



## McStas sample overview

Presenters: Emmanuel Farhi &  
Peter Willendrup



# Agenda

- General concepts
- ***Most important samples:***
  - (Incoherent scatterer)
  - Powder and Single Crystal SANS
  - Isotropic\_sqw



# Samples

For a **non-thin** sample the probabilities for **absorption**, **transmission** or **scattering** are given by

$$p_A = (1 - e^{-\Sigma_T t})(\Sigma_A / \Sigma_T)$$

$$p_S = (1 - e^{-\Sigma_T t})(\Sigma_S / \Sigma_T)$$

$$p_T = 1 - p_S - p_A = e^{-\Sigma_T t}$$

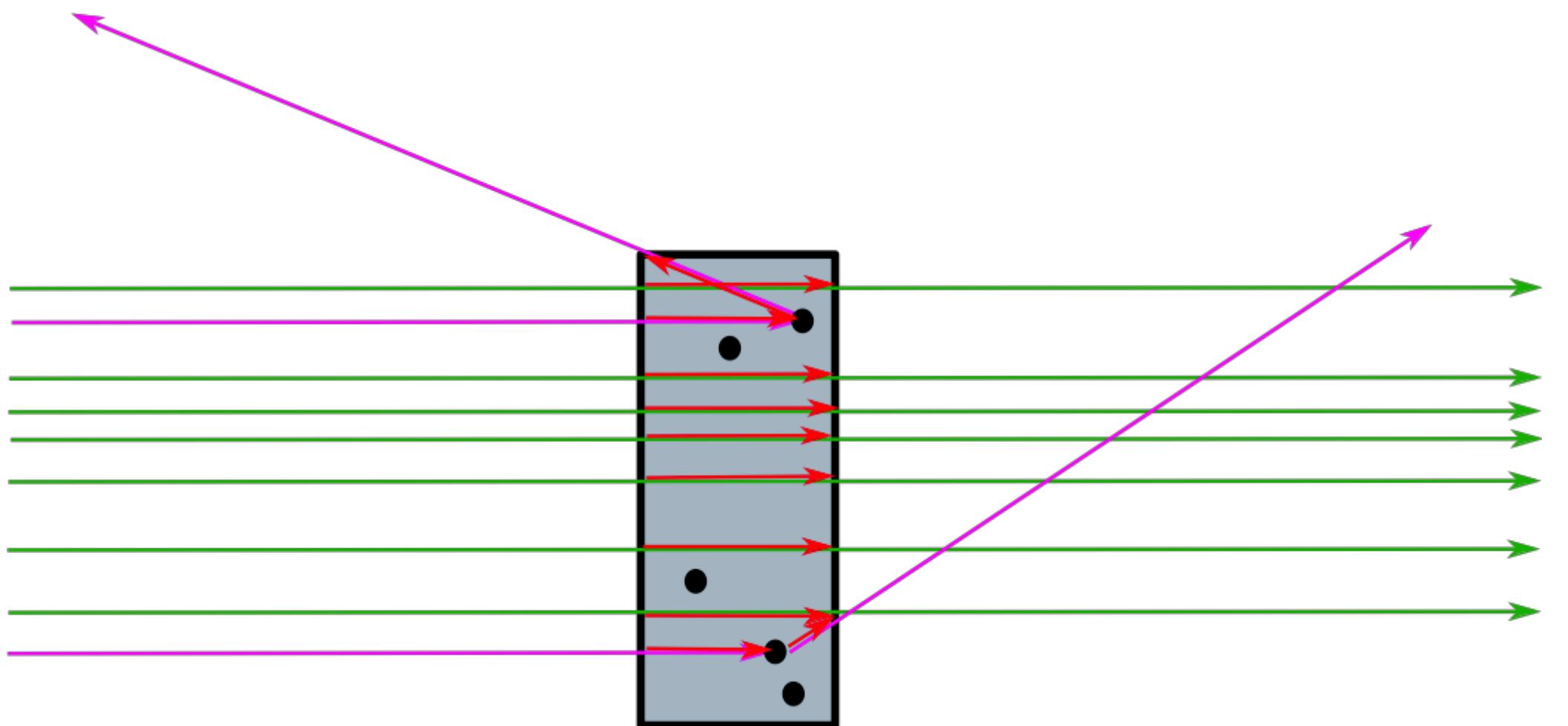
**t** = sample thickness

$$\Sigma_* = \rho \sigma_*$$

macroscopic cross section [cm<sup>-1</sup>]      microscopic cross section [barn/atom]  
 number density [atoms/cm<sup>3</sup>]      1 barn = 10<sup>-24</sup>cm<sup>2</sup>



# Samples in General in McStas

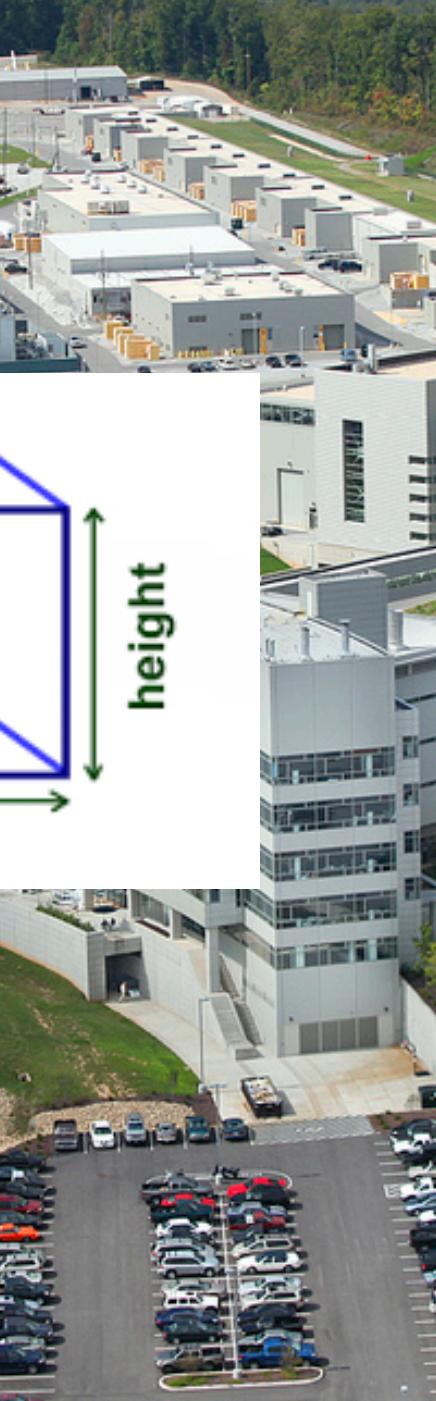
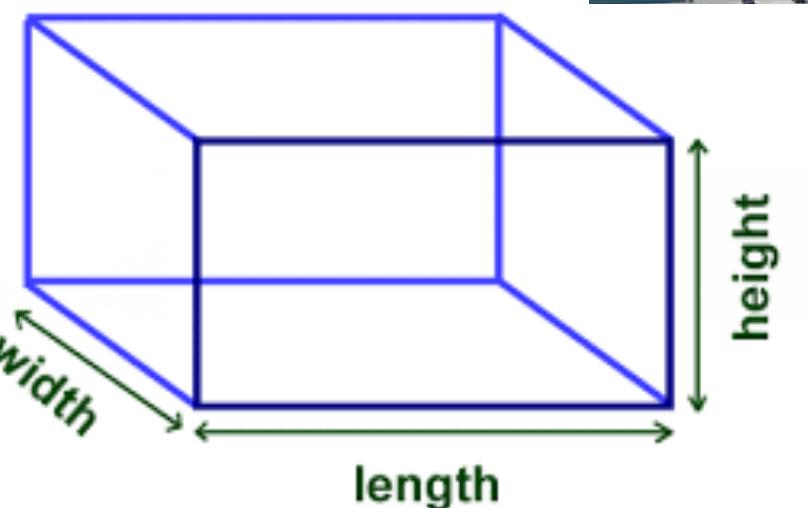
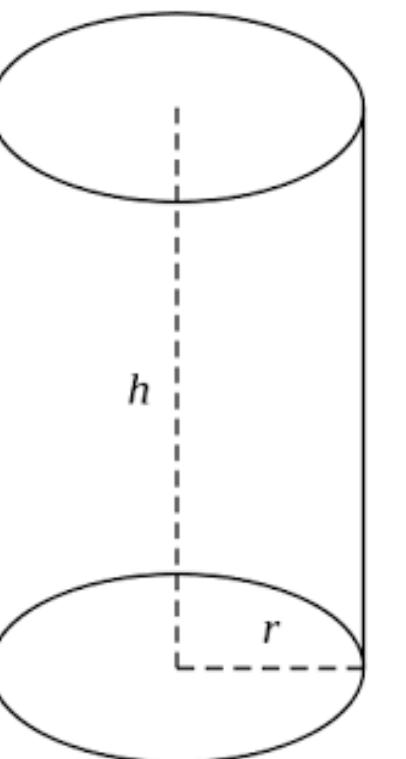
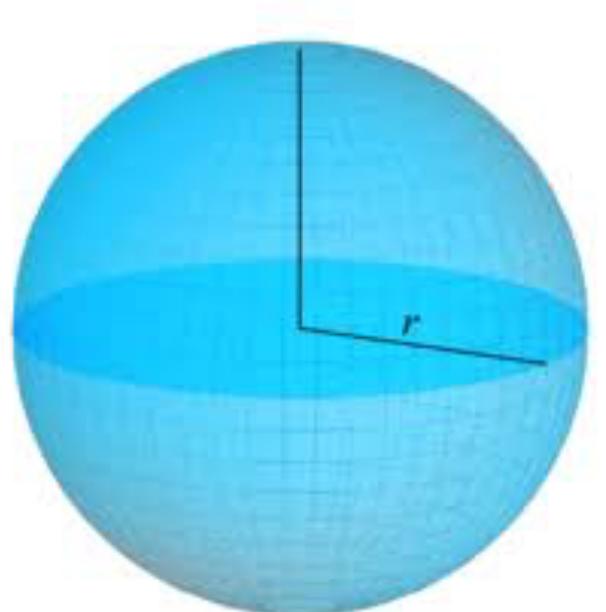


A neutron ray hitting a sample can be:  
**transmitted+absorption**, or **scattered+absorption**



