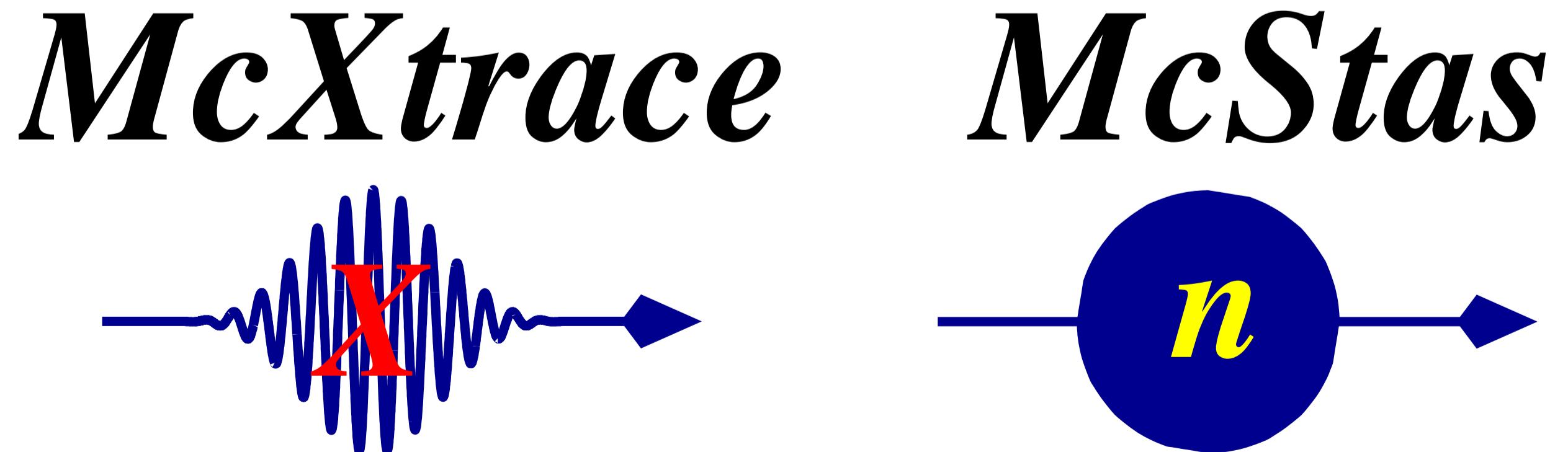


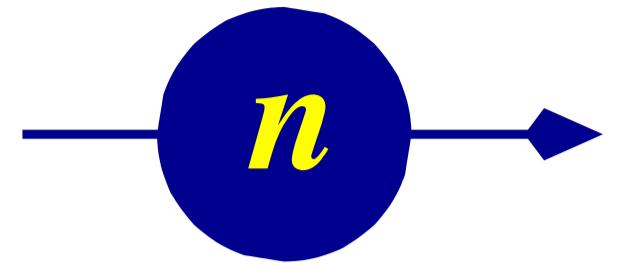
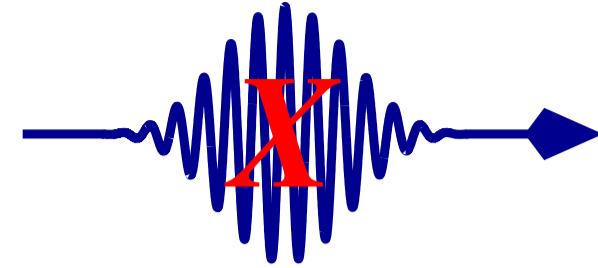
McStas and McXtrace: simulation tools for neutron- and X-ray instruments

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¹**NEXMAP, Physics Department, Technical University of Denmark, Denmark**

²**ESS 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

- In some sense you already “know” these codes... They are what you have been running in the elearn1 “simulator”

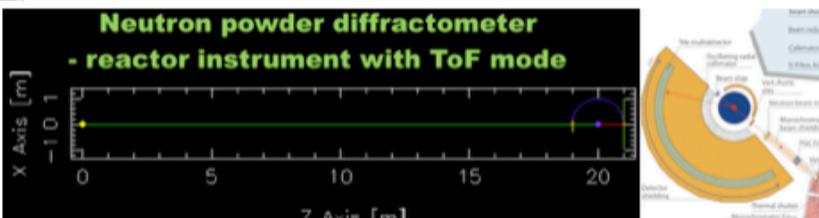
Instrument



N_diffractometer

Logged in as pkwi (see recent simruns)

Neutron powder diffractometer - reactor instrument with ToF mode



Parameters for N_diffractometer

lambda [AA]:	10	Central wavelength produced by the source (10)
dlambda [AA]:	9.5	Width +/- of wavelength band around central wavelength (9.5)
powderfile [string]:	Na2Ca3Al2F14.laz	"Structure" datafile for studied material (Na2Ca3Al2F14.laz)
d_phi [deg]:	180	When d_phi == 180 deg, the sample illuminates "all angles around the scattering plane". When d_phi scattering will be restricted directionally to "hit" the banana-shaped detectors (180)
TOF [1]:	0	"Reactor" or "Time-of-Flight" mode (0)
NU [Hz]:	100	Frequency of the chopper. (100)
THETA [deg]:	10	Angular opening of the chopper window. (10)
ANGLE [deg]:	0	Grazing angle of the monochromator crystal. (0)

Runtime configuration

neutron rays:	1000000
simulation steps:	1
random seed:	0

Start simulation run:

A web-based interface for [McStas](#).

All contents is provided under the terms of 

Instrument

e-neutrons

N_diffractometer

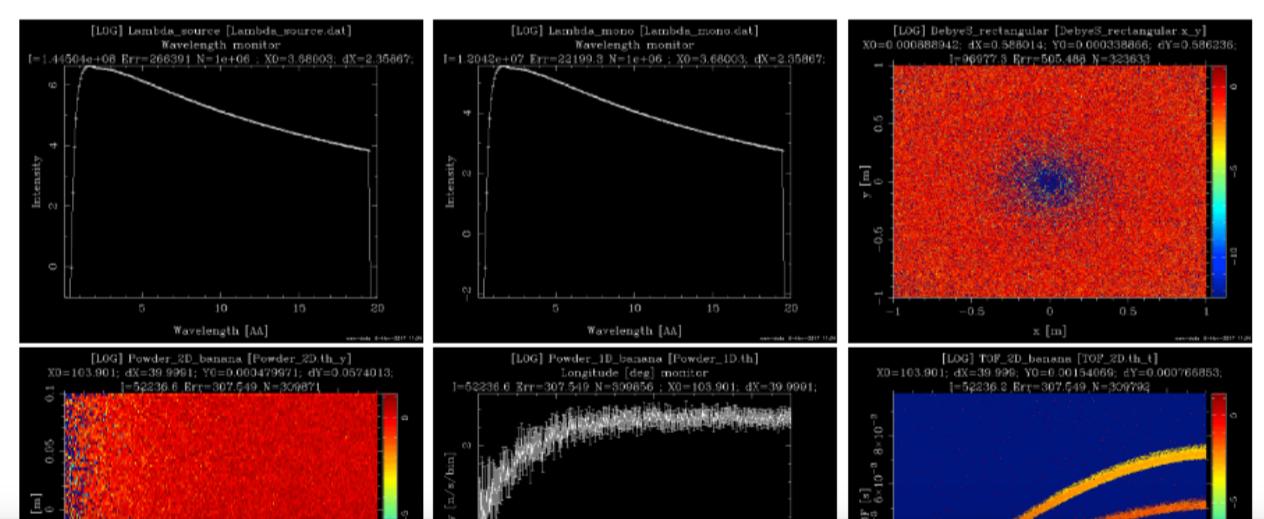
Completed 11:34:20, 09/11/2017

[Reconfigure](#)

Simulation

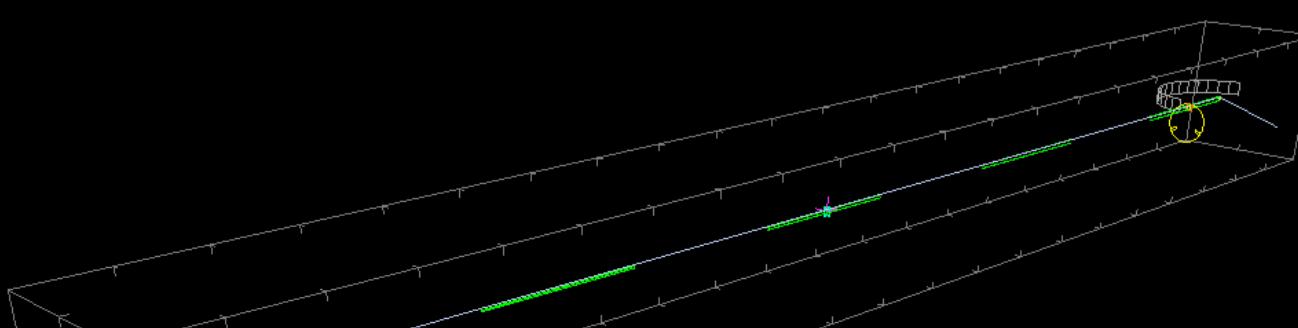
```
params: lambda=10 dilambda=9.5 powderfile=Na2Ca3Al2F14.laz d_phi=180 TOF=1 NU=100 THETA=10 ANGLE=0
neutron rays: 1000000
random seed: 0
simulation steps: 1
```

Data plots (click here for lin-scale)



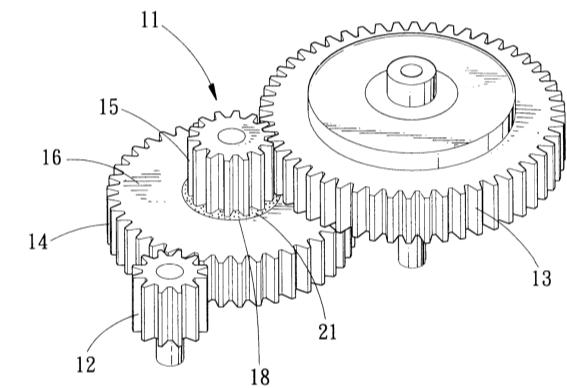
mcrun N_diffractometer.instr --no-output-files --trace --ncount=300 --dir=mcdisplay lambda=10 dilambda=9.5 powderfile=Na2Ca3Al2F14.laz d_phi=180 TOF=1 NU=100 THETA=10 ANGLE=0

Ray index 124 / 299 Keep rays Scatter Markers Reset view:

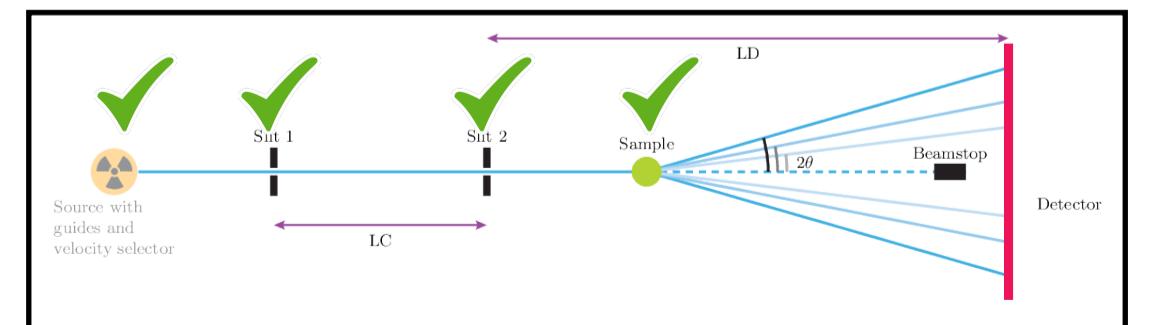


Purpose of today's activities

- See what is “under the hood” in the simulator - and work with it!



- Produce an instrument model



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 homepage. The left sidebar contains links for "About McStas", "Download", "Mailing list", "Documentation", "Workshops/conferences", "Developments", "Links", "Report bugs", "SVN", and "McStas Ubuntu live-dvd". The main content area features a heading "McStas - A neutron ray-trace simulation package" and a sub-section titled "McStas - A neutron ray-trace simulation package". It includes a plot showing the intensity of scattered neutrons from a sample, with a caption explaining the shadowing effect and non-symmetric geometry. Below the plot, there is a section for "Recent news" and a link to the release notes for McStas 2.1.

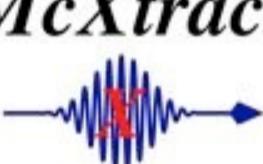
McXtrace - same idea, but for X-rays (2009-)

McXtrace homepage - Mozilla Firefox

File Edit View History Bookmarks Tools Help

McXtrace homepage www.mcxtrace.org Google

Most Visited Getting Started A/B Trøjborg 1 Latest Headlines latex-lab projec... publications.li Viewing Feed McCode: {8} A... Import to Mendeley

McXtrace  **McXtrace - An X-ray ray-trace simulation package**   

McXtrace
Project Status
Project Partners
Project People
Goal
Mailing List
Links
Publications
Minutes of Meetings
McXtrace Art
Documentation
Installation
Download Components
Search

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

     **SAXS LAB**

This site is undergoing reorganization. Inconsistencies and broken links may occur. Please do report any findings to erkn_AT_fysik.dtu.dk if you have the time. Thanks in advance.

Funding from NABIIT, [DSF](#) and the above parties.

McStas 

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 – level of scattering and atomic no.

