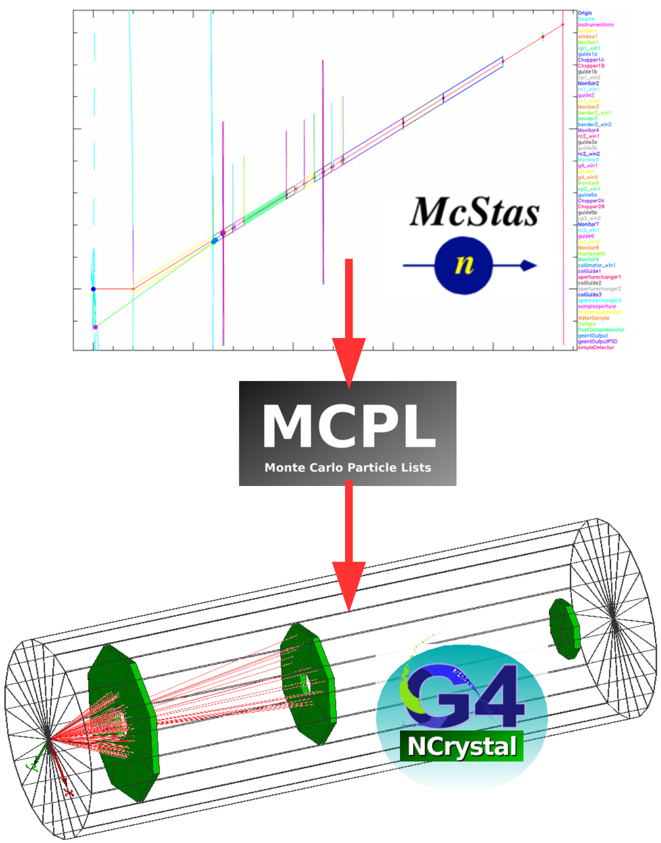
https://mctools.github.io/mcpl/

MCPL
Monte Carlo Particle Lists

- Well defined efficient & flexible format for particle exchange
- Standard browsing/editing tools
- C++/C/Python bindings
- T Kittelmann *et al* 2017 *Comput. Phys. Commun.* **218**, 17-42

For ESS detector simulations we mostly use this to hook up McStas instr. model with Geant4 detector model





T. Kittelmann, E. Klinkby, E.B. Knudsen, P. Willendrup, X.X. Cai, K. Kanaki

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NCrystal

X. X. Cai & T. Kittelmann

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

Advances earlier efforts in older "NXSG4" plugin

- T Kittelmann and M Boin 2015 *Comput. Phys. Commun.* **189**, 114-118
- Geant4-specific plugin for polycrystals, no proper bkgd, no tools/bindings
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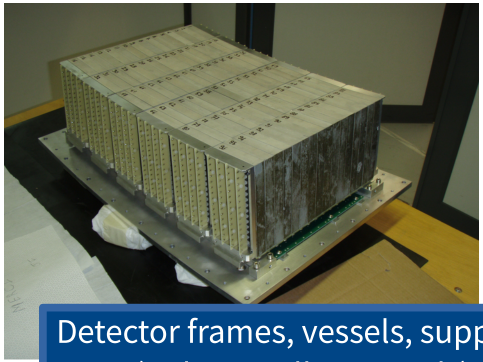

Crystalline samples

Detector frames, vessels, supports (polycrystalline metals)

Monochromators, analysers (single crystals. layered crystals)

Filters (single- or poly-crystals)

The NCrystal project

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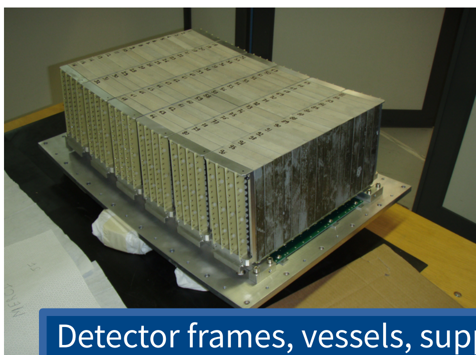
Scope has expanded beyond Geant4

- We can reach a wider and more relevant community
- We also have use-cases outside Geant4 ourselves
- As a service to the community in general



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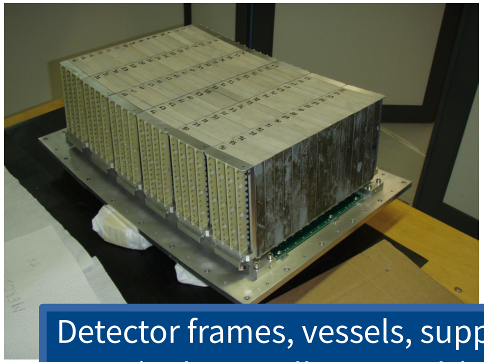

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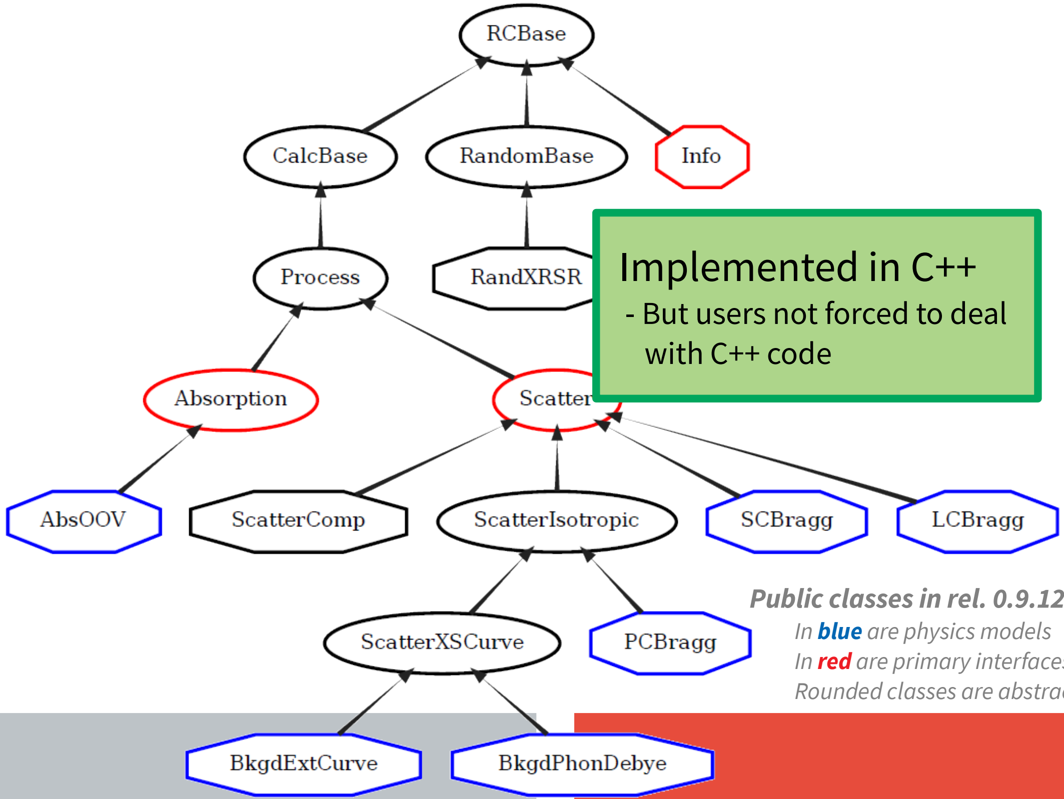


Implemented in C++

- But users not forced to deal with C++ code

Public classes in rel. 0.9.12

*In **blue** are physics models*

*In **red** are primary interfaces*

Rounded classes are abstract

Many available interfaces

Can share configurations and data files across them all

NCrystal

X. X. Cai & T. Kittelmann

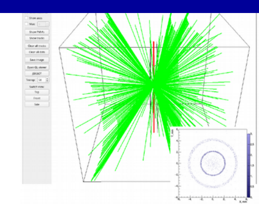
NCrystal

McStas

- *Plugin (component) ships with NCrystal release.*
- *Supports multiple scattering + a few basic sample shapes*
- *McStas devs (P. Willendrup+E. B. Knudsen) working on availability out-of-the-box.*

ANTS2

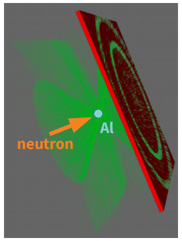
- *Available out-of-the-box (thanks to A. Morozov)*



Direct/standalone usage

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

GEANT4 A SIMULATION TOOLKIT



- *Plugin ships with NCrystal release.*
- *ESS-DG's Geant4 framework has NCrystal built in.*
- *Goal is availability out-of-the-box for all Geant4 users.*

NCrystal aims to be hassle-free:

- *Robust modelling over large range of setups*
- *No required dependencies.*
- *Linux, OSX, Windows*
- *C++98, C++03, C++11, C++14, C++17*
- *C89, C99 or C11*
- *Python2.7+, Python3.3+*
- *Unrestrictive Apache 2.0 license*
- *RNG streams, error reporting etc. can be controlled by calling code.*
- *In the pipeline: MT safety.*

OpenMC

- *Plugin is work in progress (thanks to J. I. Márquez Damián)*

NJOY

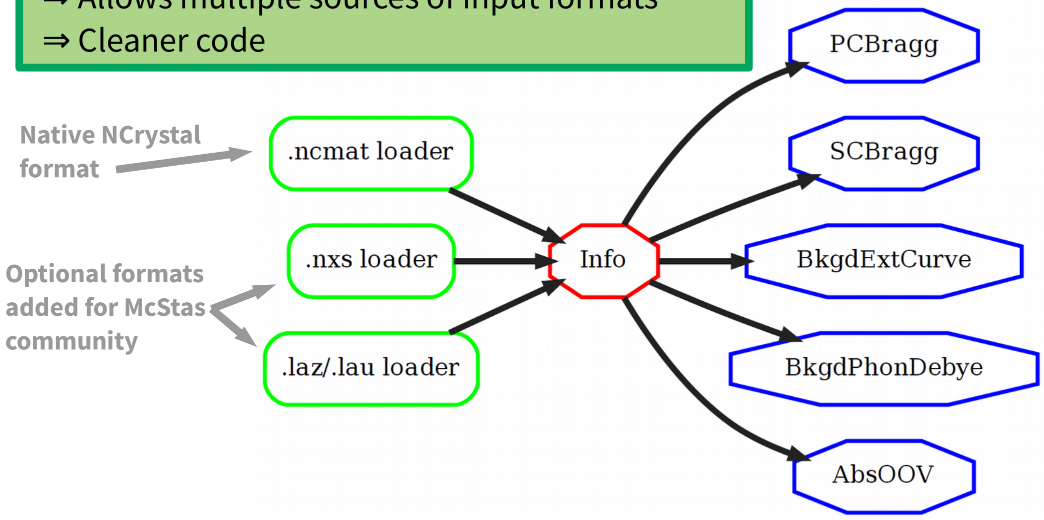
- *Can use NCrystal results when generating ENDF files for various MC applications (like MCNP).*
- *(thanks to J. I. Márquez Damián)*

Sources of crystallographic info

Can be extended if needed

NCrystal
X. X. Cai & T. Kittelmann

Well defined interface for loaded data
⇒ Allows multiple sources of input formats
⇒ Cleaner code



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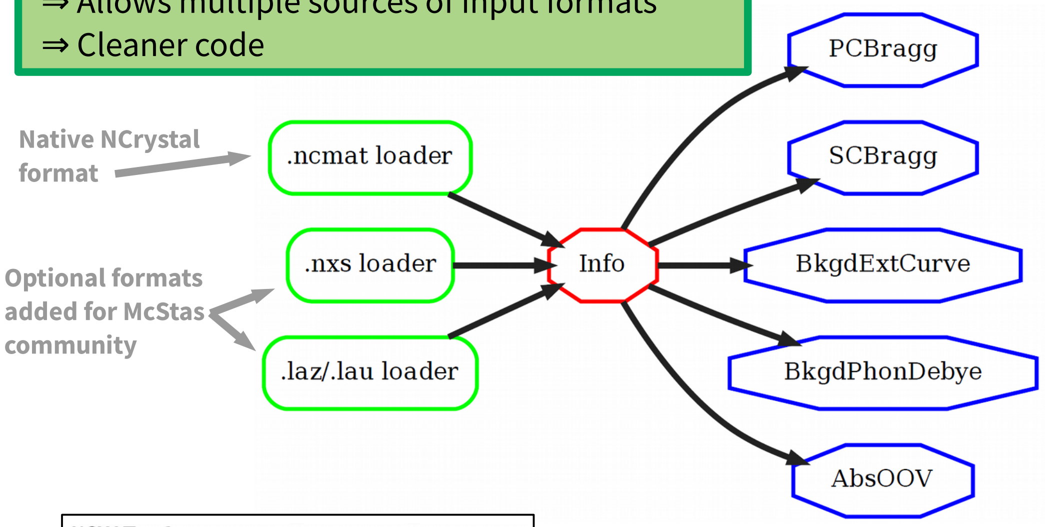


```
NCMAT v1
#Some comment here...
@CELL
    lengths 5.65735 5.65735 5.65735
    angles 90. 90. 90.
@SPACEGROUP
    227
@ATOMPOSITIONS
    Ge 0.75 0.75 0.25
    Ge 0.5  0.5  0.
    Ge 0.75 0.25 0.75
    Ge 0.5  0.   0.5
    Ge 0.25 0.75 0.75
    Ge 0.   0.5  0.5
    Ge 0.25 0.25 0.25
    Ge 0.   0. 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

Ge_sg227.ncmat

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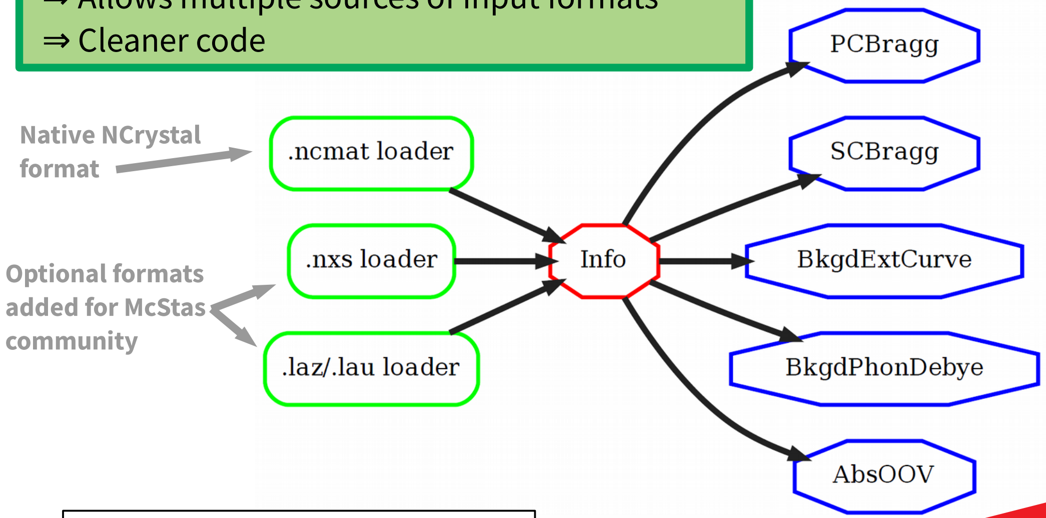