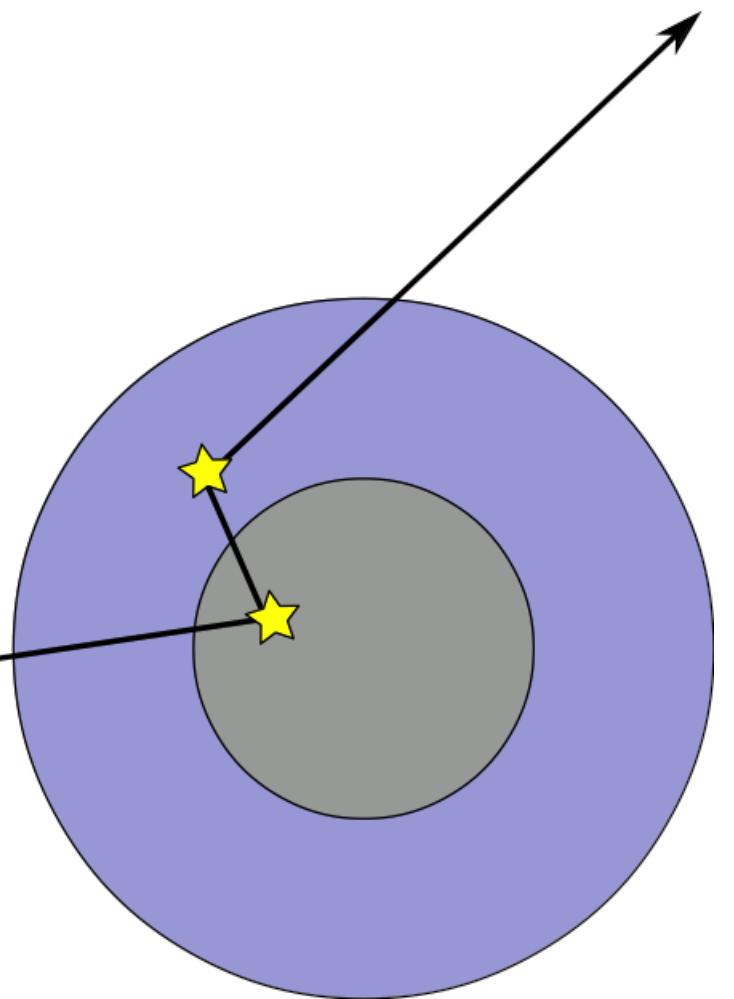
# Sample shapes

## *Simple geometrical shapes*



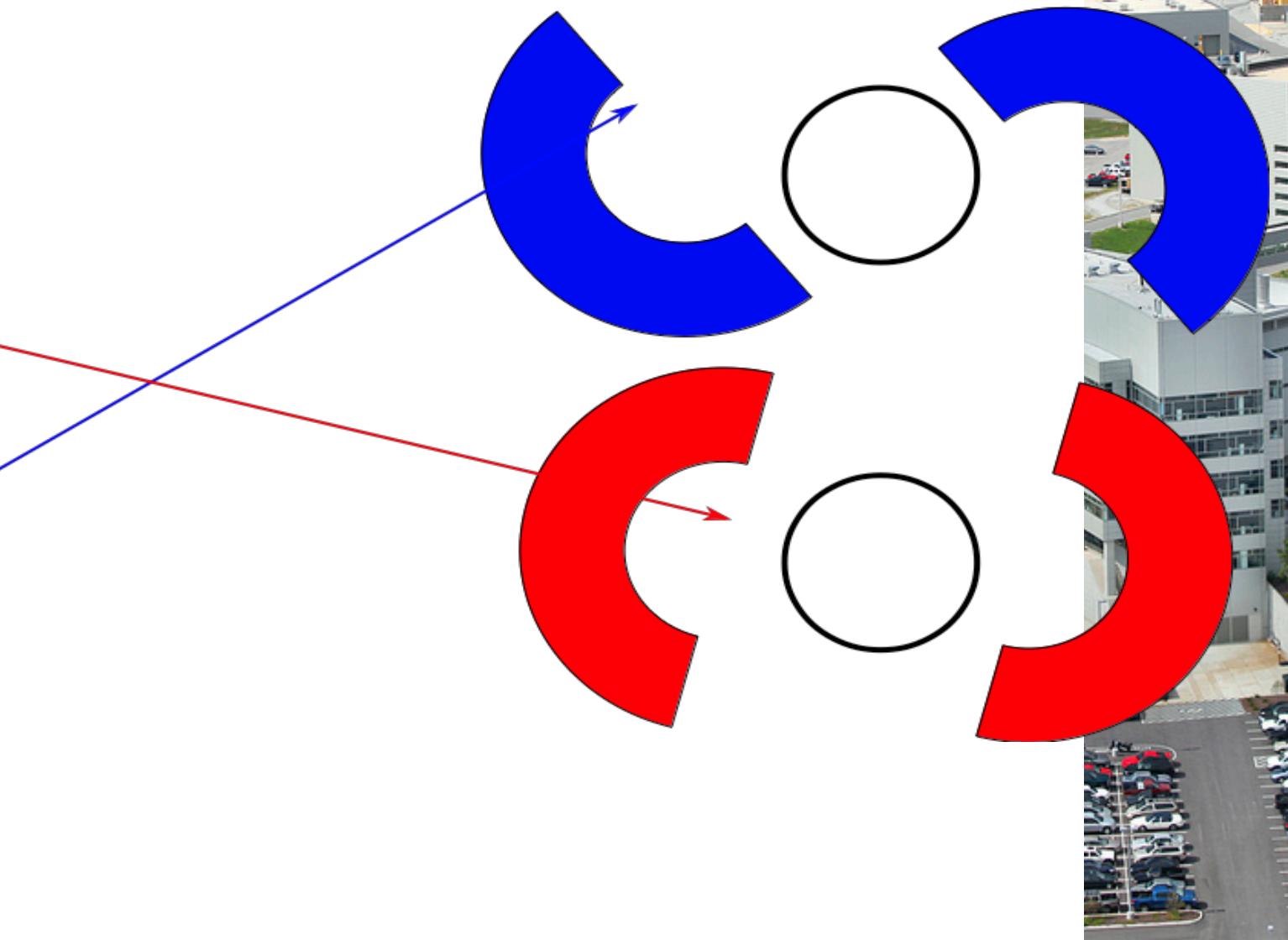
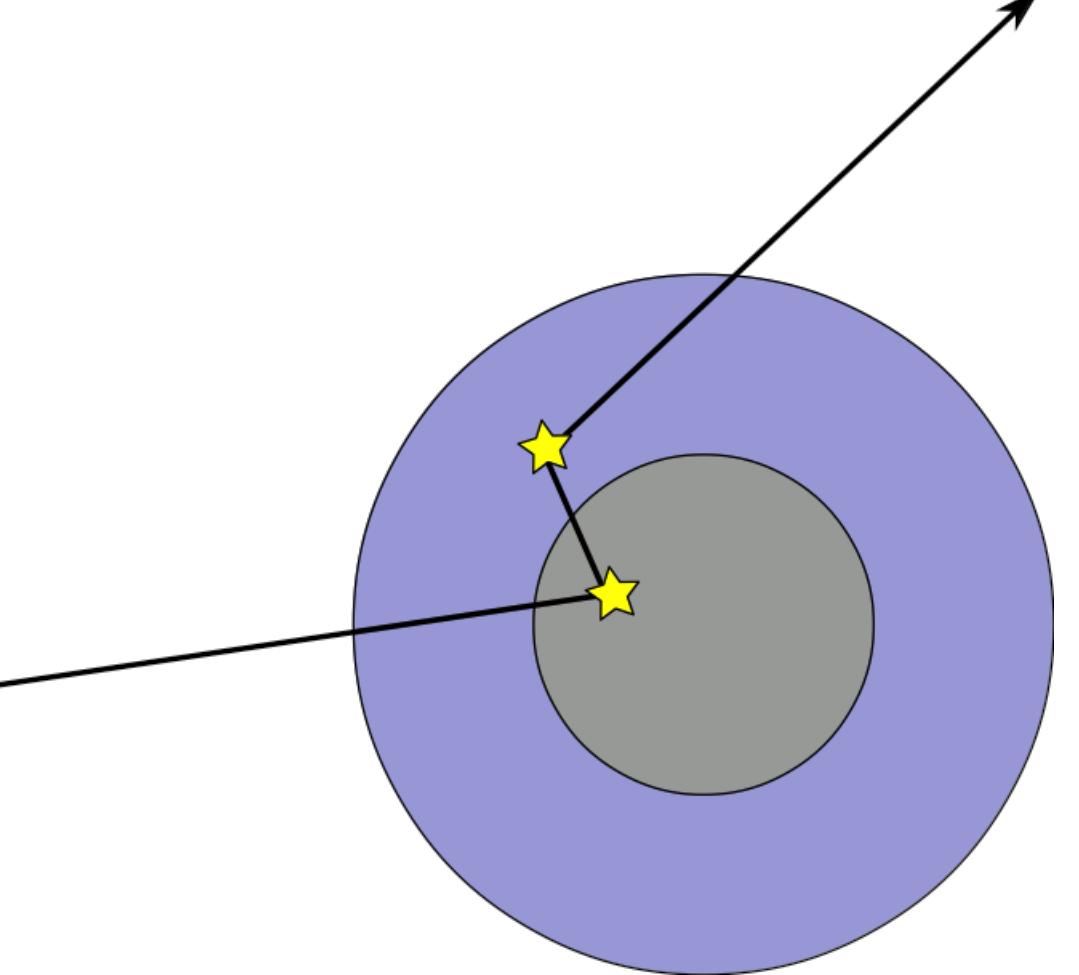
# Sample shapes

*For isotropic materials these can be "concentric",  
i.e. something can be put "inside"*



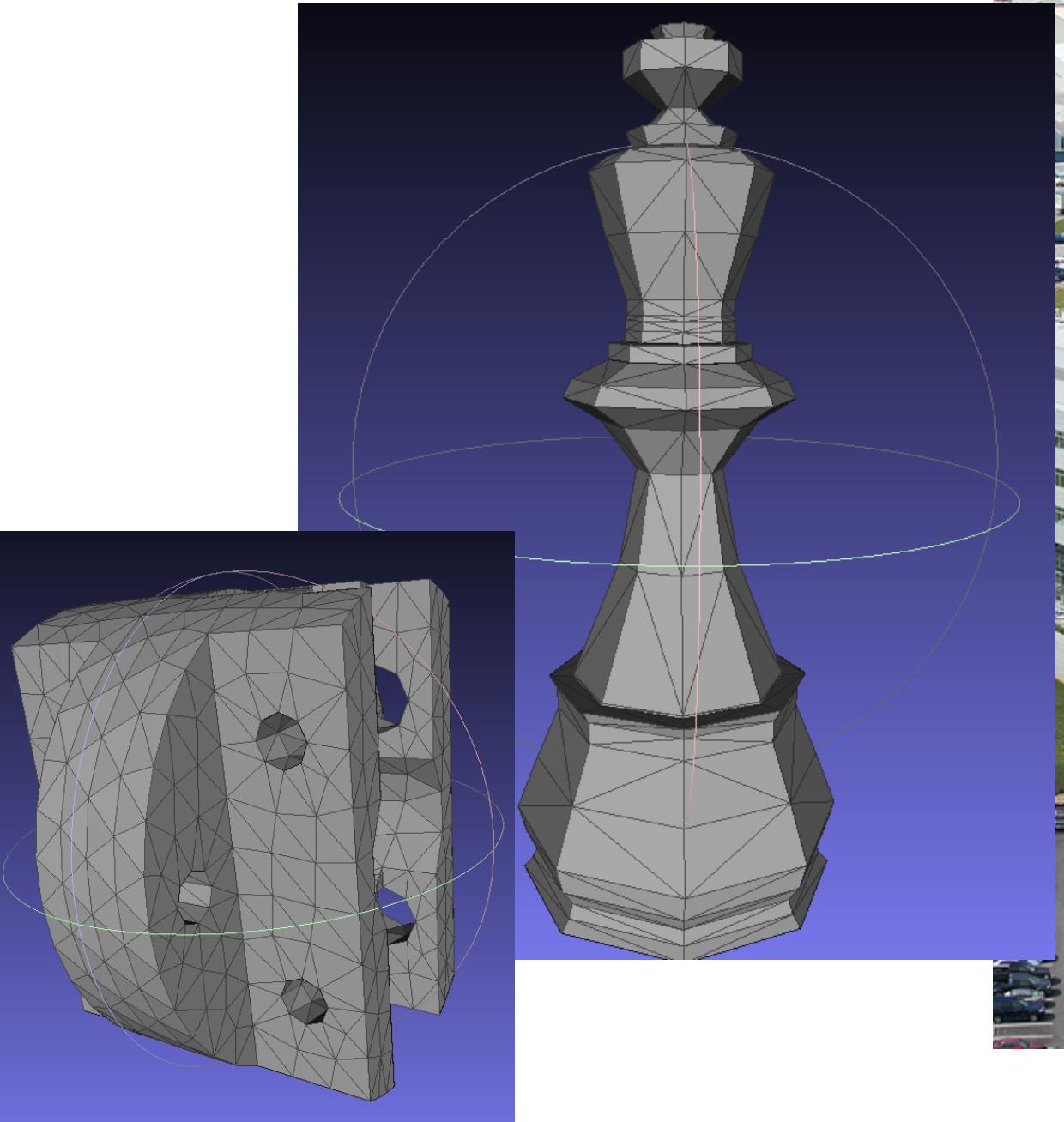
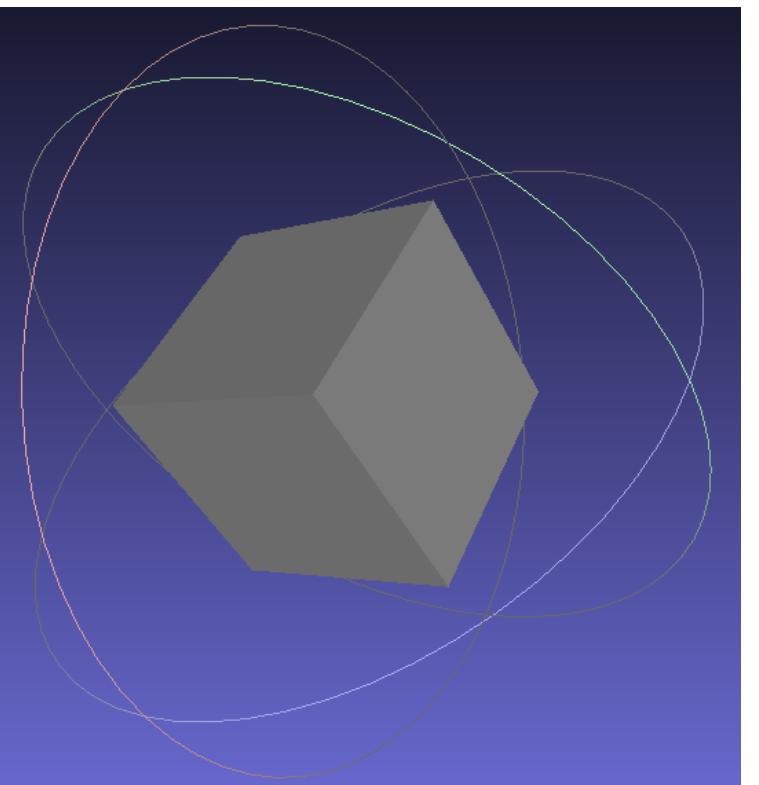
# Sample shapes