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

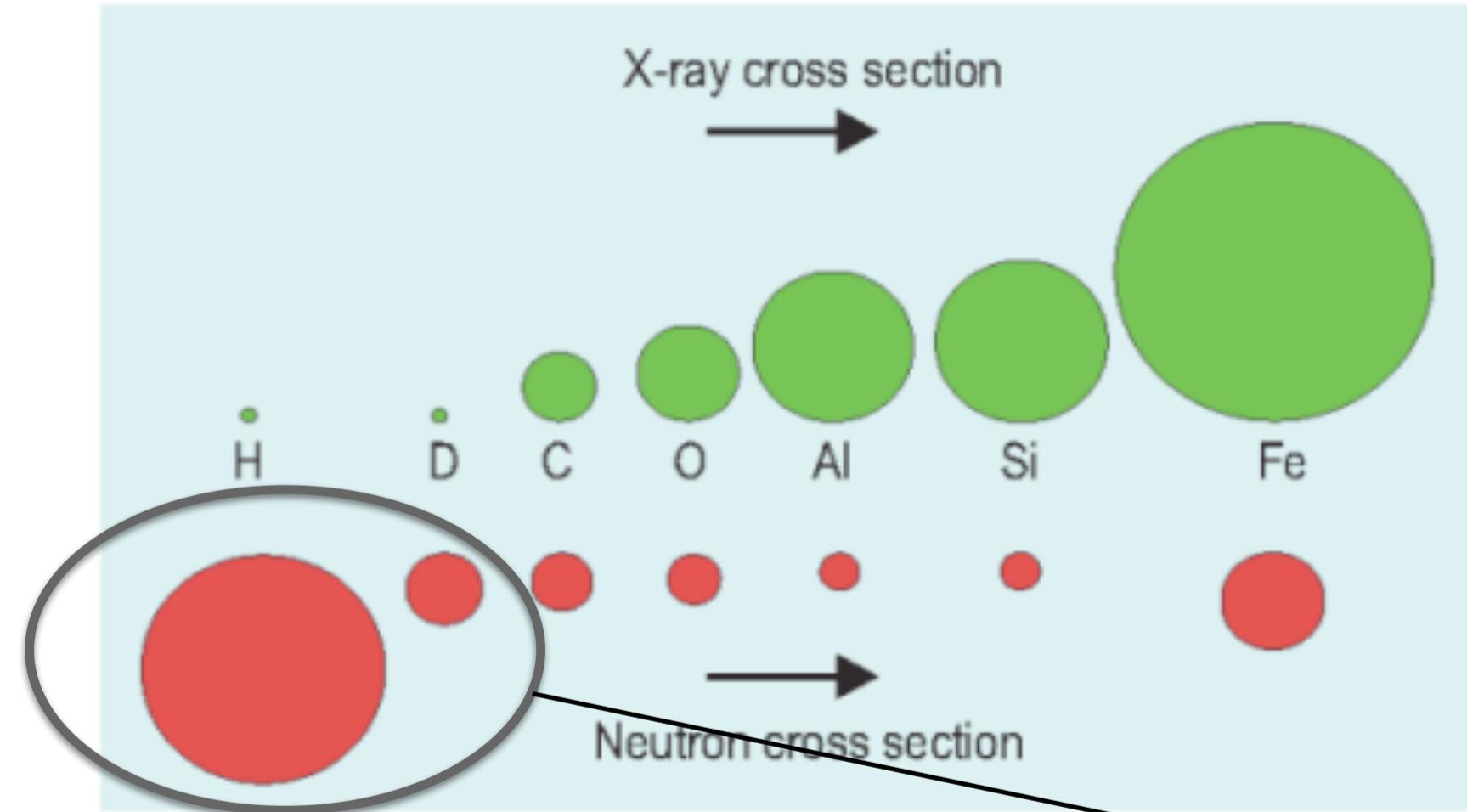


Fig. 2. Neutron and x-ray scattering cross-sections compared. Note that neutrons penetrate through Al much better than x rays do, yet are strongly scattered by hydrogen.

- Result: Two very different response/contrasts

1A	2A	About Chemistry										8A					
1 H 1s ¹	4 Be 1s ² 2s ²	5 B 1s ² 2s ¹ p ¹	6 C 1s ² 2s 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 ⁴ s ²	21 Sc [Ar]3d ⁴ s ²	22 Ti [Ar]3d ⁴ s ²	23 V [Ar]3d ⁴ s ²	24 Cr [Ar]3d ⁴ s ²	25 Mn [Ar]3d ⁴ s ²	26 Fe [Ar]3d ⁴ s ²	27 Co [Ar]3d ⁴ s ²	28 Ni [Ar]3d ⁴ s ²	29 Cu [Ar]3d ¹⁰ 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 ² 5s ¹	42 Mo [Kr]4d ² 5s ¹	43 Tc [Kr]4d ² 5s ¹	44 Ru [Kr]4d ² 5s ¹	45 Rh [Kr]4d ² 5s ¹	46 Pd [Kr]4d ¹⁰	47 Ag [Kr]4d ⁹ 5s ¹	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 ² 6s ²	73 Ta [Xe]4f ¹ 5d ² 6s ²	74 W [Xe]4f ¹ 5d ² 6s ²	75 Re [Xe]4f ¹ 5d ² 6s ²	76 Os [Xe]4f ¹ 5d ² 6s ²	77 Ir [Xe]4f ¹ 5d ² 6s ²	78 Pt [Xe]4f ¹ 5d ² 6s ²	79 Au [Xe]4f ¹ 5d ⁹ 6s ¹	80 Hg [Xe]4f ¹ 5d ⁹ 6s ¹	81 Tl [Xe]4f ¹ 5d ⁹ 6s ¹	82 Pb [Xe]4f ¹ 5d ⁹ 6s ¹	83 Bi [Xe]4f ¹ 5d ⁹ 6s ¹	84 Po [Xe]4f ¹ 5d ⁹ 6s ¹	85 At [Xe]4f ¹ 5d ⁹ 6s ¹	86 Rn [Xe]4f ¹ 5d ⁹ 6s ¹
87 Fr [Rn]7s ¹	88 Ra [Rn]7s ²	89-103 Actinides [Rn]5f ¹ 6d ¹ 7s ²	104 Rf [Rn]5f ¹ 6d ¹ 7s ²	105 Db [Rn]5f ¹ 6d ¹ 7s ²	106 Sg [Rn]5f ¹ 6d ¹ 7s ²	107 Bh [Rn]5f ¹ 6d ¹ 7s ²	108 Hs [Rn]5f ¹ 6d ¹ 7s ²	109 Mt [Rn]5f ¹ 6d ¹ 7s ²	110 Ds [Rn]5f ¹ 6d ¹ 7s ²	111 Rg [Rn]5f ¹ 6d ¹ 7s ²	112 Cn [Rn]5f ¹ 6d ¹ 7s ²	113 Uut [Rn]5f ¹ 6d ¹ 7s ²	114 Fl [Rn]5f ¹ 6d ¹ 7s ²	115 Uup [Rn]5f ¹ 6d ¹ 7s ²	116 Lv [Rn]5f ¹ 6d ¹ 7s ²	117 Uus [Rn]5f ¹ 6d ¹ 7s ²	118 Uuo [Rn]5f ¹ 6d ¹ 7s ²
Lanthanides																	
Actinides																	
* values are based on theory and are not verified																	

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

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.

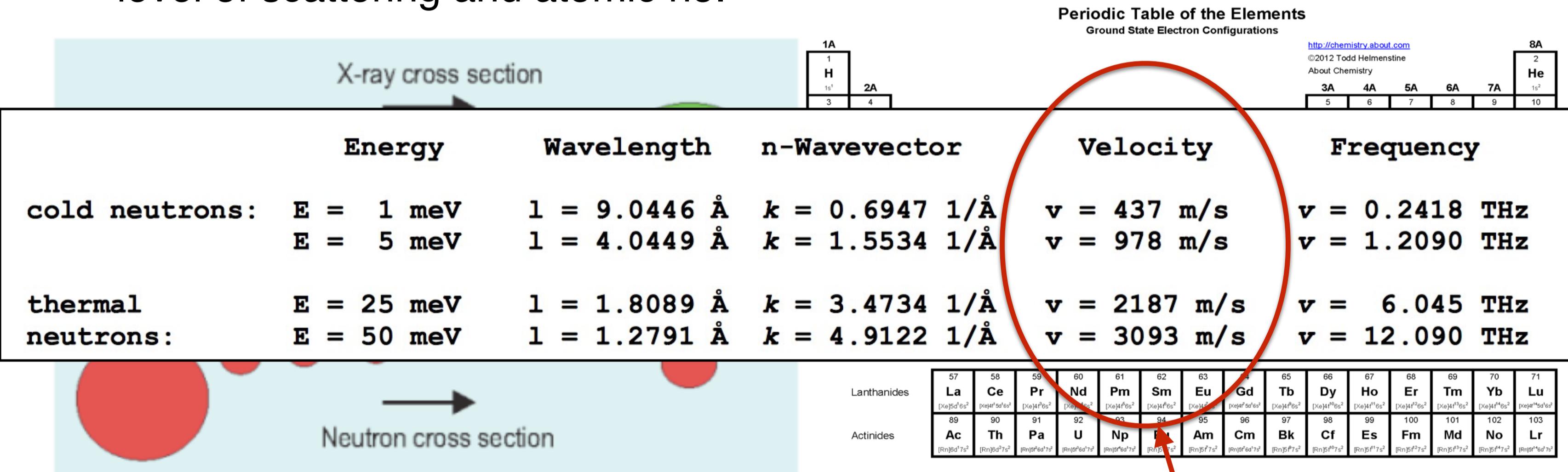


Fig. 2. Neutron and x-ray scattering cross-sections compared. Note that neutrons penetrate through Al much better than x rays do, yet are strongly scattered by hydrogen.

Low velocities makes beam-tailoring using mechanical devices feasible

- Result: Two very different response/contrasts

Monte Carlo techniques

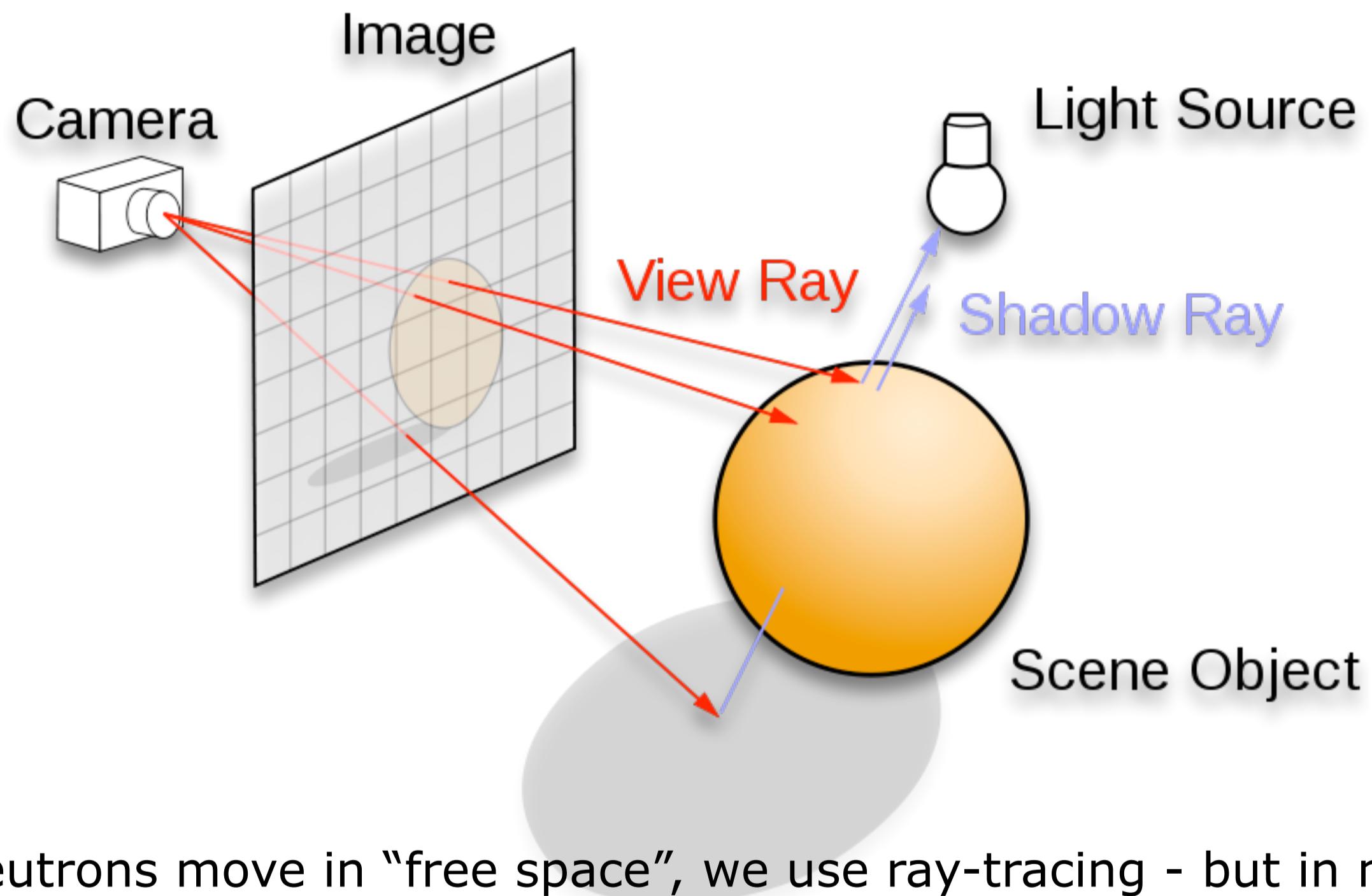


- During WW2, “numerical experiments” were applied at Los Alamos for solving mathematical complications of computing fission, criticality, neutronics, hydrodynamics, thermonuclear detonation etc.



