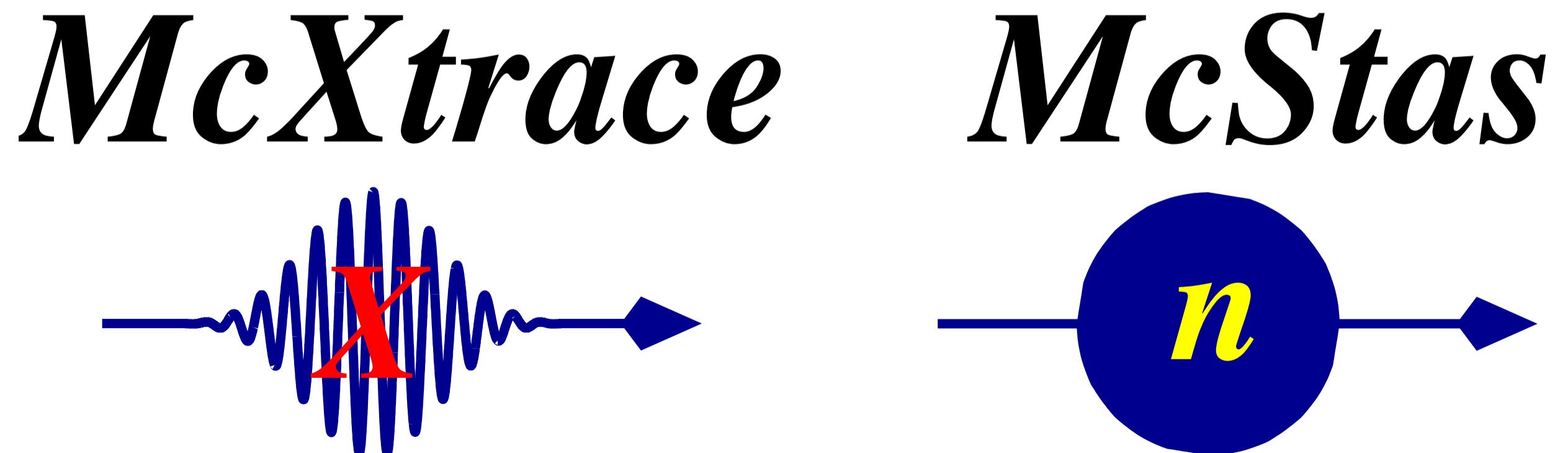


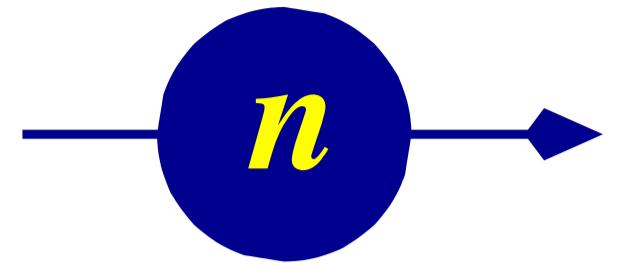
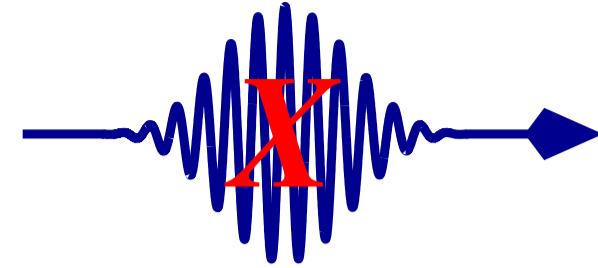
McStas and McXtrace: simulation tools for neutron- and X-ray instruments

Peter Willendrup^{1,2},

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²ESS Data Management & Software Center, Denmark



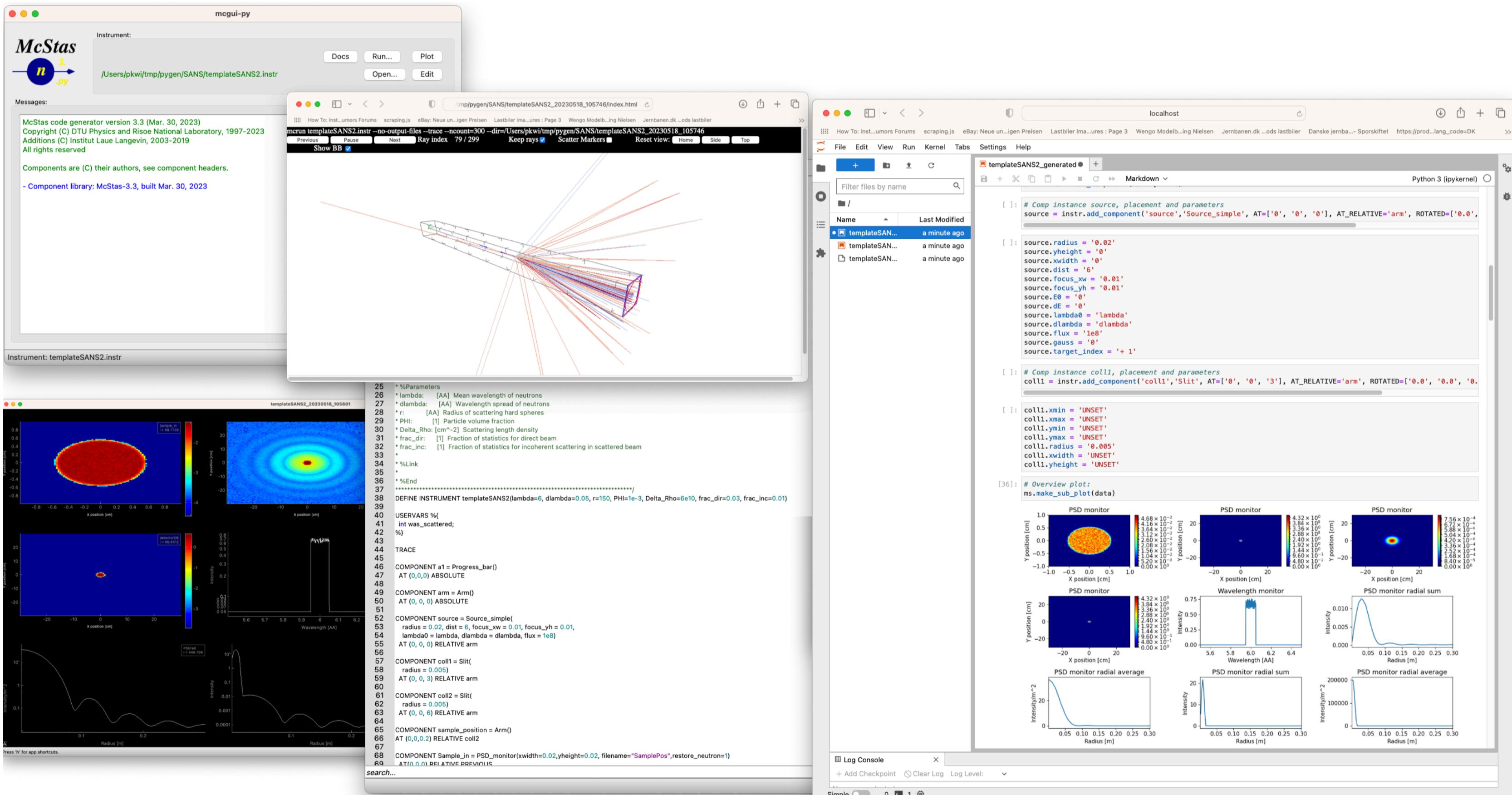


Agenda

- Introduction to McStas & McXtrace
- Neutrons and X-rays
- Monte Carlo method
- Ray-tracing
- Components of scattering instruments
- A short description of this afternoons exercise

McStas & McXtrace

- Neutron- and X-ray simulation tools for instruments and experiments



McStas Introduction

- Flexible, general simulation utility for neutron scattering experiments.
- Original design for **Monte carlo Simulation of triple axis spectrometers**
- Developed at DTU Physics, ILL, PSI, Uni CPH, **ESS**
- V. 1.0 by K Nielsen & K Lefmann (1998) RISØ
- Currently ~ 4 people full time plus students



GNU GPL
license
Open Source

Project website at
<http://www.mcstas.org>

mcstas-users@mcstas.org mailinglist

The screenshot shows the official McStas website. At the top, there's a navigation bar with links for "About McStas", "Download", "Mailing list", "Search", and "Links". The main content area features a banner for the "25 year anniversary 1998 - 2023" with logos for ESS, PSI, ILL, NEXMAP, and DTU. Below the banner, a section titled "McStas - A neutron ray-trace simulation package" contains text about the tool's purpose and support from various institutions. It includes a diagram of a neutron beam hitting a sample and a 3D intensity plot. To the right, there's a "Recent news" section with a link to "Migrating from McStas 2.x to 3.x? - Use the wiki-based guides". At the bottom, there are instructions for starting the software via a web browser or terminal.

McXtrace - same idea, but for X-rays (2009-)

The screenshot shows a web browser window with the URL mcxtrace.org in the address bar. The page content is as follows:

McXtrace

McXtrace - An X-ray ray-trace simulation package

McXtrace

About McXtrace
Publications
Project Partners
Project People
Goal

Download
Components

Documentation
Manual
Commands
Wiki (GitHub)
Tutorial

Mailing list

Links

Search

Code-repository (GitHub)

Report bugs (GitHub)

McXtrace - Monte Carlo Xray Tracing, is a joint venture by

McStas

Our code is based on technology from

Code repository (shared with 'McStas') is located at github.com/McStasMcXtrace

For information on our progress, please subscribe to our [user mailinglist](#)..

- To download the latest release: [download area](#)
- For installation instructions :
 - [McXtrace 3.5.1 installation](#)
- For a quick list of the available commands: [commands](#)

Recent McXtrace News

Migrating from McXtrace 1.x to 3.x? - [Use the wiki-based guides](#)

September 17th, 2024: Try the new version in a binder - no installation required

Here you may access a web-desktop with McStas and McXtrace:

McStas and McXtrace: simulation tools for neutron- and X-ray instruments

Both neutrons and X-rays interact with atoms

- X-rays “see” the electron cloud surrounding the atomic nucleus – the higher atomic no. ‘Z’, the more scattering

- In contrast neutrons “see” the nucleus – no correlation between level of scattering and atomic no.

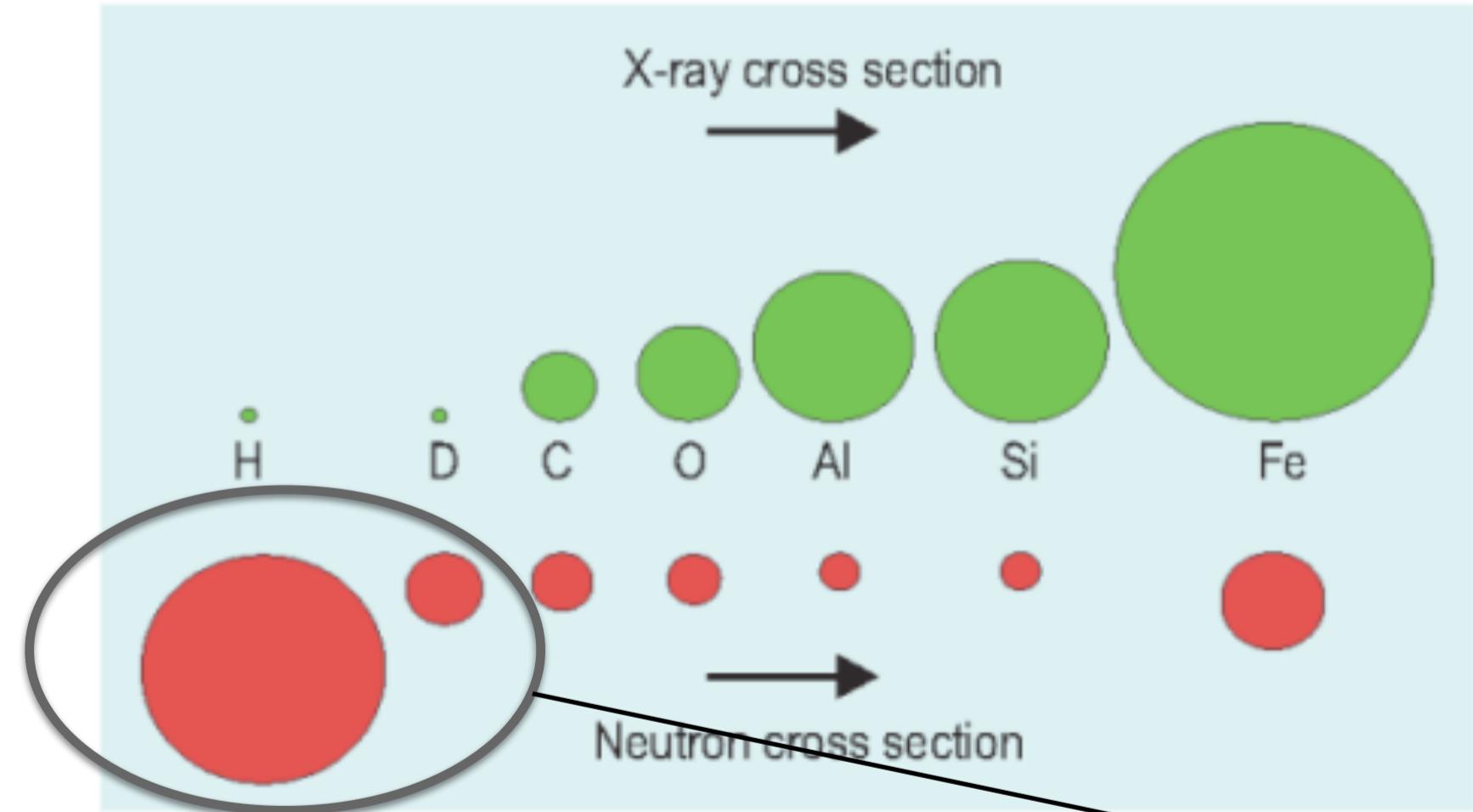


Fig. 2. Neutron and x-ray scattering cross-sections compared. Note that neutrons penetrate through Al much better than x rays do, yet are strongly scattered by hydrogen.

- Result: Two very different response/contrasts

Neutron magnetic moment,
sensitivity to magnetical structures,
polarization techniques (Larmor)

1A	2A	About Chemistry										8A					
1 H 1s ¹	4 Be 1s ² s ²	5 B 1s ² s ¹ p ¹	6 C 1s ² s ² p ²	7 N 1s ² 2s ² p ³	8 O 1s ² 2s ² p ⁴	9 F 1s ² 2s ² p ⁵	10 Ne 1s ² 2s ² p ⁶										
3 Li 1s ² 2s ¹	12 Mg [Ne]3s ²	13 Al [Ne]3s ² p ¹	14 Si [Ne]3s ² p ²	15 P [Ne]3s ² p ³	16 S [Ne]3s ² p ⁴	17 Cl [Ne]3s ² p ⁵	18 Ar [Ne]3s ² p ⁶										
19 K [Ar]4s ¹	20 Ca [Ar]3d ¹ 4s ²	21 Sc [Ar]3d ¹ 4s ²	22 Ti [Ar]3d ² 4s ²	23 V [Ar]3d ³ 4s ¹	24 Cr [Ar]3d ⁴ 4s ¹	25 Mn [Ar]3d ⁵ 4s ¹	26 Fe [Ar]3d ⁶ 4s ²	27 Co [Ar]3d ⁷ 4s ²	28 Ni [Ar]3d ⁸ 4s ²	29 Cu [Ar]3d ⁹ 4s ¹	30 Zn [Ar]3d ¹⁰ 4s ²	31 Ga [Ar]3d ¹⁰ 4s ² p ¹	32 Ge [Ar]3d ¹⁰ 4s ² p ²	33 As [Ar]3d ¹⁰ 4s ² p ³	34 Se [Ar]3d ¹⁰ 4s ² p ⁴	35 Br [Ar]3d ¹⁰ 4s ² p ⁵	36 Kr [Ar]3d ¹⁰ 4s ² p ⁶
37 Rb [Kr]5s ¹	38 Sr [Kr]4d ¹ 5s ²	39 Y [Kr]4d ¹ 5s ²	40 Zr [Kr]4d ² 5s ¹	41 Nb [Kr]4d ⁵ 5s ¹	42 Mo [Kr]4d ⁶ 5s ¹	43 Tc [Kr]4d ⁷ 5s ¹	44 Ru [Kr]4d ⁸ 5s ¹	45 Rh [Kr]4d ⁹ 5s ¹	46 Pd [Kr]4d ¹⁰ 5s ¹	47 Ag [Kr]4d ¹⁰ 5s ²	48 Cd [Kr]4d ¹⁰ 5s ²	49 In [Kr]4d ¹⁰ 5s ² p ¹	50 Sn [Kr]4d ¹⁰ 5s ² p ²	51 Sb [Kr]4d ¹⁰ 5s ² p ³	52 Te [Kr]4d ¹⁰ 5s ² p ⁴	53 Xe [Kr]4d ¹⁰ 5s ² p ⁵	
55 Cs [Xe]6s ¹	56 Ba [Xe]6s ²	57-71 Lanthanides [Xe]4f ¹ 5d ² 6s ²	72 Hf [Xe]4f ¹ 5d ⁶ 6s ²	73 Ta [Xe]4f ¹ 5d ⁶ 6s ²	74 W [Xe]4f ¹ 5d ⁶ 6s ²	75 Re [Xe]4f ¹ 5d ⁶ 6s ²	76 Os [Xe]4f ¹ 5d ⁶ 6s ²	77 Ir [Xe]4f ¹ 5d ⁶ 6s ²	78 Pt [Xe]4f ¹ 5d ⁶ 6s ²	79 Au [Xe]4f ¹ 5d ⁶ 6s ²	80 Hg [Xe]4f ¹ 5d ⁶ 6s ²	81 Tl [Xe]4f ¹ 5d ⁶ 6s ²	82 Pb [Xe]4f ¹ 5d ⁶ 6s ²	83 Bi [Xe]4f ¹ 5d ⁶ 6s ²	84 Po [Xe]4f ¹ 5d ⁶ 6s ²	85 At [Xe]4f ¹ 5d ⁶ 6s ²	86 Rn [Xe]4f ¹ 5d ⁶ 6s ²
87 Fr [Rn]7s ¹	88 Ra [Rn]7s ²	89-103 Actinides [Rn]5f ¹ 6d ² 7s ²	104 Rf [Rn]5f ¹ 6d ² 7s ²	105 Db [Rn]5f ¹ 6d ² 7s ²	106 Sg [Rn]5f ¹ 6d ² 7s ²	107 Bh [Rn]5f ¹ 6d ² 7s ²	108 Hs [Rn]5f ¹ 6d ² 7s ²	109 Mt [Rn]5f ¹ 6d ² 7s ²	110 Ds [Rn]5f ¹ 6d ² 7s ²	111 Rg [Rn]5f ¹ 6d ² 7s ²	112 Cn [Rn]5f ¹ 6d ² 7s ²	113 Uut [Rn]5f ¹ 6d ² 7s ²	114 Fl [Rn]5f ¹ 6d ² 7s ²	115 Uup [Rn]5f ¹ 6d ² 7s ²	116 Lv [Rn]5f ¹ 6d ² 7s ²	117 Uus [Rn]5f ¹ 6d ² 7s ²	118 Uuo [Rn]5f ¹ 6d ² 7s ²
Lanthanides																	
Actinides																	
57 La [Xe]5d ¹ 6s ²	58 Ce [Xe]4f ¹ 5d ¹ 6s ²	59 Pr [Xe]4f ¹ 5d ² 6s ²	60 Nd [Xe]4f ¹ 5d ³ 6s ²	61 Pm [Xe]4f ¹ 5d ⁴ 6s ²	62 Sm [Xe]4f ¹ 5d ⁵ 6s ²	63 Eu [Xe]4f ¹ 5d ⁶ 6s ²	64 Gd [Xe]4f ¹ 5d ⁷ 6s ²	65 Tb [Xe]4f ¹ 5d ⁸ 6s ²	66 Dy [Xe]4f ¹ 5d ⁹ 6s ²	67 Ho [Xe]4f ¹ 5d ¹⁰ 6s ²	68 Er [Xe]4f ¹ 5d ¹¹ 6s ²	69 Tm [Xe]4f ¹ 5d ¹² 6s ²	70 Yb [Xe]4f ¹ 5d ¹³ 6s ²	71 Lu [Xe]4f ¹ 5d ¹⁴ 6s ²			
89 Ac [Rn]8d ¹ 7s ²	90 Th [Rn]8d ² 7s ²	91 Pa [Rn]8d ³ 7s ²	92 U [Rn]8d ⁴ 7s ²	93 Np [Rn]8d ⁵ 7s ²	94 Pu [Rn]8d ⁶ 7s ²	95 Am [Rn]8d ⁷ 7s ²	96 Cm [Rn]8d ⁸ 7s ²	97 Bk [Rn]8d ⁹ 7s ²	98 Cf [Rn]8d ¹⁰ 7s ²	99 Es [Rn]8d ¹¹ 7s ²	100 Fm [Rn]8d ¹² 7s ²	101 Md [Rn]8d ¹³ 7s ²	102 No [Rn]8d ¹⁴ 7s ²	103 Lr [Rn]8d ¹⁵ 7s ²			