*For isotropic materials these can be "concentric", i.e. something can be put "inside"*



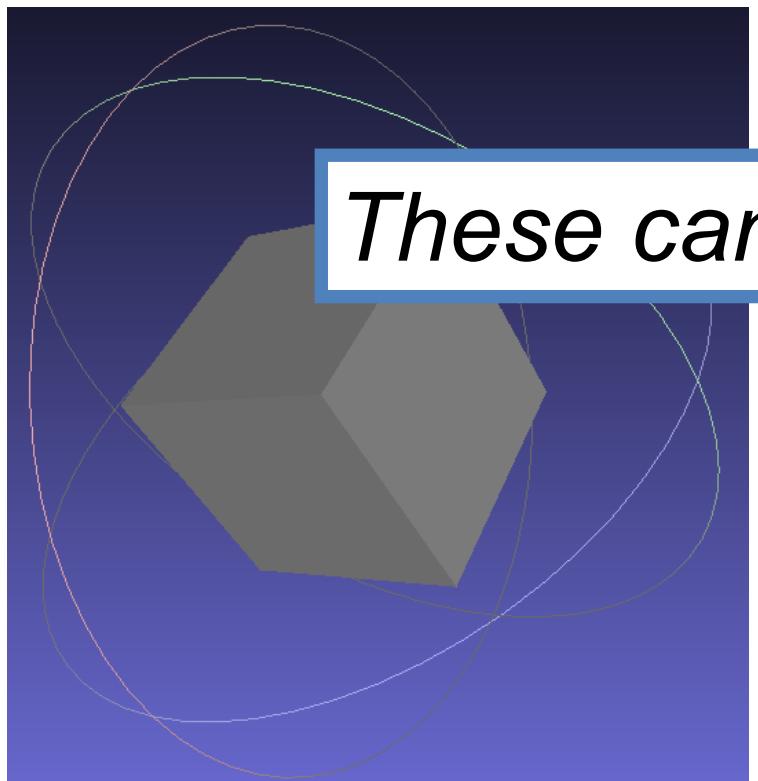
# Isotropic material samples can use OFF/PLY for "any" geometry

An additional complex geometry enables to use any point set to describe the material volume (*geomview* OFF file).

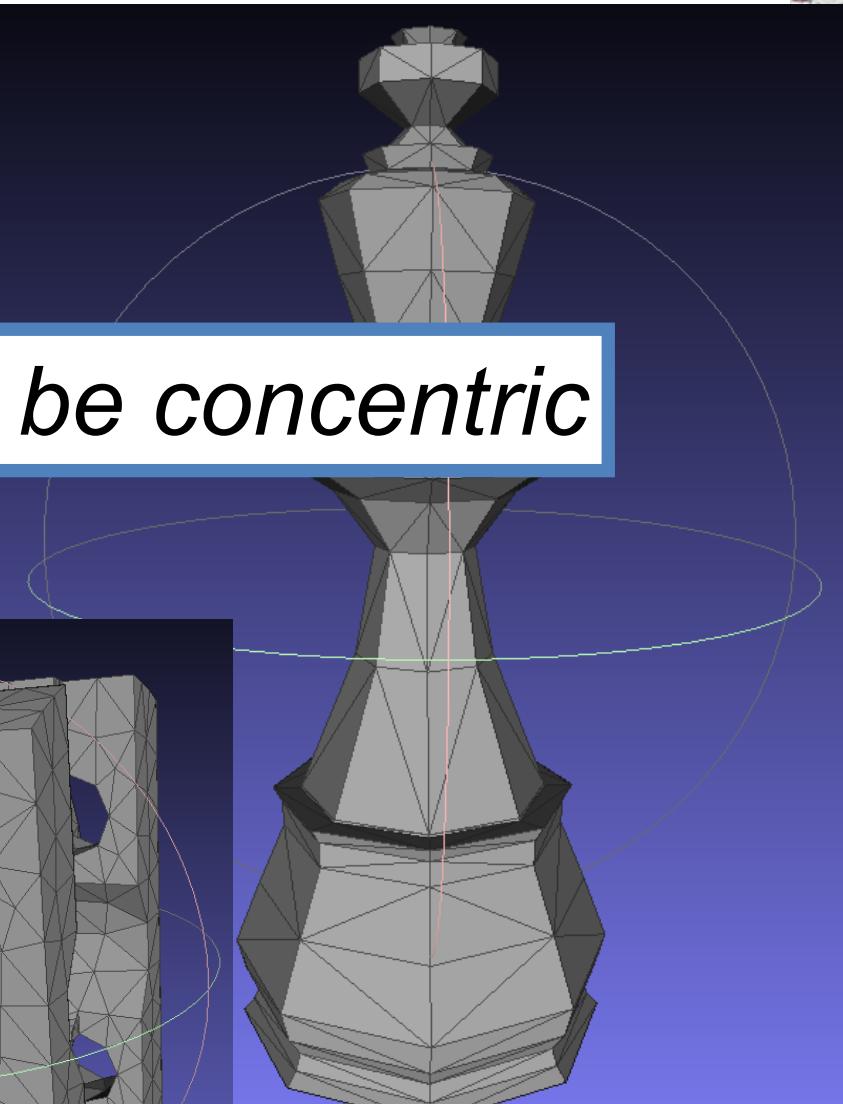
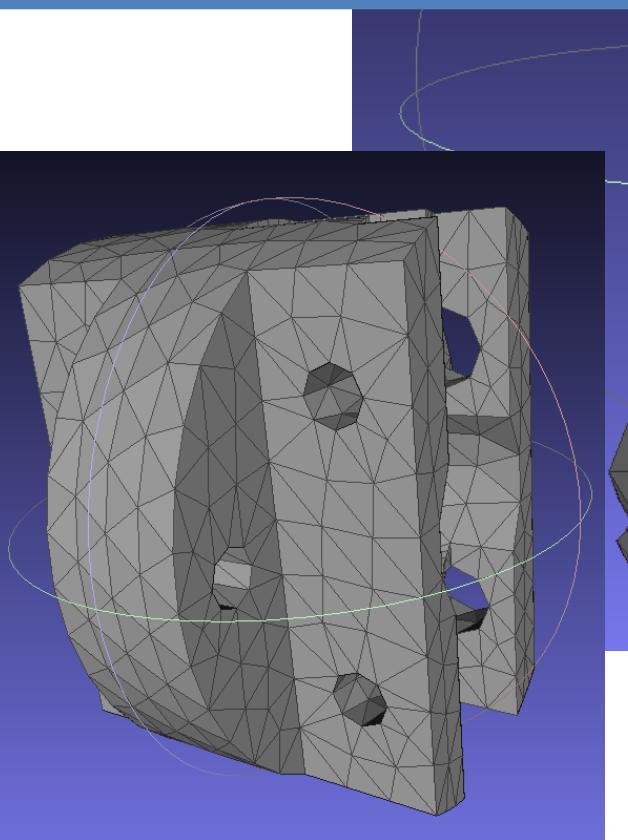


# Isotropic material samples can use OFF/PLY for "any" geometry

An additional complex geometry enables to use any point set to describe the material volume (geomview OFF file).



*These can then NOT be concentric*



# McStas sample overview table

McStas sample model functionality-matrix - McStas - ESS Confluence - Mozilla Firefox

McStas sample mod... | +

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McStas sample model functionality-matrix

Created by Peter Willendrup, last modified on Jun 19, 2018

(Master version available at the URL <https://confluence.esss.lu.se/display/MCSTAS/McStas+sample+model+functionality-matrix>)

Status of the McStas sample components, relevant for McStas 2.4.1 (Released summer 2017)

See also: [McStas sample models for Diffraction](#), [McStas sample models for Imaging](#), [McStas sample models for Large-scale Structures](#), [McStas sample models for Spectroscopy](#)

**SPACE SHORTCUTS**

- Using MCPL as source term in M...
- McStas on the ESS cluster
- How McStas works - in 2 minutes
- McStas-McXtrace developer wiki ...
- Wiki docs for the Python toolset ...

**McStas SPACE**

- Instrument model repositories
- McStas DMSC Wiki
- McStas sample model function...
- Other McStas pages
- Vitess "ESS-survival kit" via mcst...

The content of this macro can only be viewed by users who have logged in.

	McStas sample comp + author info in italic	Model description	Main use areas	Incoherent scattering	Absorption	Bragg or other elastic scattering (type)	Inelastic scattering (type)	Multiple scattering	Non-trivial sample geometry
1	Incoherent (Vanadium, Plexiglass etc.) <i>McStas team</i>	Simple incoherent scatterer	Generic, <a href="#">imaging</a>	✓	✓	✗	✗	✓	✓
2	Tunelling_sample <i>McStas team / Kim Lefmann</i>	Idem 1, plus tunneling peaks and QE broadening	Quasi-elastic scattering, backscattering	✓	✓	✗	✗✓ (Quasielastic broadening + tunnel peaks)	(✓ analytic approach)	✓
3	PowderN <i>McStas team / Peter Willendrup</i>	Debye-scherrer cones, tabular input ( <a href="#">lau</a> / <a href="#">laz</a> )	Powder <a href="#">diffraction</a> , <a href="#">Imaging</a>	✓	✓	✓ (Debye-Scherrer cones)	✗	✗	✓
4	Sample_nxs <i>Mirko Boin, HZB</i>	Debye-scherrer cones, unit-cell / atom input list	Powder <a href="#">diffraction</a> , (future: <a href="#">imaging</a> )	✓	✓	✓ (Debye-Scherrer cones)	✗✓	✓	✗
5	Single_crystal <i>McStas team</i>	Bragg spots, tabular input ( <a href="#">lau</a> ). "Perfect imperfect" single crystal with mosaicity / lattice variation	Single crystal and MX <a href="#">diffraction</a>	✓	✓	✓ (Bragg spots)	✗	✓	✓
6	Sans_spheres (and other similar) <i>McStas team and Martin Cramer Pedersen, KU</i>	Hard spheres in thin solution and other models, defined per-component...	SANS	✓	✓	"✓" - SANS	✗	✗	✗
7	SANS_benchmark2 (and a few other stand-alone models) <i>Heinrich Frielinghaus, FZJ/JCNS</i>	Experimentally-benchmarked model set for SANS	SANS	✓	✓	"✓" - SANS	✗	✓ up to 10 orders	✗
8	SASview_models !yet unreleased! <i>McStas team</i>	"Any" model from SASview / SASmodels	SANS	✓	✓	"✓" - SANS	✗	✗ at this point	✗

# McStas sample table overview

McStas sample model functionality-matrix - McStas - ESS Confluence - Mozilla Firefox