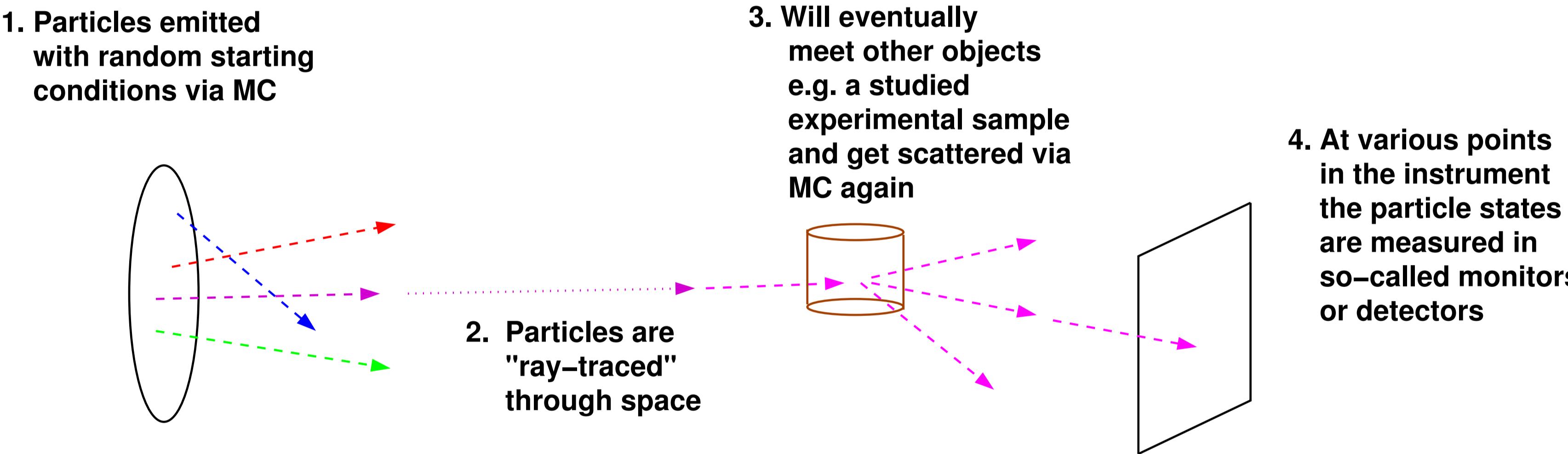
- Notable fathers: John v. Neumann Stanislav Ulam Nicholas Metropolis
- Named “Monte Carlo” after Ulam’s fathers frequent visits to the Monte Carlo casino in Las Vegas
- Initially “implemented” by letting large numbers of women use tabularized random numbers and hand calculators for individual particle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

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

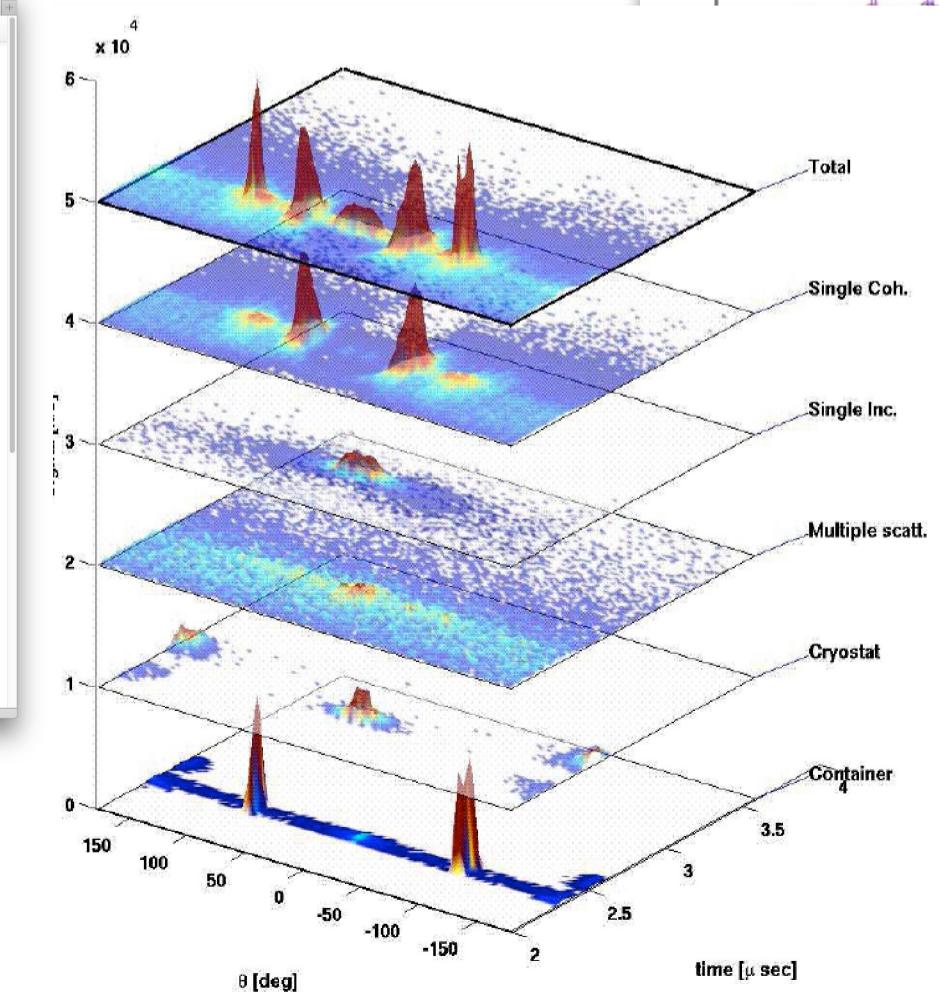
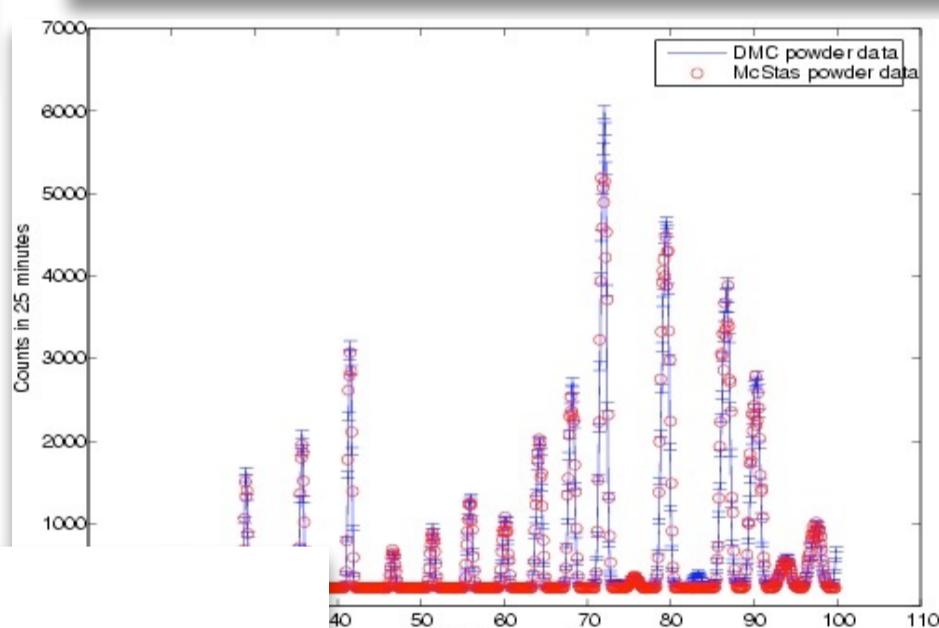
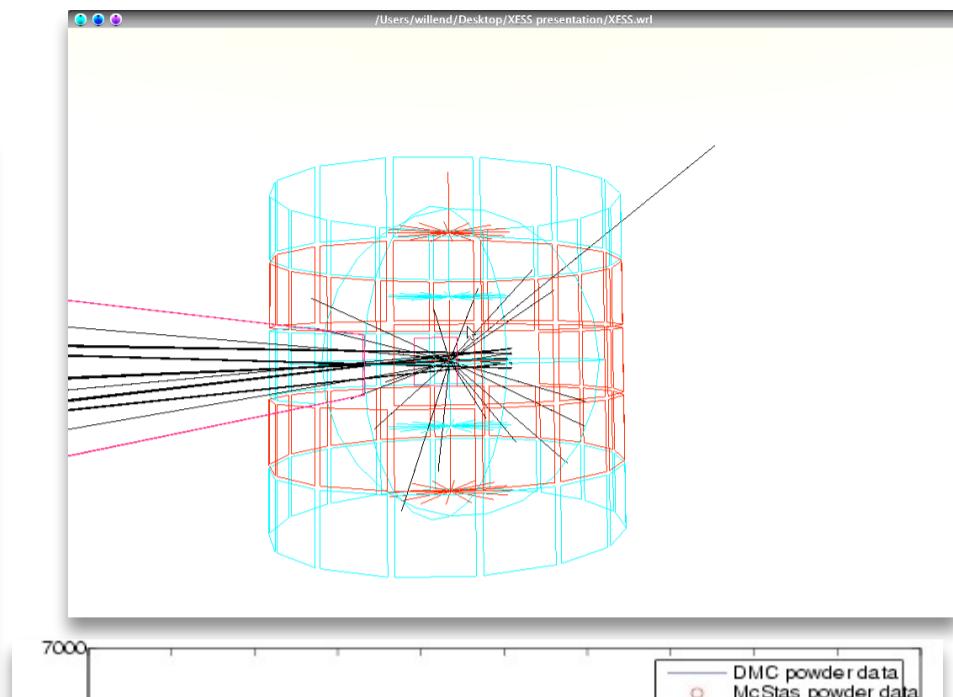
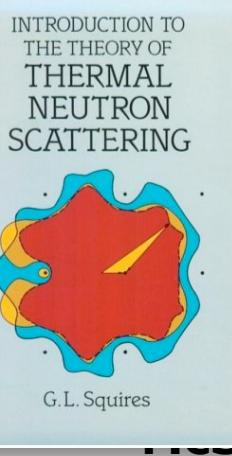
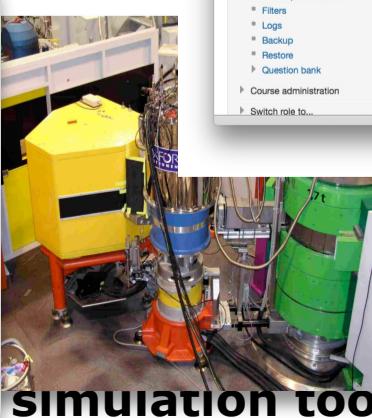


- Important efficiency mechanisms:
 - “Focusing” - e.g. source to beamport only (4π vs. limited solid angle only)
 - Rather vs. single particle description, absorption handled through statistics and downscaling the ray weight

What are the codes used for?

- Instrumentation
- Virtual experiments
- Data analysis
- Teaching

(KU, DTU)



Neutron ray/package:

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

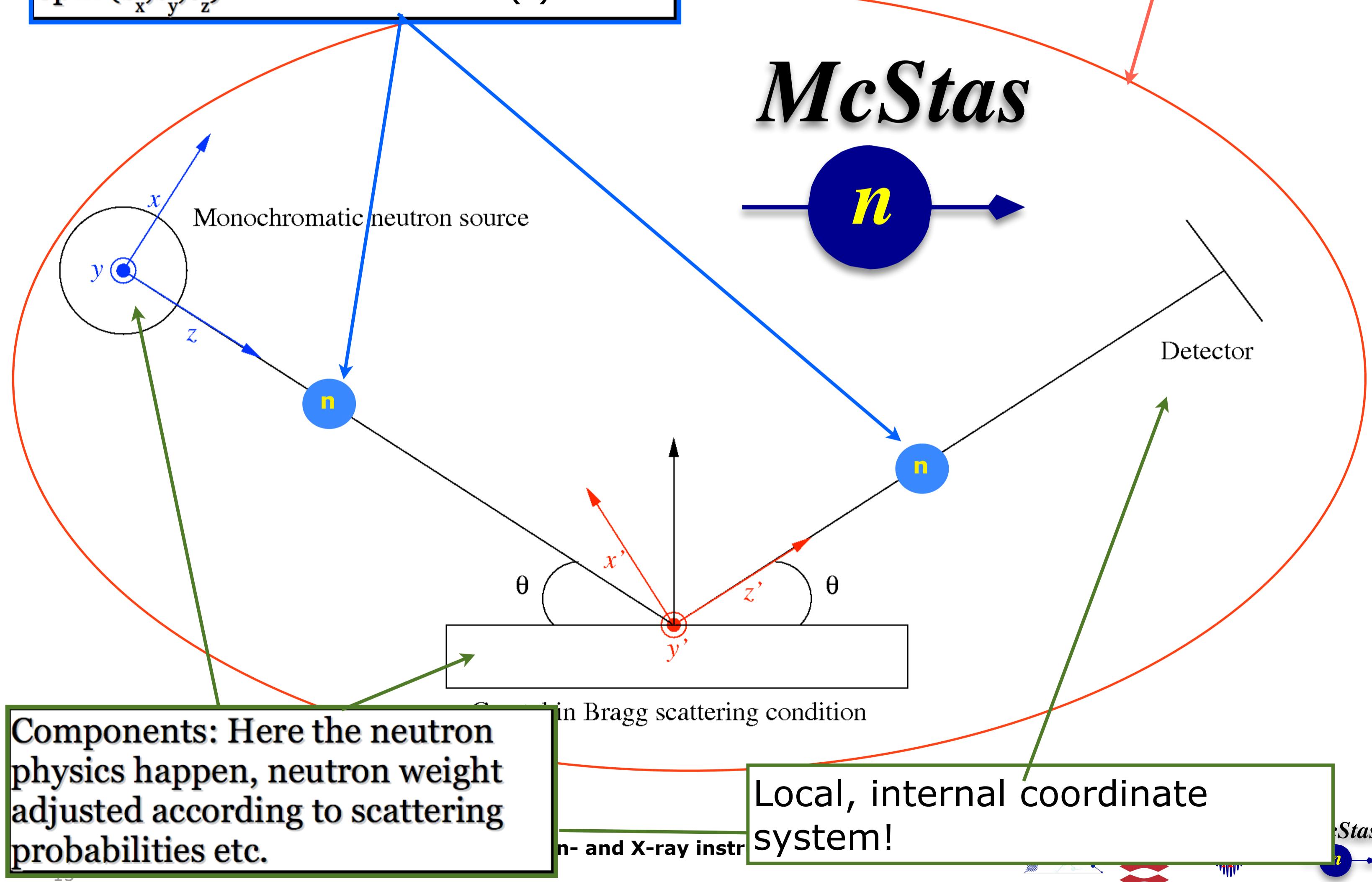
Coordinates (x, y, z)

Velocity (v_x, v_y, v_z)

Spin (s_x, s_y, s_z)

Time (t)