* values are based on theory and are not verified

Large contrast H vs D,
ideal for biological systems,
via deuteration

- Result: Two very different response/contrasts

Both neutrons and X-rays interact with atoms

- X-rays “see” the electron cloud surrounding the atomic nucleus – the higher atomic no. ‘Z’, the more scattering
- In contrast neutrons “see” the nucleus – no simple connection between level of scattering and atomic no.

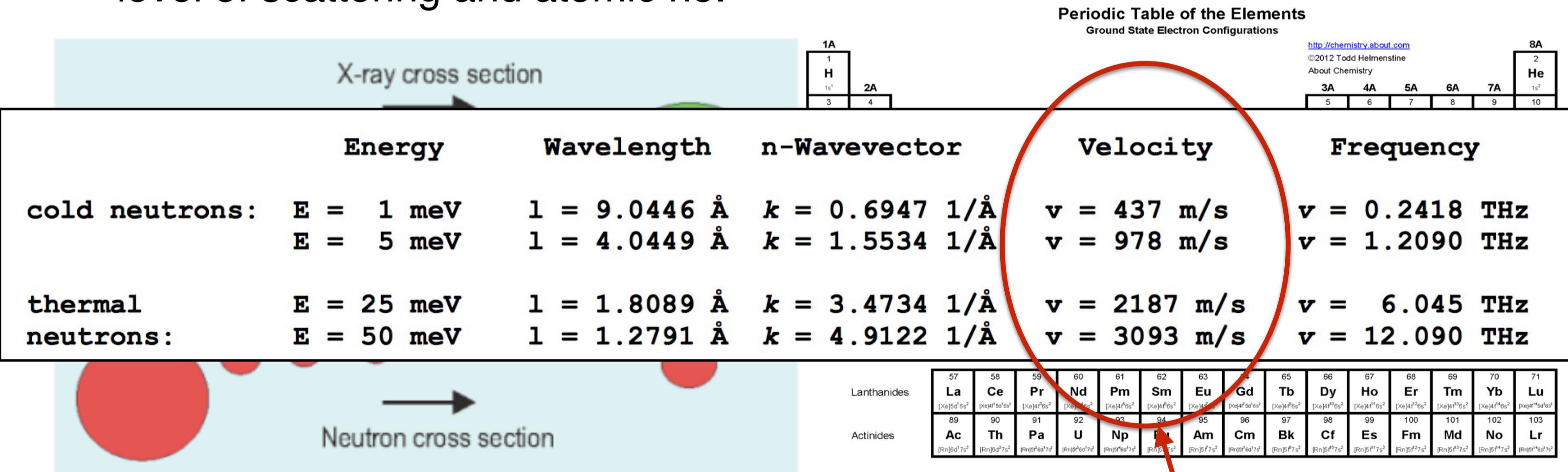


Fig. 2. Neutron and x-ray scattering cross-sections compared. Note that neutrons penetrate through Al much better than x rays do, yet are strongly scattered by hydrogen.

- Result: Two very different response/contrasts

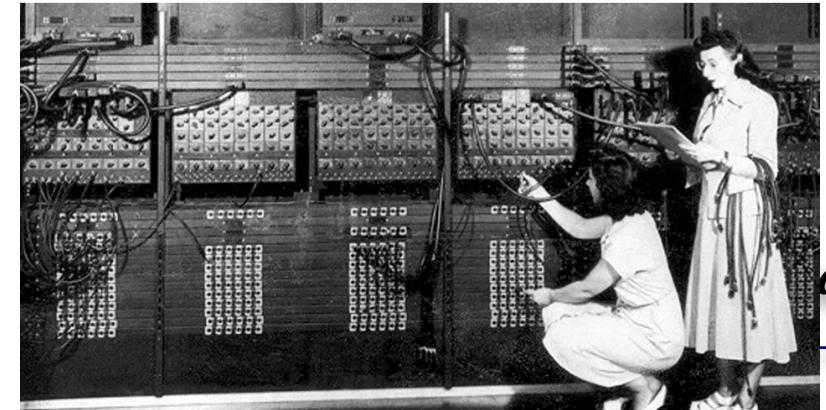
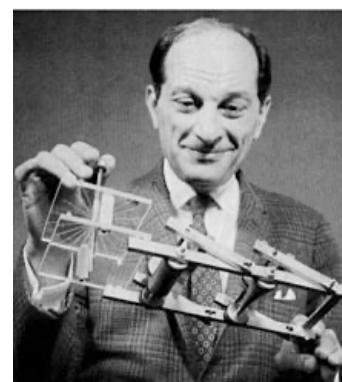
Monte Carlo techniques



- During WW2, “numerical experiments” were applied at Los Alamos for solving mathematical complications of computing fission, criticality, neutronics, hydrodynamics, thermonuclear detonation etc.

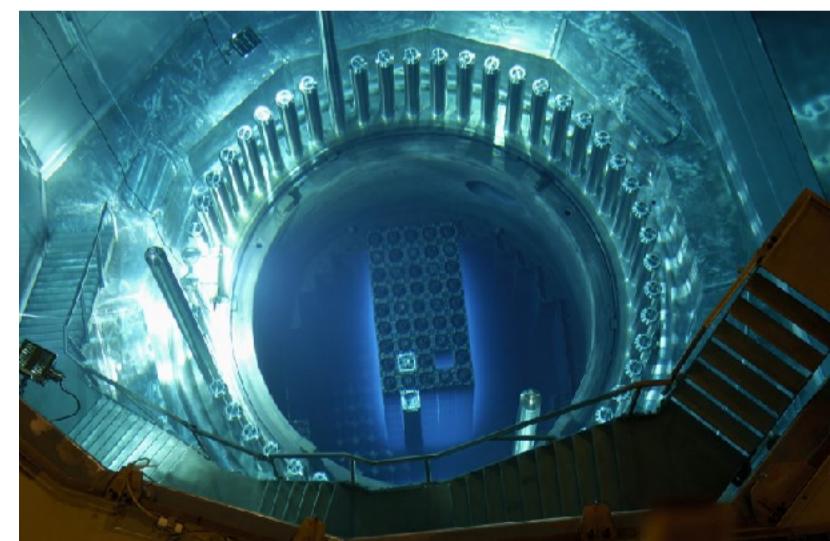
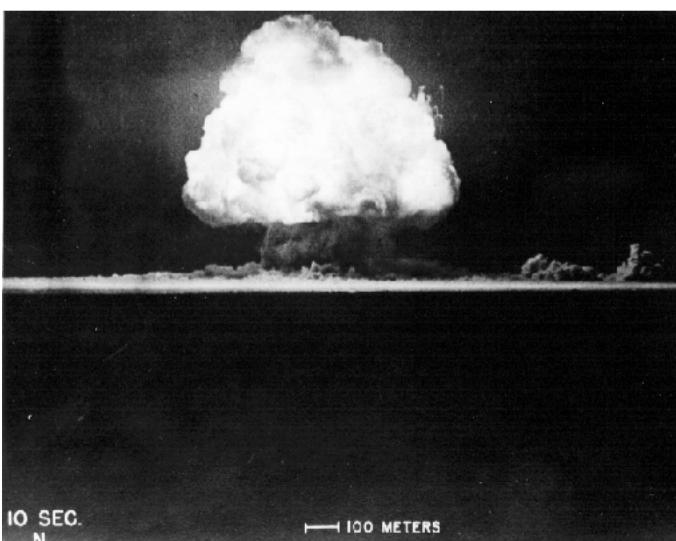


- Notable fathers: John v. Neumann Stanislav Ulam Nicholas Metropolis
- Named “Monte Carlo” after Ulam’s fathers frequent visits to the Monte Carlo casino in Las Vegas
- Initially “implemented” by letting large numbers of women use tabularized random numbers and hand calculators for individual particle calculations
- Later, analogue and digital computing devices were used

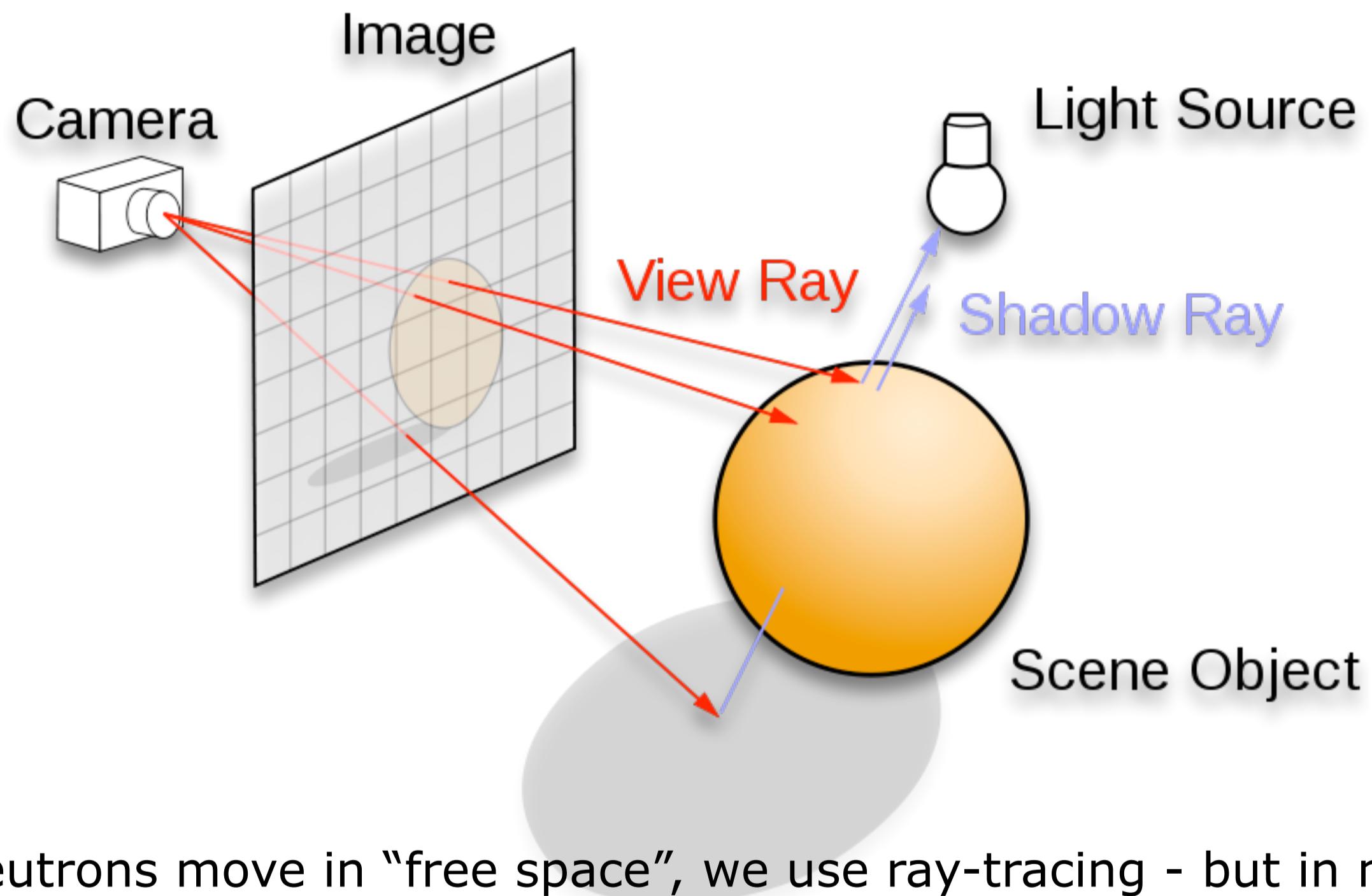


Monte Carlo techniques

- Los Alamos has since then developed and perfected many different monte carlo codes leading to what is today known as the codes MCNP5 and MCNPX
- State of the art is MCNP6 that features numerous (even exotic) particles
- MCNP was originally Monte Carlo Neutron Photon, later N-Particle
- Mainly used for high-energy particle descriptions in weapons, power reactors and routinely used for estimating dose rates and needed shielding
- Not much focus on crystalline / ordered material and coherent scattering of neutrons due to the focus on high energies