McStas sample mod... + https://confluence.esss.lu.se/display/MCSTAS/McStas+sample+model+functionality-matrix

McStas sample comp + author info in italic	Model description	Main use areas	Incoherent scattering	Absorption	Bragg or other elastic scattering (type)	Inelastic scattering (type)	Multiple scattering	Non-trivial sample geometry
<i>McStas team</i>								
9 <a href="#">Multilayer_sample</a> <i>Rob Dalglish, ISIS STFC</i>	Multilayer-sample (dynamic scattering theory) with incoherent background	Reflectometry	✓	✓	"✓" - Reflectivity curve	✗	✗	✗
10 <a href="#">Phonon_simple</a> <i>McStas team / Kim Lefmann</i>	Single-branch acoustic phonon in FCC lattice	Inelastic scattering phonons	✗	✗	✗	✓ (phonon, at this point FCC lattice only)	✗	✗

16	Below this line not yet available in repo	Below this line not yet available in repo	Below this line not yet available in repo	Below this line not yet available in repo	Below this line not yet available in repo	Below this line not yet available in repo	Below this line not yet available in repo	Below this line not yet available in repo
17	"4D S(\vec{Q}),\omega)" Duc Le - soon at ISIS STFC?	Ala Isotropic_Sqw, but with crystal lattice	Elastic and inelastic experiments with crystals	✓	✓	✓	✓	✓
18	"Polycrystal" <i>Alberto Cereser + Erik Knudsen, DTU Physics</i>	Engineering-diffraction / imaging oriented multigrain sample	Engineering-diffraction / imaging	✓	✓	✓ (Bragg spots)	✗	✓
19	"Magnetic single crystal" <i>Linda Udy KU, + Erik Knudsen, DTU</i>	Bragg spots from lattice ala Single_crystal plus magnetic lattice. Tabular input ( <a href="#">lau</a> )	Single crystal magnetic diffraction	✓	✓	✓ (Bragg spots)	✗	✓ / ?✓?
20	"Reflectometry sample" <i>Jochen Stahn, PSI</i>	Reflectivity-curve sample	Reflectometry	✓	✓	"✓" - Reflectivity curve	✗	✗

But since it is impossible to read this table – here's where it's at:

<https://confluence.esss.lu.se/display/MCSTAS/McStas+sample+model+functionality-matrix>

... or take a look in the Dropbox for at PDF-version.

# Samples – elastic, structure

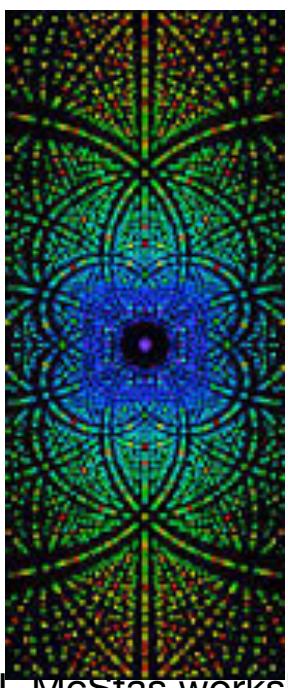


- ★ ( *Incoherent.comp*: Incoherent scattering (and absorption) )
- ★ *PowderN.comp* : Elastic Bragg scattering from an ideal powder
- ★ *Single\_crystal.comp* : Bragg scattering from single crystals
- ★ Small Angle Scattering

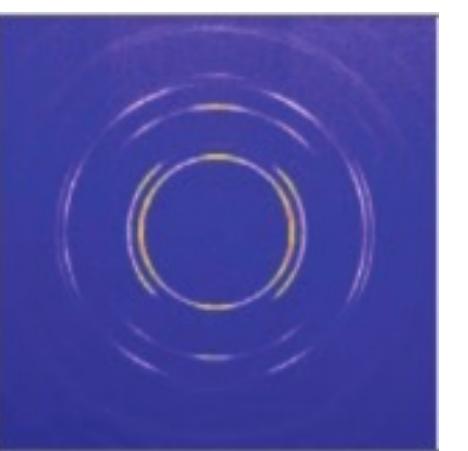
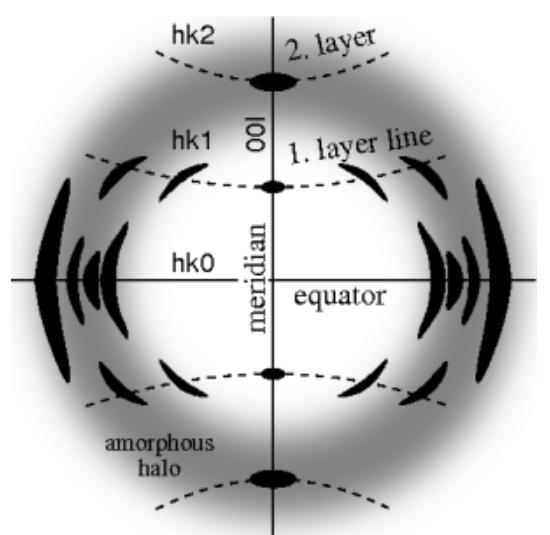


# From single crystal / crystallites to powder....

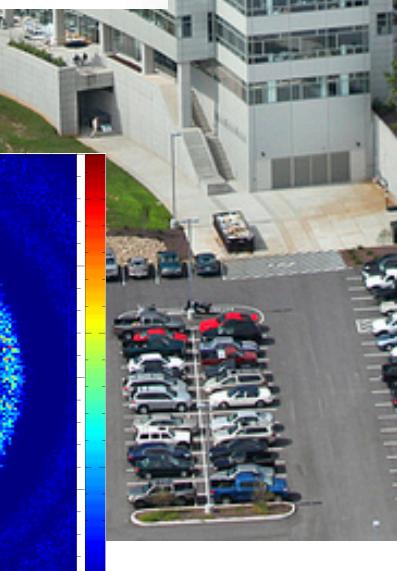
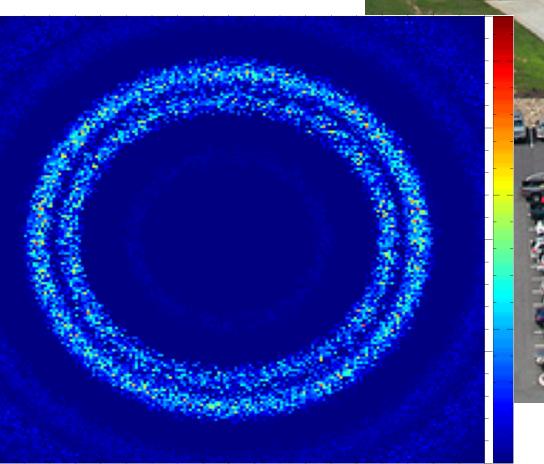
Single crystal



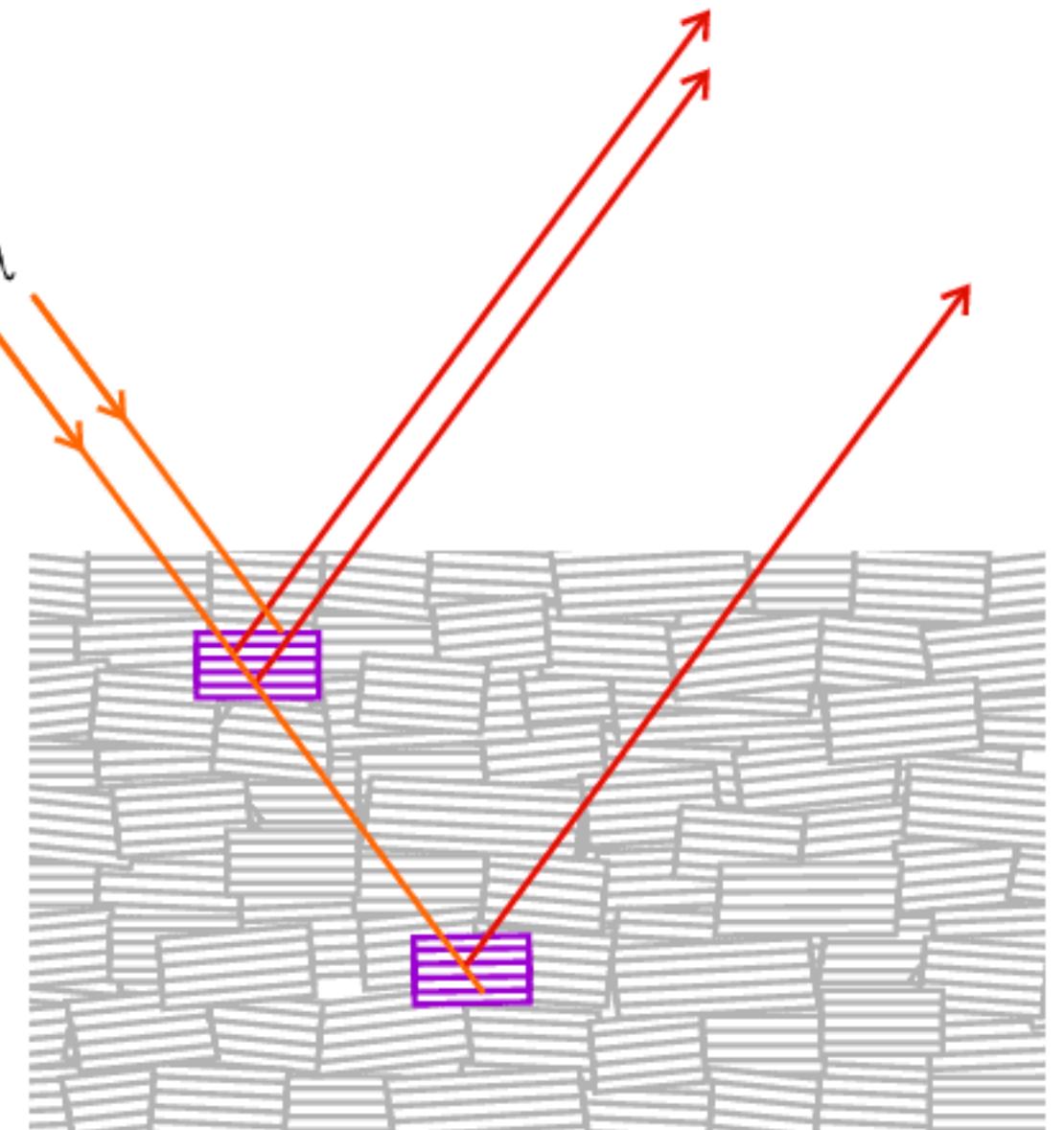
Polycrystal with a little disorder,  
i.e. a *preferred orientation, texture*



Powder with complete disorder



# Single Crystal model



- Models *ideally imperfect crystal*:
- Peak broadening is dominated by mosaic => not appropriate for highly perfect crystals.
- “Space group symmetries” considered out of scope.
  - Optimized for small unit cells but...
  - No assumption about unit cell, orientation etc.
  - Gaussian model for mosaic (see later)



Courtesy University College London

# Single Crystal



## Input parameters

Parameters in **boldface** are required; the others are optional.