```
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@CELL
    lengths 5.65735 5.65735 5.65735
    angles 90. 90. 90.
@SPACEGROUP
    227
@ATOMPOSITIONS
    Ge 0.75 0.75 0.25
    Ge 0.5  0.5  0.
    Ge 0.75 0.25 0.75
    Ge 0.5  0.   0.5
    Ge 0.25 0.75 0.75
    Ge 0.   0.5  0.5
    Ge 0.25 0.25 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  -7  -1  0.792187           48        13.2885 1,-7,-1 | -1,7,1 | 1,
  2  -6  -4  0.755995           48        25.3595 2,-6,-4 | -2,6,4 | 2,
```

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Can be extended if needed

NCrystal

X. X. Cai & T. Kittelmann

Well d
⇒ Allov
⇒ Clear

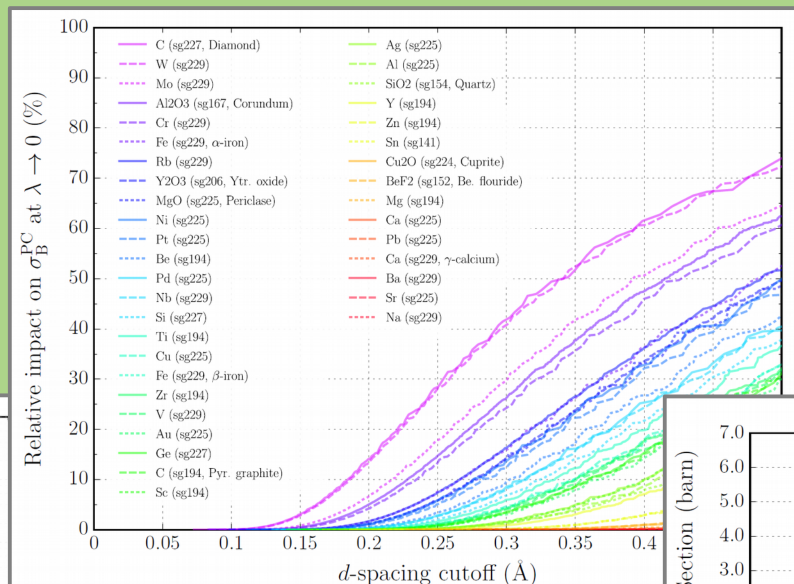
Native NCr
format

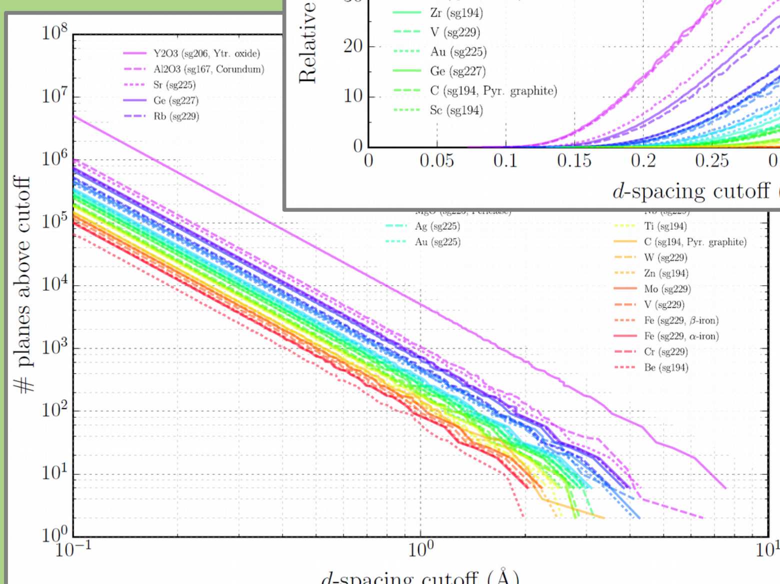
Optional for
added for M
community

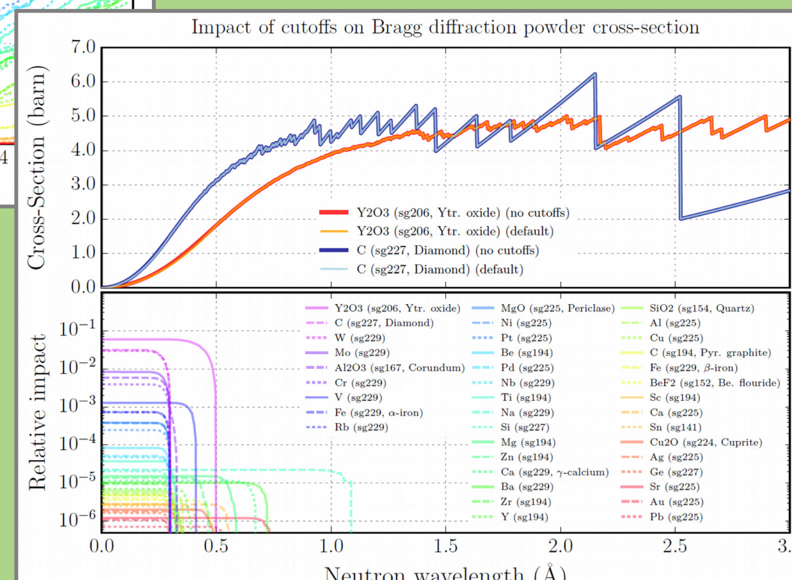
```
NCMAT
#Some
@CELL
    le
    ar
@SPACE
    22
@ATOMP
    Ge
    Ge
    Ge
    Ge
    Ge
    Ge
    Ge
    Ge
@DEBYE
    Ge
```

```
ist
,1 | 1,
2 | 0,2
,1 | 1,
 | 0,4,
,3 | 1,
,2 | 2,
,1 | 1,
4 | 0,4
,3 | 1,
6 | 0,2
,3 | 3,
,4 | 4,
,1 | 1,
```

Default .ncmat cutoffs tuned to give both short O(10-100ms) load times and realistic total x-sects at shorter wavelengths







NCrystal data library

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

NCrystal

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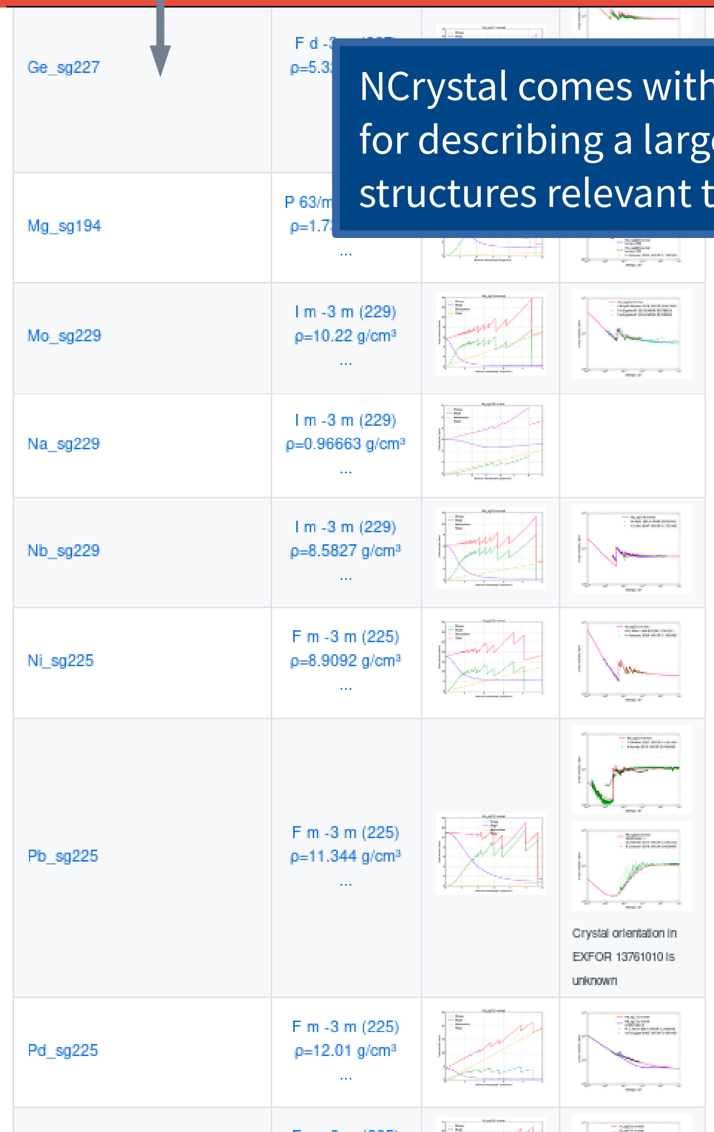
NCrystal comes with library of validated data files, for describing a large number of crystal structures relevant to neutron scattering.