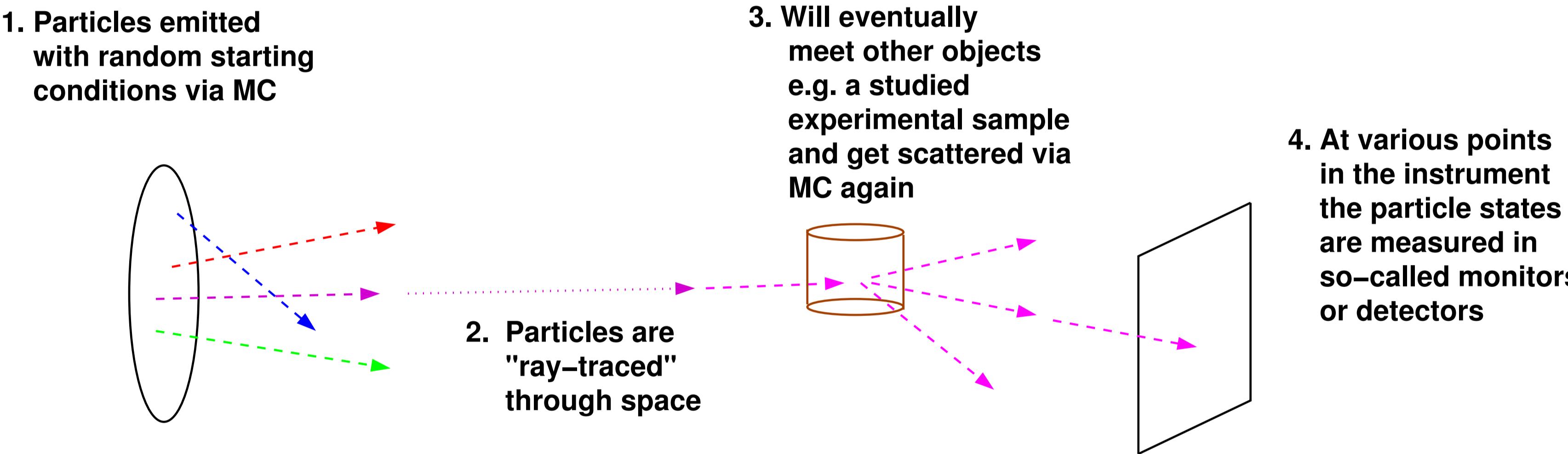


Ray-tracing methods



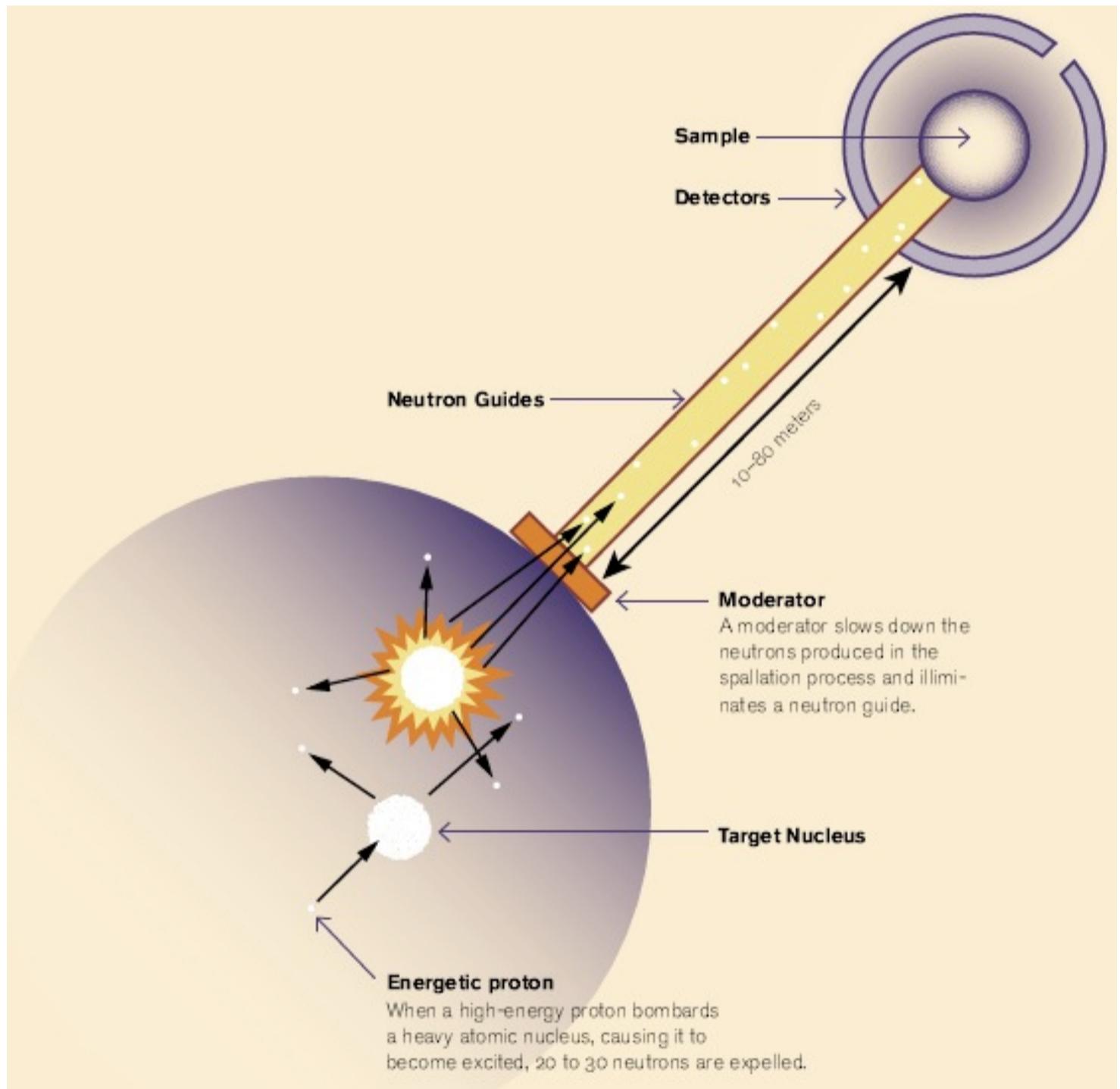
- When neutrons move in “free space”, we use ray-tracing - but in most cases in direction source -> detector
- Of course parabolas rather than straight lines are used to implement gravity

Overall picture: Monte Carlo Ray-Tracing

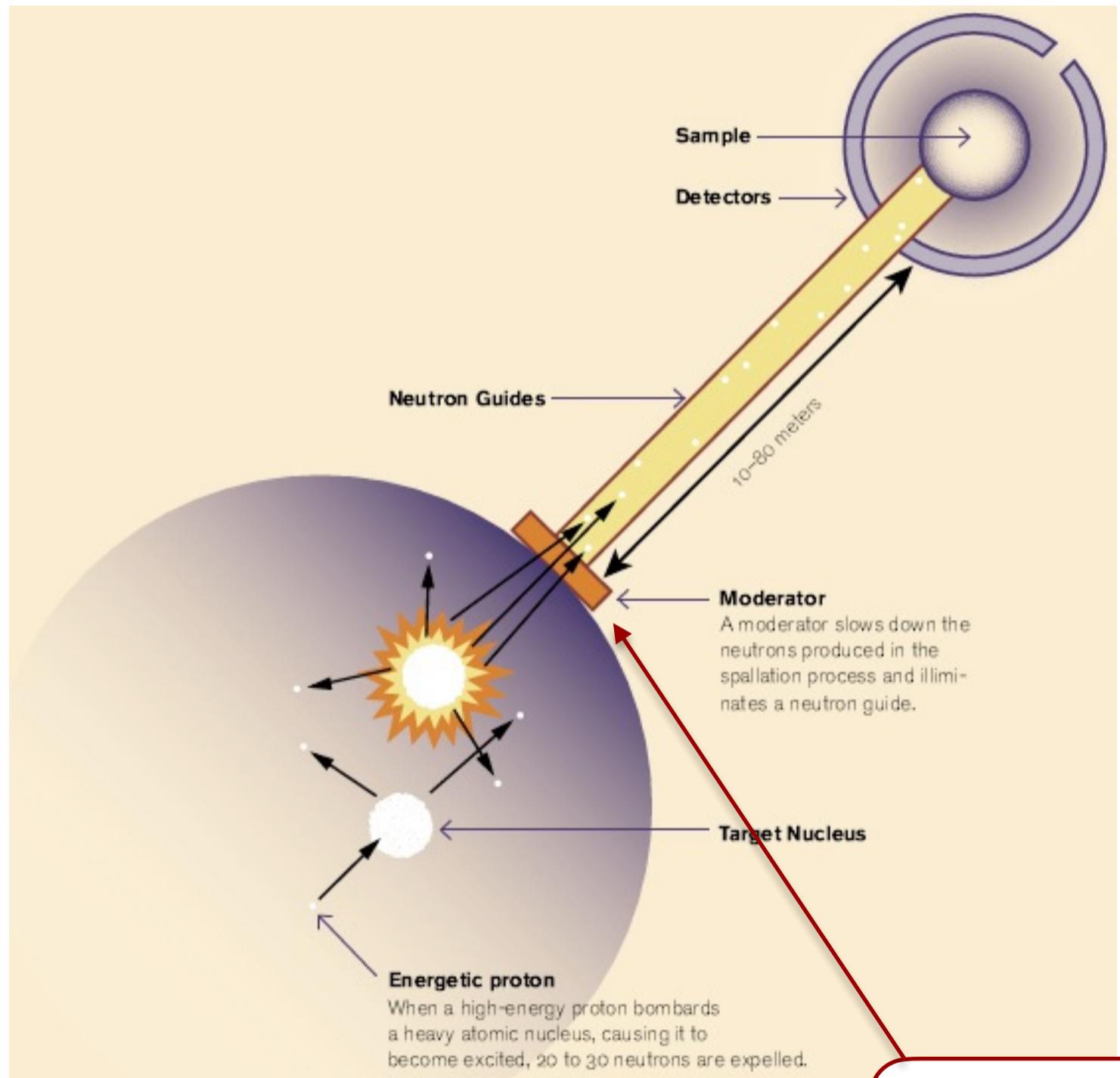


- Important efficiency mechanisms:
 - “Focusing” - e.g. source to beamport only (4π vs. limited solid angle only)
 - Rather vs. single particle description, absorption handled though statistics and downscaling the ray weight

Components of neutron instruments

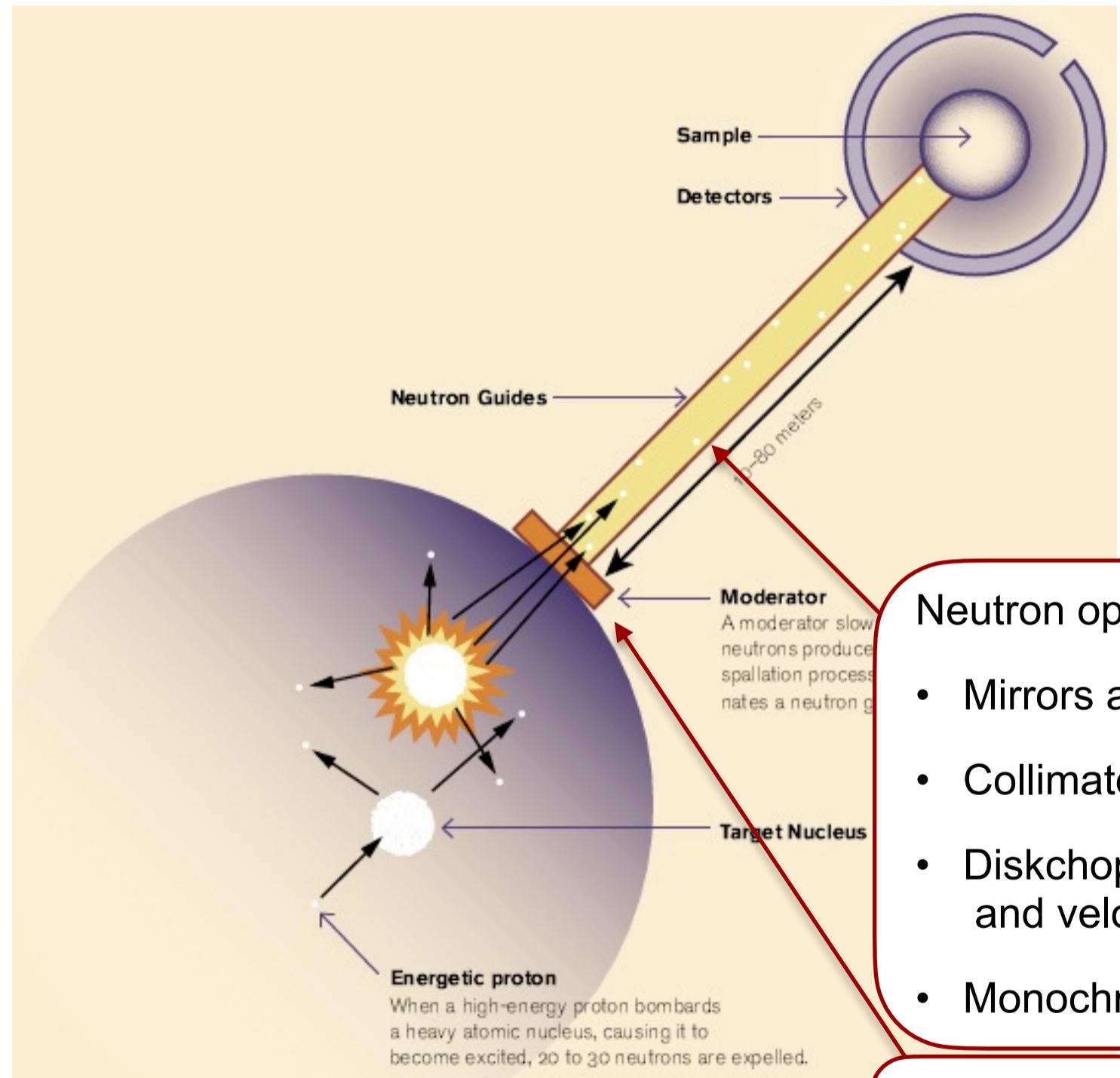


Components of neutron instruments



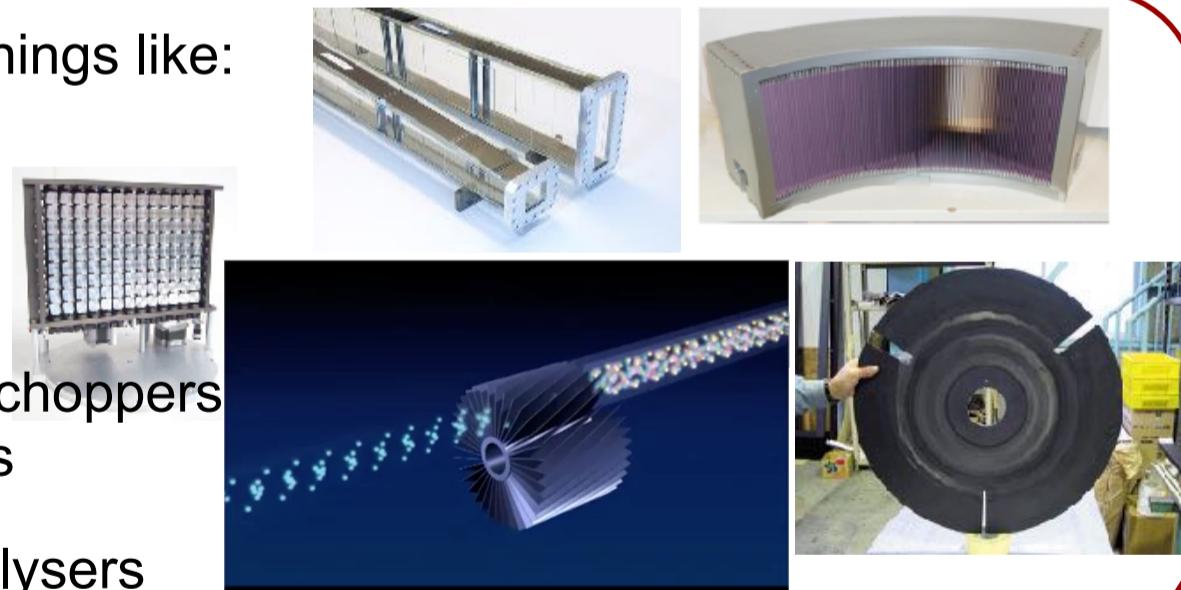
In McStas the moderator is the
“source”

Components of neutron instruments



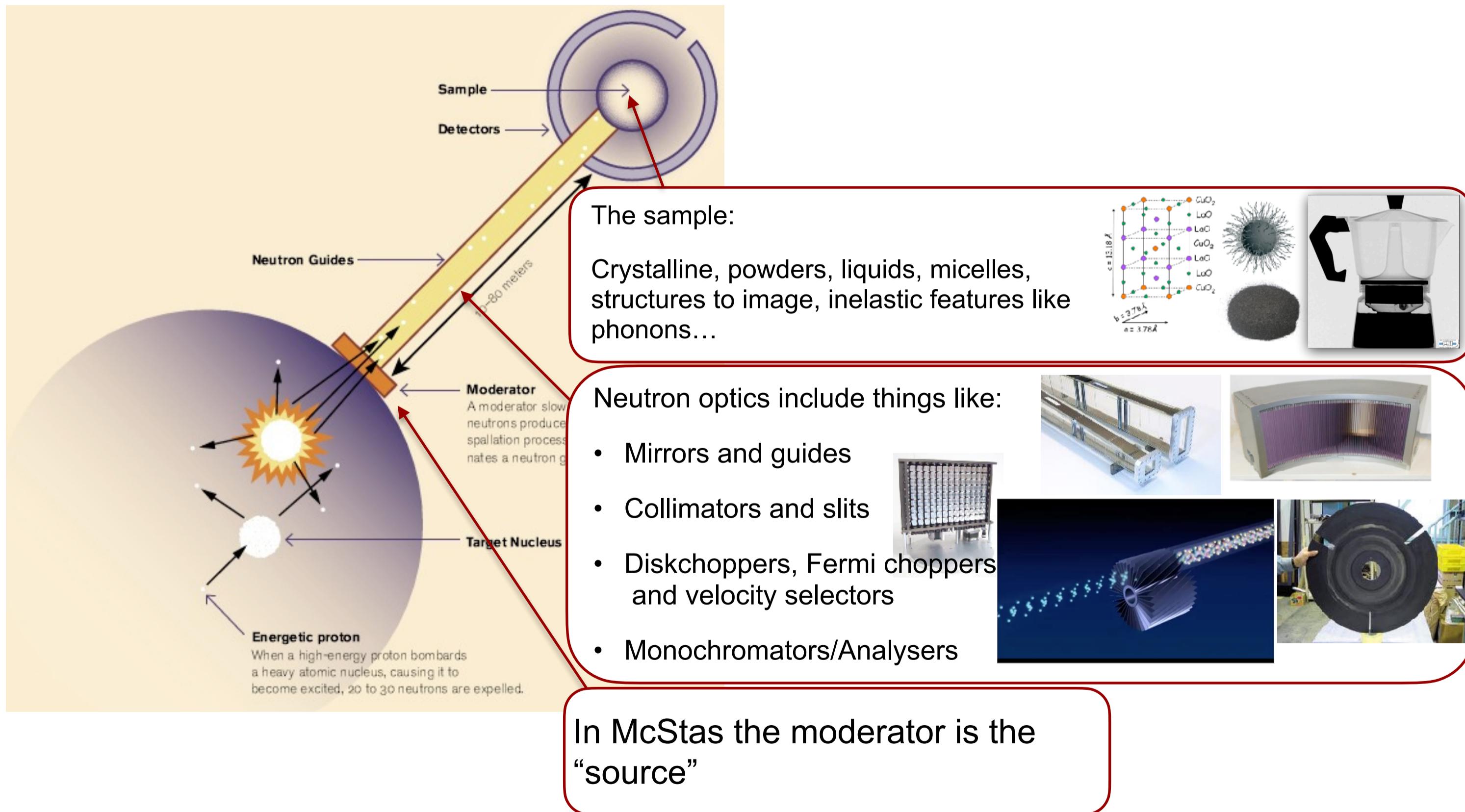
Neutron optics include things like:

- Mirrors and guides
- Collimators and slits
- Diskchoppers, Fermi choppers and velocity selectors
- Monochromators/Analysers