Name	Unit	Description
mosaic_AB	arc_minutes, arc_minutes,1, 1, 1, 1, 1, 1	In Plane mosaic rotation and plane vectors (anisotropic), mosaic_A, mosaic_B, A_h,A_k,A_l, B_h,B_k,B_l. Puts the crystal in the in-plane mosaic state. Vectors A and B define plane in which the crystal roation is defined, and mosaic denotes the resp. mosaicities (gaussian RMS) with respect to the two reflections chosen by A and B (Miller indices).
reflections	string	File name containing structure factors of reflections. Use empty ("") or NULL for incoherent scattering only
geometry	str	Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust
xwidth	m	Width of crystal
yheight	m	Height of crystal
zdepth	no extinction simulated	[m] Depth of crystal
radius	m	Outer radius of sample in (x,z) plane
delta_d_d	1	Lattice spacing variance, gaussian RMS
mosaic	arc minutes	Crystal mosaic (isotropic), gaussian RMS. Puts the crystal in the isotropic mosaic model state, thus disregarding other mosaicity parameters.
mosaic_a	arc minutes	Horizontal (rotation around lattice vector a) mosaic (anisotropic), gaussian RMS. Put the crystal in the anisotropic crystal vector state. I.e. model mosaicity through rotation around the crystal lattice vectors. Has precedence over in-plane mosaic.
mosaic_b	arc minutes	Vertical (rotation around lattice vector b) mosaic (anisotropic), gaussian RMS.
mosaic_c	arc minutes	Out-of-plane (Rotation around lattice vector c) mosaic (anisotropic), gaussian RMS
recip_cell	1	Choice of direct/reciprocal (0/1) unit cell definition
barns	1	Flag to indicate if $ F ^2$ from 'reflections' is in barns or fm <sup>2</sup> . barns=1 for laz and isotropic constant elastic scattering (reflections=NULL), barns=0 for lau type files
ax	AA or AA <sup>-1</sup>	Coordinates of first (direct/recip) unit cell vector
ay		
az		
bx	AA or AA <sup>-1</sup>	Coordinates of second (direct/recip) unit cell vector
by		
bz		
cx	AA or AA <sup>-1</sup>	Coordinates of third (direct/recip) unit cell vector
cy		
cz		
p_transmit	1	Monte Carlo probability for neutrons to be transmitted without any scattering. Used to improve statistics from weak reflections
sigma_abs	barns	Absorption cross-section per unit cell at 2200 m/s
sigma_inc	barns	Incoherent scattering cross-section per unit cell Use -1 to unactivate
aa	deg	Unit cell angles alpha, beta and gamma. Then uses norms of vectors a,b and c as lattice parameters
bb	deg	Beta angle
cc	deg	Gamma angle
order	0: all, 1: first, 2: second, ...	[1] Limit multiple scattering up to given order
RX	m	Radius of horizontal along X lattice curvature. flat for 0
RY	m	Radius of vertical lattice curvature. flat for 0
RZ	m	Radius of horizontal along Z lattice curvature. flat for 0
powder	1	Flag to indicate powder mode, for simulation of Debye-Scherrer cones via random crystallite orientation. A powder texture can be approximated with 0
PG	1	Flag to indicate "Pyrolytic Graphite" mode, only meaningful with choice of Graphite.lau, models PG crystal. A powder texture can be approximated with 0

# Single Crystal



## Input parameters

Parameters in **boldface** are required; the others are optional.

Name	Unit	Description
mosaic_AB	arc_minutes, arc_minutes, 1, 1, 1, 1, 1, 1	In Plane mosaic rotation and plane vectors (anisotropic), mosaic_A, mosaic_B, A_h,A_k,A_l, B_h,B_k,B_l. Puts the crystal in the in-plane mosaic state. Vectors A and B define plane in which the crystal roation is defined, and mosaic denotes the resp. mosaicities (gaussian RMS) with respect to the two reflections chosen by A and B (Miller indices).
reflections	string	File name containing structure factors of reflections. Use empty ("") or NULL for incoherent scattering only
geometry	str	Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust
xwidth	m	Width of crystal
yheight	m	Height of crystal
zdepth	no extinction simulated	[m] Depth of crystal
radius	m	Outer radius of sample in (x,z) plane
delta_d_d	1	Lattice spacing variance, gaussian RMS
mosaic	arc minutes	Crystal mosaic (isotropic), gaussian RMS. Puts the crystal in the isotropic mosaic model state, thus disregarding other mosaicity parameters.
mosaic_a	arc minutes	Horizontal (rotation around lattice vector a) mosaic (anisotropic), gaussian RMS. Put the crystal in the anisotropic crystal vector state. I.e. model mosaicity through rotation around the crystal lattice vectors. Has precedence over in-plane mosaic.
mosaic_b	arc minutes	Vertical (rotation around lattice vector b) mosaic (anisotropic), gaussian RMS.
mosaic_c	arc minutes	Out-of-plane (Rotation around lattice vector c) mosaic (anisotropic), gaussian RMS
recip_cell	1	Choice of direct/reciprocal (0/1) unit cell definition
barns	1	Flag to indicate if $ F ^2$ from 'reflections' is in barns or fm <sup>2</sup> . barns=1 for laz and isotropic constant elastic scattering (reflections=NULL), barns=0 for lau type files
ax	AA or AA <sup>-1</sup>	
ay		
az		
bx	AA or AA <sup>-1</sup>	
by		
bz		
cx	AA or AA <sup>-1</sup>	
cy		
cz		
p_transm	1	
sigma_pos	barns	
sigma_inc	barns	Incoherent scattering cross-section per unit cell Use -1 to unactivate
aa	deg	Unit cell angles alpha, beta and gamma. Then uses norms of vectors a,b and c as lattice parameters
bb	deg	Beta angle
cc	deg	Gamma angle
order	0: all, 1: first, 2: second, ...	[1] Limit multiple scattering up to given order
RX	m	Radius of horizontal along X lattice curvature. flat for 0
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RZ	m	Radius of horizontal along Z lattice curvature. flat for 0
powder	1	Flag to indicate powder mode, for simulation of Debye-Scherrer cones via random crystallite orientation. A powder texture can be approximated with 0
PG	1	Flag to indicate "Pyrolytic Graphite" mode, only meaningful with choice of Graphite.lau, models PG crystal. A powder texture can be approximated with 0

Unit cell vectors (ax,ay,az, bx, by,bz, cx,cy, cz).  
 Encodes the crystal orientation relative to the  
 Component's orientation



# Single Crystal

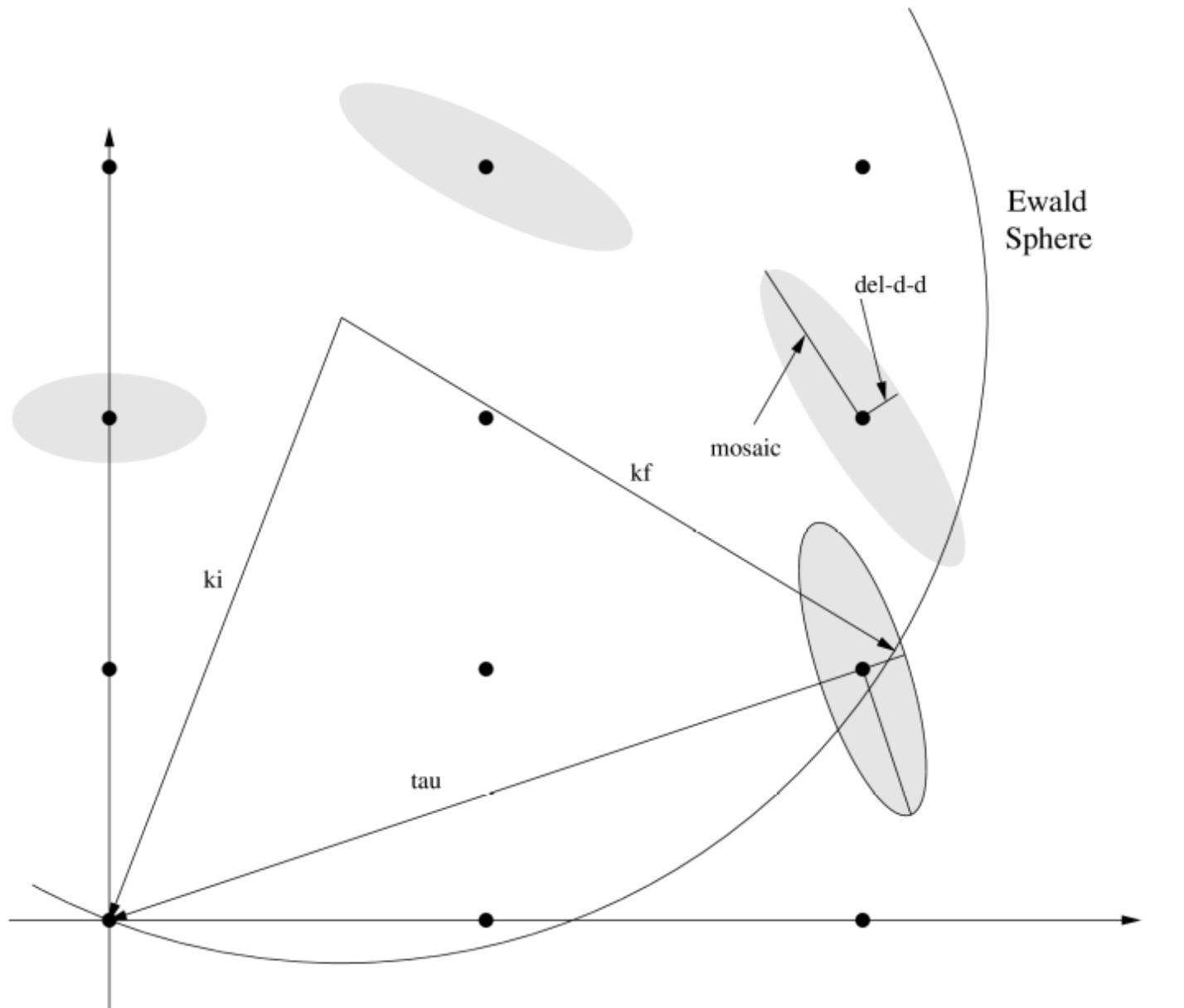
## Input parameters

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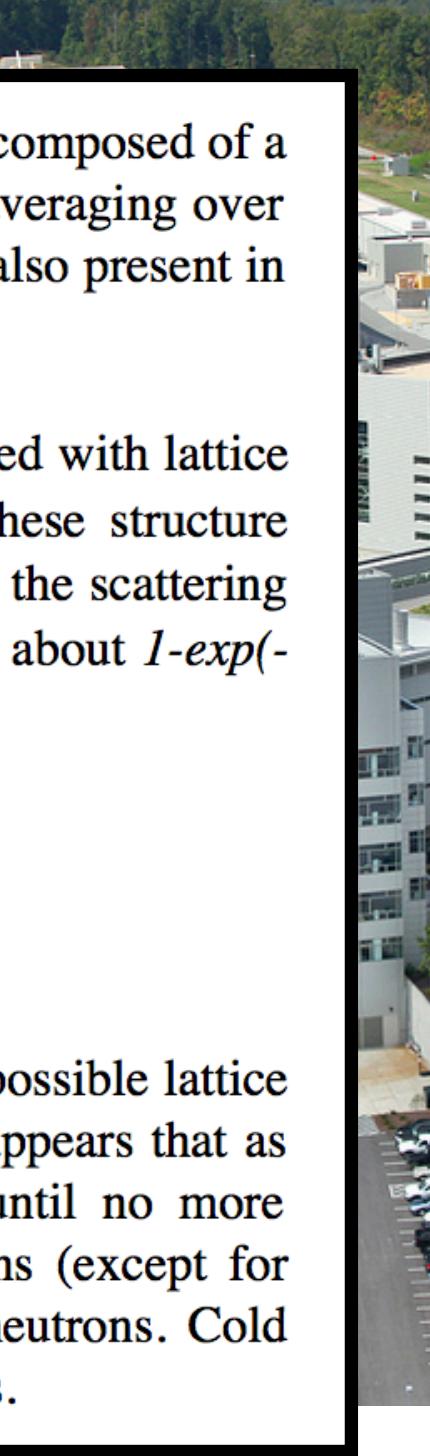
Name	Unit	Description
mosaic_AB	arc_minutes, arc_minutes,1, 1, 1, 1	In Plane mosaic rotation and plane vectors (anisotropic), mosaic_A, mosaic_B, A_h,A_k,A_l, B_h,B_k,B_l. Puts the crystal in the in-plane mosaic state. Vectors A and B define plane in which the crystal roation is defined, and mosaic_A, m
reflections	string	File name containing structure factors of reflections. Use empty ("") or NULL for incoherent scattering only
geometry	str	Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust
xwidth	m	Width of crystal
yheight	m	
zdepth	no extinction simulated	
radius	m	
area_d	1	
mosaic	arc minutes	
mosaic_a	arc minutes	
mosaic_b	arc minutes	
mosaic_c	arc minutes	
recip_cell	1	
barns	1	
rx	AA or AA^-1	
ay		
az		
bx	AA or AA^-1	Coordinates of second (direct/recip) unit cell vector
by		
bz		
cx	AA or AA^-1	Coordinates of third (direct/recip) unit cell vector
cy		
cz		
p_transmit	1	Monte Carlo probability for neutrons to be transmitted without any scattering. Used to improve statistics from weak reflections
sigma_abs	barns	Absorption cross-section per unit cell at 2200 m/s
sigma_inc	barns	Incoherent scattering cross-section per unit cell Use -1 to unactivate
aa	deg	Unit cell angles alpha, beta and gamma. Then uses norms of vectors a,b and c as lattice parameters
bb	deg	Beta angle
cc	deg	Gamma angle
order	0: all, 1: first, 2: second, ...	[1] Limit multiple scattering up to given order
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PG	1	Flag to indicate "Pyrolytic Graphite" mode, only meaningful with choice of Graphite.lau, models PG crystal. A powder texture can be approximated with 0

Mosaicity parameters: mosaic, mosaic\_a, mosaic\_b, mosaic\_c, mosaic\_AB

# Single Crystal mosaicity



## 9.2 PowderN



Among the most common materials measured with neutron scattering techniques are powders, which are composed of a large number of tiny single crystals. The scattering intensity, by means of constructive interference and averaging over all crystallites, appears as well defined rings around the out-going direct beam direction. These rings are also present in liquids, but are much smoother, as we shall see in next section.