```
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#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
@DEBYETEMPERATURE
    Al 410.35
```

Al_sg225.ncmat

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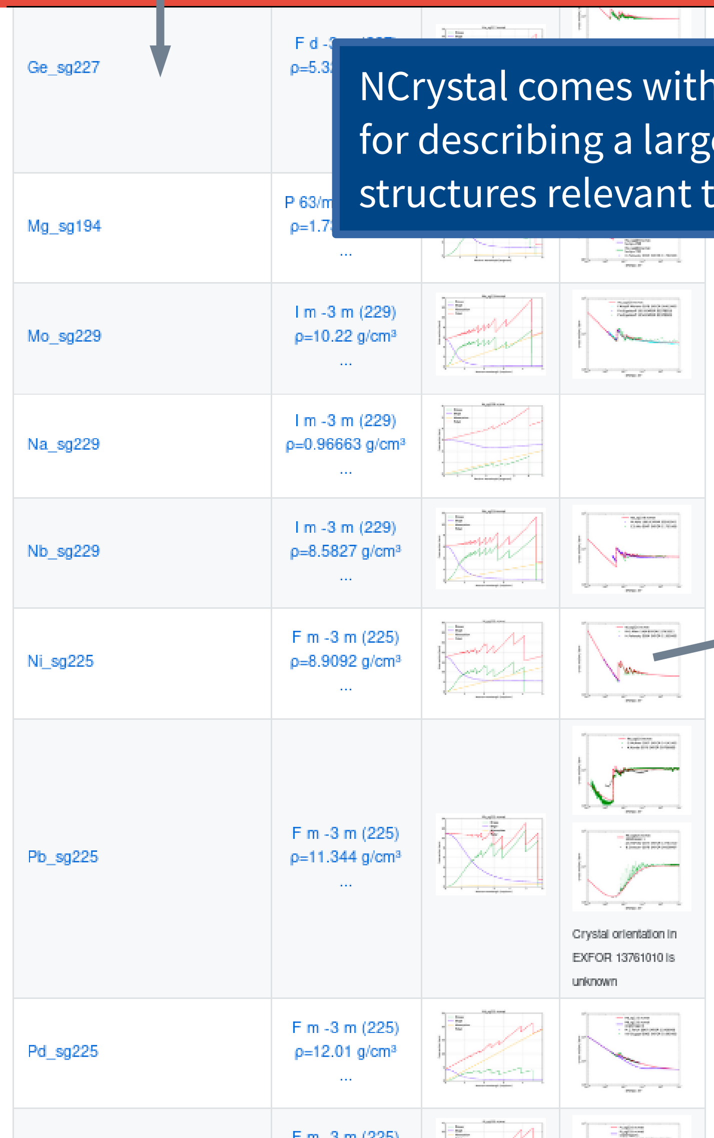


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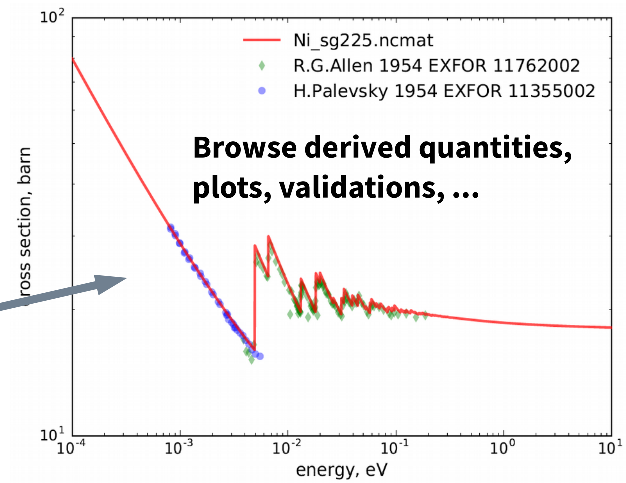
Al_sg225.ncmat



Browse derived quantities, plots, validations, ...

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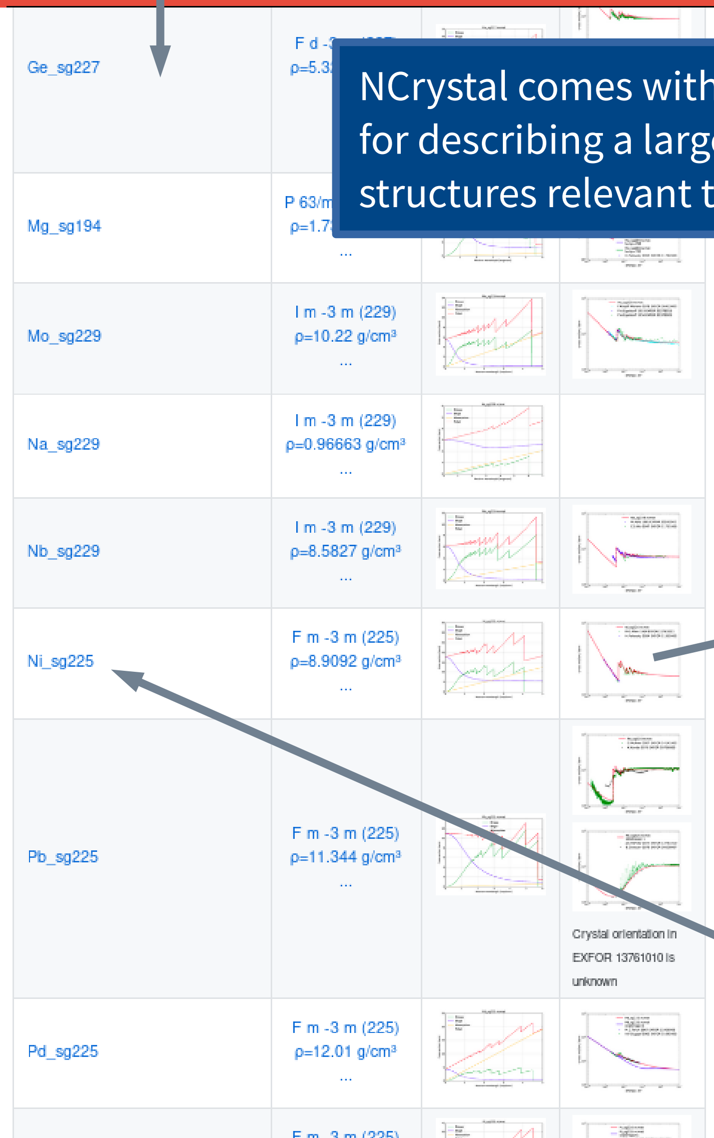

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    Al 0.5 0. 0.5
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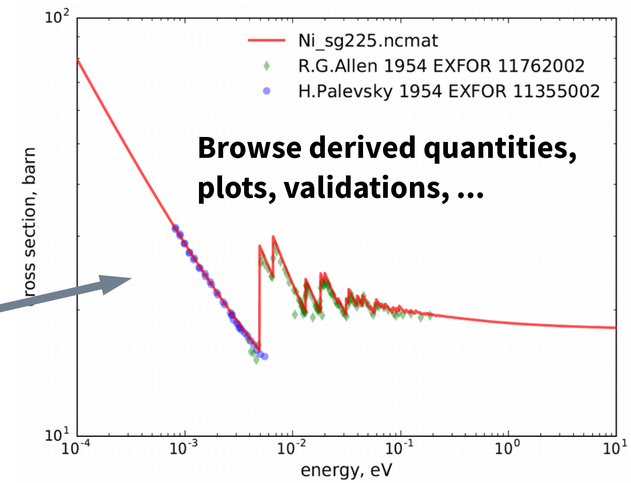


Browse derived quantities, plots, validations, ...

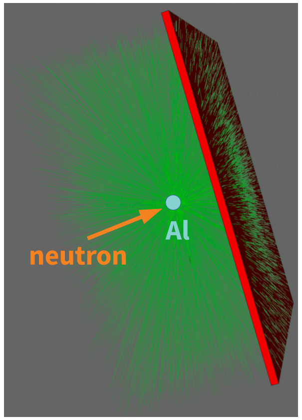
To use in Geant4 or McStas (or ...), simply supply name of material file, along with relevant parameters like temperature, orientation of single crystal, etc.

Bragg diffraction in polycrystals and powders

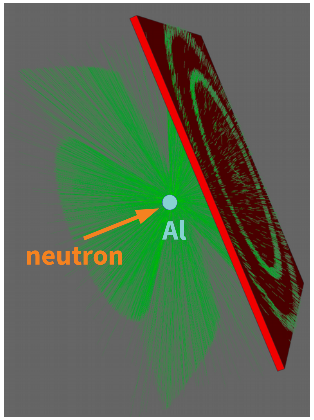
NCrystal
X. X. Cai & T. Kittelmann

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

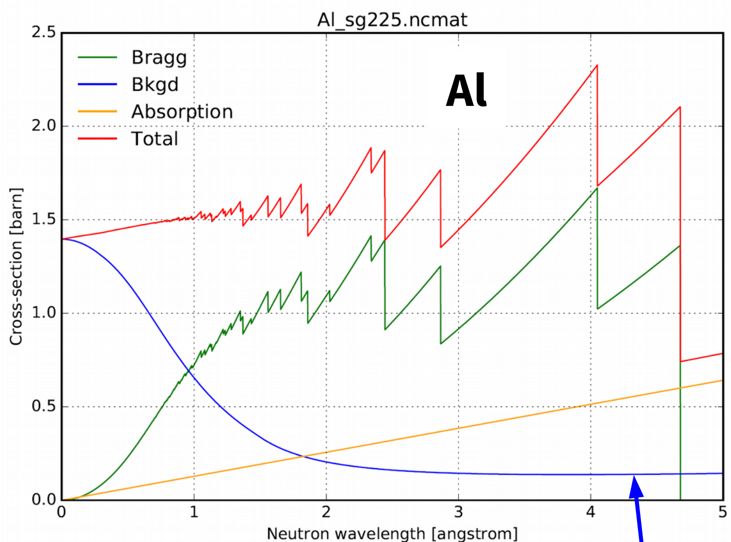
Care is taken to be extremely fast O(ns/call), even in case of huge number of planes.



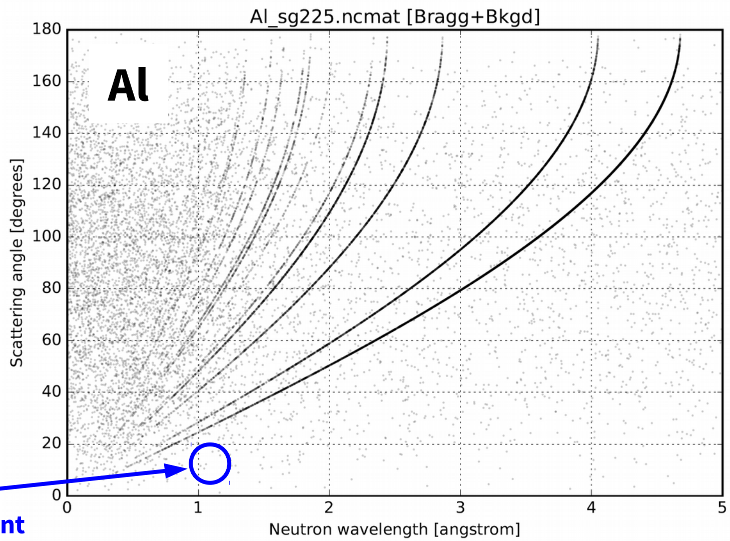
Geant4 free-gas model (wrong MFP, wrong scatter)



Geant4 with NCrystal ⇒Debye-Scherrer cones



Provides cross-sections

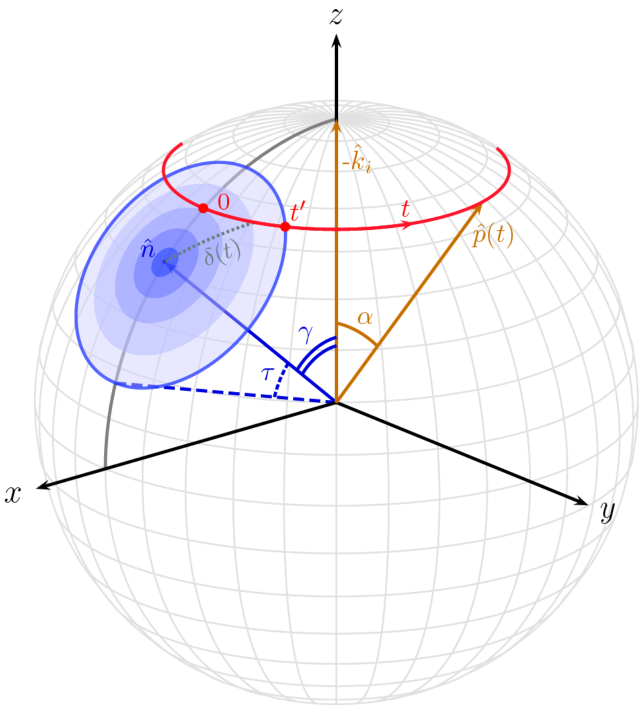


And scatter angles

Non-Bragg "Bkgd" component discussed on later slide

Single Crystals with Gaussian mosaicity

Can model monochromators, analysers, SC samples



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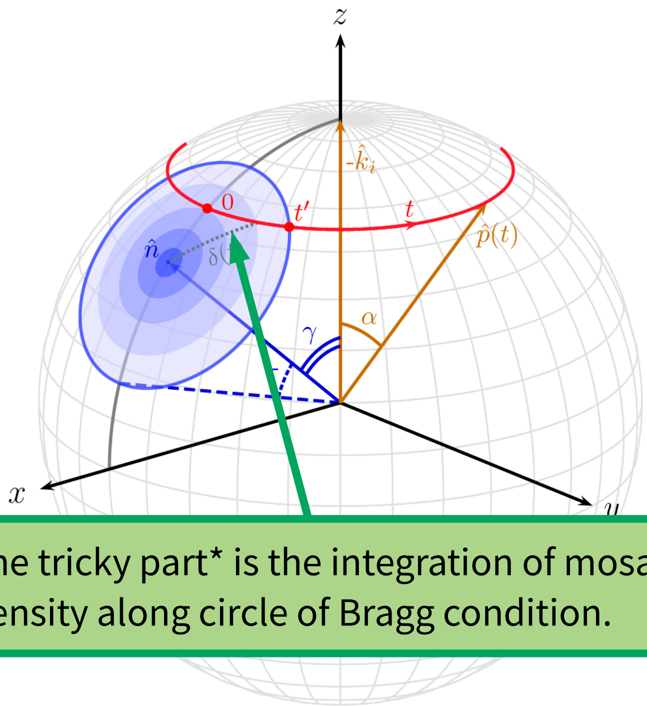

The tricky part* is the integration of mosaic density along circle of Bragg condition.

**: Once contributing normals Have been identified.*

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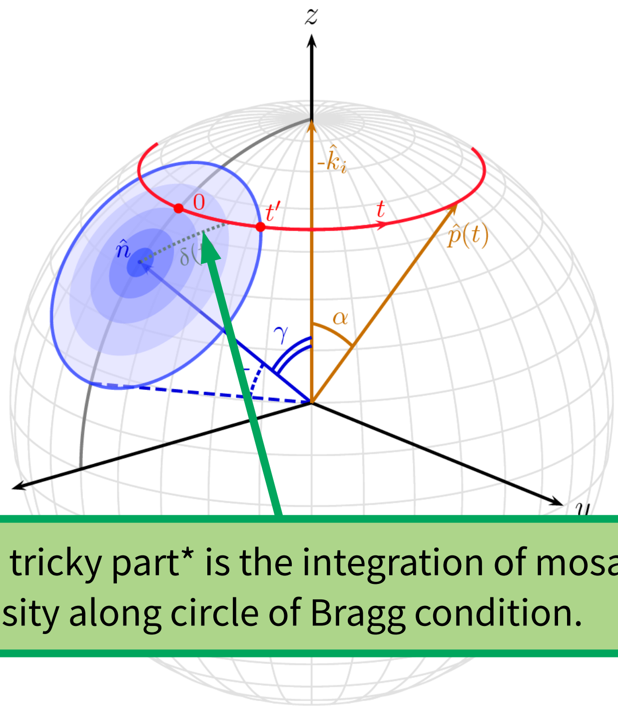