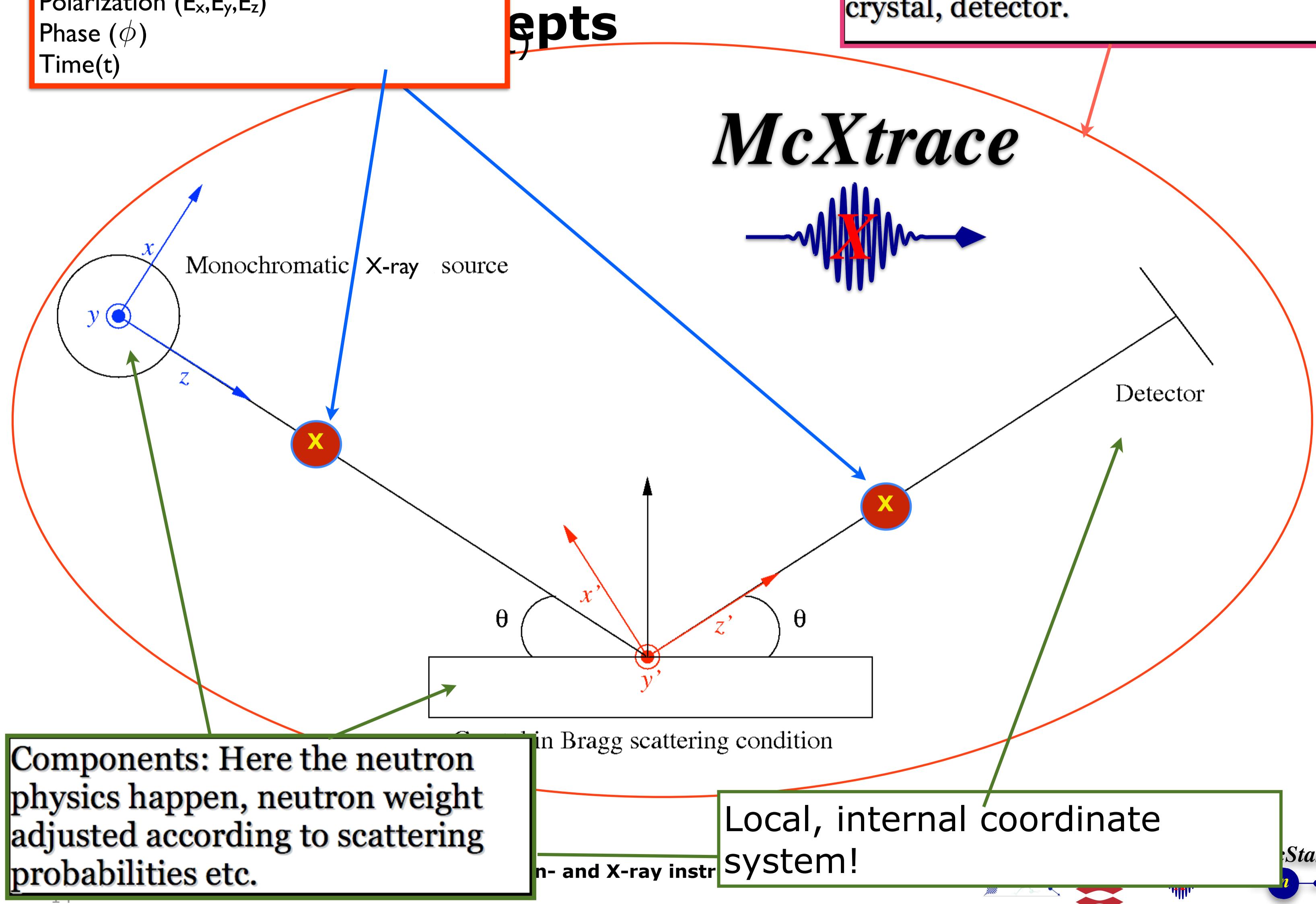
Instrument: positioning + transformation between sequential component coordinate systems, e.g. neutron source, crystal, detector.



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)



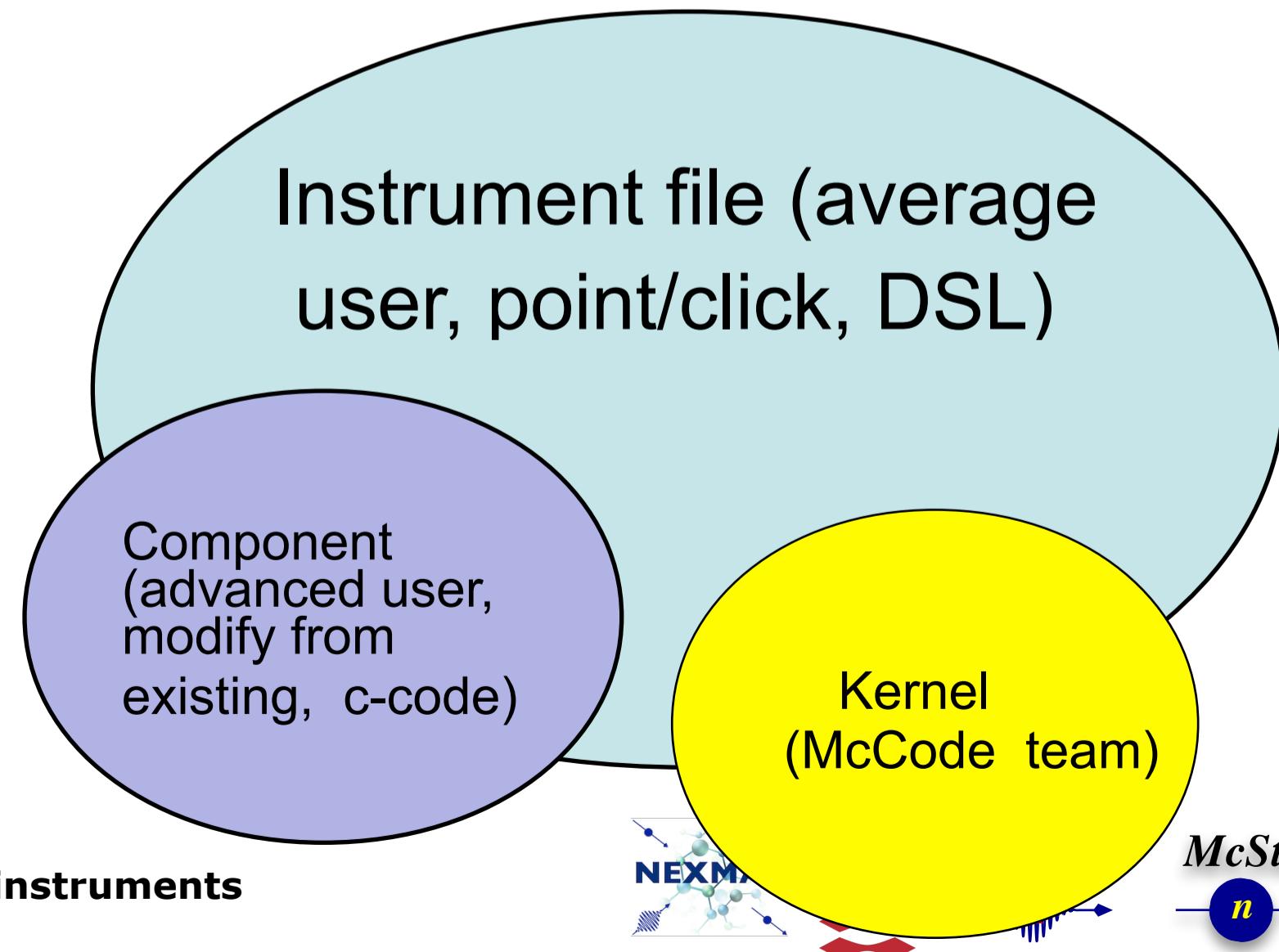
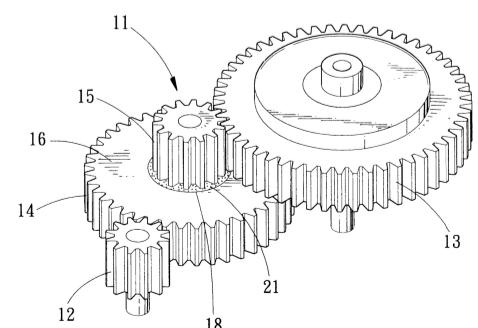
- Ran on everything from iPhone to 1000+ node cluster!



- 'Component' files (~150/~40) inserted from library

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

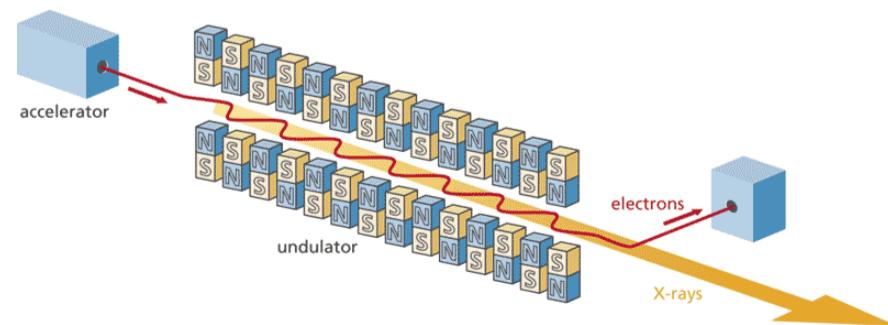
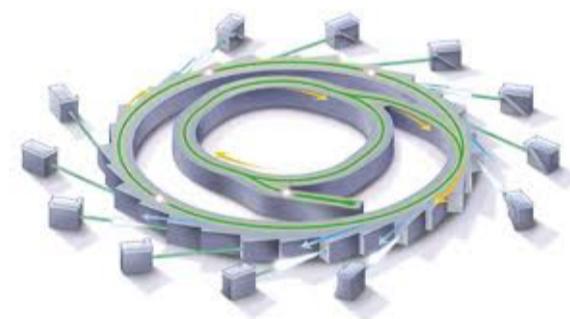
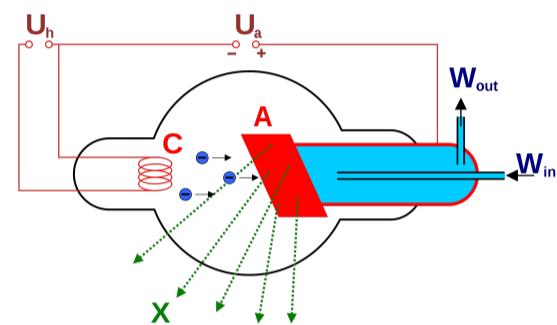
- DSL + ISO-C code gen.



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

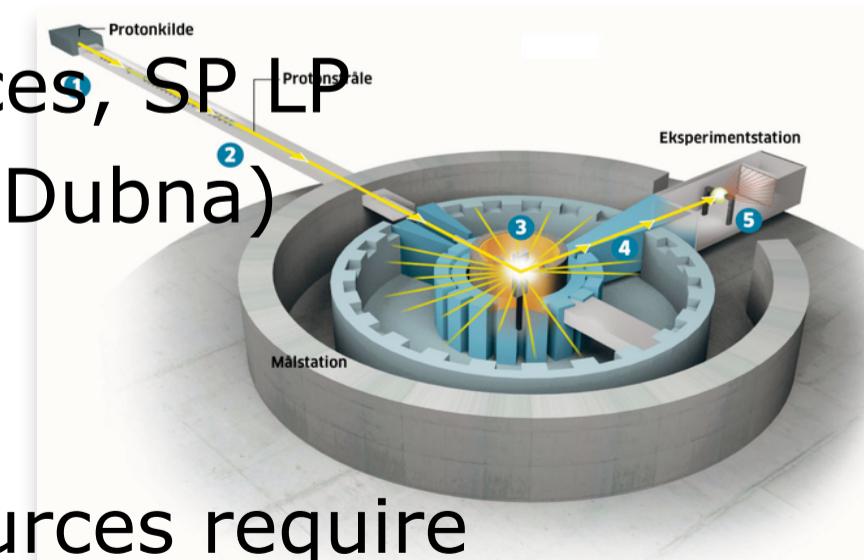
- Lab equipment
 - Radioisotope-based
 - CANS (Compact acclererator based)



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



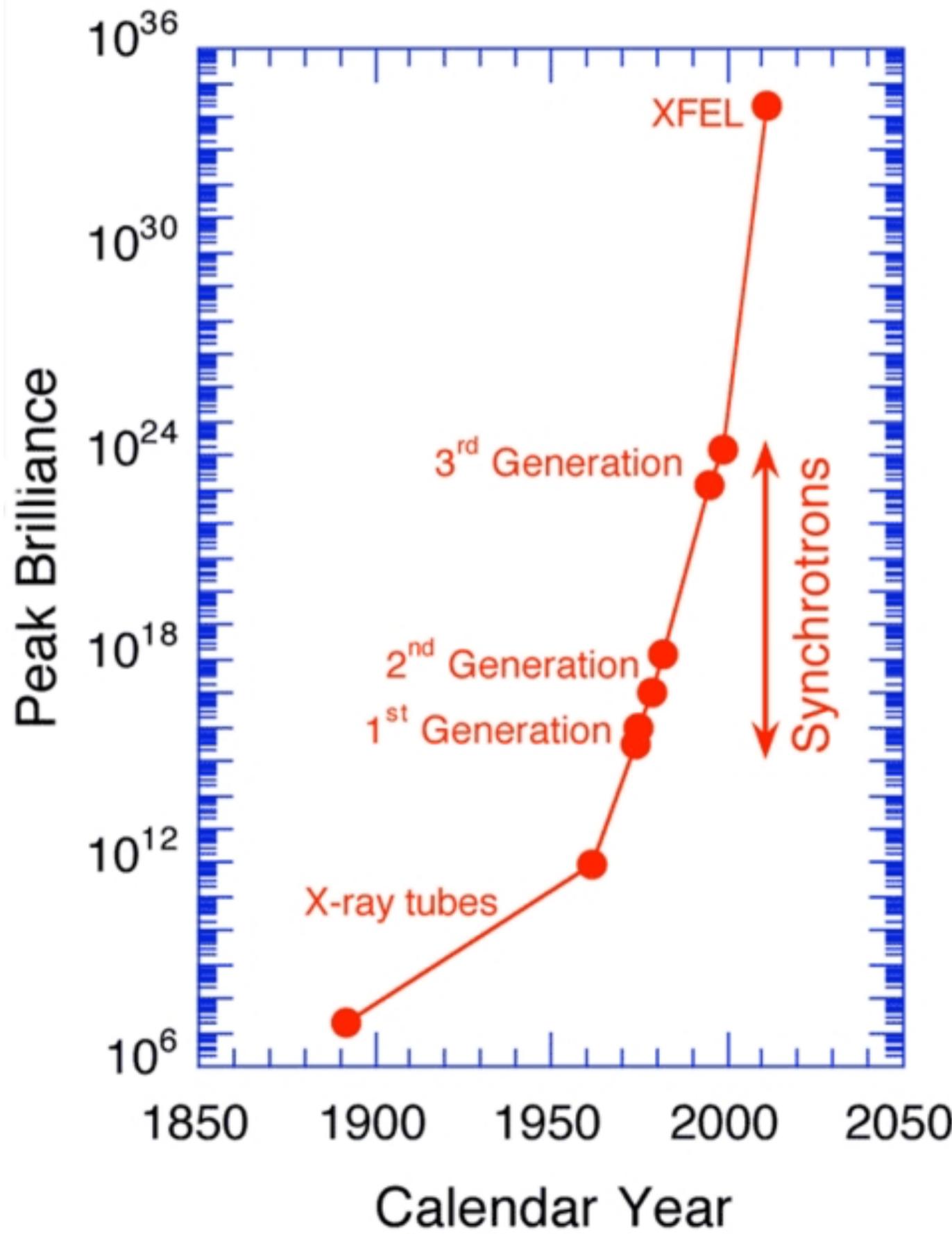
- Pulsed sources
 - Spallation sources, SP, LP
 - Pulsed reactor (Dubna)