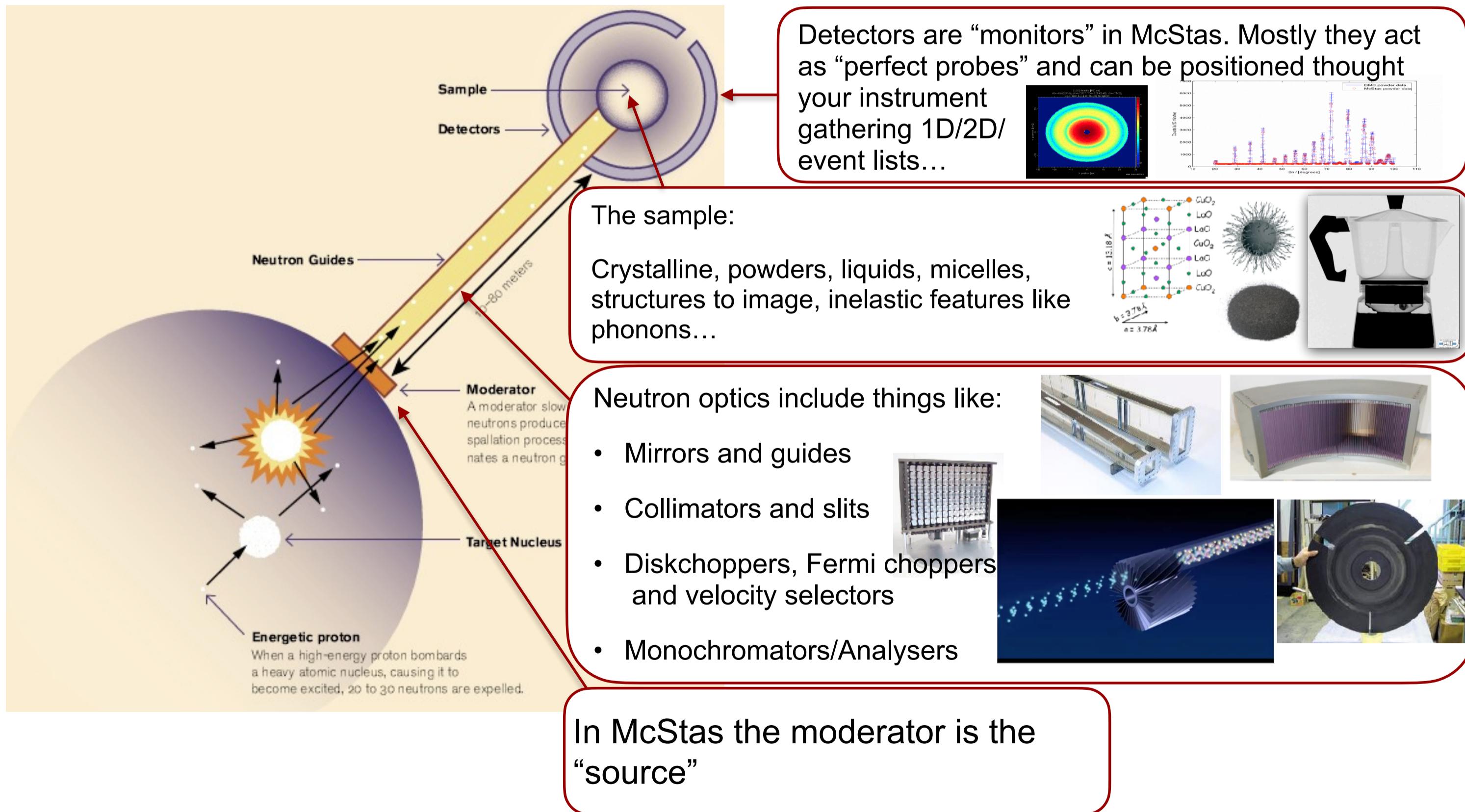


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Components of neutron instruments



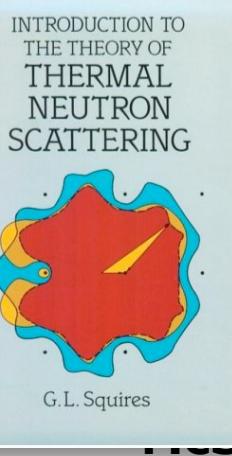
Components of neutron instruments



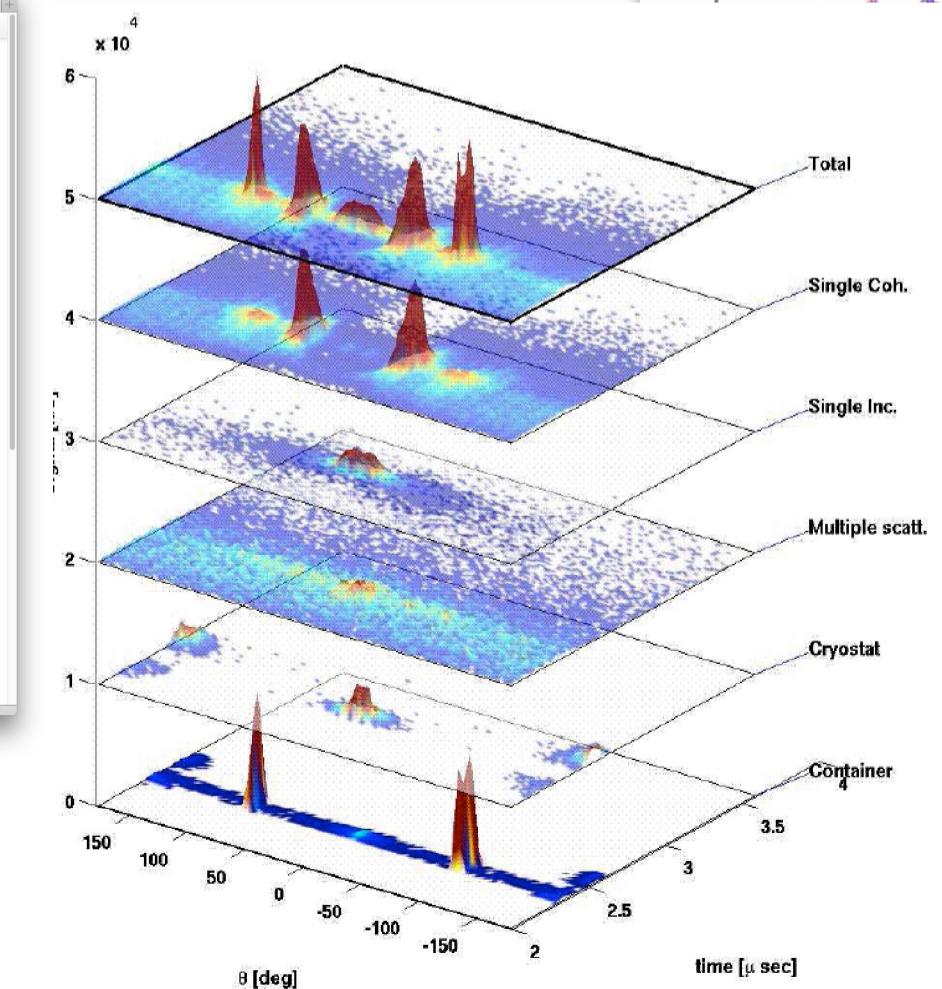
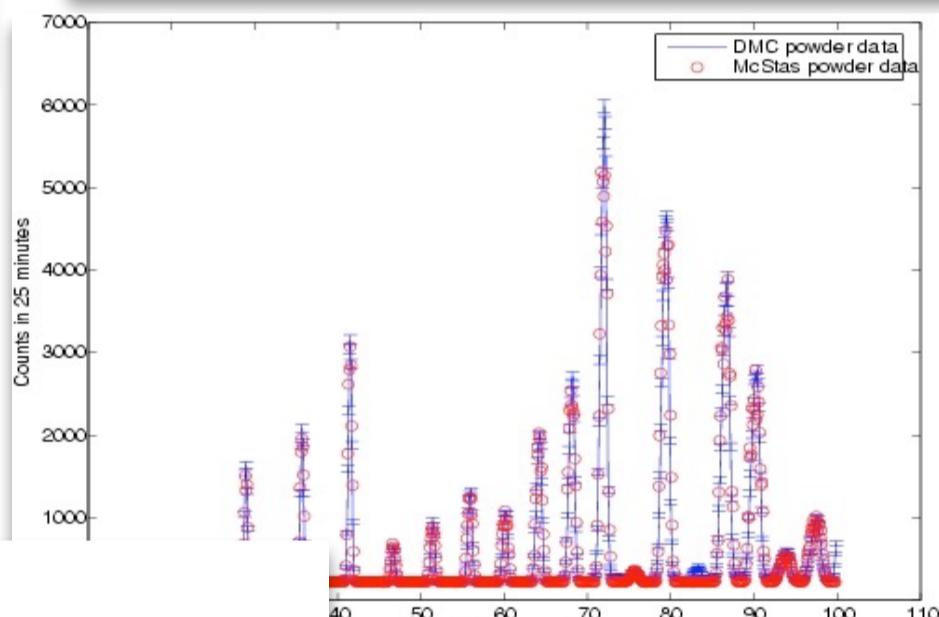
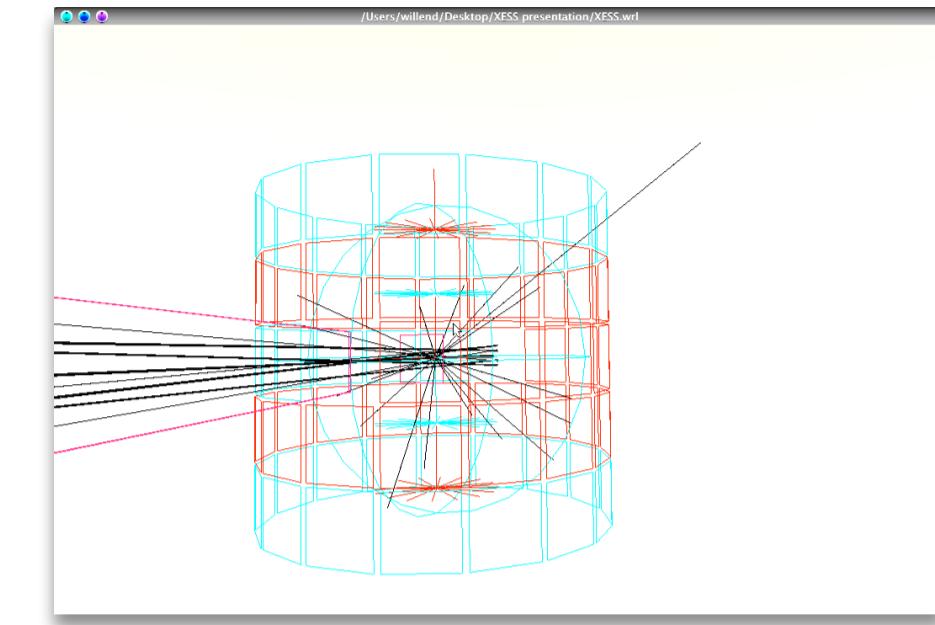
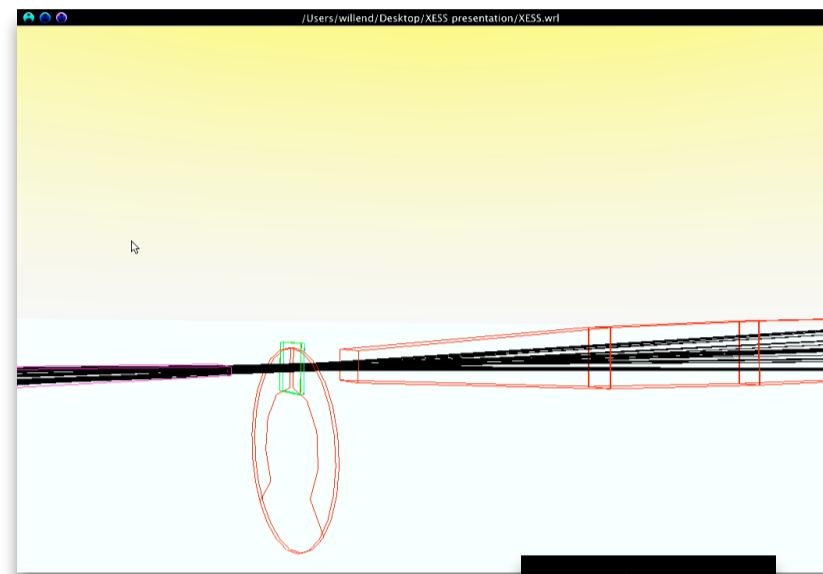
What are the codes used for?

- Instrumentation
- Virtual experiments
- Data analysis
- Teaching

(KU, DTU)



simulation tools for neutron- and X-ray in...



Neutron ray/package:

Weight (p): # neutrons (left) in the package

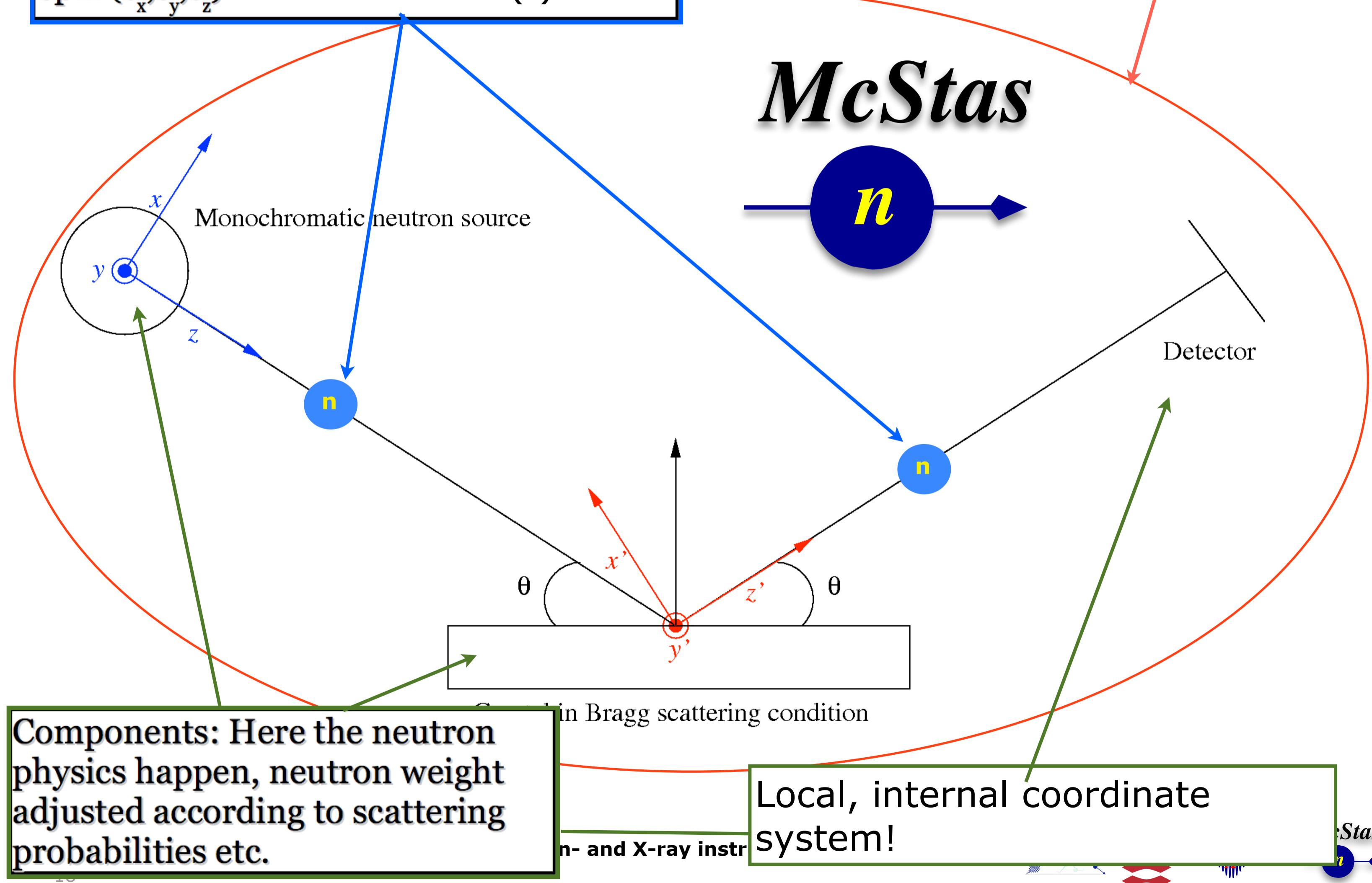
Coordinates (x, y, z)

Velocity (v_x, v_y, v_z)

Spin (s_x, s_y, s_z)

Time (t)

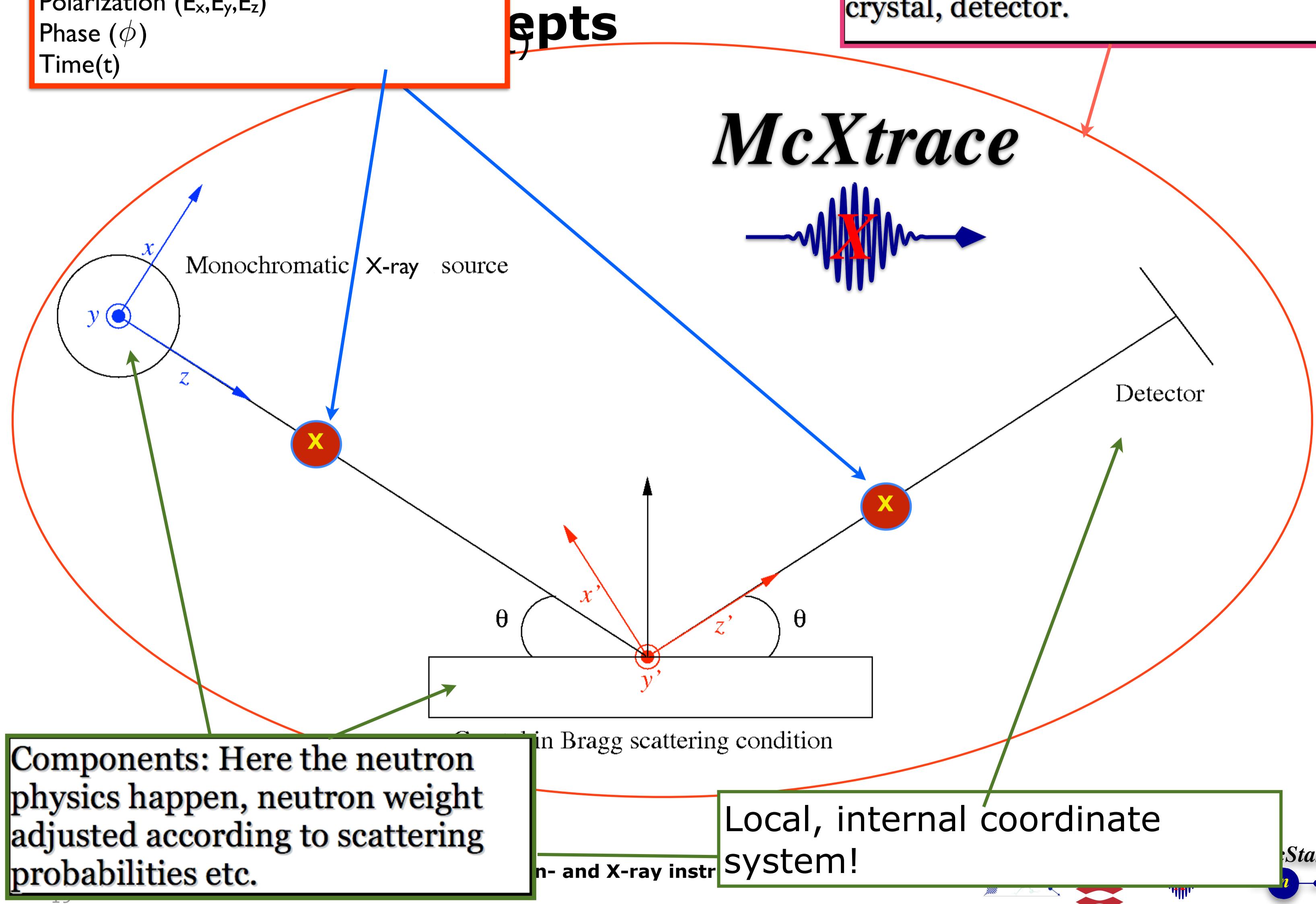
Instrument: positioning + transformation between sequential component coordinate systems, e.g. neutron source, crystal, detector.