Let us consider a material of density  $\rho$  made of  $N$  scattering units each with a unit cell volume  $V_0$  arranged with lattice spacings  $d_Q=2\pi/Q$  associated to structure factors  $F(Q)$  with equivalent reflection multiplicities  $j_Q$ . These structure factors characterize the efficiency of the reflection with momentum exchange  $Q$ . Following Squires [14] the scattering probability for an incoming neutron with wavelength  $\lambda$  penetrating along a distance  $x$  into the material is about  $1-\exp(-\rho\sigma_{cone}x)$  where  $\sigma_{cone}$  is the so-called coherent elastic cross-section of the ring,

$$\sigma_{cone} = \frac{N \pi \lambda^2 j_Q |F(Q)|^2}{V_0 Q} .$$

This relation is only valid under certain conditions, among which  $d_Q > 1/2$ , from the Bragg law. As the possible lattice spacings  $d$  in the material can not exceed a maximum value (for instance the inter-atomic distance), it appears that as the neutron wavelength increases, the number of visible rings in the diffractogram will decrease, until no more scattering is possible above the so-called *Bragg edge*, where materials become transparent to neutrons (except for absorption and incoherent scattering). This is why most of the diffractometers use thermal and hot neutrons. Cold neutrons can only scatter on large distance arrangements in materials, *e.g.* in larger molecules and proteins.

# PowderN inputs

## Input parameters

Parameters in **boldface** are required; the others are optional.

Name	Unit	Description	Default
format	no quotes	Name of the format, or list of column indexes (see Description).	Undefined
reflections			"NULL"
geometry	str	Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust	"NULL"
radius	m	Outer radius of sample in (x,z) plane	0
yheight	m	Height of sample y direction	0
xwidth	m	Horiz. dimension of sample, as a width	0
zdepth	m	Depth of box sample	0
thickness			0
pack	1	Packing factor	1
Vc	AA^3	Volume of unit cell=nb atoms per cell/density of atoms	0
sigma_abs	barns	Absorption cross section per unit cell at 2200 m/s. Use a negative value to unactivate it	0
sigma_inc	barns	Incoherent cross section per unit cell. Use a negative value to unactivate it	0
delta_d_d	0/1	Global relative delta_d/d broadening when the 'w' column is not available. Use 0 if ideal.	0
p_inc	1	Fraction of incoherently scattered neutron rays	0.1
p_transmit	1	Fraction of transmitted (only attenuated) neutron rays	0.1
DW	1	Global Debye-Waller factor when the 'DW' column is not available. Use 1 if included in F2	0
nb_atoms	1	Number of sub-unit per unit cell, that is ratio of sigma for chemical formula to sigma per unit cell	1
d_phi	deg	Angle corresponding to the vertical angular range to focus to, e.g. detector height. 0 for no focusing	0
p_interact	1	Fraction of events interacting with sample, e.g. 1-p_transmit-p_inc	0
concentric	only for box, cylinder, sphere	[1] Indicate that this component has a hollow geometry and may contain other components. It should then be duplicated after the inside part	0
density	g/cm^3	Density of material. rho=density/weight/1e24*N_A.	0
weight	g/mol	Atomic/molecular weight of material	0
barns	1	Flag to indicate if  F ^2 from 'reflections' is in barns or fm^2 (barns=1 for laz, barns=0 for lau type files).	1
Strain	ppm	Global relative delta_d/d shift when the 'Strain' column is not available. Use 0 if ideal.	0
focus_flip	1	Controls the sense of d_phi. If 0 d_phi is measured against the xz-plane. If !=0 d_phi is measured against zy-plane.	0



# PowderN inputs

## Input parameters

Parameters in **boldface** are required; the others are optional.

Name	Unit	Description	Default
format	no quotes	Name of the format, or list of column indexes (see Description).	Undefined
reflections			"NULL"
geometry	str	Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust	"NULL"
radius	m	Outer radius of sample in (x,z) plane	0
yheight	m	Height of sample y direction	0
xwidth	m	Horiz. dimension of sample, as a width	0
zdepth	m	Depth of box sample	0
thickness			0
pack	1	Packing factor	1
Vc	AA^3	Volume of unit cell=nb atoms per cell/density of atoms	0
sigma_abs	barns		0
sigma_inc	barns		0
delta_u_d	0/1		0
p_inc	1	Fraction of incoherently scattered neutron rays	0.1
p_transmit	1	Fraction of transmitted (only attenuated) neutron rays	0.1
DW	1	Global Debye-Waller factor when the 'DW' column is not available. Use 1 if included in F2	0
nb_atoms	1	Number of sub-unit per unit cell, that is ratio of sigma for chemical formula to sigma per unit cell	1
d_phi	deg	Angle corresponding to the vertical angular range to focus to, e.g. detector height. 0 for no focusing	0
p_interact	1	Fraction of interacted neutrons	0
concentric	only for box, cylinder, sphere	[1] Indicate if concentric shell	0
density	g/cm^3	Density of sample	0
weight	g/mol	Atomic weight of sample	0
barns	1	Flag to indicate barns units (barns=0 for lau type files).	1
Strain	ppm	Global strain	0
focus_flip	1	Controls the sense of d_phi. If 0 d_phi is measured against the xz-plane. If !=0 d_phi is measured against zy-plane.	0

Sampling parameters

Concentric = Hollow Powder [cylinder]



# PowderN inputs

## Input parameters

Parameters in **boldface** are required; the others are optional.

Name	Unit	Description	Default
format	no quotes	Name of the format, or list of column indexes (see Description).	Undefined
reflections			"NULL"
geometry	str	Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust	"NULL"
radius	m	Outer radius of sample in (x,z) plane	0
yheight	m	Height of sample y direction	0
xwidth	m	Horiz. dimension of sample, as a width	0
zdepth	m	Depth of box sample	0
thickness			0
pack	1	Packing factor	1
Vc	AA^3	Volume of unit cell=nb atoms per cell/density of atoms	0
sigma_abs	barns	Absorption cross section per unit cell at 2200 m/s. Use a negative value to unactivate it	0
sigma_inc	barns	Incoherent cross section per unit cell. Use a negative value to unactivate it	0
delta_d_d	0/1	Global relative delta_d/d broadening when the 'w' column is not available. Use 0 if ideal.	0
p_inc	1	Fraction of incoherently scattered neutron rays	0.1
p_transmit	1	Fraction of transmitted (only attenuated) neutron rays	0.1
DW	1	Global Debye-Waller factor when the 'DW' column is not available. Use 1 if included in F2	0
nb_atoms	1	Number of sub-unit per unit cell, that is ratio of sigma for chemical formula to sigma per unit cell	1
d_phi	deg	Angle corresponding to the vertical angular range to focus to, e.g. detector height. 0 for no focusing	0
p_interact	1	Fraction of events interacting with sample, e.g. 1-p_transmit-p_inc	0
concentric	only for box, cylinder,	onents. It should then be duplicated after the inside part	0
density	g/cm^3		0
weight	g/mol		0
barns	1		1
Strain	ppm	(0 for lau type files).	0
focus_flip	1	ideal.	0
		i is measured against zy-plane.	0

Only scatter into a part of  $4\pi$



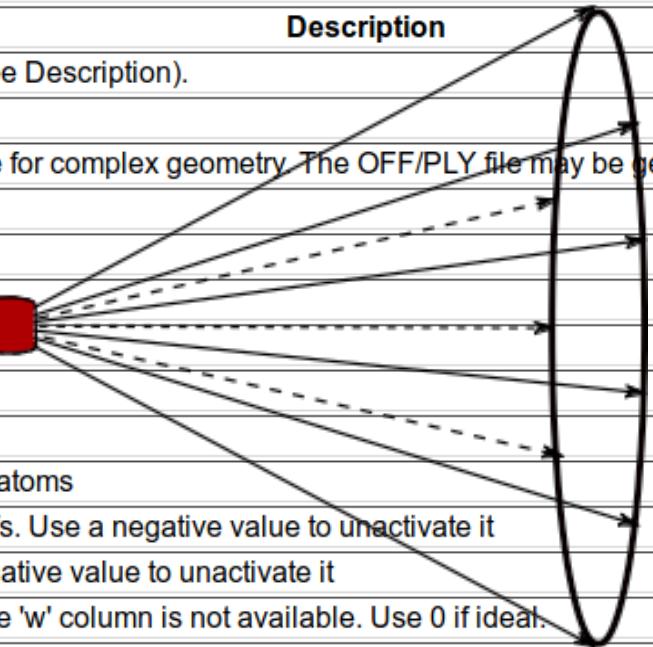
# PowderN inputs

## Input parameters

Parameters in **boldface** are required; the others are optional.

Name	Unit	Description	Default
format	no quotes	Name of the format, or list of column indexes (see Description).	Undefined
reflections			"NULL"
geometry	str	Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust	"NULL"
radius	m	Outer radius of sample in (x,z) plane	0
yheight	m	Height of sample y direction	0
xwidth	m	Horiz. dimension of sample, as a width	0
zdepth	m	Depth of box sample	0
thickness			0
pack	1	Packing factor	1
Vc	AA^3	Volume of unit cell=nb atoms per cell/density of atoms	0
sigma_abs	barns	Absorption cross section per unit cell at 2200 m/s. Use a negative value to unactivate it	0
sigma_inc	barns	Incoherent cross section per unit cell. Use a negative value to unactivate it	0
delta_d_d	0/1	Global relative delta_d/d broadening when the 'w' column is not available. Use 0 if ideal.	0
p_inc	1	Fraction of incoherently scattered neutron rays	0.1
p_transmit	1	Fraction of transmitted (only attenuated) neutron rays	0.1
DW	1	Global Debye-Waller factor when the 'DW' column is not available. Use 1 if included in F2	0
nb_atoms	1	Number of sub-unit per unit cell, that is ratio of sigma for chemical formula to sigma per unit cell	1
d_phi	deg	Angle corresponding to the vertical angular range to focus to, e.g. detector height. 0 for no focusing	0
p_interact	1	Fraction of events interacting with sample, e.g. 1-p_transmit-p_inc	0
concentric	only for box, cylinder,	Only scatter into a part of $4\pi$	0
density	g/cm^3	Only scatter into a part of $4\pi$	0
weight	g/mol	Only scatter into a part of $4\pi$	0
barns	1	Only scatter into a part of $4\pi$	1
Strain	ppm	Only scatter into a part of $4\pi$	0
focus_flip	1	Only scatter into a part of $4\pi$	0

Only scatter into a part of  $4\pi$



# PowderN inputs

## Input parameters

Parameters in **boldface** are required; the others are optional.