The tricky part* is the integration of mosaic density along circle of Bragg condition.

**: Once contributing normals Have been identified.*

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

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

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

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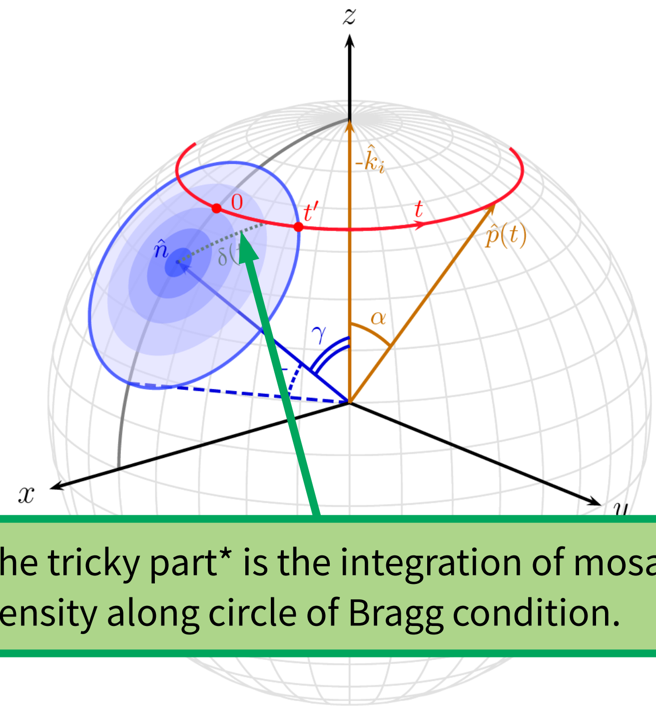

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*: Once contributing normals
Have been identified.

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

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

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

Improved form extends validity to much larger mosaicities

Single Crystals with Gaussian mosaicity

Can model monochromators, analysers, SC samples

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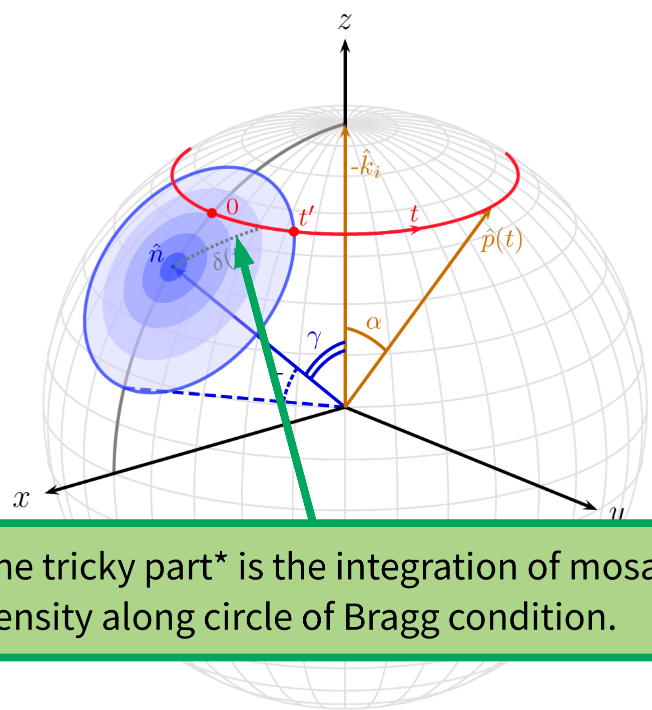

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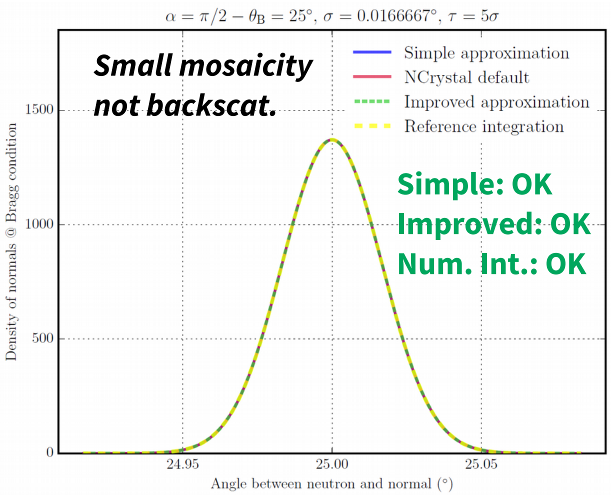

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$$\sigma_{\text{Bragg}}(\alpha,\gamma) = Q \times \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\tfrac{1}{2}\delta_0^2/\sigma^2\right] \times \text{erf}\left[\sqrt{\frac{\tau^2-\delta_0^2}{2\sigma^2}}\right] \times \sqrt{\frac{\sin\alpha}{\sin\gamma}} \times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

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

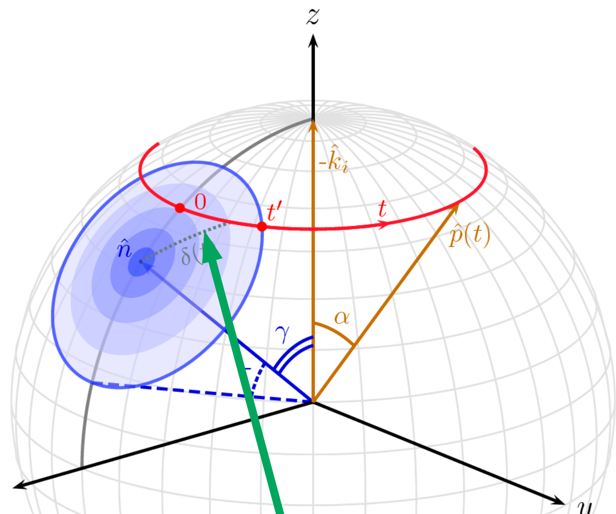
Improved form extends validity to much larger mosaicities

Single Crystals with Gaussian mosaicity

Can model monochromators, analysers, SC samples

NCrystal

X. X. Cai & T. Kittelmann



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

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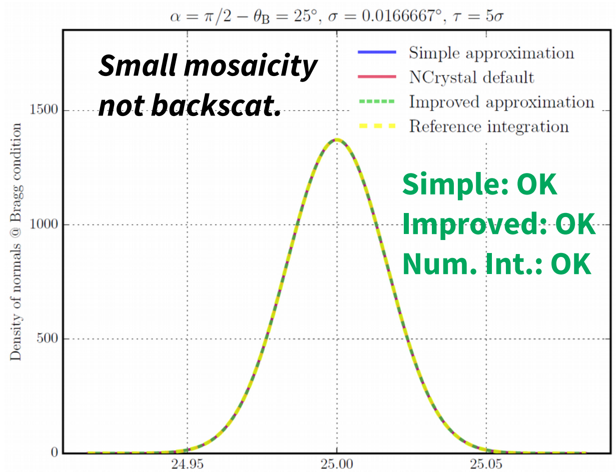

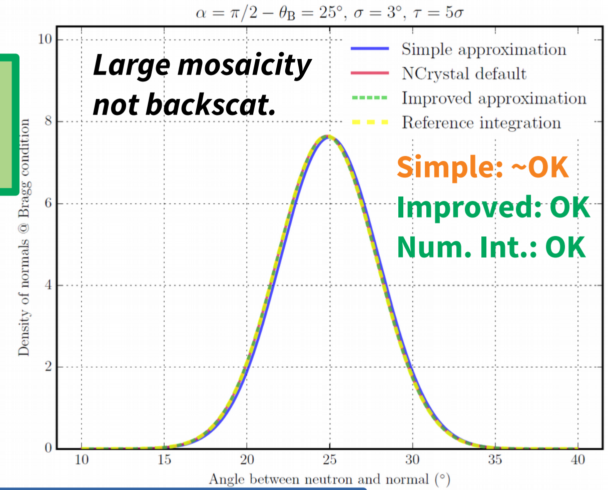

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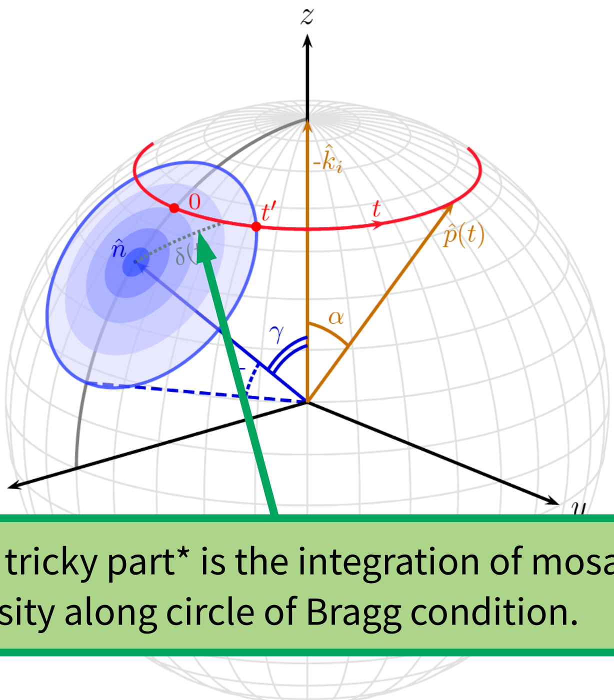