X-ray package:

Weight (p), # photons (left) in the package
Coordinates (x, y, z)
Wavevector (k_x, k_y, k_z)
Polarization (E_x, E_y, E_z)
Phase (ϕ)
Time(t)

Instrument: positioning + transformation between sequential component coordinate systems, e.g. neutron source, crystal, detector.



McStas/McXtrace tech overview

- Portable code (Unix/Linux/Mac/Windoze)

CPU's



+ NVIDIA GPU's



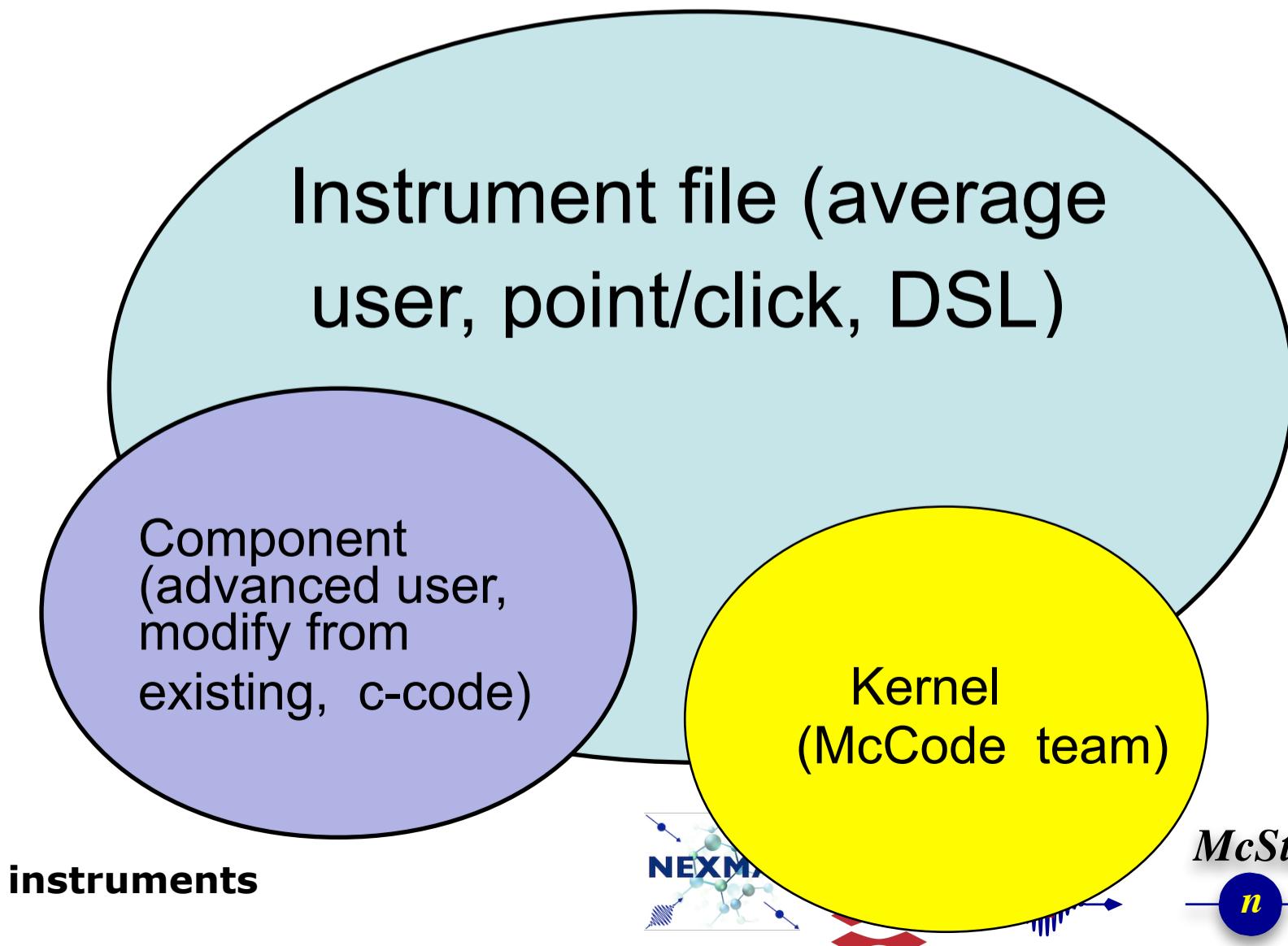
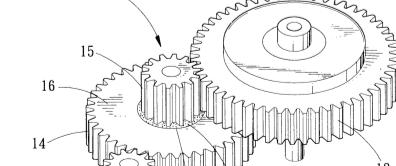
- Ran on everything from iPhone to 1000+ node cluster!



- 'Component' files (~259/~105) inserted from library

- Sources
- Optics
- Samples
- Monitors
- If needed, write your own comps

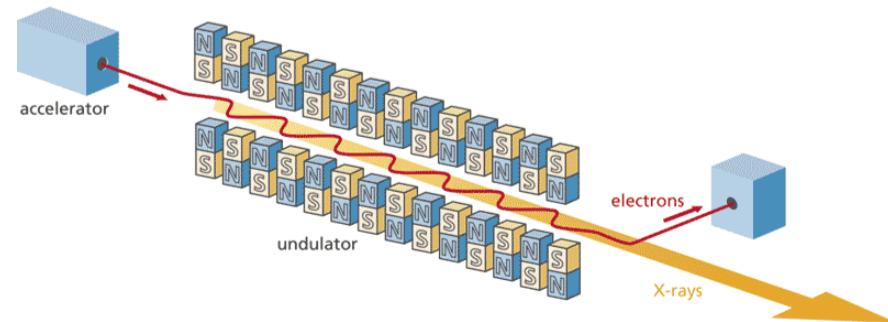
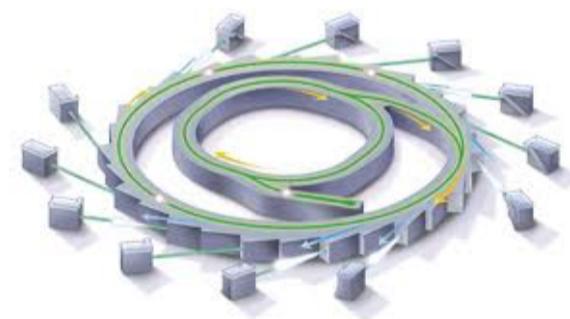
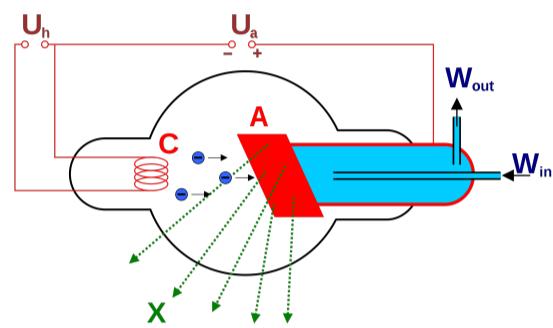
- DSL + ISO-C code gen.



Sources - 1

• X-ray sources

- Lab equipment
 - X-ray tube
 - Rotating anode
 - Liquid jet anode
- Synchrotron
 - Bending magnet
 - Wiggler
 - Undulator
- XFEL
 - SASE (very long undulator)

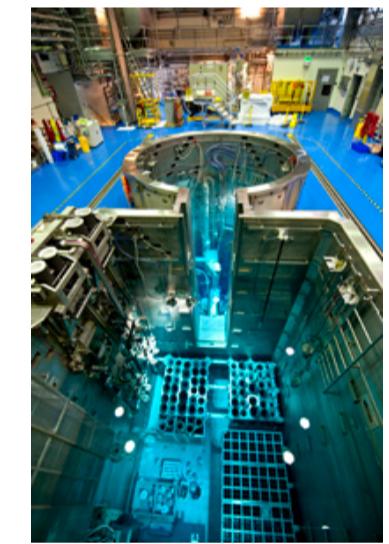


• Neutron sources

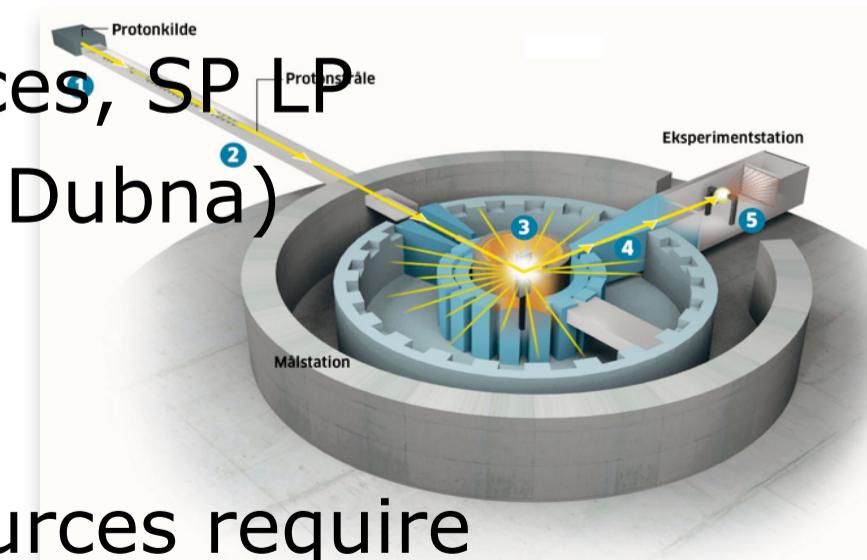
- Lab equipment
 - Radioisotope-based
 - CANS (Compact acclererator based)



- Steady state sources
 - Research reactors
 - Spallation source at PSI



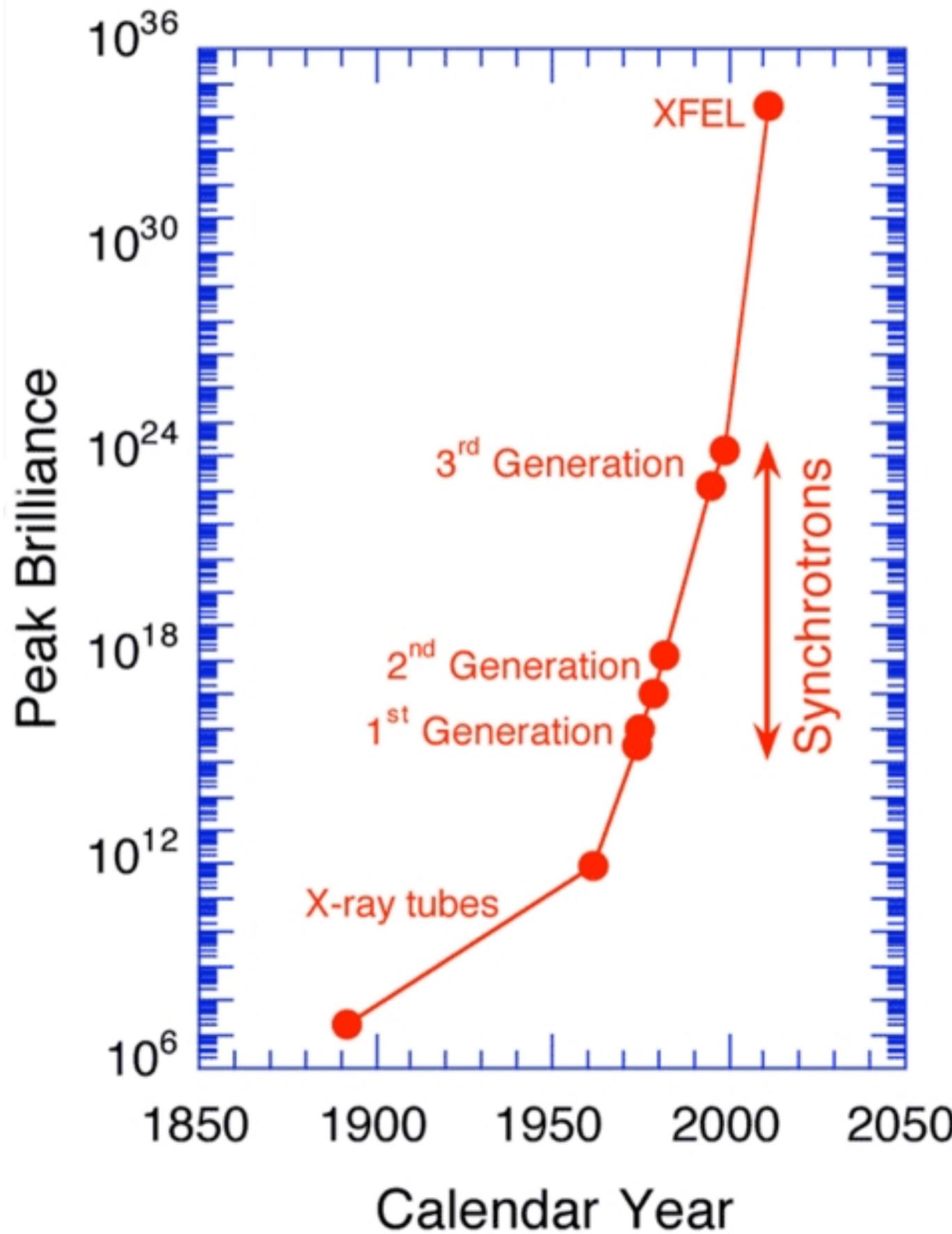
- Pulsed sources
 - Spallation sources, SP LP
 - Pulsed reactor (Dubna)



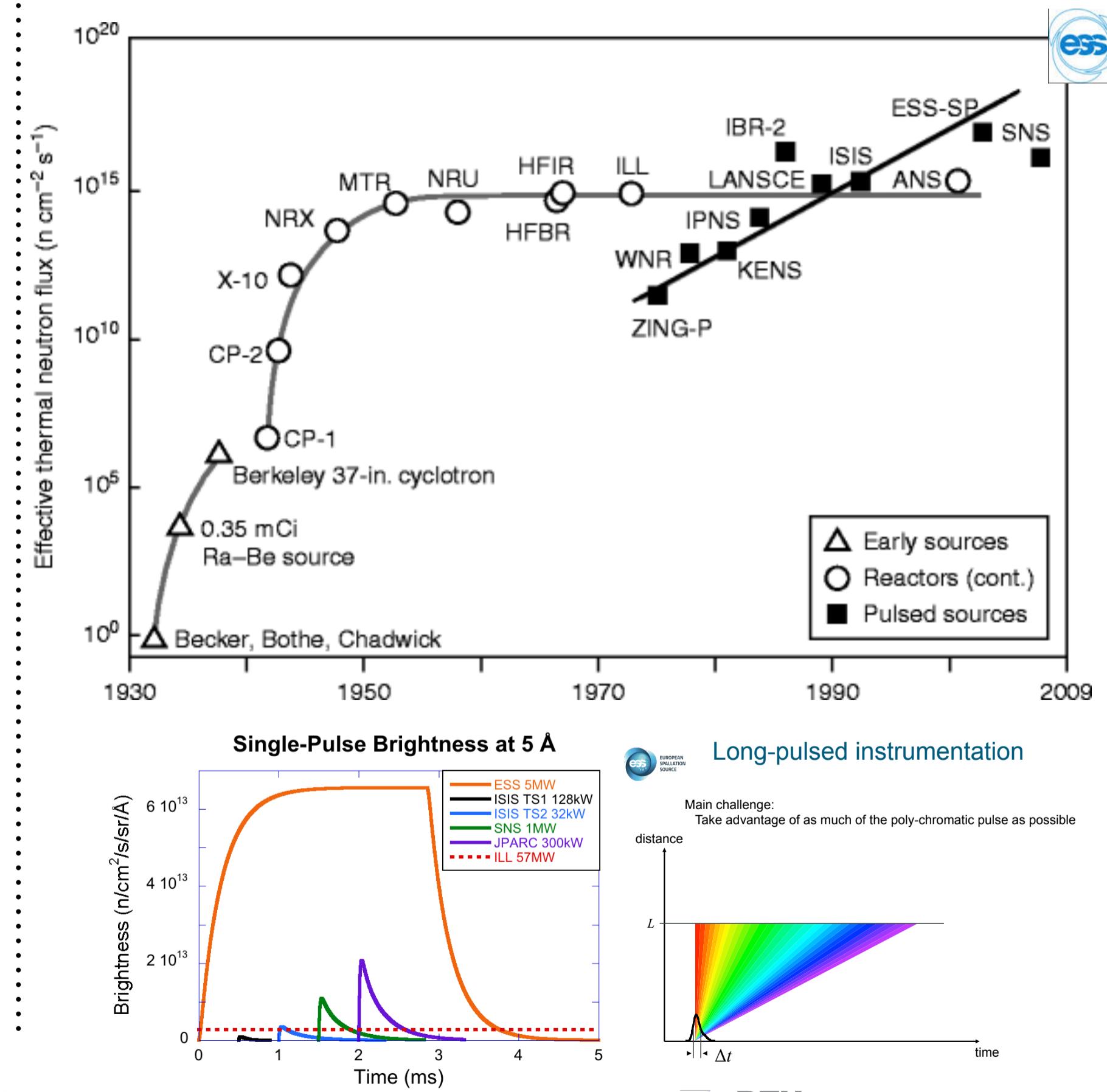
- Most neutron sources require moderation of the neutron energy