Name	Unit	Description	Default
format	no quotes	Name of the format, or list of column indexes (see Description).	Undefined
reflections			"NULL"
geometry	str	Name of an Object File Format (OFF) or PLY file for complex geometry. The OFF/PLY file may be generated from XYZ coordinates using qhull/powercrust	"NULL"
radius	m	Outer radius of sample in (x,z) plane	0
yheight	m	Height of sample y direction	0
xwidth	m	Horiz. dimension of sample, as a width	0
zdepth	m	Depth of box sample	0
thickness			0
pack	1	Packing factor	1
Vc	AA^3	Volume of unit cell=nb atoms per cell/density of atoms	0
sigma_abs	barns	Absorption cross section per unit cell at 2200 m/s. Use a negative value to unactivate it	0
sigma_inc	barns	Incoherent cross section per unit cell. Use a negative value to unactivate it	0
delta_d_d	0/1	Global relative delta_d_d/d broadening when the 'w' column is not available. 0 if ideal.	0
p_inc	1	Fraction of incoherently scattered neutron rays	0.1
p_transmit	1	Fraction of transmitted (only attenuated) neutron rays	0.1
DW	1	Global Debye-Waller factor when the 'DW' column is not available. Use 1 if included in F2	0
nb_atoms	1	Number of sub-unit per unit cell, that is ratio of sigma for chemical formula to sigma per unit cell	1
d_phi	deg	Angle corresponding to the vertical angular range to focus to, e.g. detector height. 0 for no focusing	0
p_interact	1	Fraction of events interacting with sample, e.g. 1-p_transmit-p_inc	0
concentric	only for box, cylinder,	Only scatter into a part of $4\pi$	0
density	g/cm^3	Components. It should then be duplicated after the inside part	0
weight	g/mol		0
barns	1		1
Strain	ppm	(0 for lau type files).	0
focus_flip	1	ideal.	0
		i is measured against zy-plane.	0

Only scatter into a part of  $4\pi$



# Reflection files for Single\_crystal and PowderN

---

```
# TITLE *Aluminum-Al-[FM3-M] Miller, H.P.jr.;DuMond, J.W.M.[1942] at 298 K
# CELL 4.049320 4.049320 4.049320 90.000000 90.000000 90.000000
# SPCGRP F M 3 M CUBIC STRUCTURE
# ATOM AL 1 0.000000 0.000000 0.000000
# SCATTERING FACTOR COEFFICIENTS: AL F= 0.345 CM-12
# Reference: Physical Review (1940) 57, 198-206
#
# Physical parameters:
# sigma_coh 1.495 coherent scattering cross section (single atom) in [barn]
# sigma_inc 0.0082 incoherent scattering cross section (single atom)in [barn]
# sigma_abs 0.231 absorption scattering cross section (single atom) in [barn]
# density 2.70 in [g/cm^3]
# weight 26.98 in [g/mol] (single atom)
# multiplicity 4 in [atoms/unit cell]
# Vc 66.4 volume of unit cell in [A^3]
# v_sound 5100 in [m/s]
# v_sound_l 6420 velocity of longitudinal sound in [m/s]
# v_sound_t 3040 velocity of transversal sound in [m/s]
# T_m 933.5 melting temperature in [K]
# T_b 2792.2 boiling temperature in [K]
# At_number 13 atomic number Z
# lattice_a 4.04932 lattice parameter a in [Angs]
#
# Format parameters: Crystallographica format
# column_j 4 multiplicity 'j'
# column_d 5 d-spacing 'd' in [Angs]
# column_F2 7 norm of scattering factor |F|^2 in [fm^2]
# column_h 1
# column_k 2
# column_l 3
#
# h k l Mult. d-space 2Theta F-squared
-1 -1 1 8 2.338 24.6973 21.3
-1 -1 1 8 2.338 24.6973 21.3
...

```

Lau datafiles  
header  
+  
reflection list

Can be used with  
Single\_crystal, PowderN,  
Isotropic\_Sqw



# Input for the PowderN

```

# TITLE *Corundum-Al2O3-[R3-CH] Graafsma, H.;Souhassou, M.;Harkem[1998] [corundum saphire:blue, ruby:red]
# CELL 4.757000 4.757000 12.987700 90.000000 90.000000 120.000000
# SPCGRP R -3 C TRIGONAL STRUCTURE
# ATOM AL 1 0.000000 0.000000 0.352110
# ATOM O 1 0.306260 0.306260 0.250000
# SCATTERING FACTOR COEFFICIENTS: AL F= 0.345 CM-12 ; O F= 0.581 CM-12
# Reference: Acta Crystallographica B (1998) 54, 193-195
#
# Physical parameters:
# sigma_coh 15.683 coherent scattering cross section for Al2O3 in [barn]
# sigma_inc 0.0188 incoherent scattering cross section for Al2O3 in [barn]
# sigma_abs 0.4625 absorption scattering cross section for Al2O3 in [barn]
# density 4.05 in [g/cm^3]
# weight 101.96 in [g/mol] for Al2O3
# multiplicity 6 in [Al2O3/unit cell]
# Vc 254.52 volume of unit cell in [A^3]
# T_m 2273 melting temperature in [K]
# T_b 3773 boiling temperature in [K]
# lattice_a 4.757 lattice parameter a in [Angs]
# lattice_c 12.9877 lattice parameter c in [Angs]
# lattice_cc 120 lattice angle gamma in [deg]
#
# Format parameters: Lazy format <http://icsd.ill.fr>
# column_j 17 multiplicity 'j'
# column_d 6 d-spacing 'd' in [Angs]
# column_F 13 norm of scattering factor |F| in [barn]
# column_h 1
# column_k 2
# column_l 3
#
#H K L THETA 2THETA D VALUE 1/D**2 SIN2*1000 H K L INTENSITY /F(HKL)/ A(HKL) B(HKL) PHA.ANG. MULT LPG
 1 0 1 6.35 12.71 4.5175 0.0490 12.25 1 0 1 367.0 4.1 -4.08 0.00 180.00 6 82.14
 0 0 3 7.10 14.20 4.0467 0.0611 15.27 0 0 3 110.0 4.3 4.32 0.00 0.00 2 66.01
 0 1 2 7.57 15.13 3.7972 0.0694 17.34 0 1 2 10.9 0.8 0.84 0.00 0.00 6 58.18
...

```

Laz + Lau datafiles  
header  
+  
reflection list

Can be used with PowderN,  
Isotropic\_Sqw

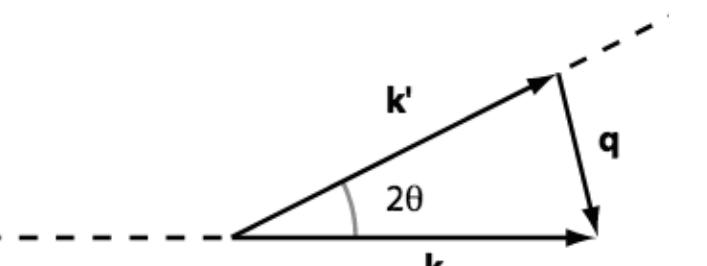
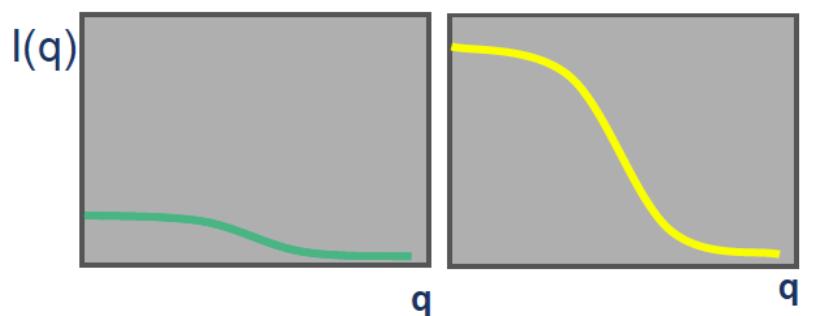
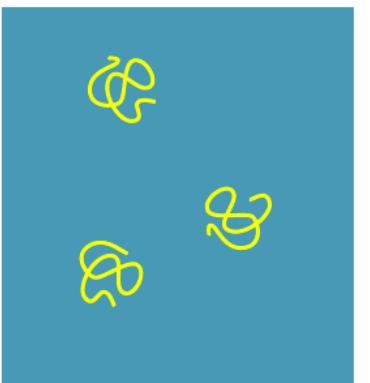
# Where to get these files...

- | \$MCSTAS/data
  - | Windows: c:\mcstas-2.2a\lib\data
  - | Linux: /usr/(local)/share/mcstas/2.2a/data
  - | OS X: /Applications/McStas-2.2a/Contents/Resources/mcstas/2.2a/data
- | - Or make your own via
  - | Finding a CIF file for the given structure
    - | e.g. from ICSD <http://icsd.fiz-karlsruhe.de>
    - | Build one using VESTA
  - | Process it using
    - | cif2hkl tool that comes preinstalled with McStas
    - | Crystallographica, using the guide
      - | <https://github.com/McStasMcXtrace/McCode/wiki/Single-crystal---and-generating-its-input>



# Small angle scattering SANS

- SANS method can be used for many samples
- Specific sample: Molecule + Liquid (buffer solution)
- Isotropic scattering



# SANS spheres

## Input parameters

Parameters in **boldface** are required; the others are optional.

Name	Unit	Description	Default
R	AA	Radius of scattering hard spheres	100
Phi	1	Particle volume fraction	1e-3
Delta_rho	fm/AA^3	Excess scattering length density	0.6
sigma_abs	m^-1	Absorption cross section density at 2200 m/s	0.05
xwidth	m	horiz. dimension of sample, as a width	0
yheight	m	vert. dimension of sample, as a height for cylinder/box	0
zdepth	m	depth of sample	0
radius	m	Outer radius of sample in (x,z) plane for cylinder/sphere	0
target_x			0
target_y	m	position of target to focus at	0
target_z			6
target_index	1	Relative index of component to focus at, e.g. next is +1	0
focus_xw	m	horiz. dimension of a rectangular area	0
focus_yh	m	vert. dimension of a rectangular area	0
focus_aw	deg	horiz. angular dimension of a rectangular area	0
focus_ah	deg	vert. angular dimension of a rectangular area	0
focus_r	m	Detector (disk-shaped) radius	0

Dilute, monodisperse, hard spheres in solution, with given contrast and radius



# SasView\_models

## Input parameters

Parameters in **boldface** are required; the others are optional.

Name	Unit	Description	Default
model_index			21
model_scale			1.0
model_pars			{60}
model_abs	1/m	Absorption cross section density at 2200 m/s	0.5
xwidth	m	horiz. dimension of sample, as a width	0
yheight	m	vert . dimension of sample, as a height for cylinder/box	0
zdepth	m	depth of sample	0
radius	m	Outer radius of sample in (x,z) plane for cylinder/sphere	0
target_x	m	relative focus target position	0
target_y	m	relative focus target position	0
target_z	m	relative focus target position	6
target_index	1	Relative index of component to focus at, e.g. next is +1	0
focus_xw	m	horiz. dimension of a rectangular area	0
focus_yh	m	vert. dimension of a rectangular area	0
focus_aw	deg	horiz. angular dimension of a rectangular area	0
focus_ah	deg	vert. angular dimension of a rectangular area	0
focus_r	m	Detector (disk-shaped) radius	0



# SasView\_models

---



47	<a href="#">parallelepiped</a>	(sld, solvent_sld, a_side, b_side, c_side)
48	<a href="#">parallelepiped_xy</a>	(sld, solvent_sld, a_side, b_side, c_side, theta, phi, psi)
49	<a href="#">pearl_necklace</a>	(radius, edge_separation, string_thickness, number_of_pearls, sld, string_s
50	<a href="#">pearl_necklace_xy</a>	(radius, edge_separation, string_thickness, number_of_pearls, sld, string_s
51	<a href="#">sphere</a>	(sld, solvent_sld, radius)
52	<a href="#">sphere_xy</a>	(sld, solvent_sld, radius)
53	<a href="#">star_polymer</a>	(radius2, arms)
54	<a href="#">star_polymer_xy</a>	(radius2, arms)
55	<a href="#">stickyhardsphere</a>	(effect_radius, volfraction, perturb, stickiness)
56	<a href="#">stickyhardsphere_xy</a>	(effect_radius, volfraction, perturb, stickiness)
57	<a href="#">triaxial_ellipsoid</a>	(sld, solvent_sld, req_minor, req_major, rpolar)
58	<a href="#">triaxial_ellipsoid_xy</a>	(sld, solvent_sld, req_minor, req_major, rpolar, theta, phi, psi)