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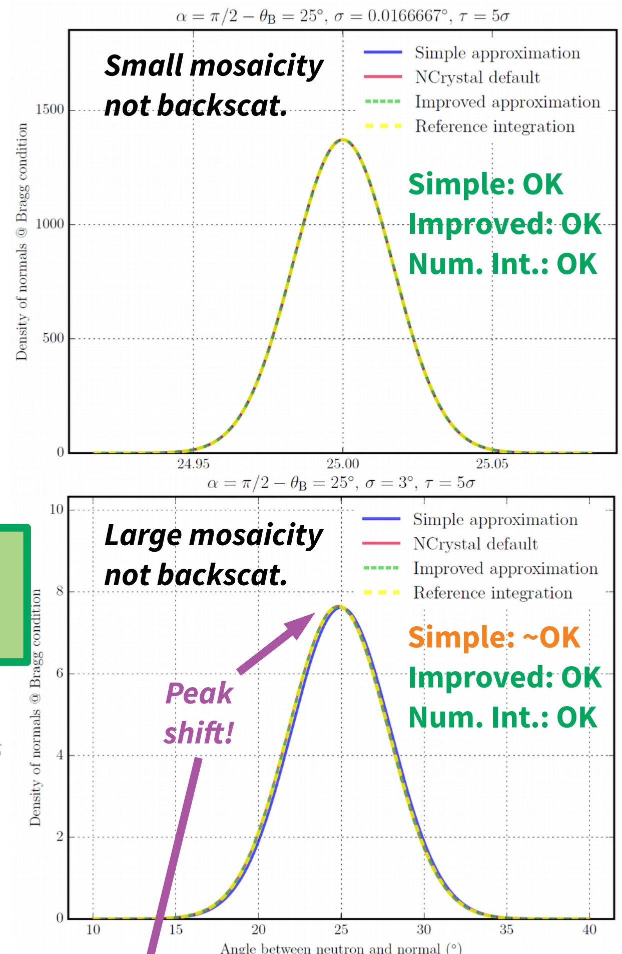

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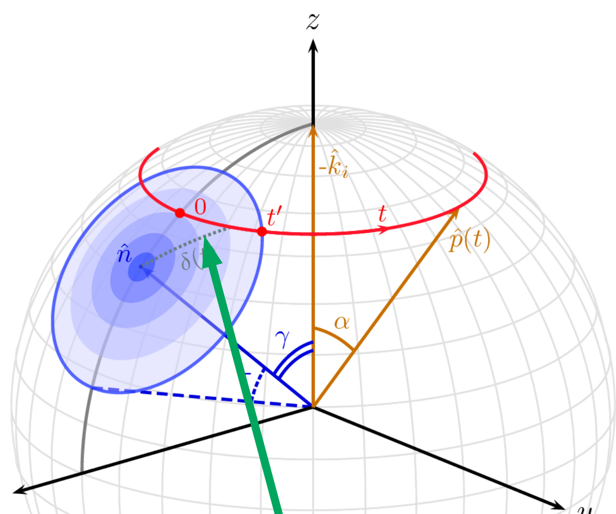

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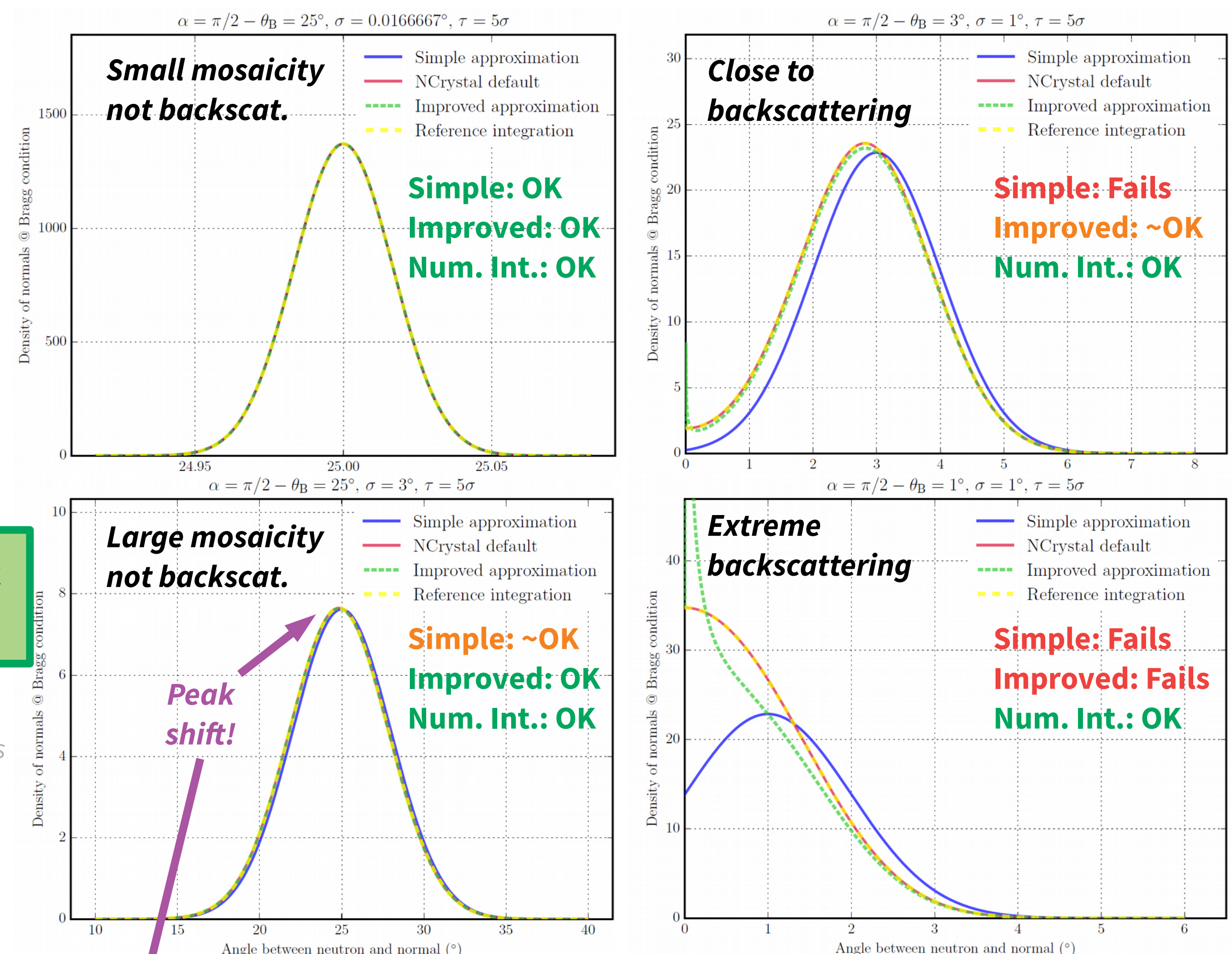

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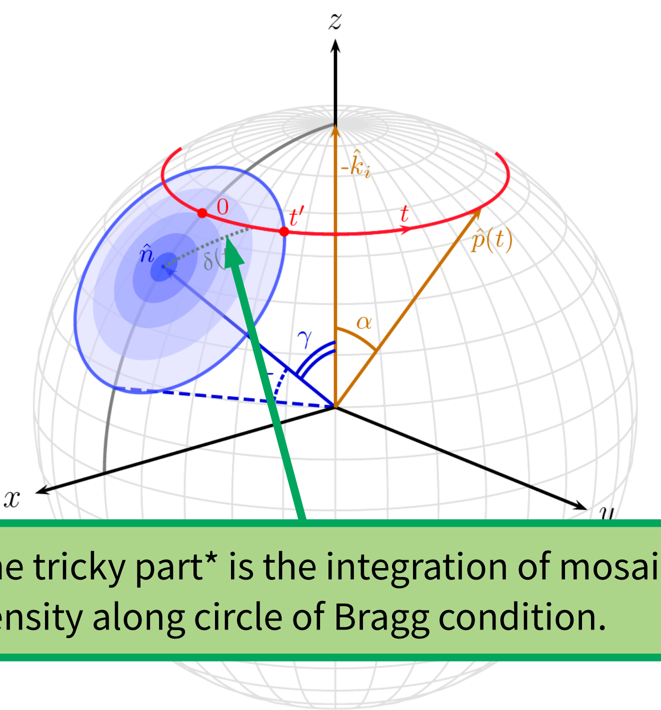

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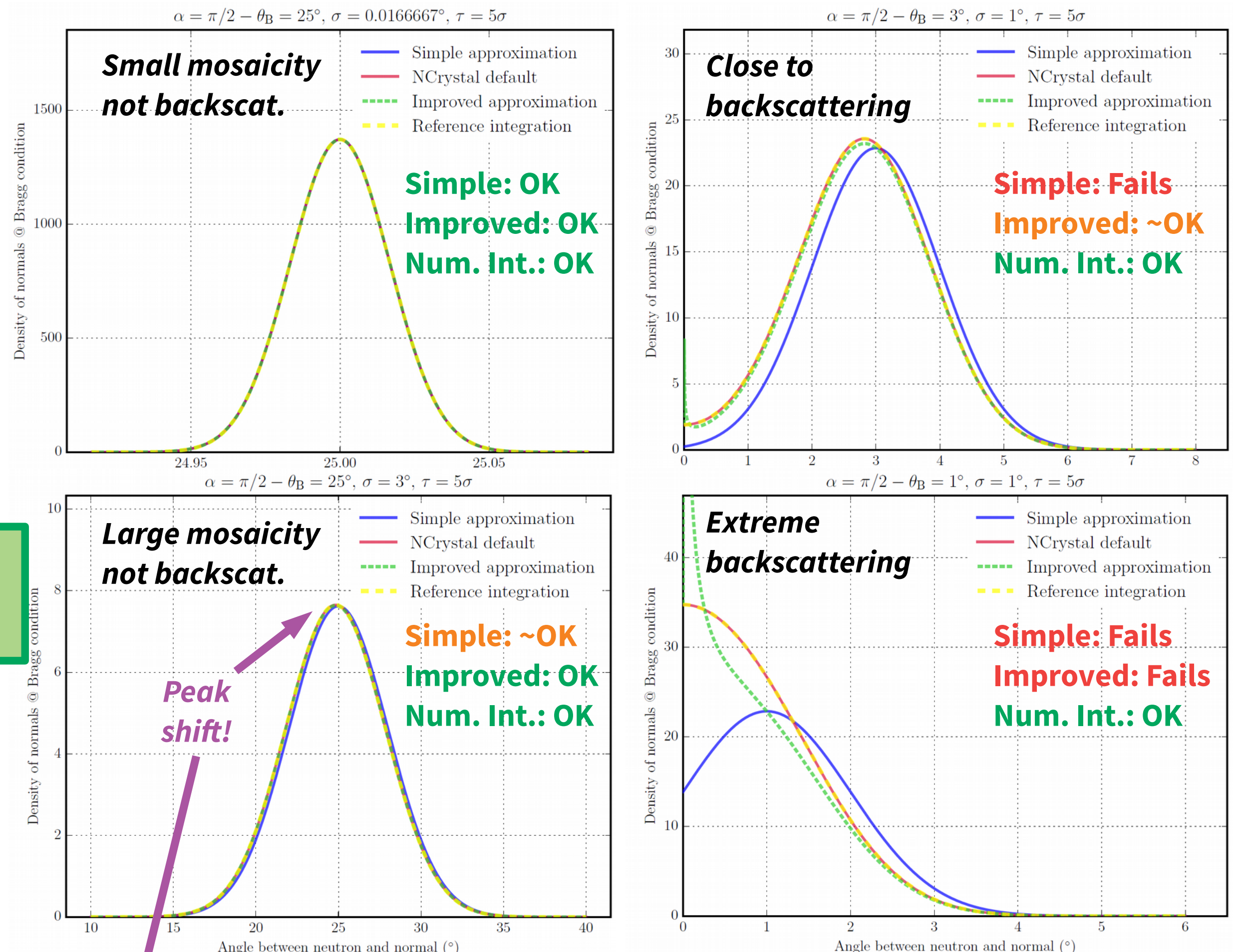

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Improved form extends validity to much larger mosaicities

Code automatically picks appropriate method

Pyrolythic Graphite

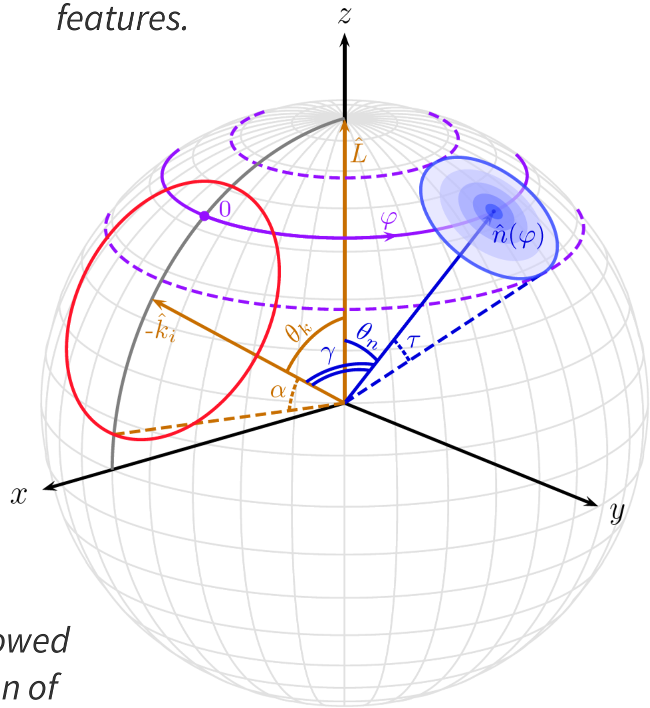
Special anisotropic model

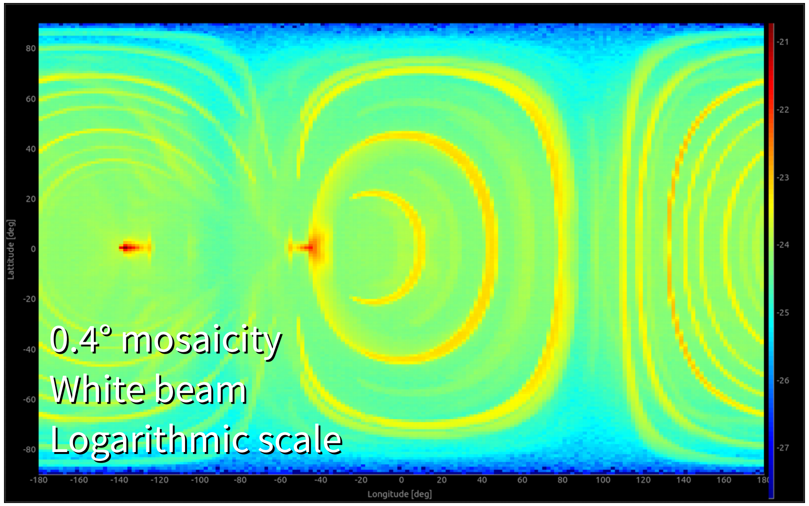
NCrystal

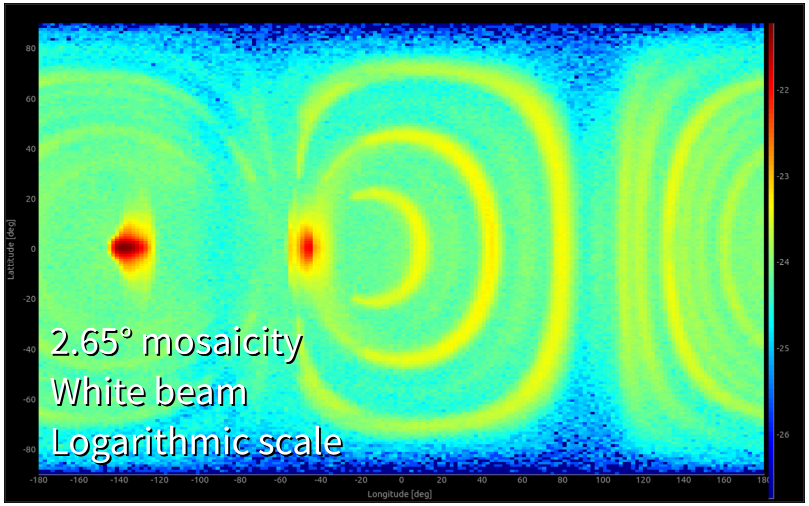
X. X. Cai & T. Kittelmann

Layered crystal model:

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







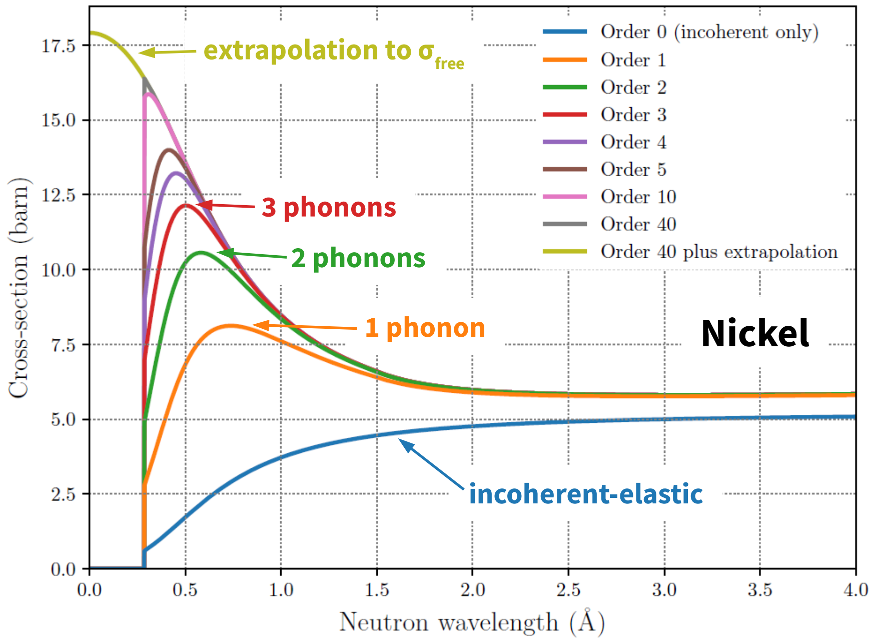
Features:

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

NCrystal physics

Inelastic/incoherent scattering (“Bkgd”)

Inelastic cross-section estimated by multi-phonon expansion, calculated via custom FFT code during the Initialisation stage:



NCrystal physics

Inelastic/incoherent scattering ("Bkgd")

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X. X. Cai & T. Kittelmann

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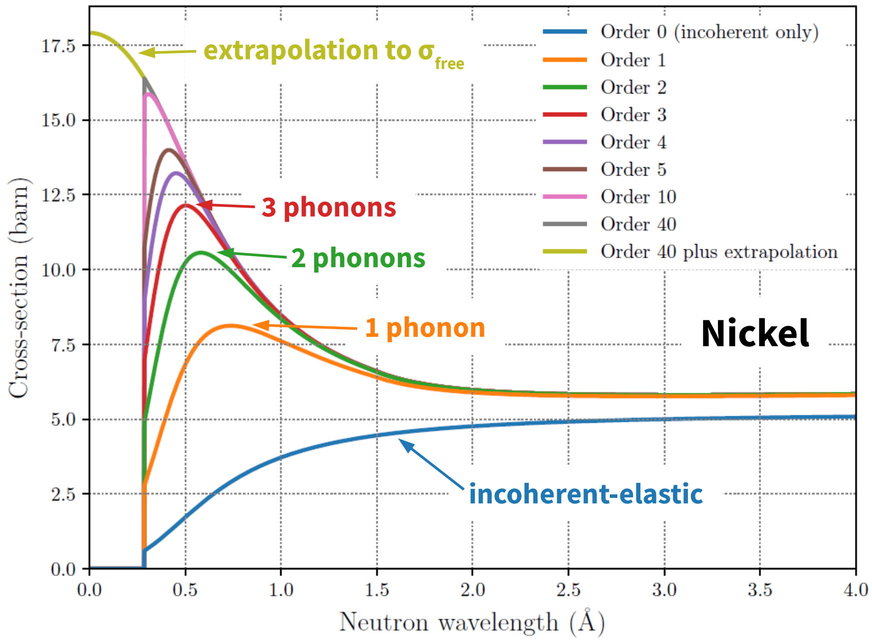
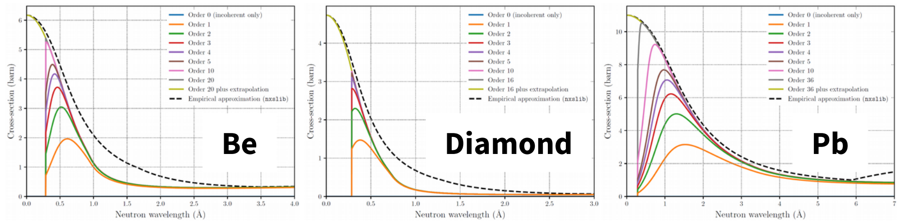




NCrystal physics

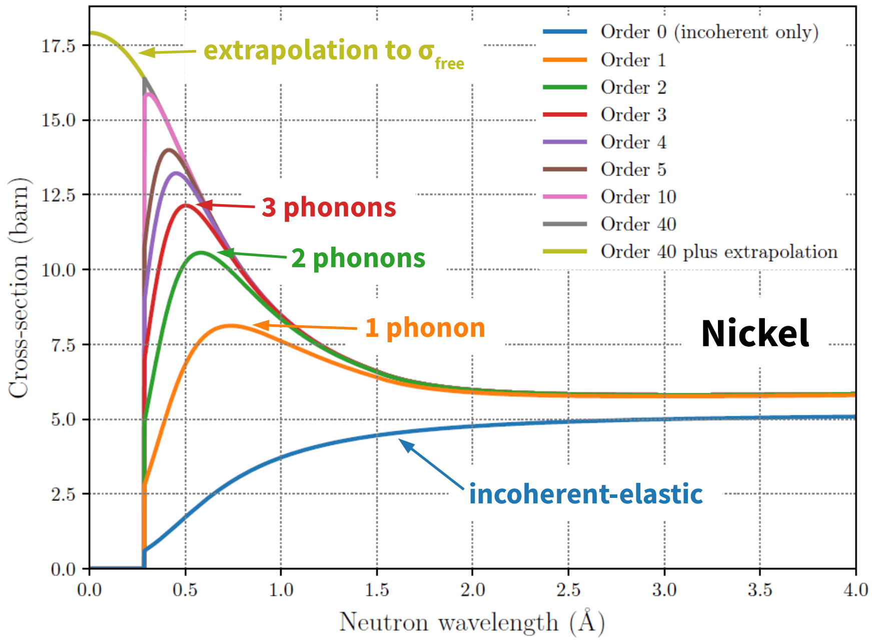
Inelastic/incoherent scattering (“Bkgd”)

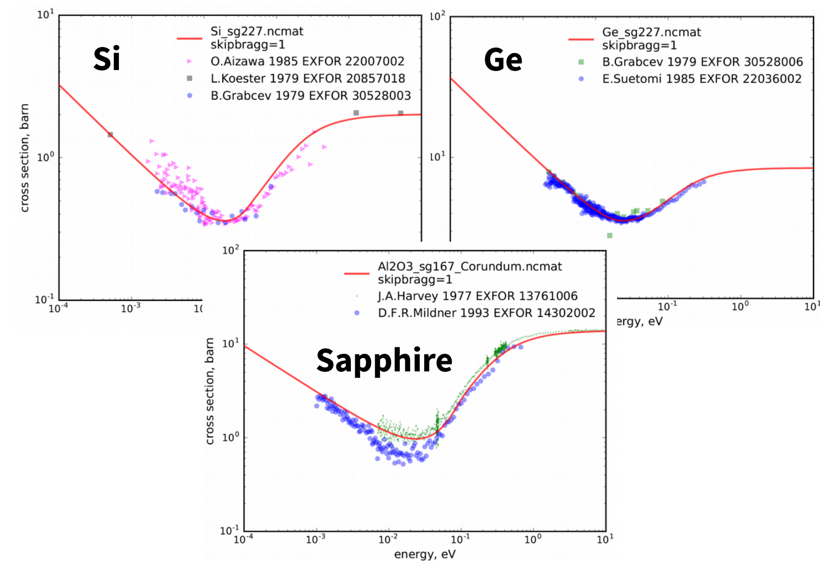
NCrystal

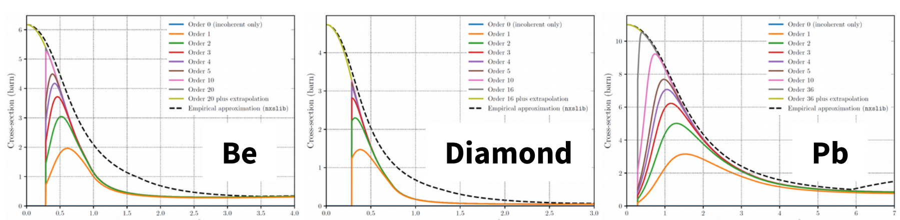
X. X. Cai & T. Kittelmann

Inelastic cross-section estimated by multi-phonon expansion, calculated via custom FFT code during the Initialisation stage:

This approach much more reliable than any of the various empirical formulas people typically employ (e.g. Cassels 1950, Freund 1983, Einstein model, ...)







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NCrystal

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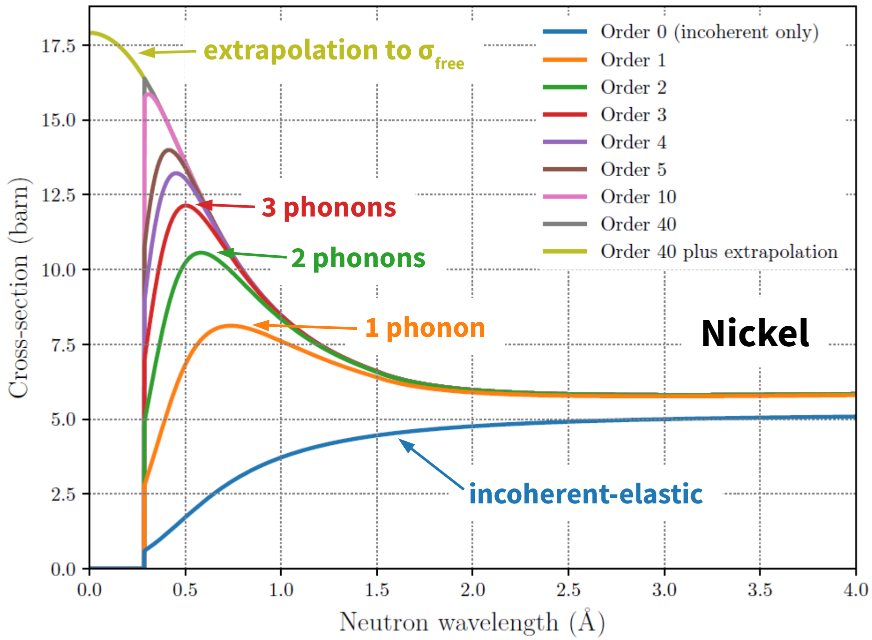
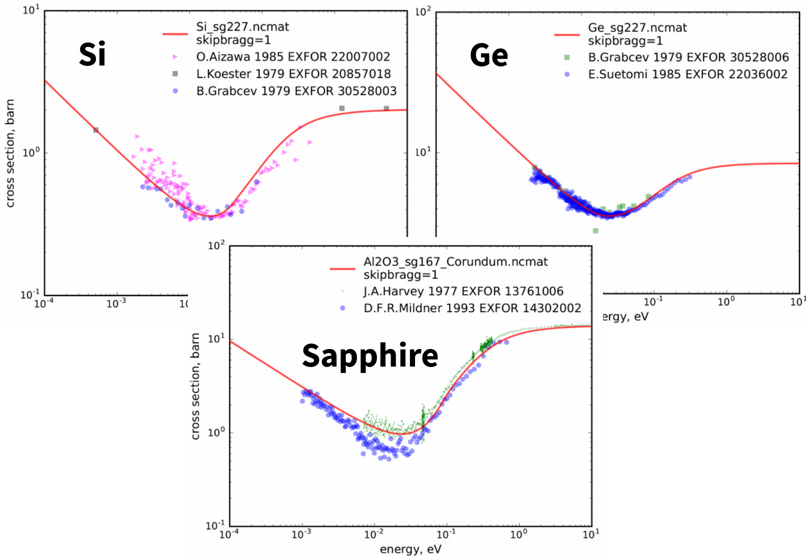
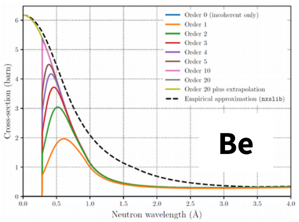
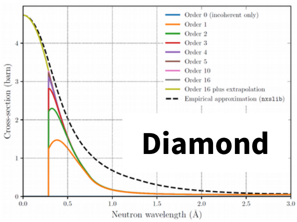
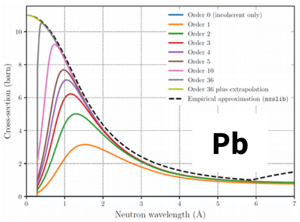










Advantage: Works without extra input (such as scatter kernels)!
Limitation: No specific modelling of energy transfers & scatter-angles.
Work in progress: Trying to mitigate limitation somewhat.

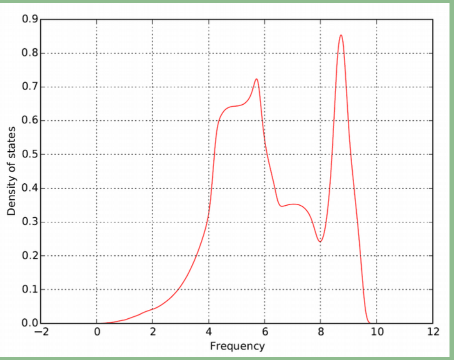
…but will in any case not always be precise enough…

NCrystal physics

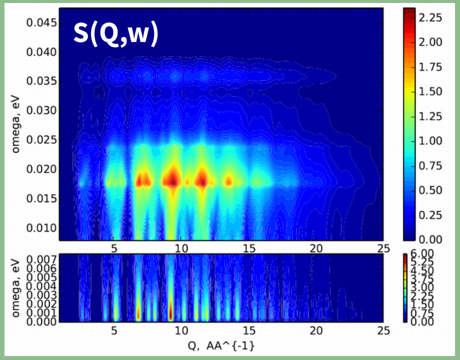
Planned support for detailed inelastic/incoherent data

X. X. Cai & T. Kittelmann

In the pipeline is ability to use more detailed data where available



1D phonon spectrum



2D scattering kernel

NCrystal physics

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NCrystal

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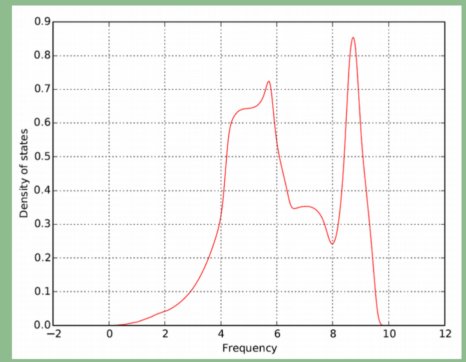
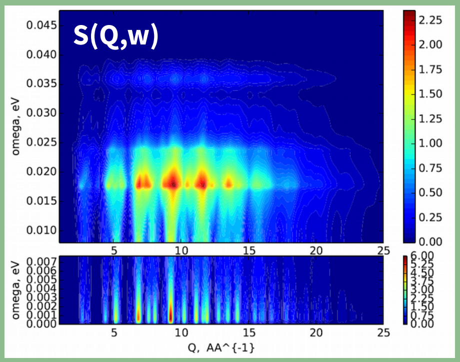


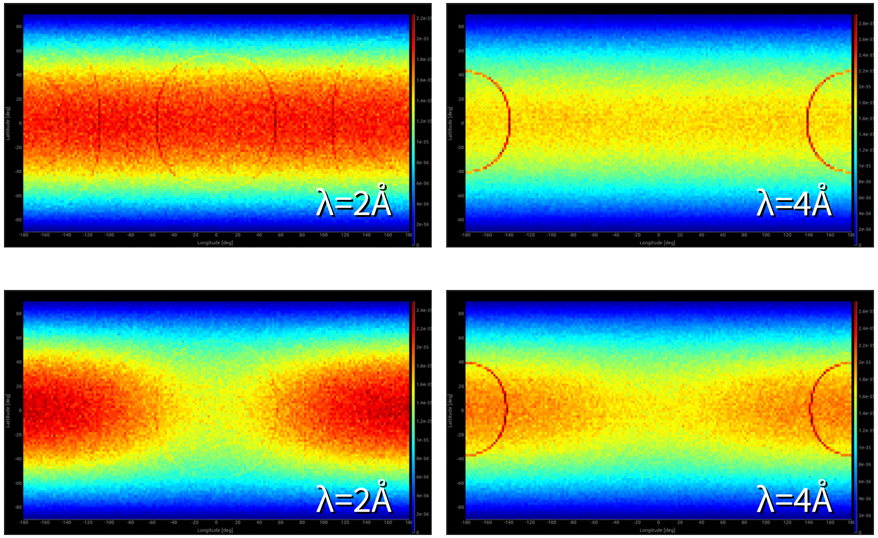
1D phonon spectrum



2D scattering kernel

4π vanadium scatter patterns (no kernel)

Same patterns with dedicated scatter kernels



NCrystal physics

Planned support for detailed inelastic/incoherent data

NCrystal

X. X. Cai & T. Kittelmann

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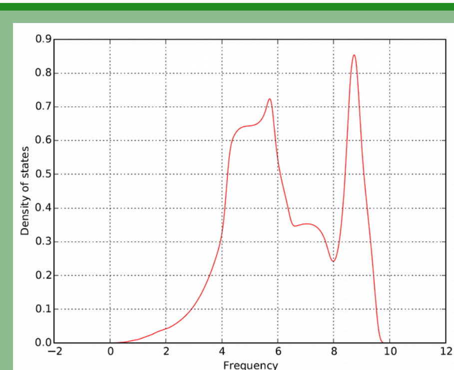
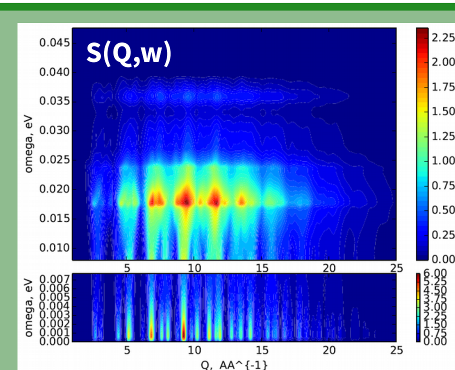


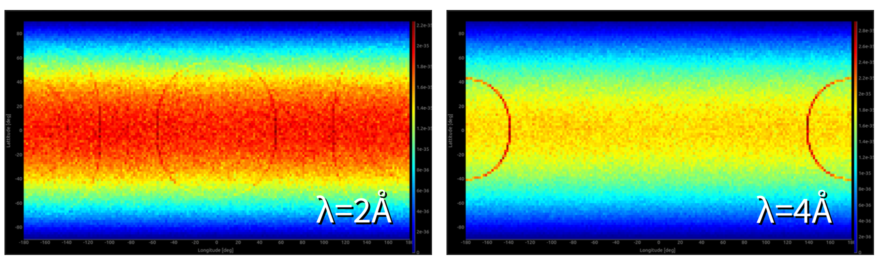
1D phonon spectrum



2D scattering kernel

Aim is ability to model individual scatterings precisely, not just many-scattering effects. Improving algorithms where needed:

4π vanadium scatter patterns (no kernel) →