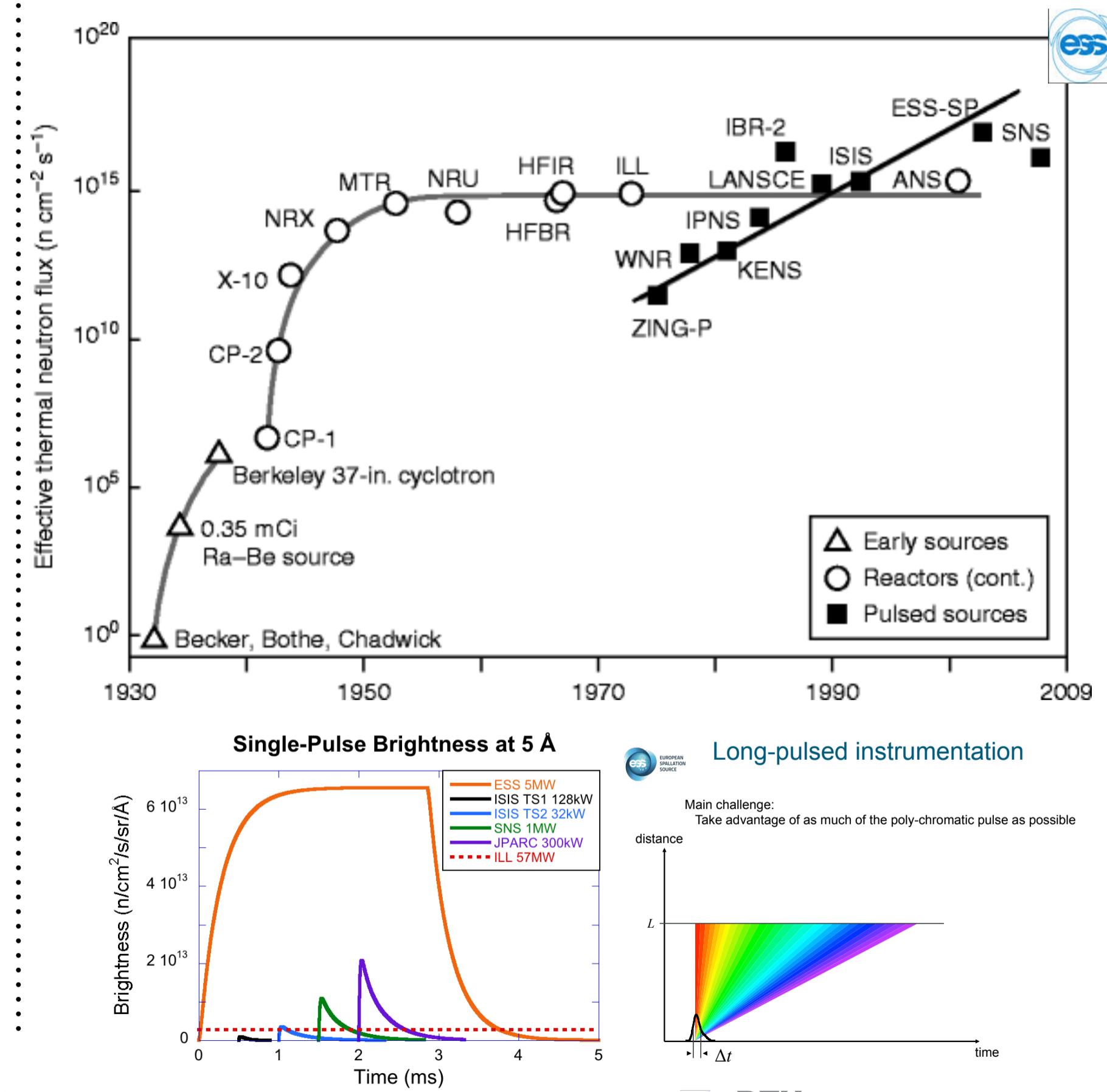
- Most neutron sources require moderation of the neutron energy

Sources - 2

• X-ray sources



• Neutron sources



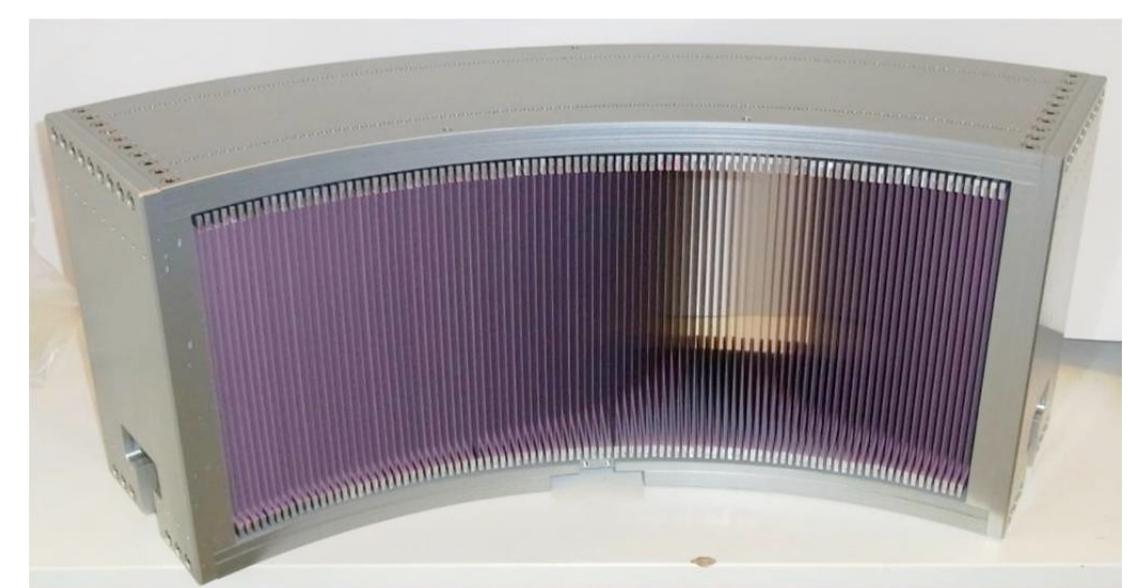
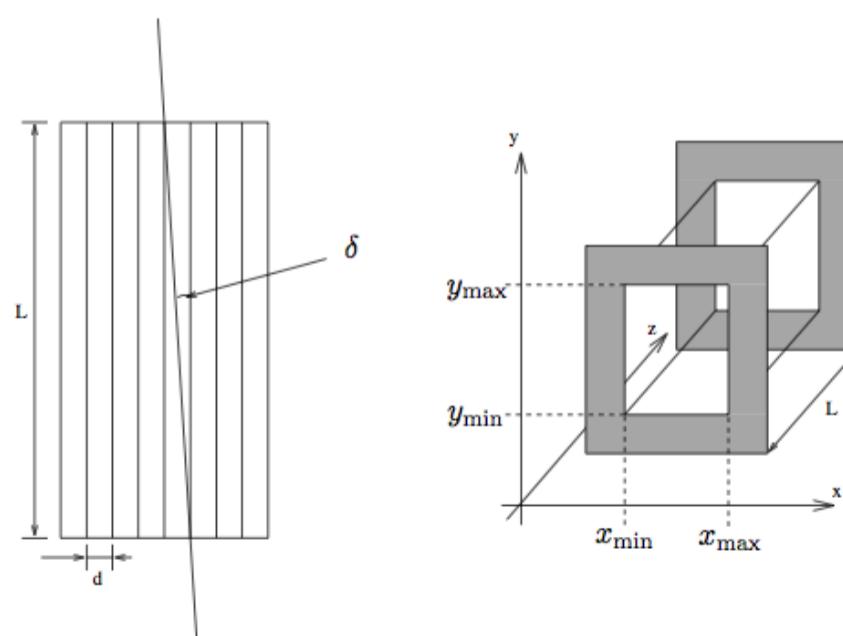
Spatial / directional beam adjustment

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



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

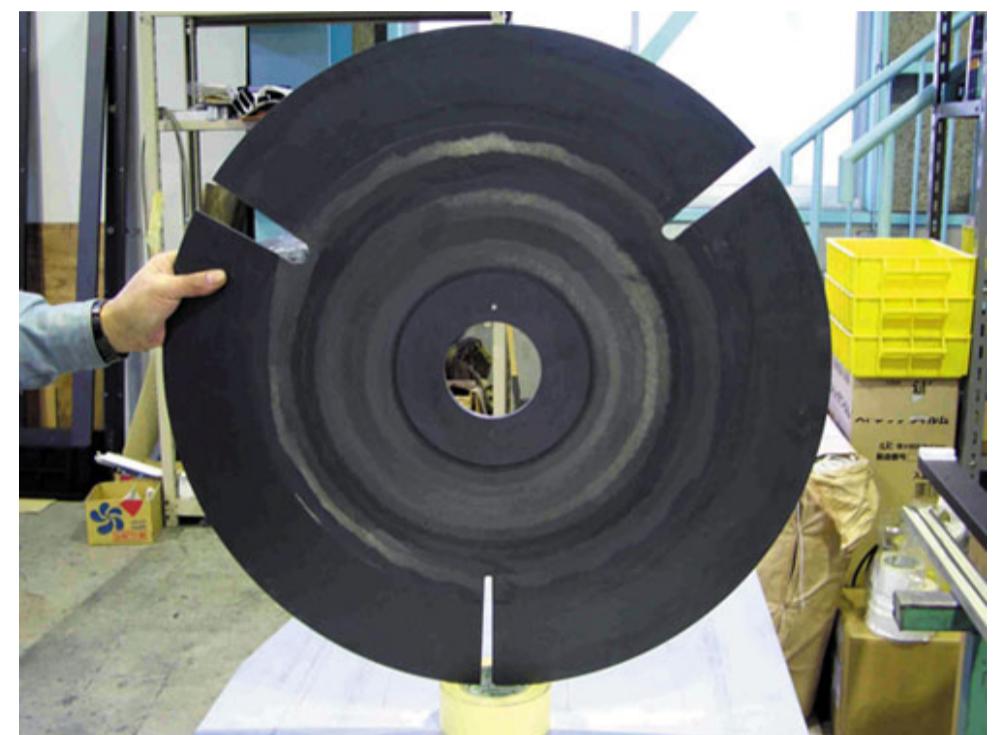
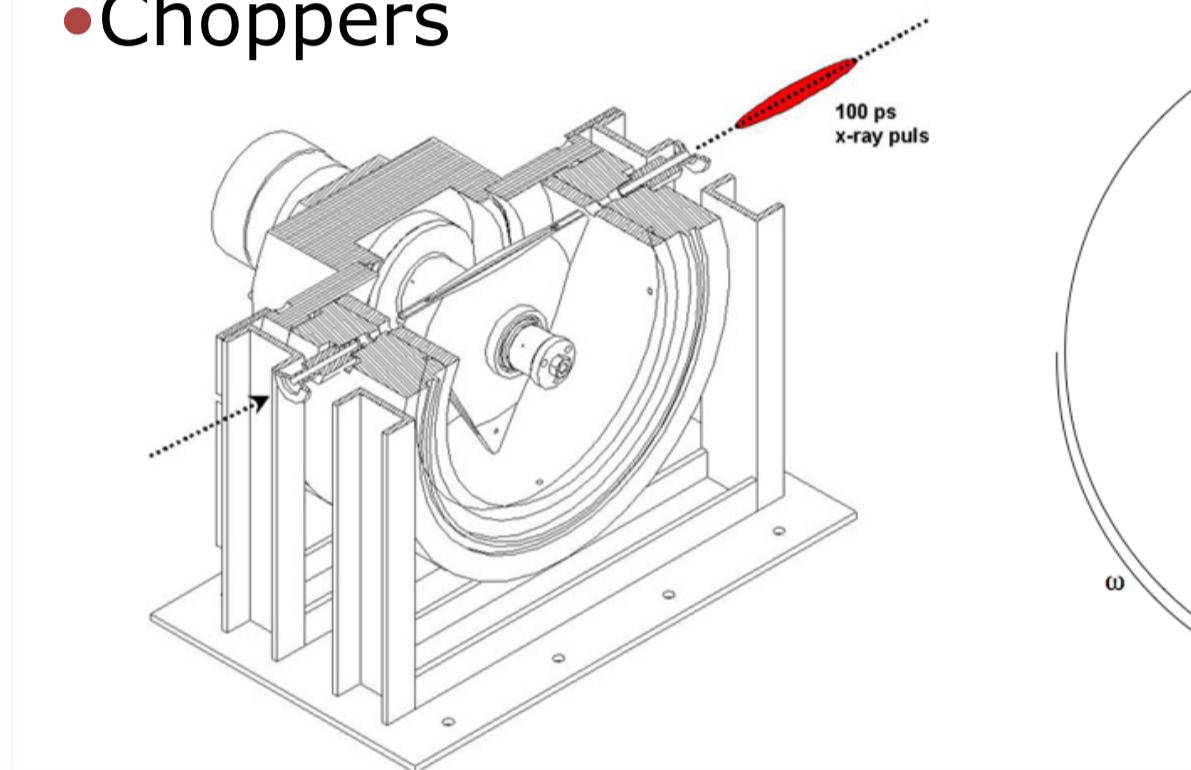
- Two or more slits defines an accepted divergence
- Collimators makes “channels”, typically with absorbing walls
- Usually static devices, but rotating radial collimators exist