# SANS other samples

McStas has a suite of SANS-models:

Try ellipsoidal and cylindrical particles  
-or-

Elliptic cylinders  
Go for Nanodiscs and Liposomes

- SANS\_AnySamp.comp
- SANS\_DebyeS.comp
- SANSCylinders.comp
- SANSEllipticCylinders.comp
- SANSGuinier.comp
- SANSLiposomes.comp
- SANSNanodiscs.comp
- SANSNanodiscsFast.comp
- SANSNanodiscsWithTags.
- SANSNanodiscsWithTagsFast
- SANSPDB.comp
- SANSPDBFAST.comp
- SANSShells.comp
- SANSSpheres.comp

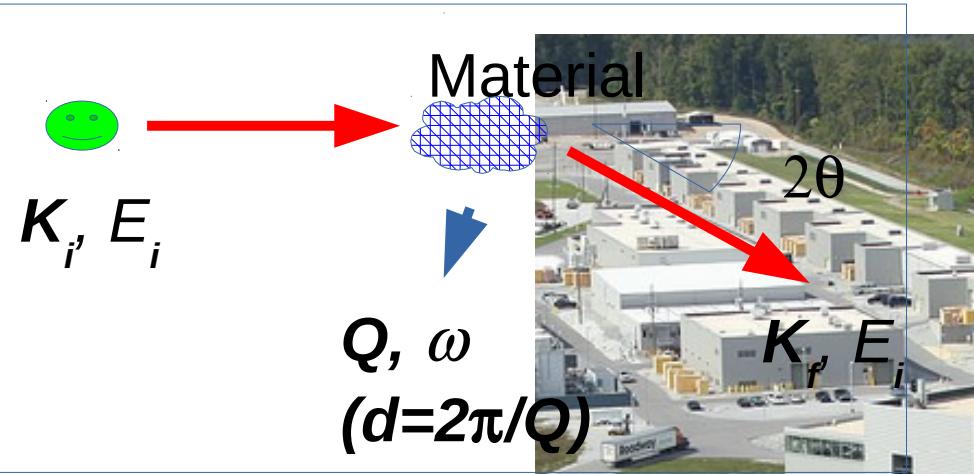


October 2018

# Neutron-matter interaction

$$K_f = K_i + Q$$

$$E_f = E_i + \omega$$



Bragg's law (diffraction on structure – atoms separated by distance  $d$ )

$$n\lambda = 2\pi / K_i = 2d \sin \theta$$

Scattering law (intensity per solid angle and energy, dynamics)

Holy Book (Squires)

$$\frac{d^2 \sigma}{d\Omega dE_f} = \frac{K_f}{K_i} \left[ \frac{\sigma}{4\pi} S(Q, \omega) \right]$$



Dynamical structure factor  $S(Q, \omega)$  is characteristic of each material

Reflects ordering of matter (atom/molecule positions – movements - domains)

# Computing the total scattering probability

The total scattering cross section is given in  $(\Omega, E_f)$  space, but  $S$  is given in  $(q, \omega)$ .  
 A variable change must be done for the integration (Jacobian).

We like to play games  
in  $(q, \omega)$  space

$$\begin{aligned}\frac{d\Omega}{d\theta} &= -2\pi \sin\theta \\ \frac{dq}{d\theta} &= -\frac{k_i k_f \sin\theta}{q}\end{aligned}$$

Effective cross section  
in  $(q, \omega)$  space

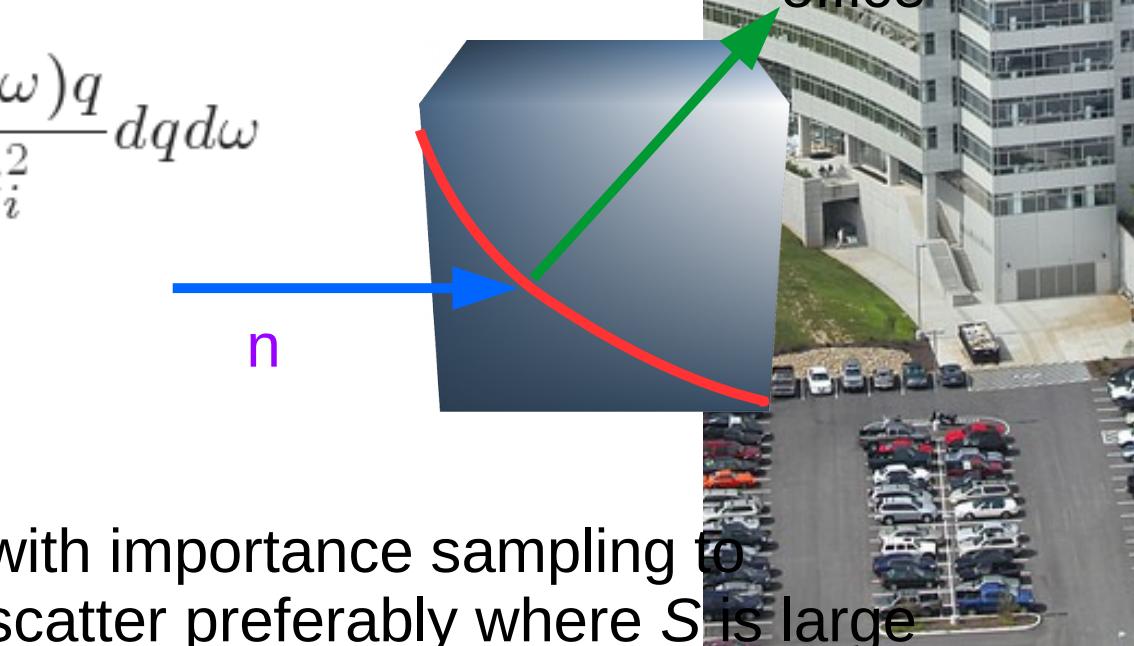
$$\hat{\sigma} = \sigma \iint \frac{S(q, \omega) q}{2k_i^2} dq d\omega$$

Probability to transmit

$$p = e^{-\rho \hat{\sigma} x}$$

Scattering distribution

$$S(q, \omega)$$



# *Isotropic\_Sqw syntax*

- ***Isotropic\_Sqw(***  
 $Sqw\_coh=FILE\_COH,$   
 $Sqw\_inc=FILE\_INC,$   
 $radius=R,$   
 $height=H)$
- More component parameters can specify geometry, physical properties, ...
- The data files specify the  $S(Q, \omega)$  or  $S(Q)$  values as a matrix with  $Q, \omega$  extent. Additional fields can be included as meta data (# lines).



# Isotropic\_Sqw data format

October 201

```

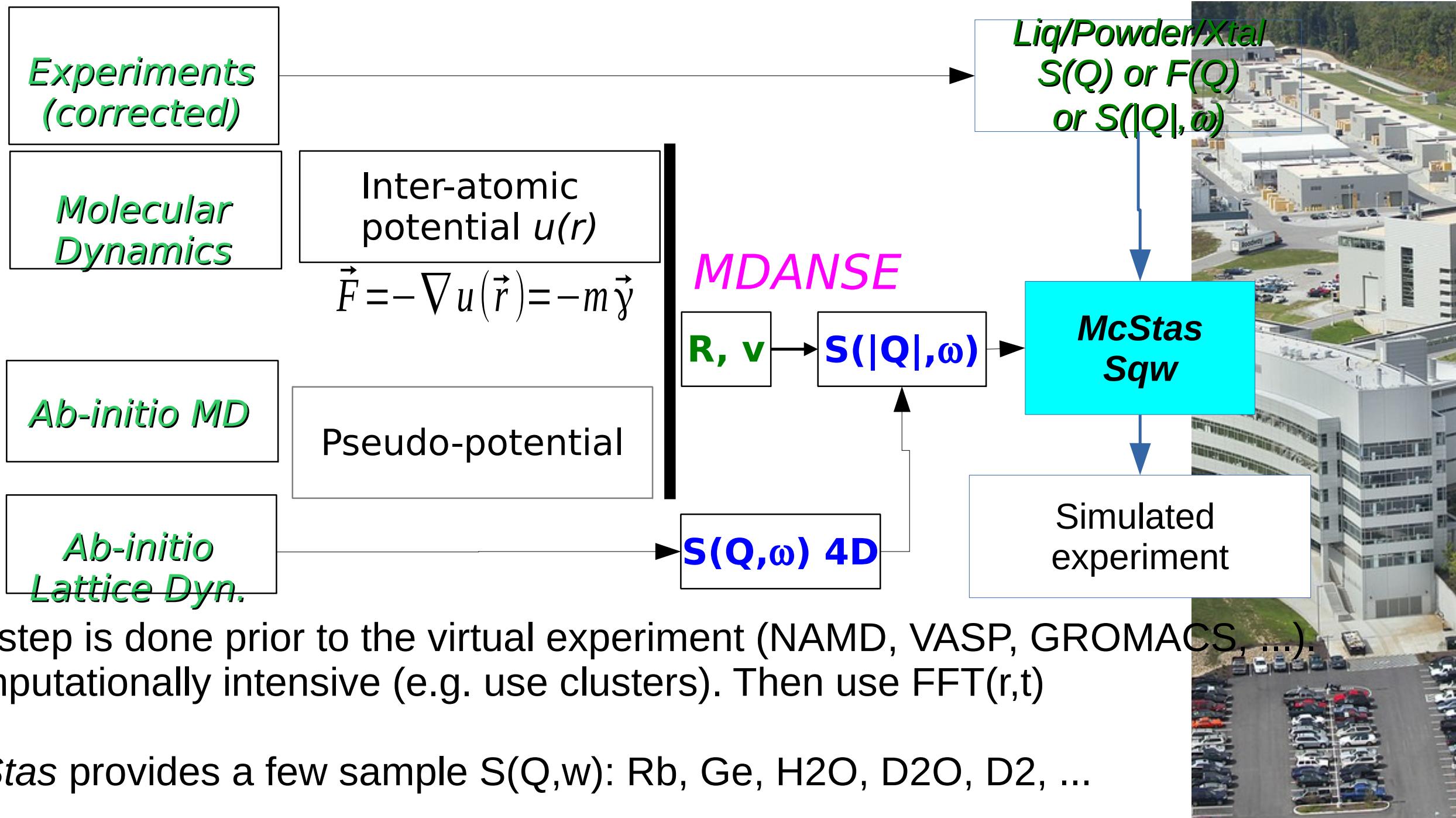
# Sqw data file for Isotropic_Sqw
# liquid He4: coherent part, no incoherent, atomic number 2
# Elementary Excitation Data by R.J. Donnelly et al., J. Low Temp. Phys., 44 (1981) 471
# WARNING: line width is constant, intensity is not right
#
# Physical parameters:
# V_rho      0.072    atom density per Angs^3
# weight      4.002    in [g/mol]
# density     0.4784   in [g/cm^3]
# sigma_abs   0.00747 absorption scattering cross section in [barn]
# sigma_coh   1.34    coherent scattering cross section in [barn]
# sigma_inc   0        incoherent scattering cross section in [barn]
# Temperature 2        in [K]
# classical   0        experimental, contains Bose factor
#
# q axis values
# vector of m values in Angstroem-1
0.001000 0.011000 0.02 ...
# w axis values
# vector of n values in meV
0.001391 0.011391 0.021391 0.0313 ...
# sqw values (one line per q axis value)
# matrix of S(q,w) values (m rows x n values), one line per q value
9.721422 10.599145 11.344954 ...

```

[He4\\_liq\\_coh.sqw](#)



# How to get $S(q,w)$ data sets



MD step is done prior to the virtual experiment (NAMD, VASP, GROMACS, ...). Computationally intensive (e.g. use clusters). Then use FFT( $r, t$ )

McStas provides a few sample  $S(Q, w)$ : Rb, Ge, H<sub>2</sub>O, D<sub>2</sub>O, D<sub>2</sub>, ...

**Isotropic\_Sqw:** Handles **elastic** and **inelastic** for both **coherent** and **incoherent** channels