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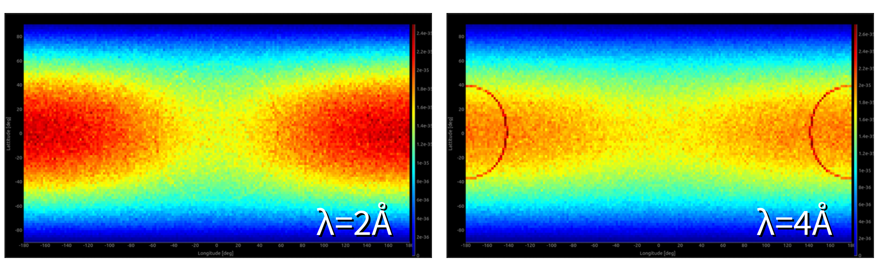

Rejection-based sampling of inelastic neutron scattering

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

Submitted to J. Comput. Phys. (arXiv:1808:02634)

Abstract

Distributions of inelastically scattered neutrons can be quantum dynamically described by a scattering kernel. We present an accurate and computationally efficient rejection method for sampling a given scattering kernel of any isotropic material. The proposed method produces continuous neutron energy and angular distributions, typically using just a single interpolation per sampling. We benchmark the results of this method

Validate PC/Powder Bragg & Inel./incoh. models with EXFOR total x-sects

NCrystal

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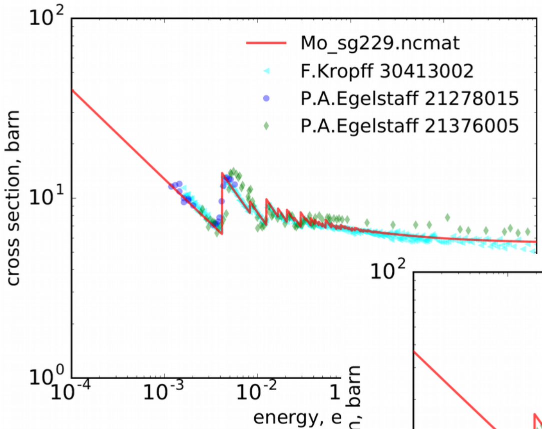
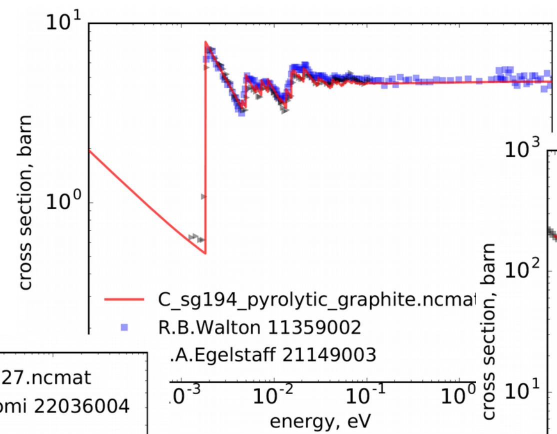
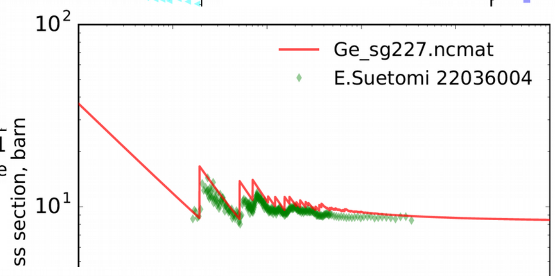
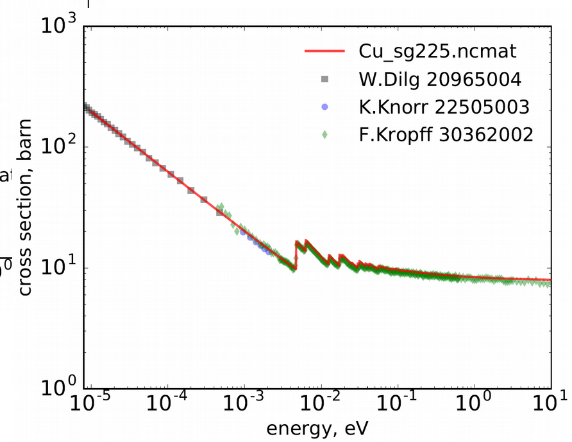
Some examples shown here,
Find all on wiki data-library page.

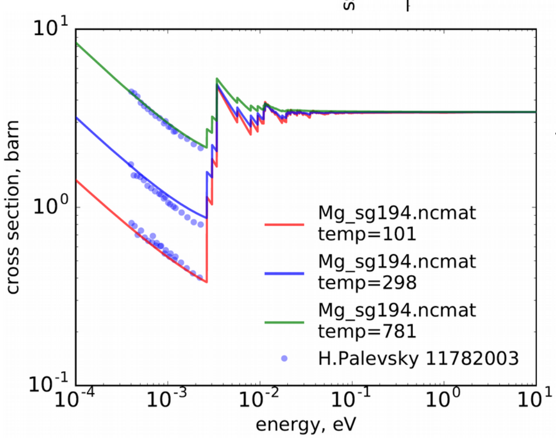
General good agreement, but data is not always perfect (doesn't agree with other data)

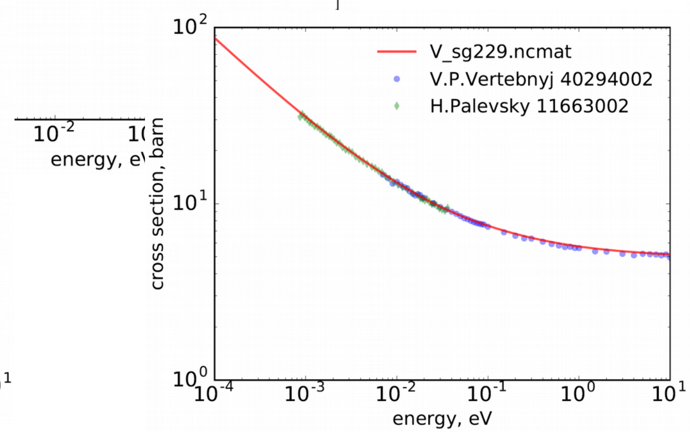


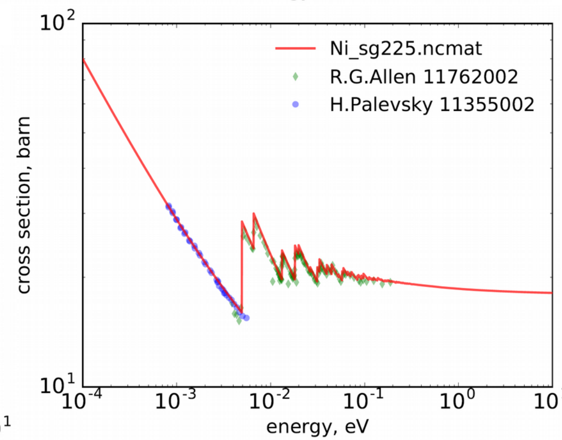












Validate Single Crystal code against analytical predictions or other codes

NCrystal

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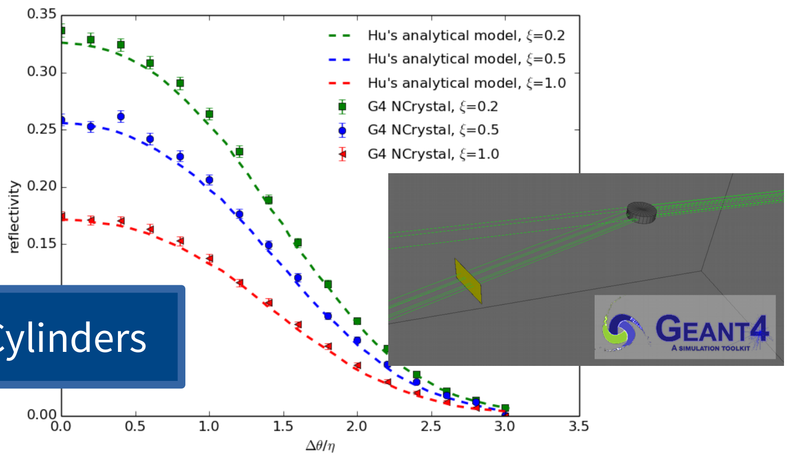
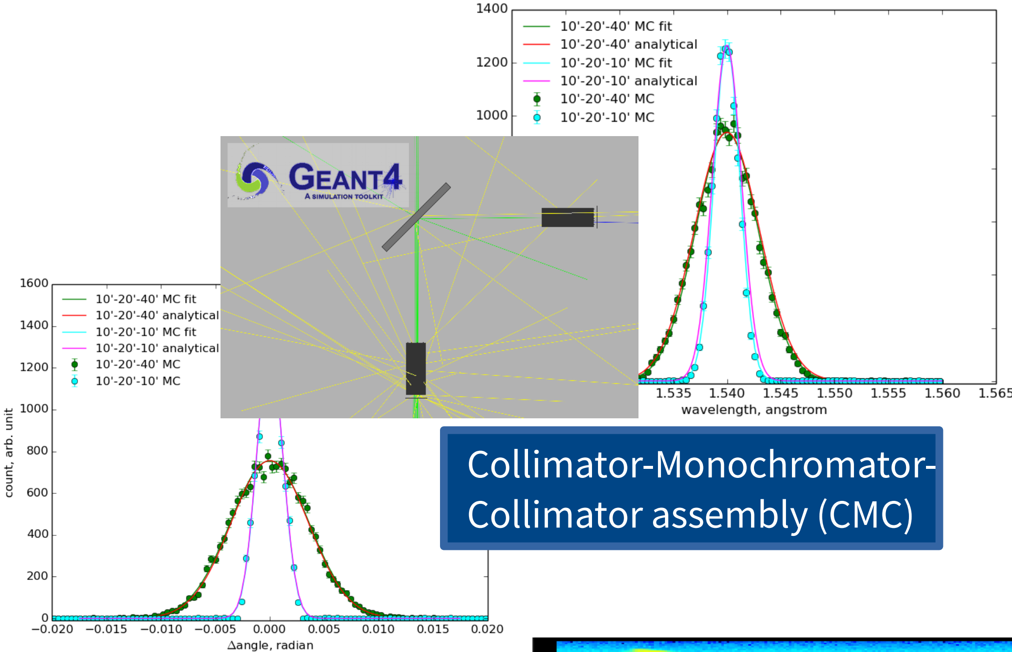
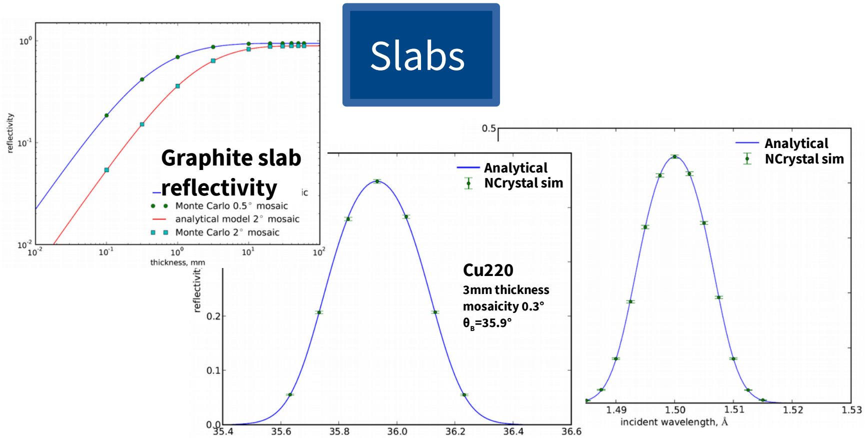


Cylinders

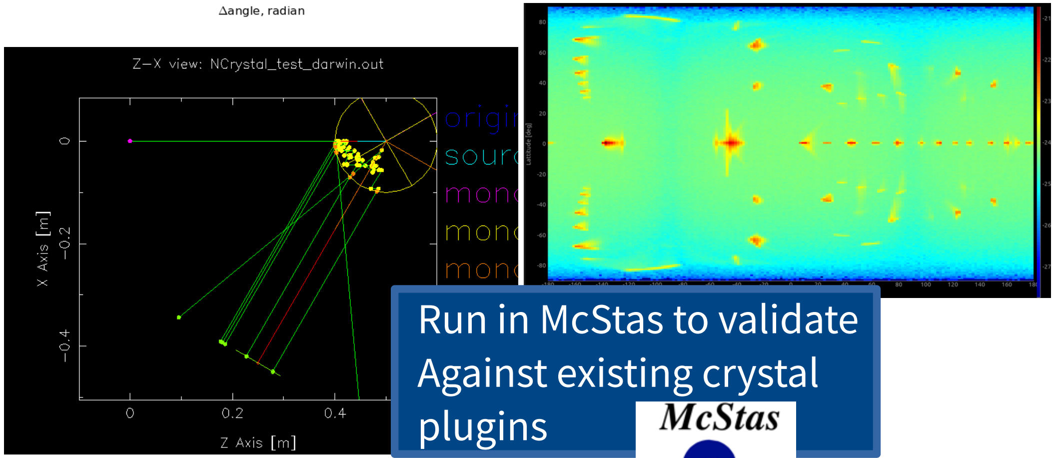


Collimator-Monochromator-Collimator assembly (CMC)

Slabs



Sample monochromator rocking curve and λ dependency



Run in McStas to validate Against existing crystal plugins

McStas

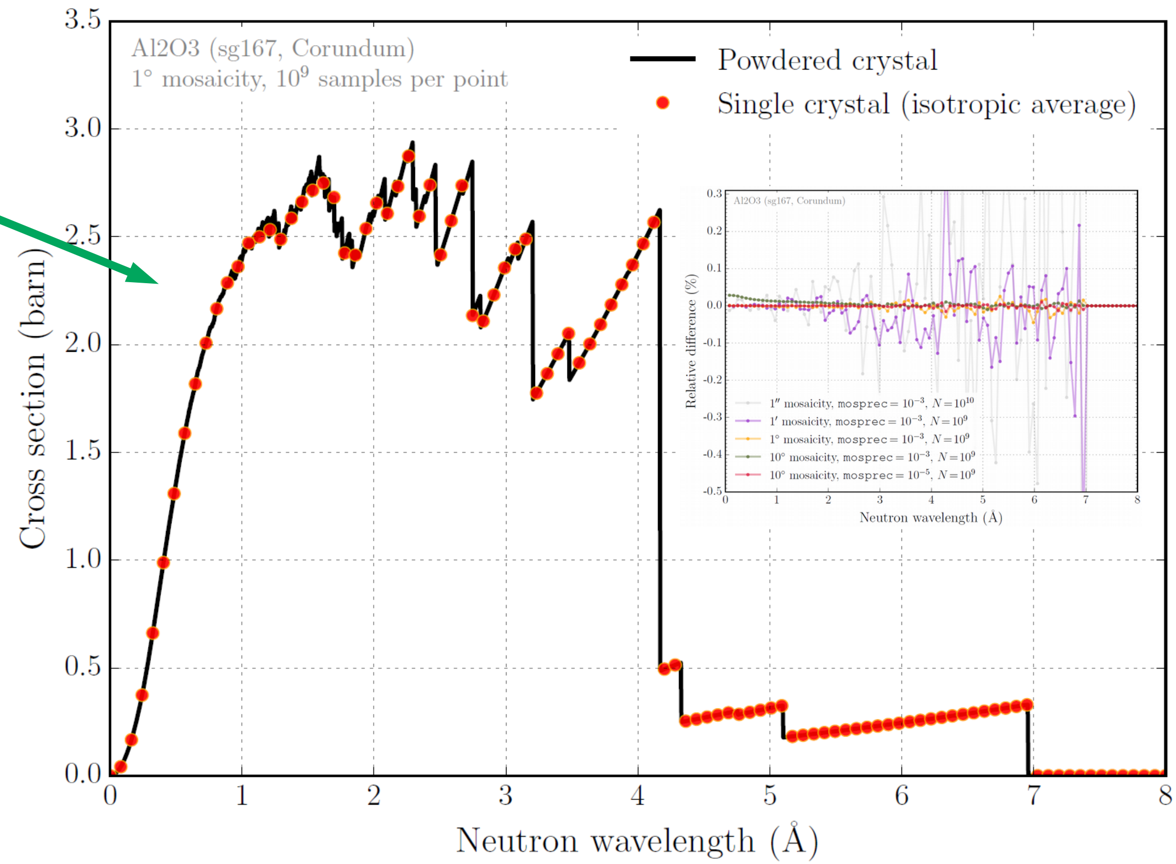
Technical check for consistency of Single Crystals codes

NCrystal

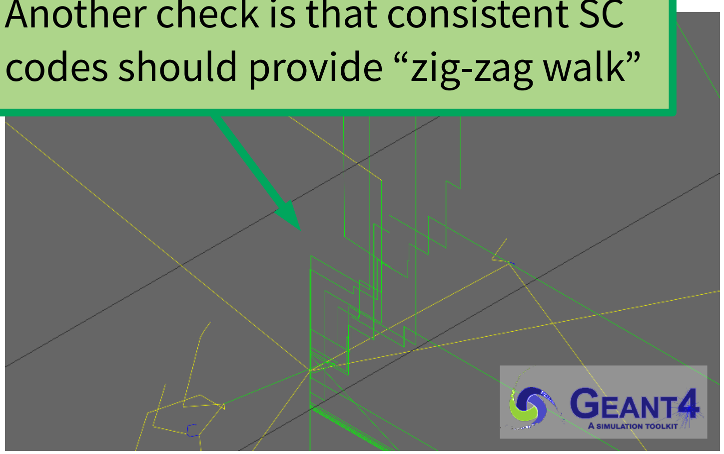
X. X. Cai & T. Kittelmann