Sources - 2

• X-ray sources



• Neutron sources



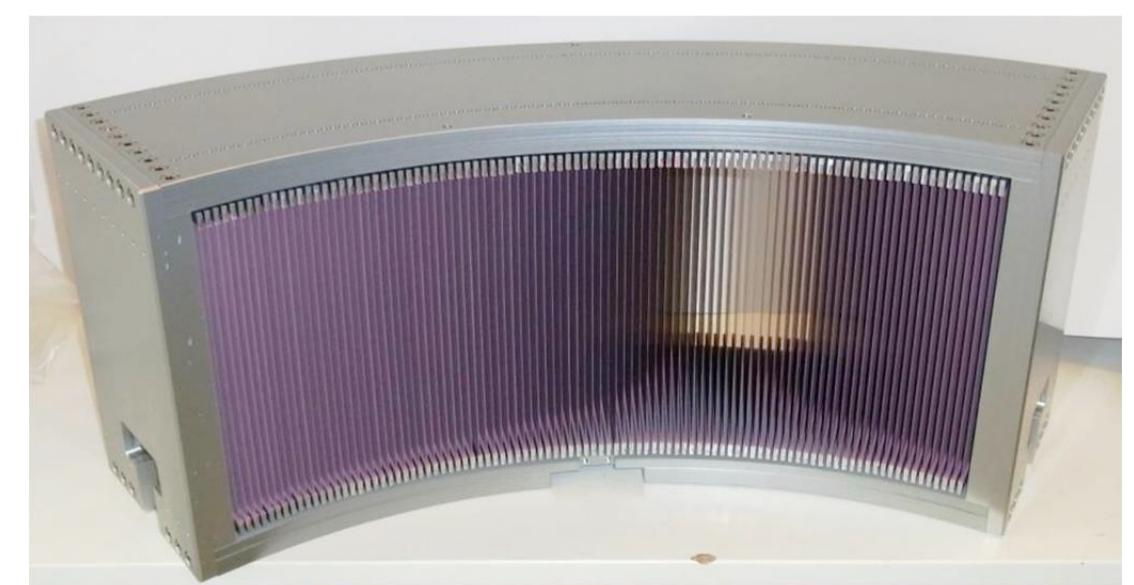
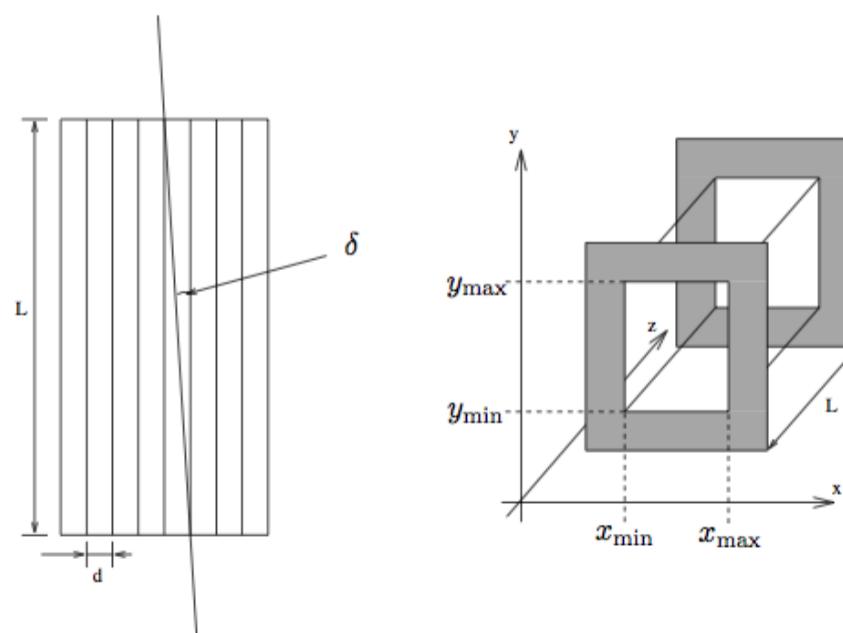
Spatial / directional beam adjustment

- **Spatial: pinholes / slits / apertures**
 - Static or adjustable “hole” in absorbing material



- **Directional: slit-assemblies or collimators**

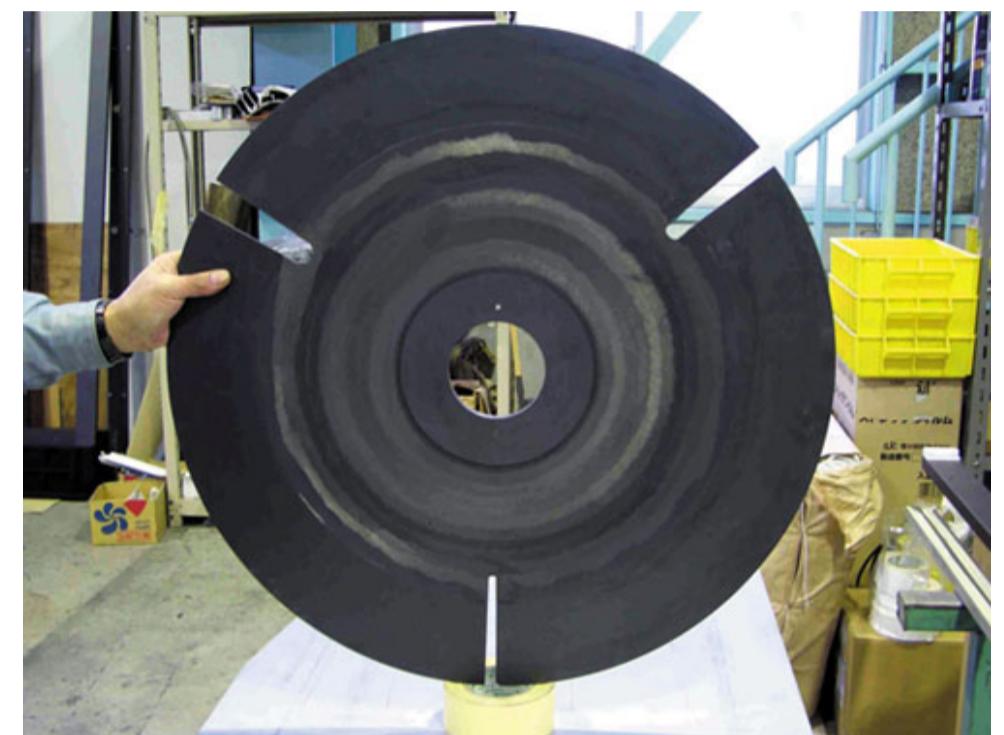
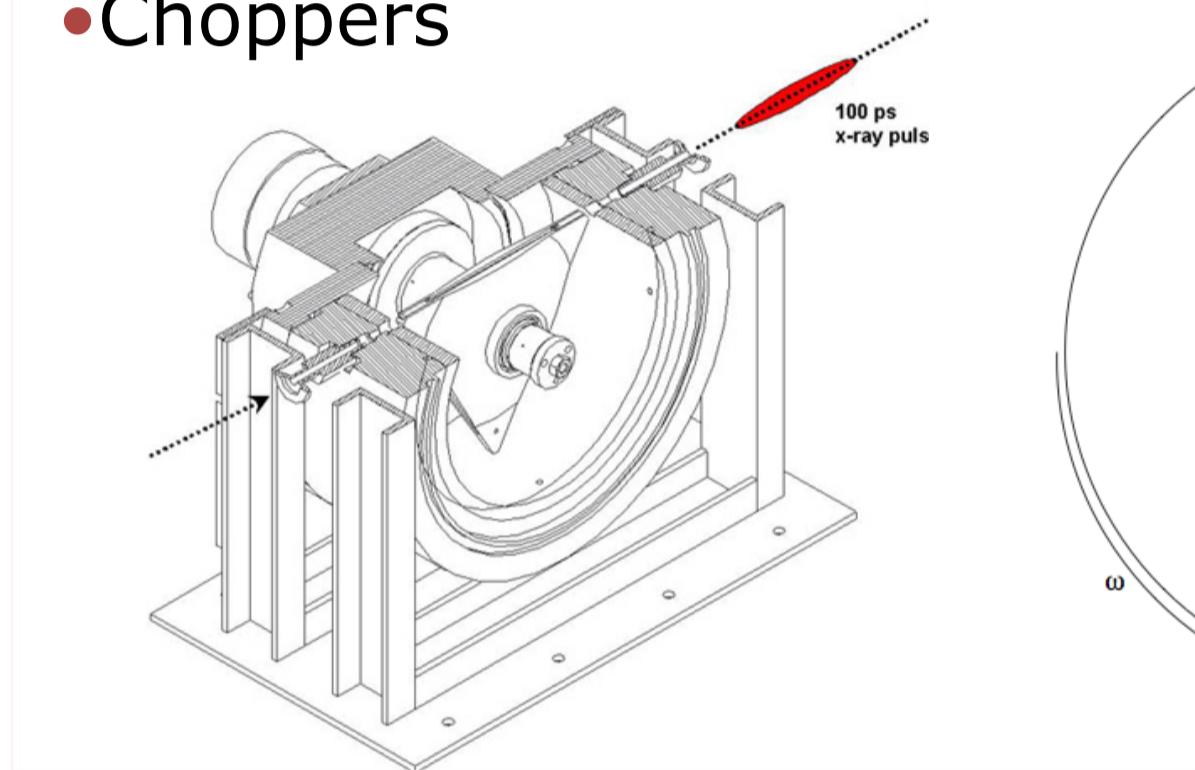
- Two or more slits defines an accepted divergence
- Collimators makes “channels”, typically with absorbing walls
- Usually static devices, but rotating radial collimators exist



Temporal beam adjustment, rotating optics

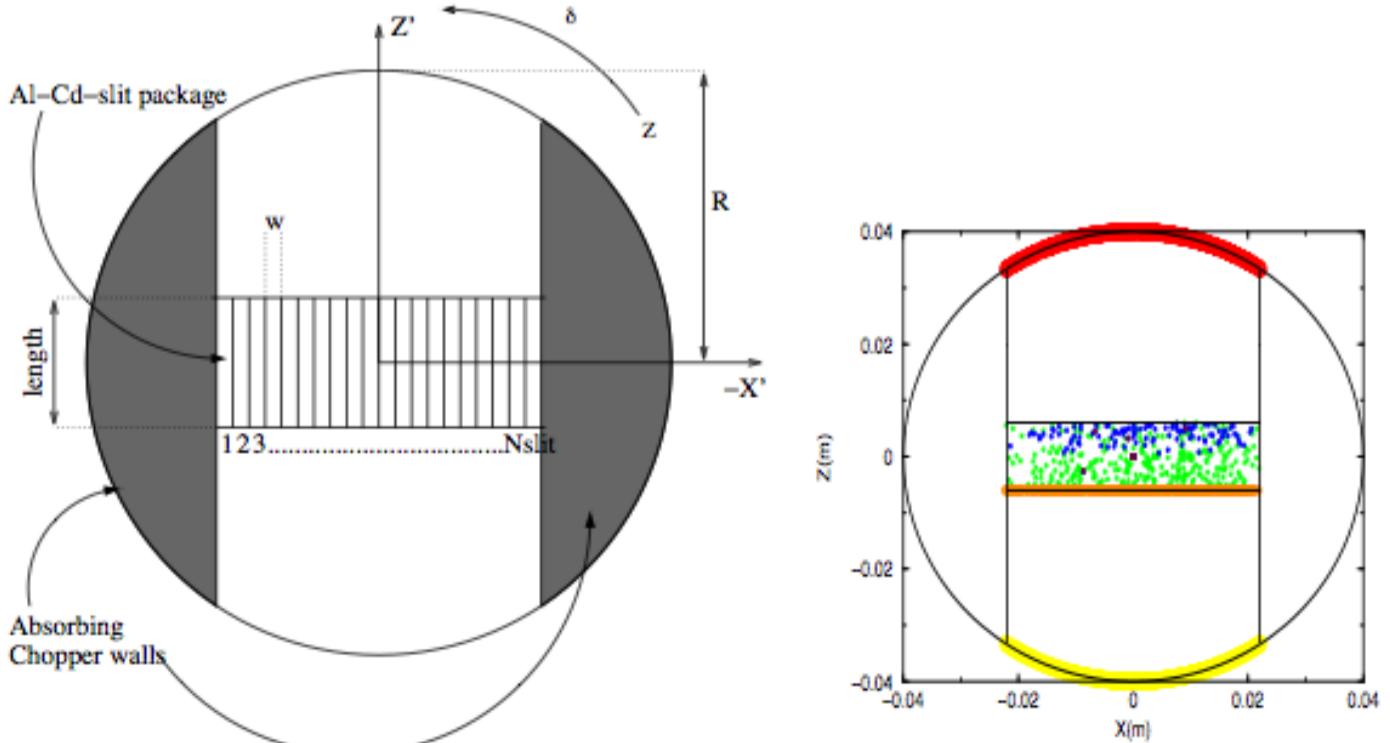
- X-ray and neutrons

- Choppers



- Neutrons only - monochromating rotating optics

- Fermi-chopper “rotating collimator”



McStas and McXtrace: simulation tools for neutron- and X-ray instruments

Velocity-selector



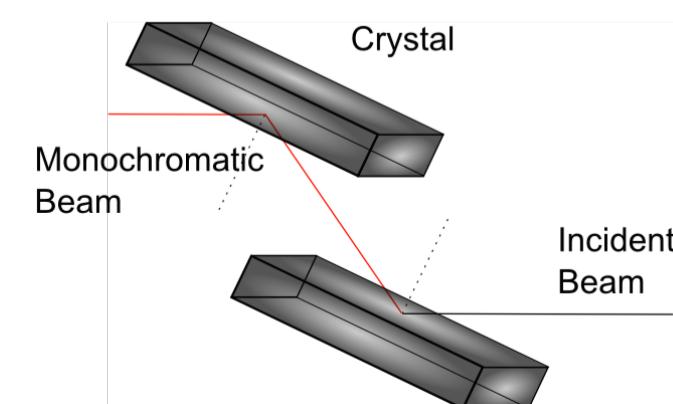
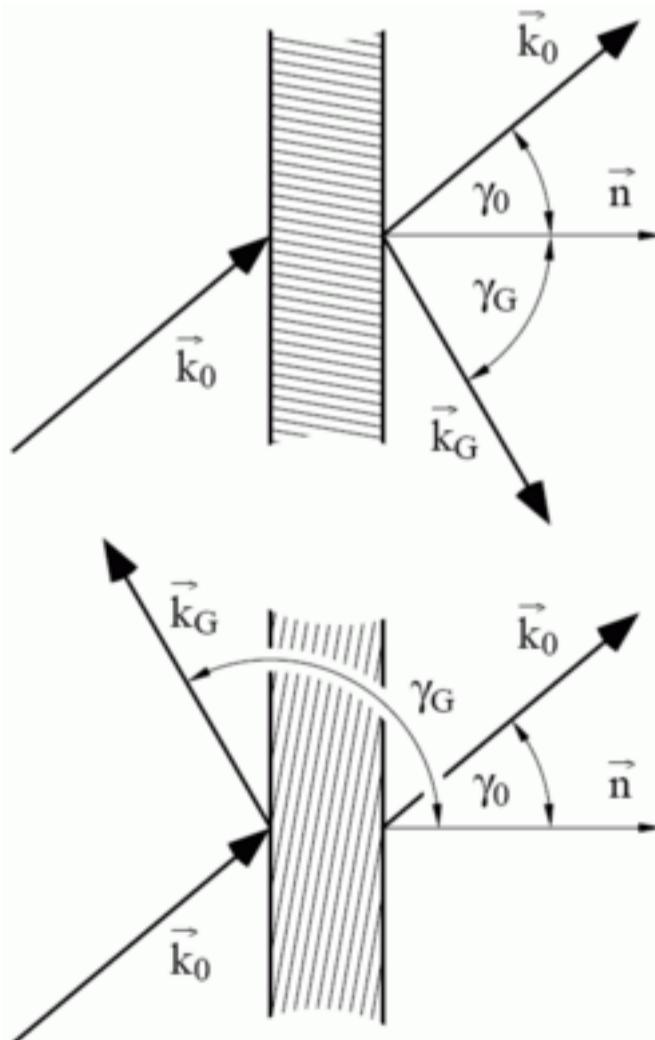
$$\frac{\delta\lambda}{\lambda} \approx 10\%$$

Crystal-based monochromators - Braggs law

- **X-ray**

$$\frac{\delta\lambda}{\lambda} \approx 0.1\%$$

- Typically very little mosaicity (perfect single crystal Si, Ge, C,...)
- Laue and Bragg geometries (transmission vs. reflection)
- Creates narrow, low-divergence monochromatic beams