Temporal beam adjustment, rotating optics

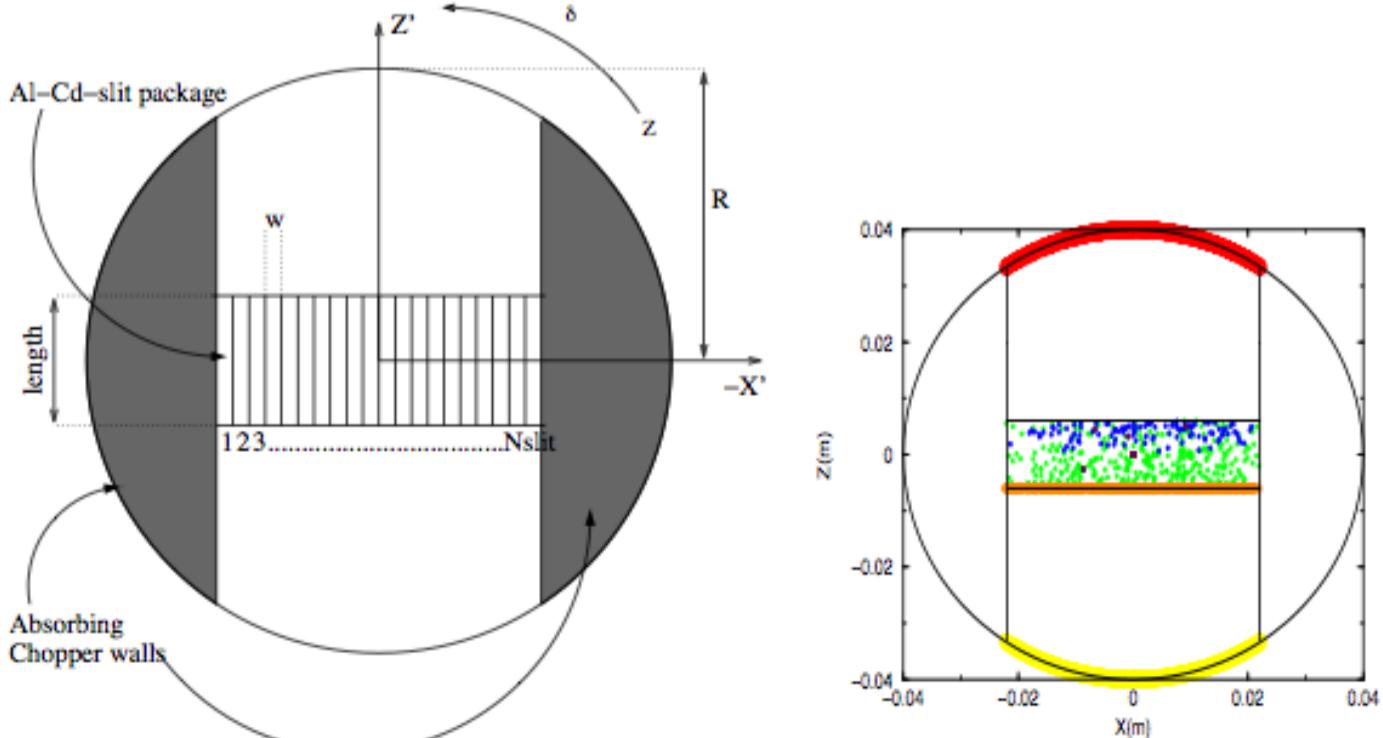
- X-ray and neutrons

- Choppers



- Neutrons only - monochromating rotating optics

- Fermi-chopper “rotating collimator”



Velocity-selector



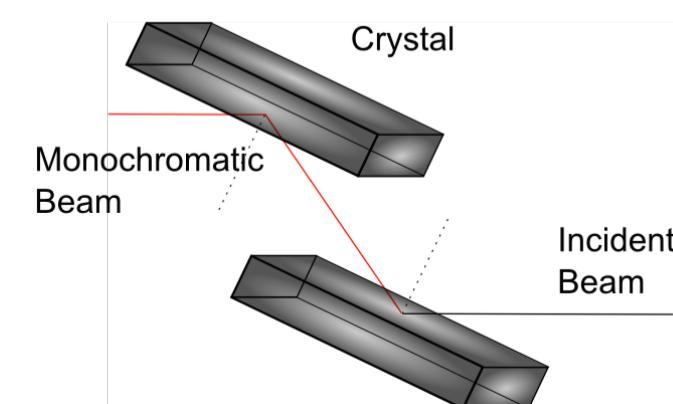
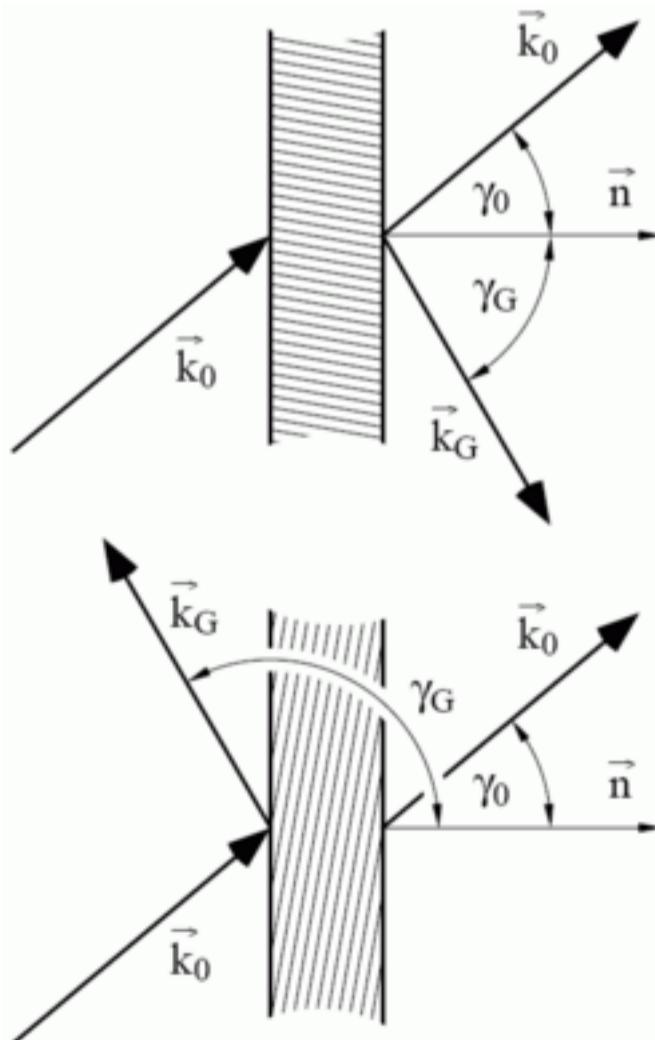
$$\frac{\delta \lambda}{\lambda} \approx 10\%$$

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**

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

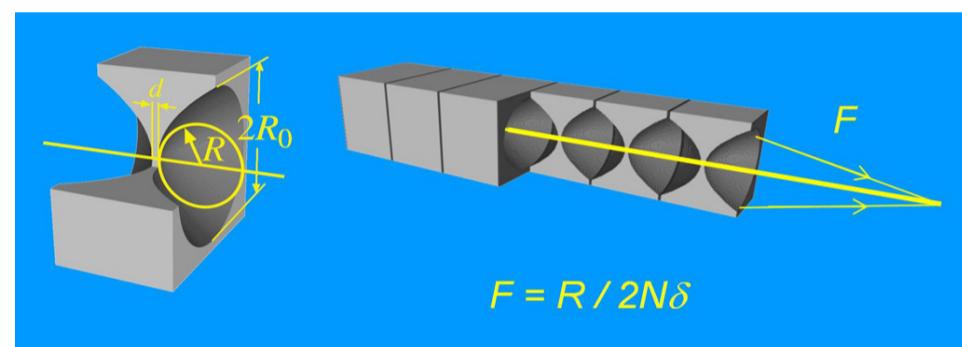
- Typically high-mosaicity (pyrolytic graphite, deformed Cu, Ge, ...)
- Often focusing, multi-crystal
- Typically Bragg geometry (reflection)
- Creates medium divergence monochromatic beams



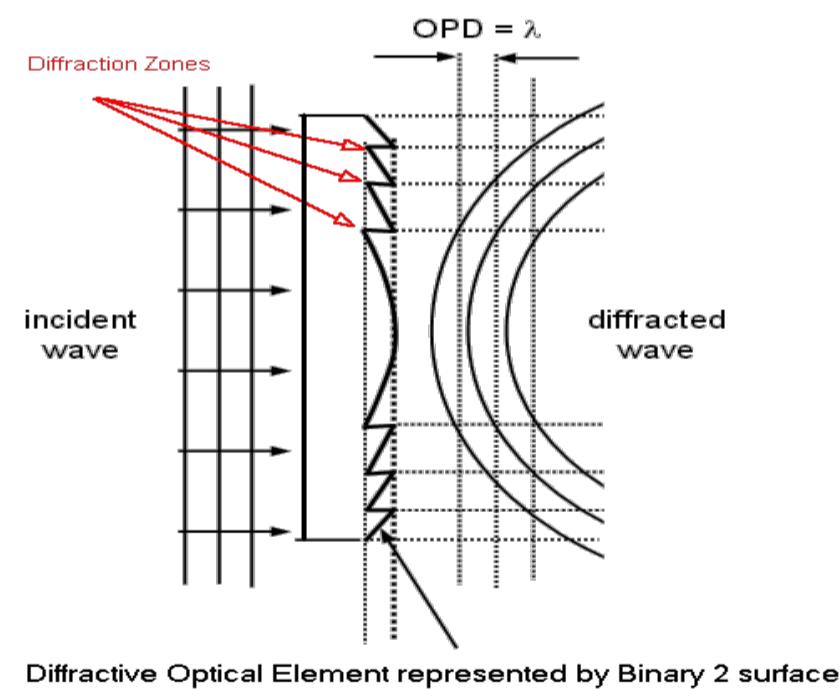
Refractive optics

· X-ray

- Refractive lenses (CRLs)

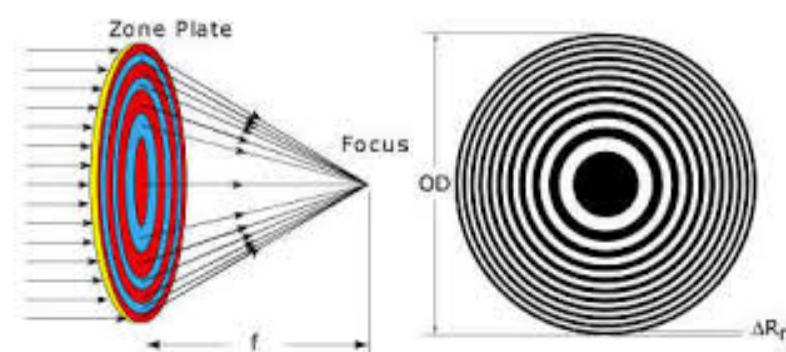


Kinoform Lens



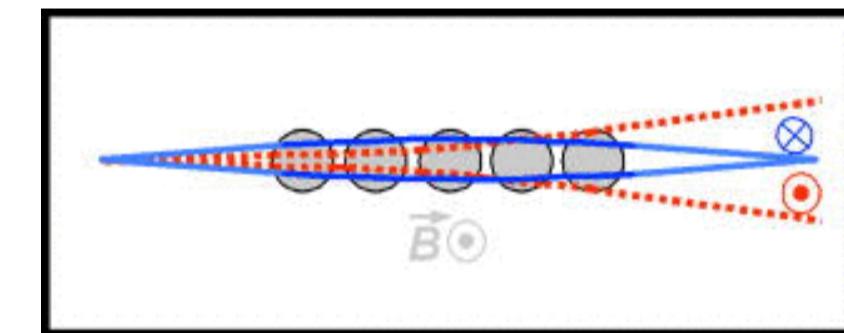
Diffractive Optical Element represented by Binary 2 surface

Fresnel Zone Plates



· Neutron

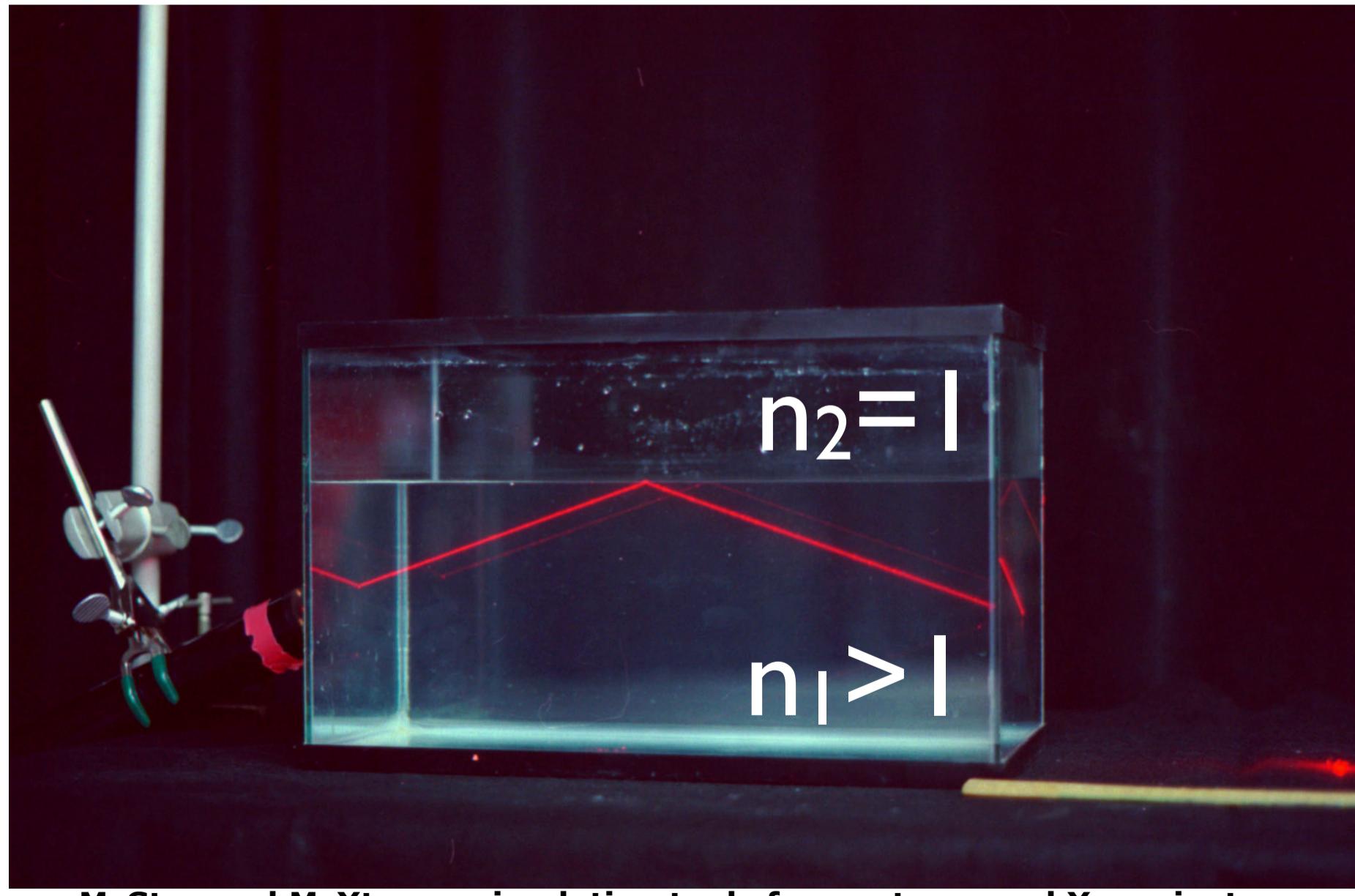
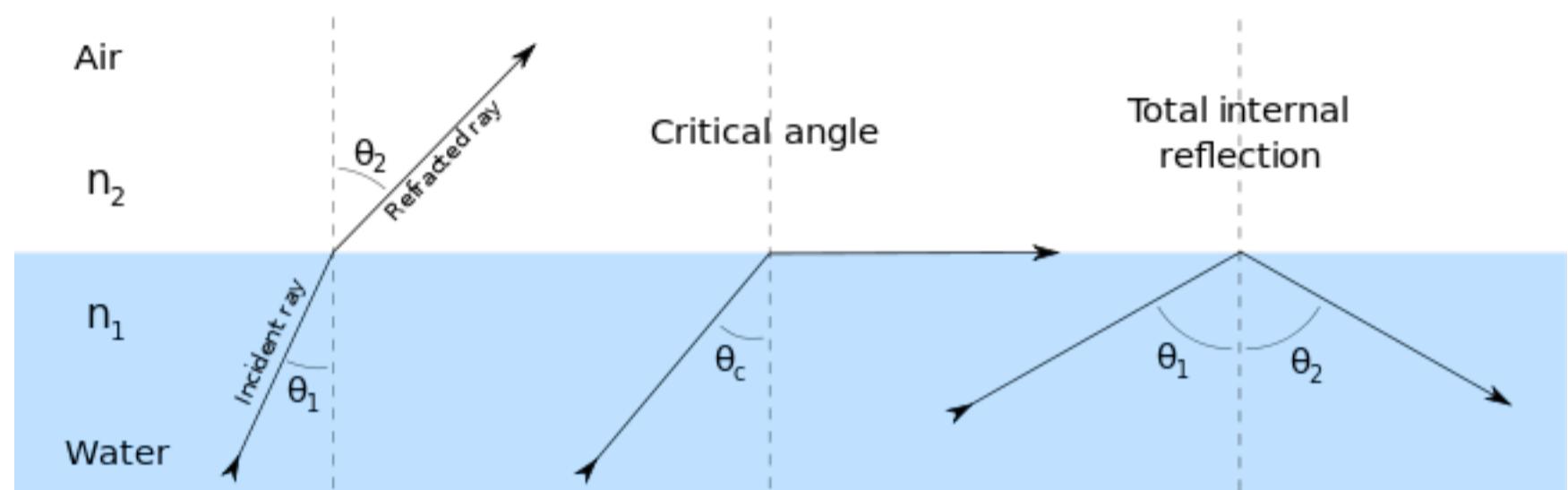
- Refractive Lenses (CRLs)