In principle an isotropically illuminated single crystal should on average give powder-like cross-sections.

In practice, a lot of edge-cases and details have to be treated correctly in the SC code before this happens!



Another check is that consistent SC codes should provide "zig-zag walk"



Thanks to the DMSC cluster for help with this brute force validation.

Large validation effort

Against measurements, formulas, other codes, …

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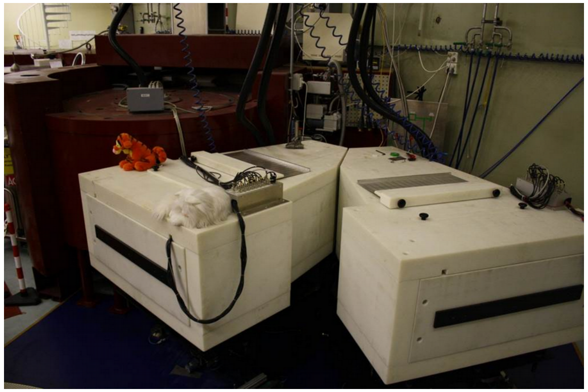
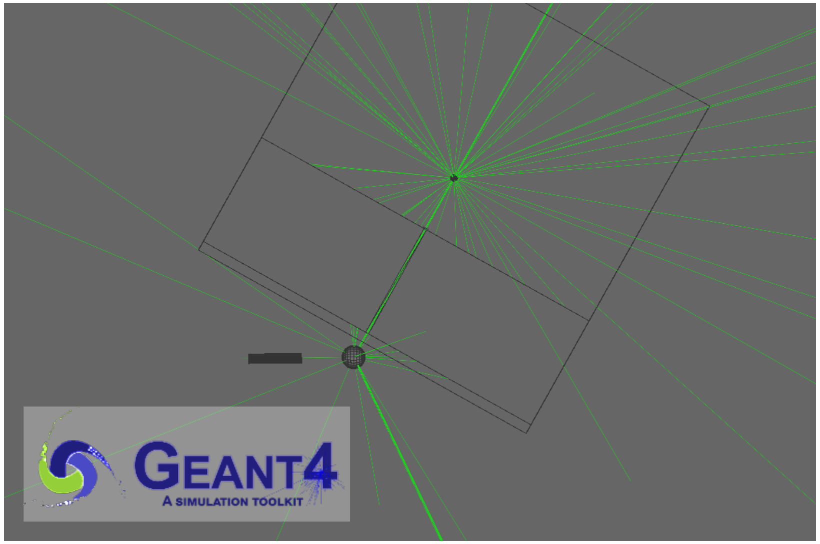
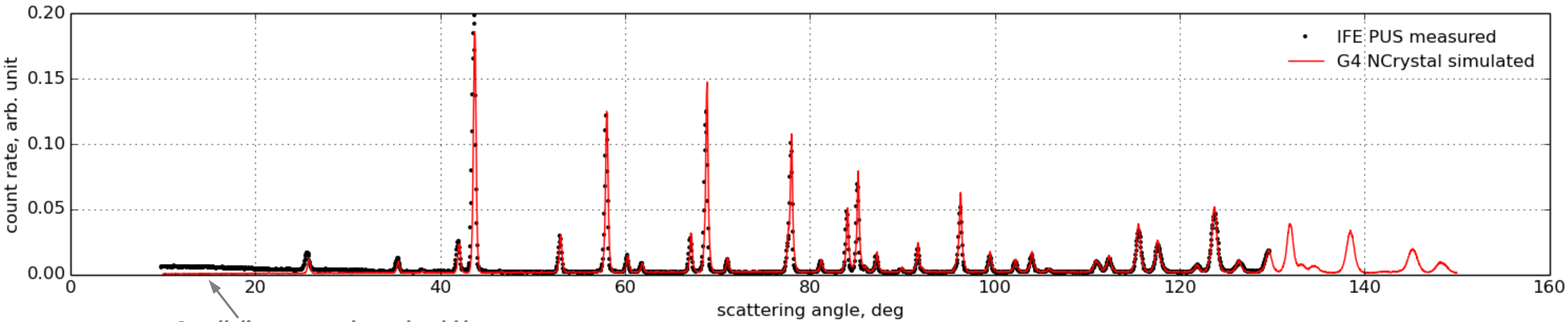
Reproduce powder data, simulating IFE PUS Instrument with collimator, monochromator and powder sample (sapphire).







Small discrepancy here should be improved with inelastic scatter kernel

Outlook and planned work

- **Most urgently: Finish and submit detailed publication (this fall)**
- **Continue work for upstream integration into Geant4, McStas, etc.**
  - Work with (or help) relevant experts
  - Must improve multi-threading support (needed for proper ANTS2+Geant4 integration)
- **Improve modelling of inelastic/incoherent components**
  - Including adding support for scatter kernels
  - But also improve modelling of materials without such extra data.
- **Support "impure" materials: multiphase alloys, dopings, contaminations, enrichments.**
- **Continue to expand data library size and capabilities**
- **Consider various (reasonable) requests:**
  - Support focusing in McStas, d-spacing deviations, asymmetric mosaicities, in-memory data files, ...
- **Expand data library and documentation**

Incomplete (sorry!) list of people who provided useful input, testing, bug reports or other support:
J. I. Márquez Damián, E. Dian, R. Hall-Wilton, K. Kanaki, M. Klausz, E. Klinkby, E.B.Knudsen, A. Morozov, P. Willendrup, …

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under grant agreement 676548