- **Neutron**

$$\frac{\delta\lambda}{\lambda} \approx 3\%$$

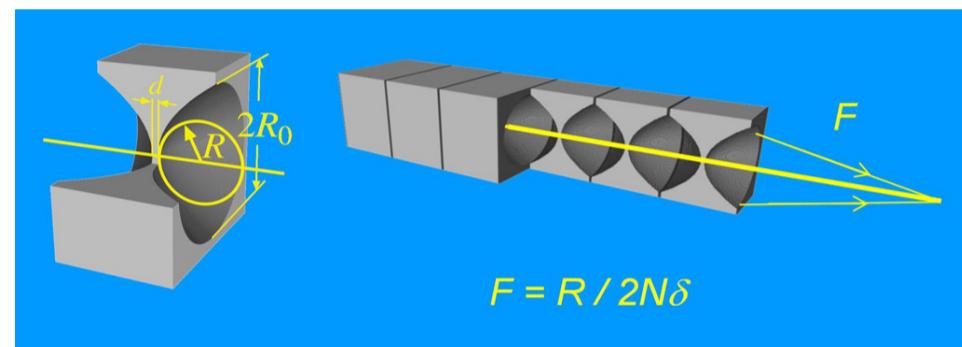
- Typically high-mosaicity (pyrolytic graphite, deformed Cu, Ge, ...)
- Often focusing, multi-crystal
- Typically Bragg geometry (reflection)
- Creates medium divergence monochromatic beams



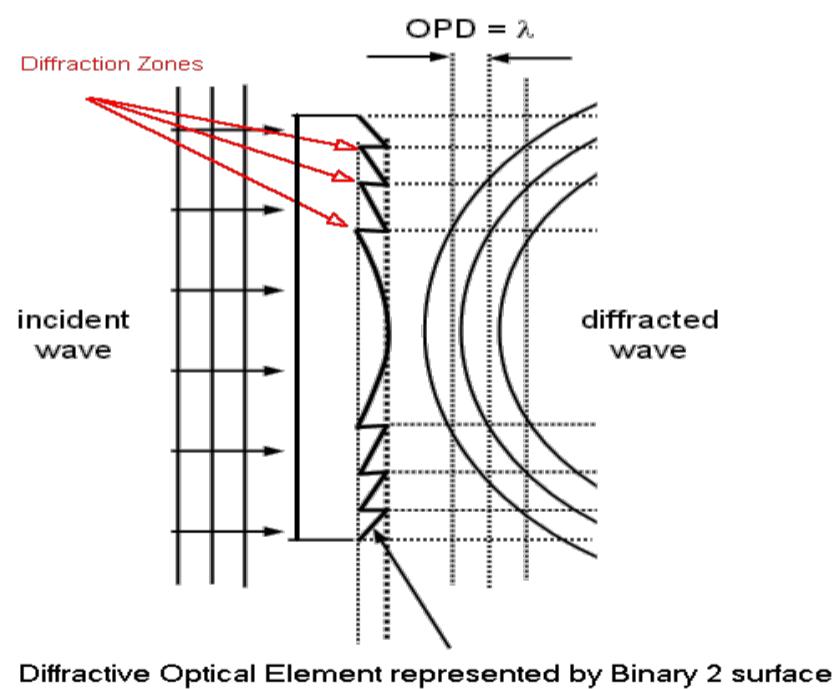
Refractive optics

· X-ray

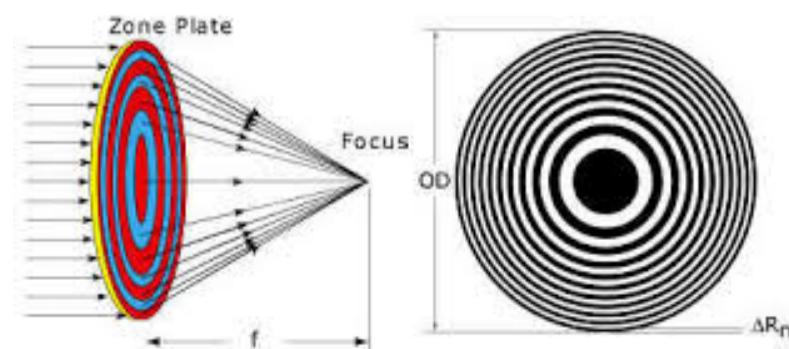
- Refractive lenses (CRLs)



Kinoform Lens

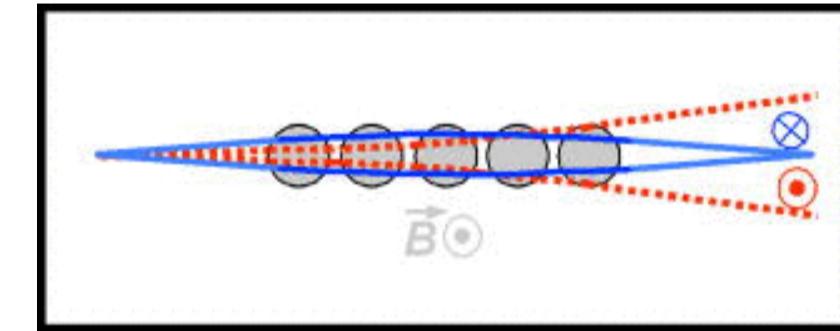


Fresnel Zone Plates



· Neutron

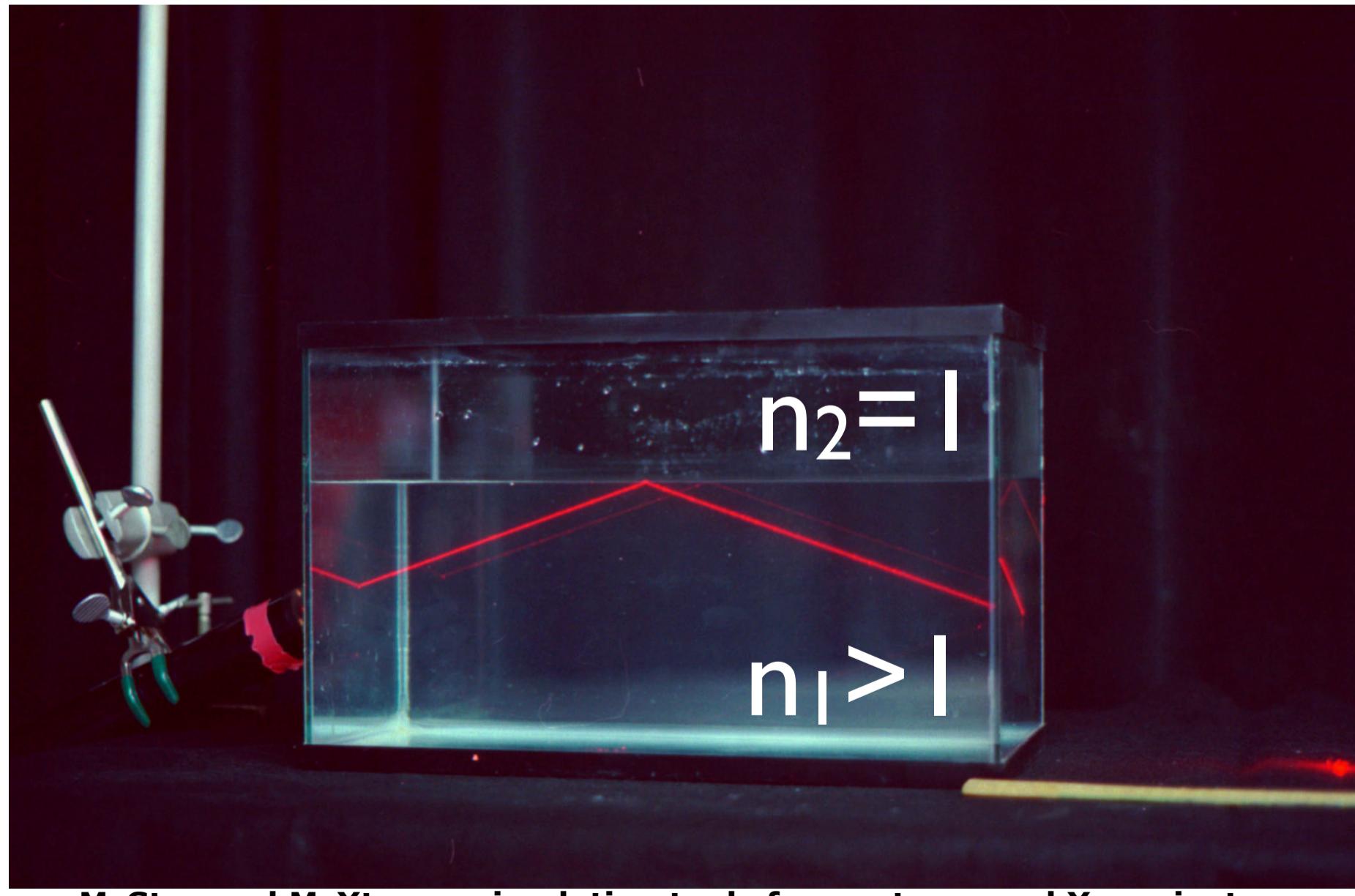
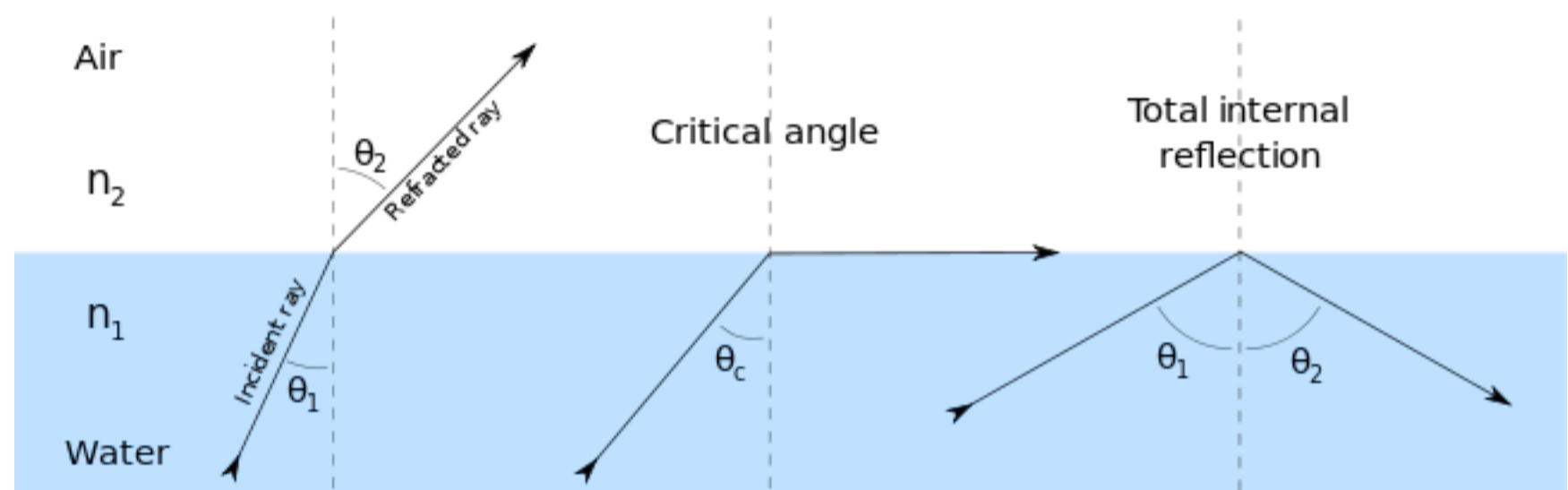
- Refractive Lenses (CRLs)



- Magnetic Materials (focusing e.g. "spin-up")

Refractive optics, total reflection - a reminder

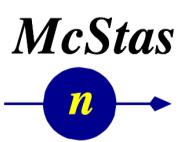
Visible light



$$n = 1 - \delta + i\beta$$

Absorption term
Refraction term

McStas and McXtrace: simulation tools for neutron- and X-ray instruments



Refractive optics

X-ray

Refractive index < 1

$$\delta_{Xray} = f(Z, \lambda, \dots)$$

$$n = 1 - \delta + i\beta$$

$$\delta_{neut} = f(b, B, \dots)$$

$$\downarrow \\ (\delta_{Xray} \propto Z)$$

$$\downarrow$$

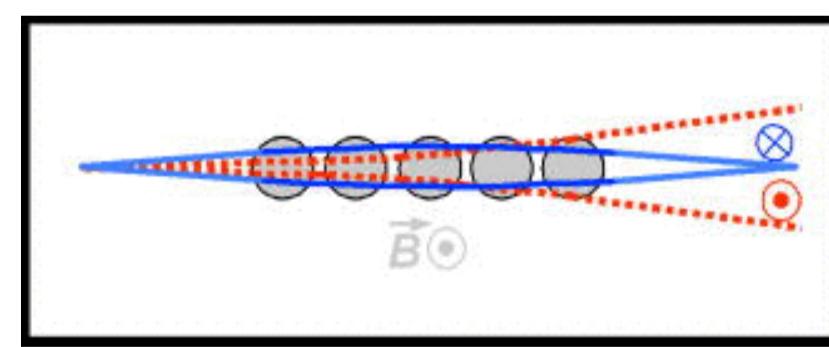
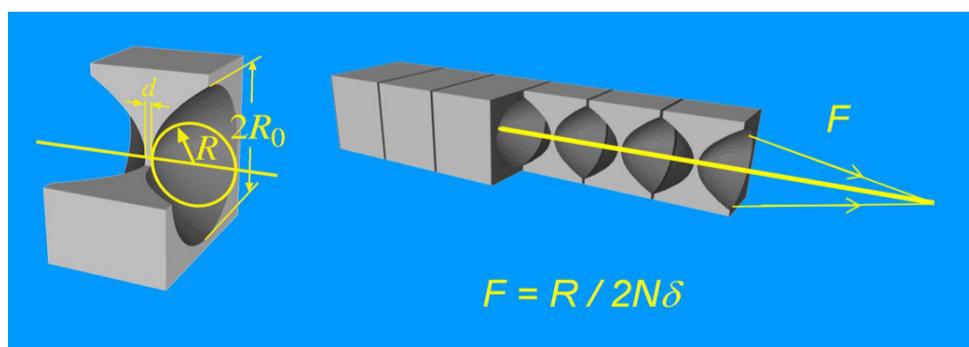
Low Z materials with low absorption. Be, Al.

High b materials with low absorption. Mg₂F

$$\downarrow$$

CRL's are a reasonable way to have low absorption with sufficient refraction

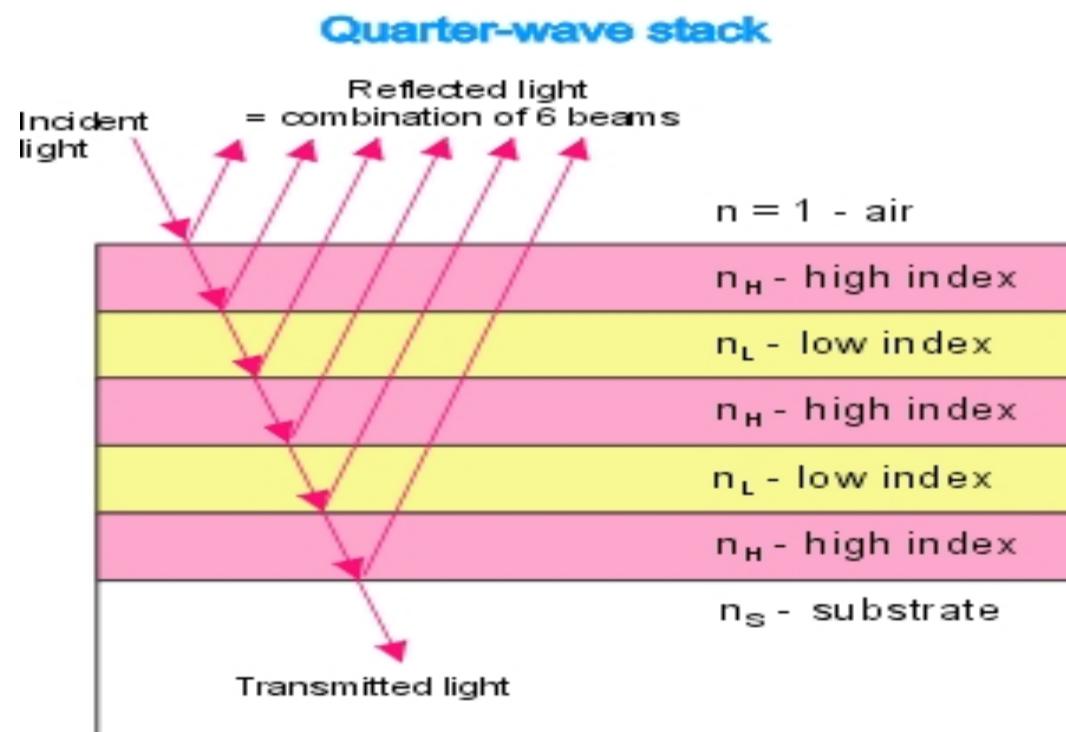
With neutrons, Lens effect from magnetism is small, hence "CRL"