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

Refractive optics, total reflection - a reminder

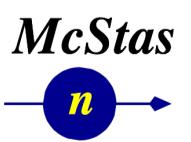
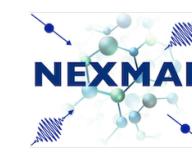
Visible light



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

Absorption term
Refraction term

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



Refractive optics

X-ray

Refractive index < 1

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

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

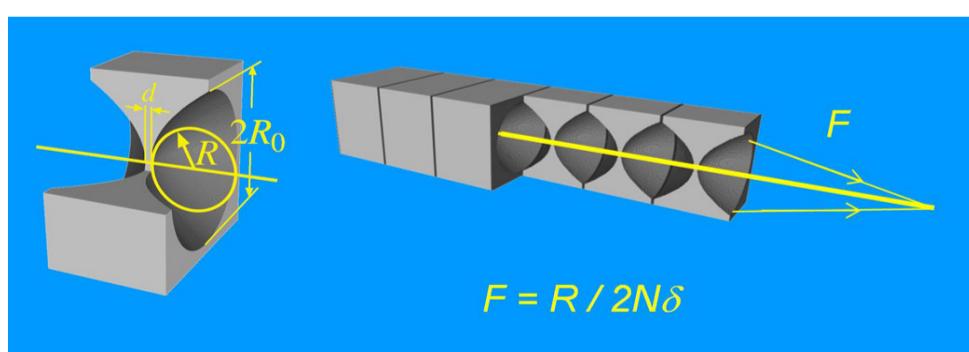
$$\delta_{neut} = f(b, B, \dots)$$

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

Low Z materials with low absorption. Be, Al.



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



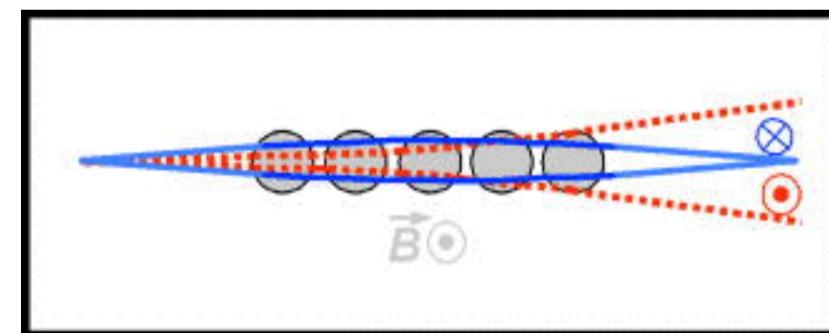
Neutron

Refractive Index < 1 for $b > 1$



High b materials with low absorption. Mg₂F

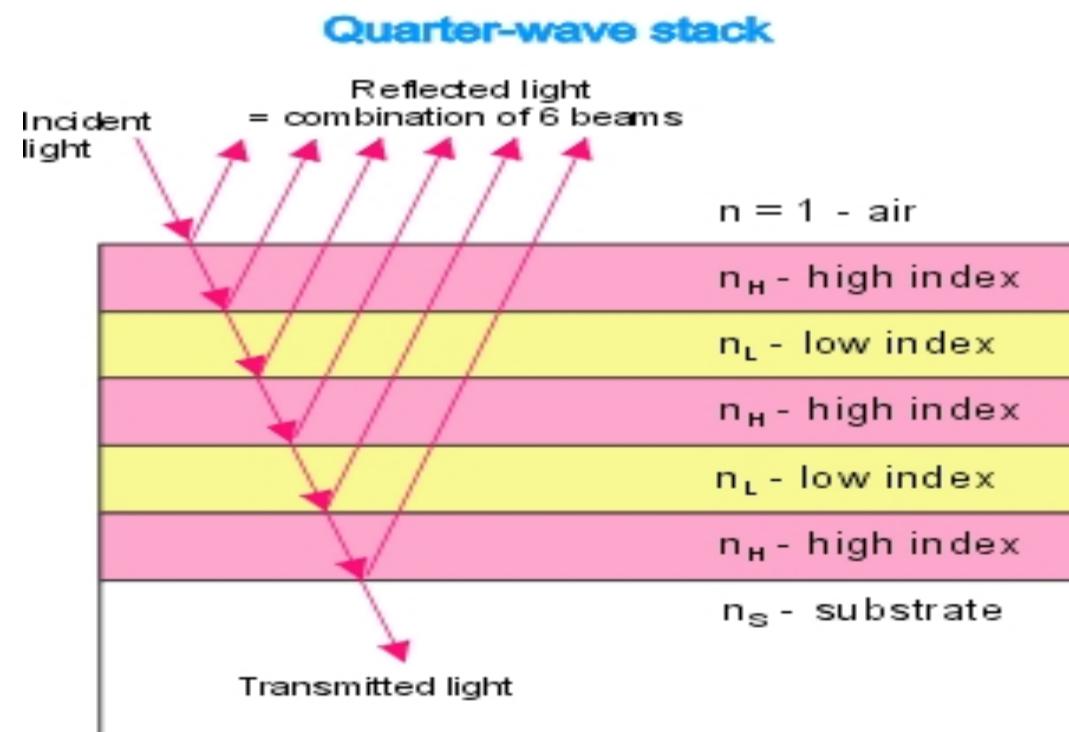
With neutrons, Lens effect from magnetism is small, hence "CRL"



Multilayers

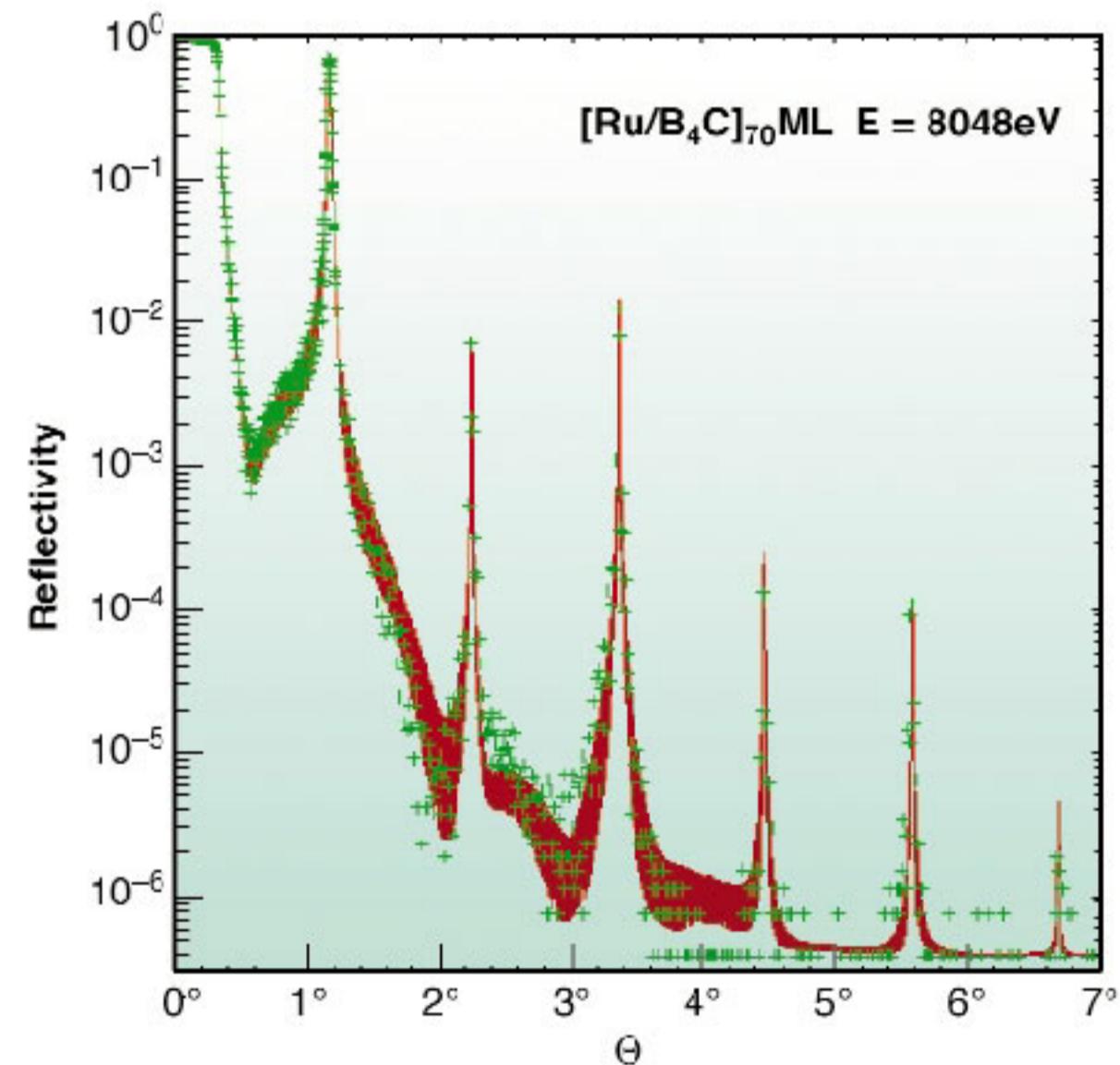
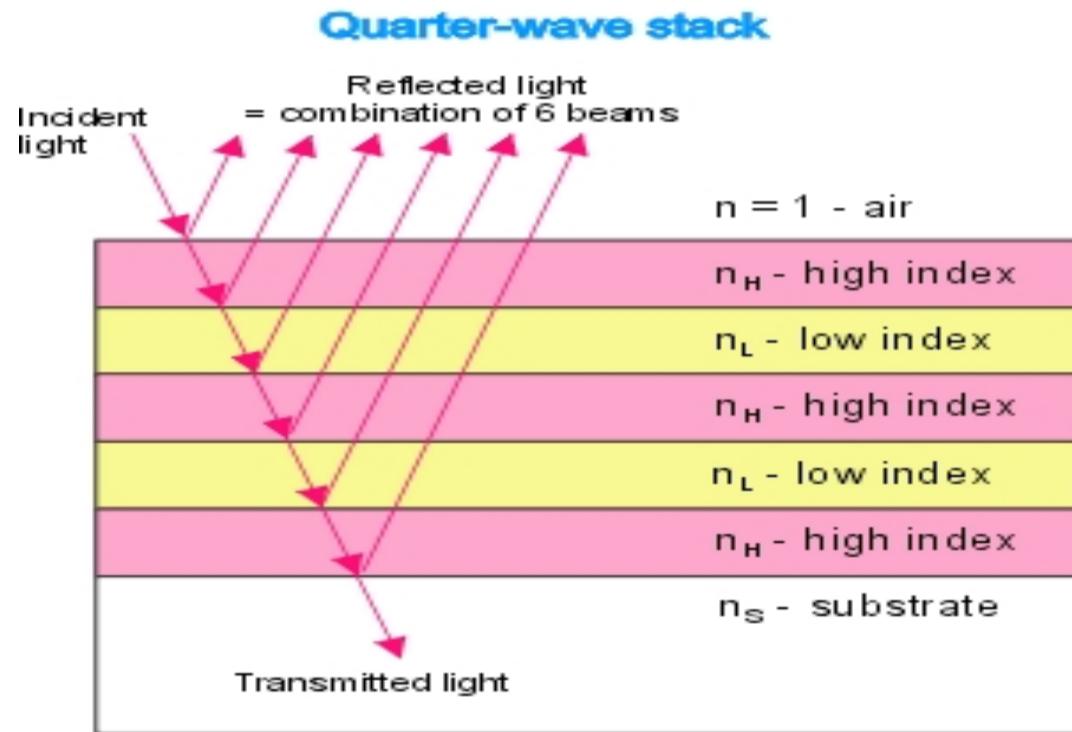
● X-ray and neutrons