Multilayers

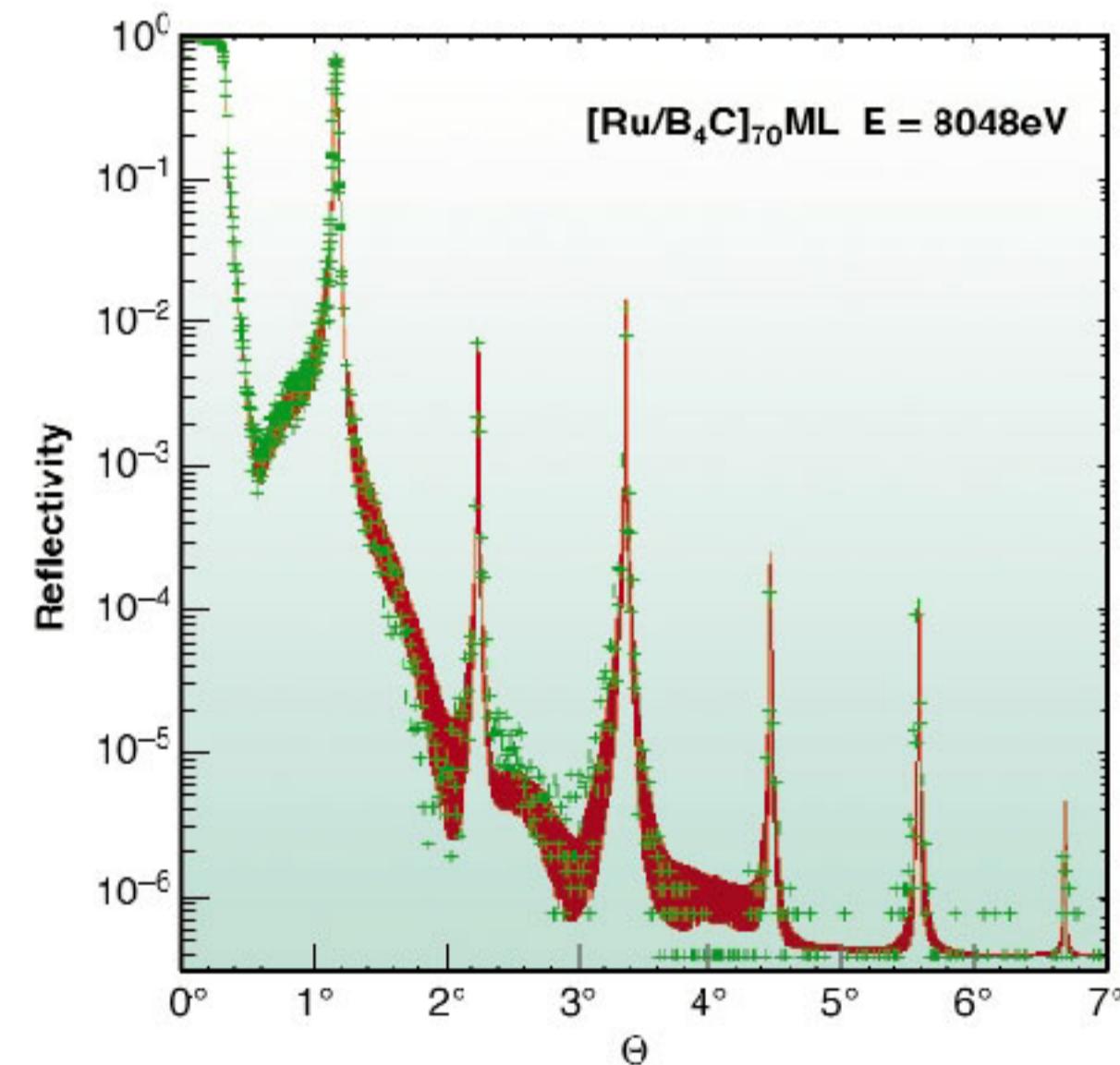
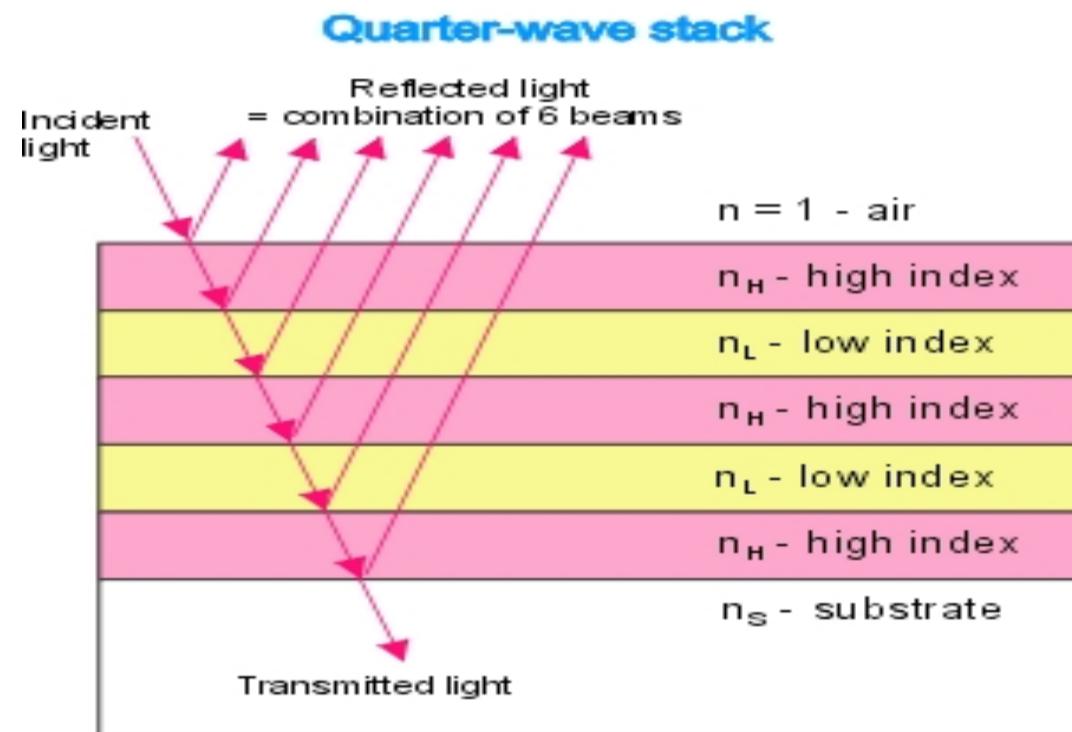
● X-ray and neutrons

Playing with phase of partial ray reflected from a given layer in the structure



Multilayers

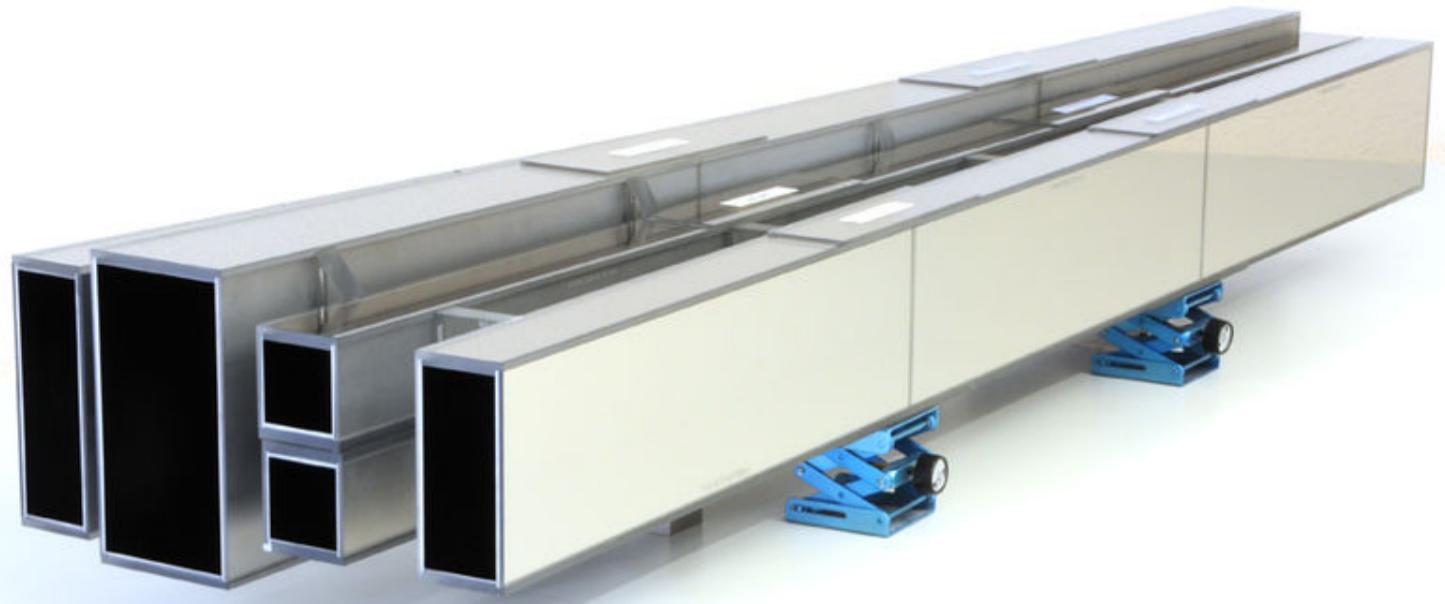
- **X-rays:**



Superstructure often used as “monochromator” - also in focusing geometry

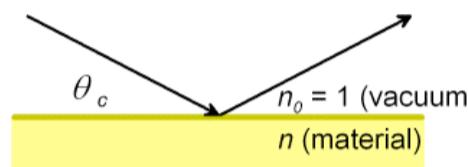
- When used as monochromator, use one of the first “side peaks” on the reflectivity curve

Multilayers



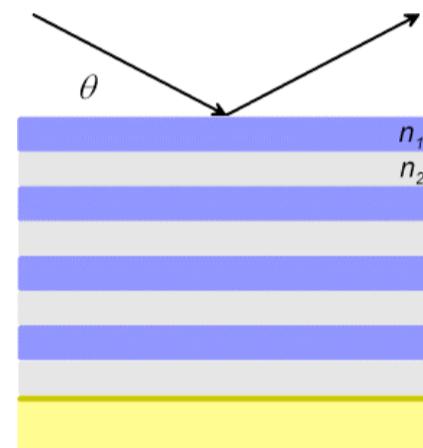
• Neutrons:

single mirror



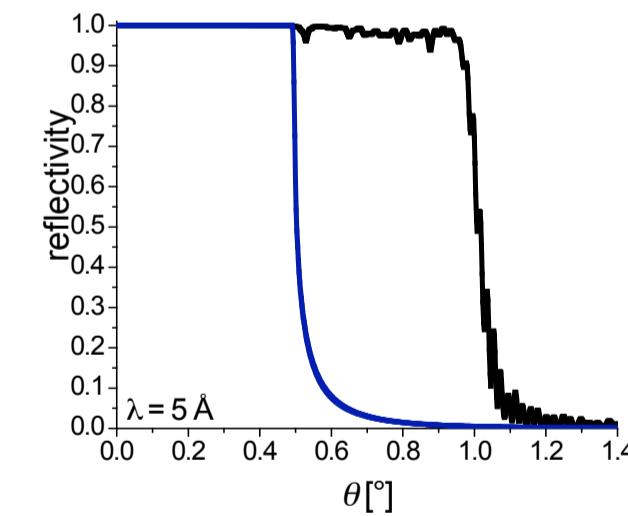
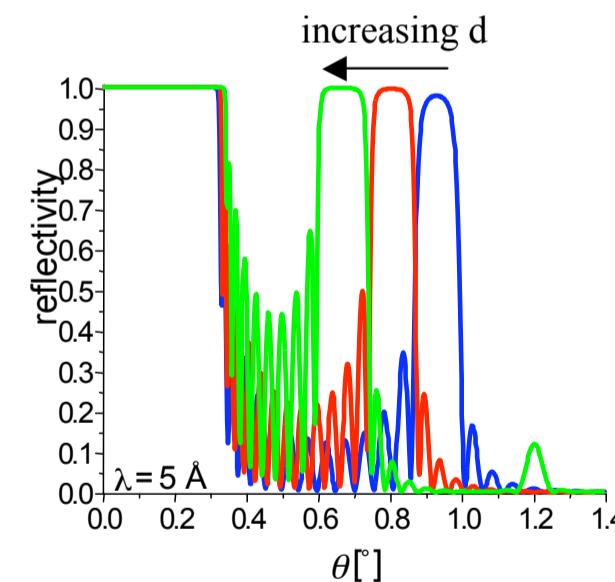
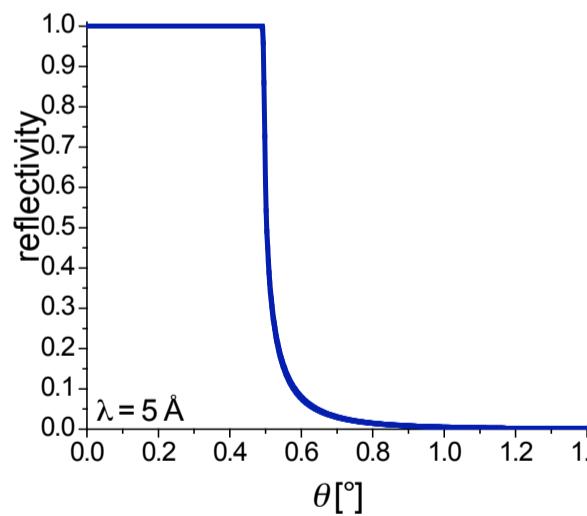
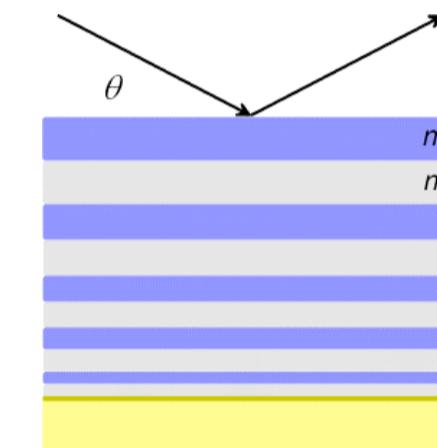
- refractive index $n < 1$
- total external reflection
e.g. Ni $\theta_c = 0.1^\circ/\text{\AA}$

multilayer



$$\lambda = 2nd \sin \theta$$

supermirror

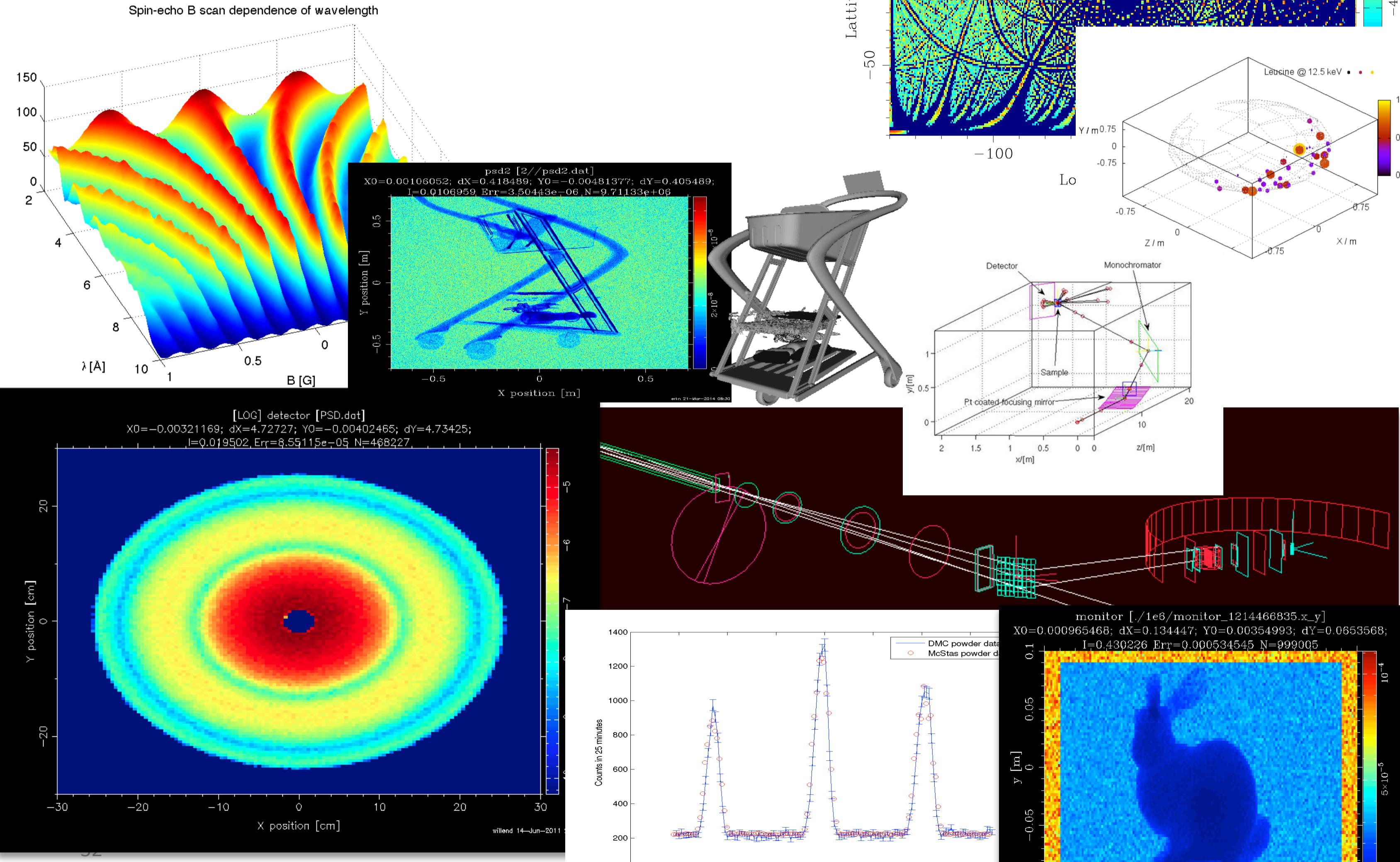


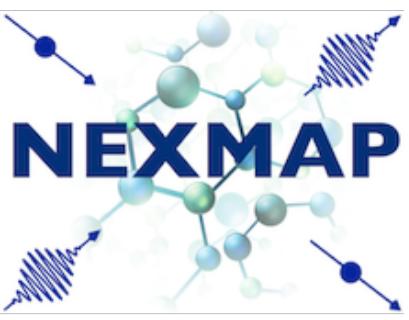
Superstructure “extends” the total-reflection range in Q by “Bragg peaks”

- ideally a wide, flat distribution
- used in all kinds of neutron optics, but specifically in guides - “optical fibre”

[LOG] det [1e9_parallel/psd.dat]
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 I=210.788 Err=0.162219 N=2.09642e+06

Example suite - instruments: 247 McStas 63 McXtrace





Questions?

Now we proceed to the simulations

- Form groups of 2 to work together, e.g.
 - Take turns @ keyboard
 - Discuss as you go along, interact and compare results
- Use <https://e-learning.pan-training.eu/course/view.php?id=104> to access McStas and McXtrace
(I demo this at first)