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



Multilayers

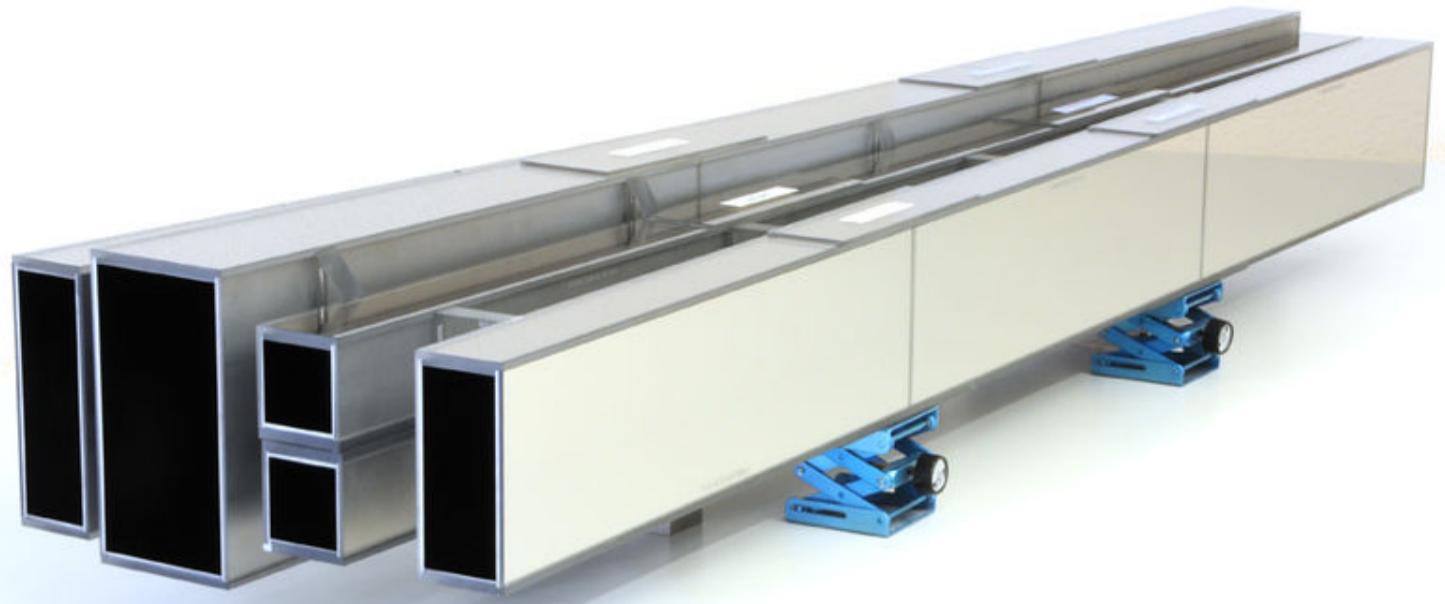
• X-rays:



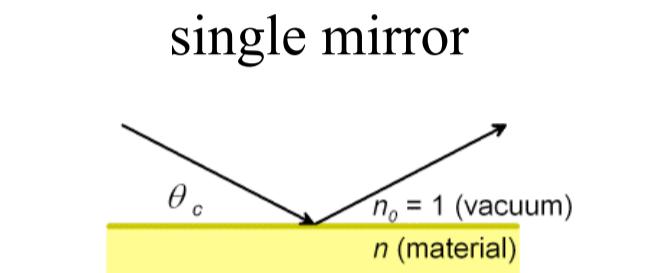
Superstructure often used as “monochromator” - also in focusing geometry

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

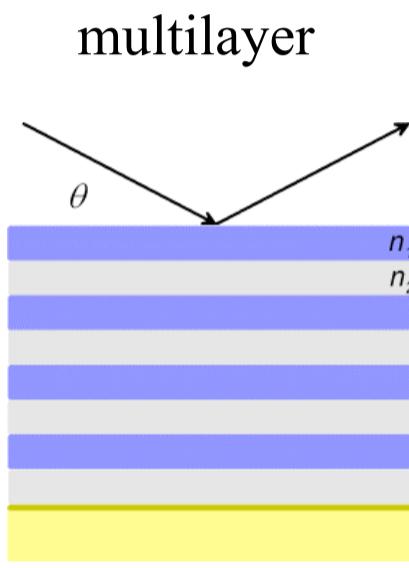
Multilayers



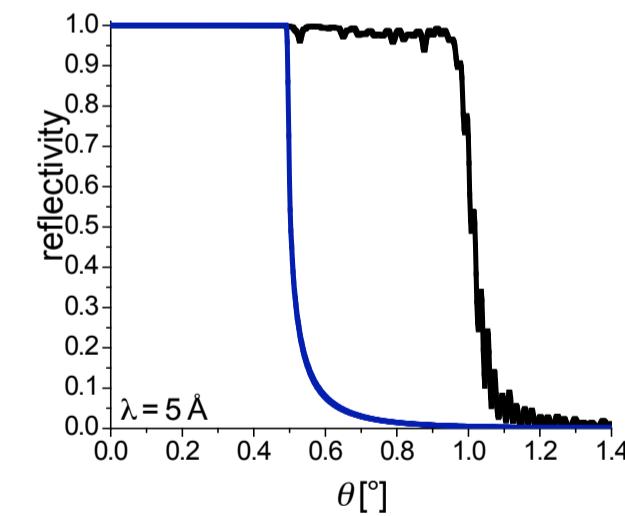
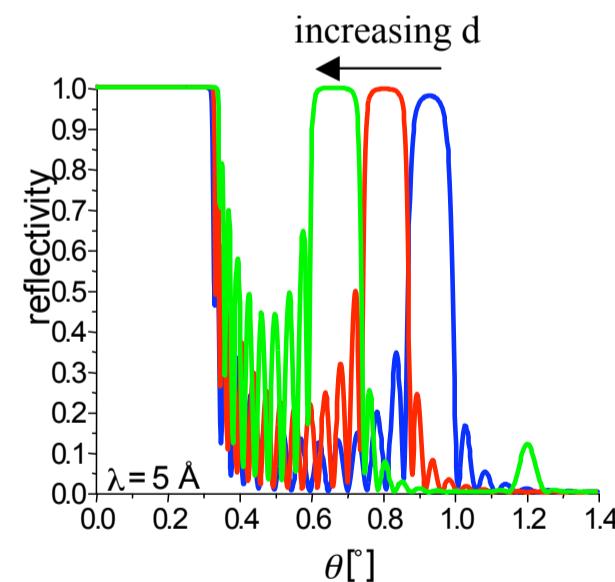
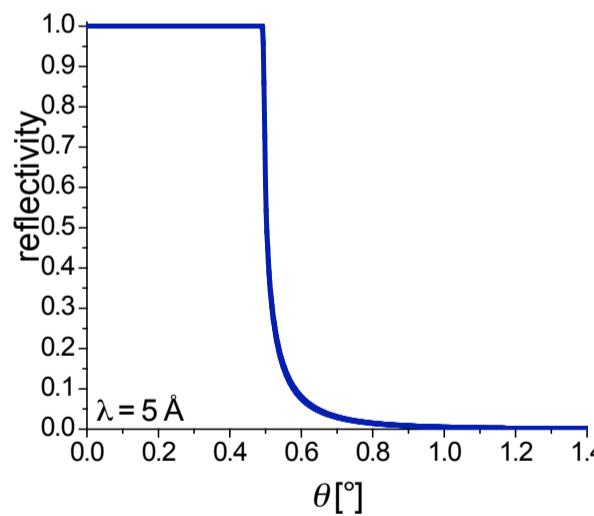
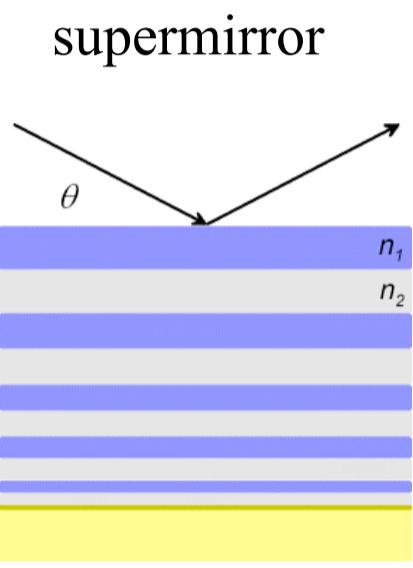
• Neutrons:



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



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

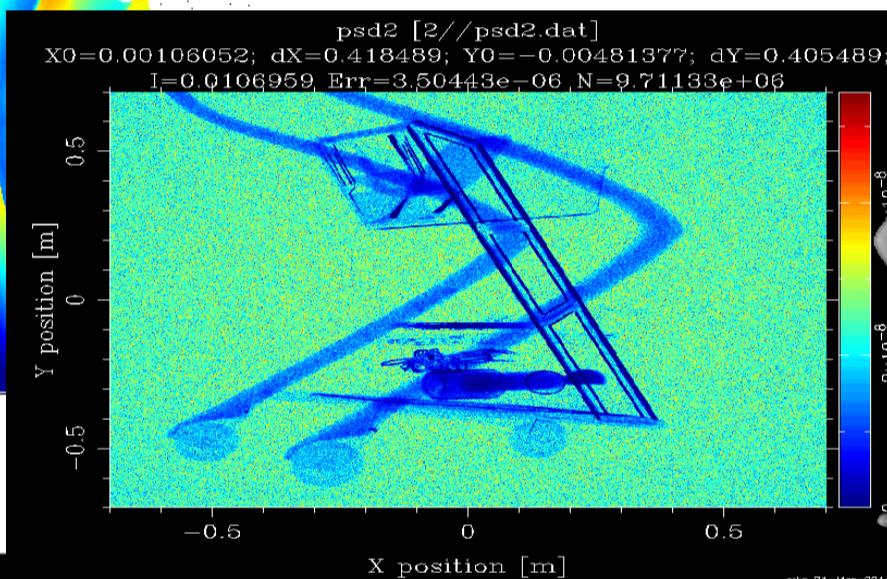
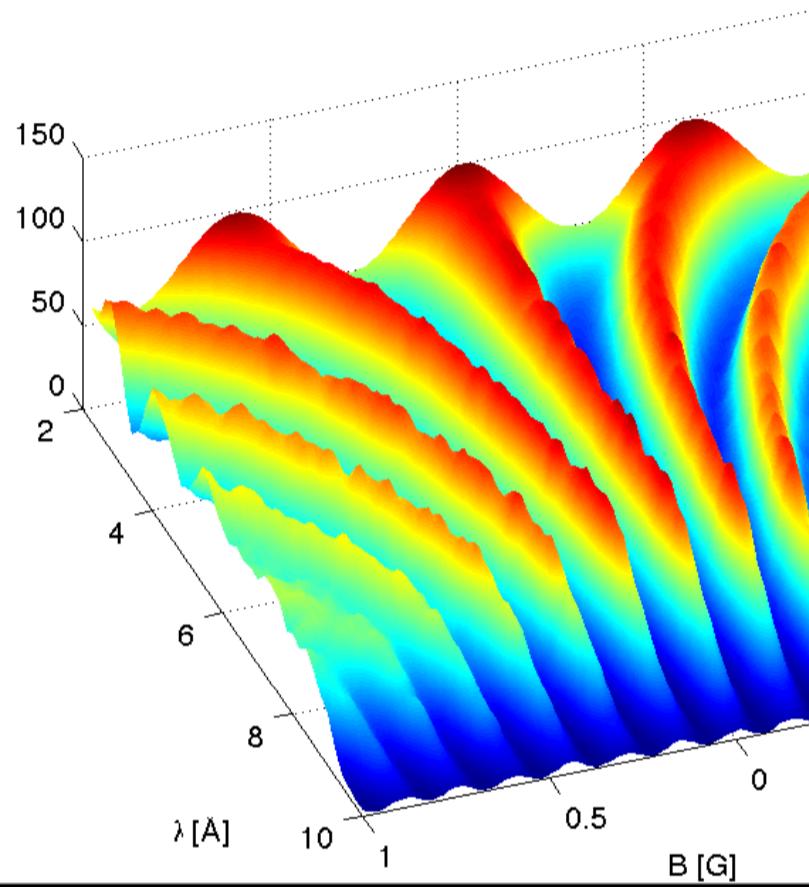


Superstructure “extends” the total-reflection range in Q by “Bragg peaks”

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

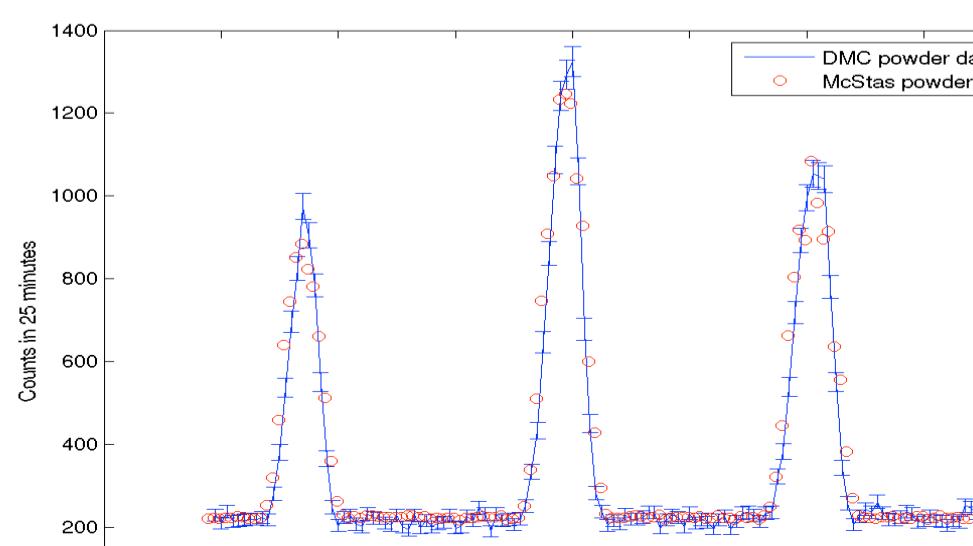
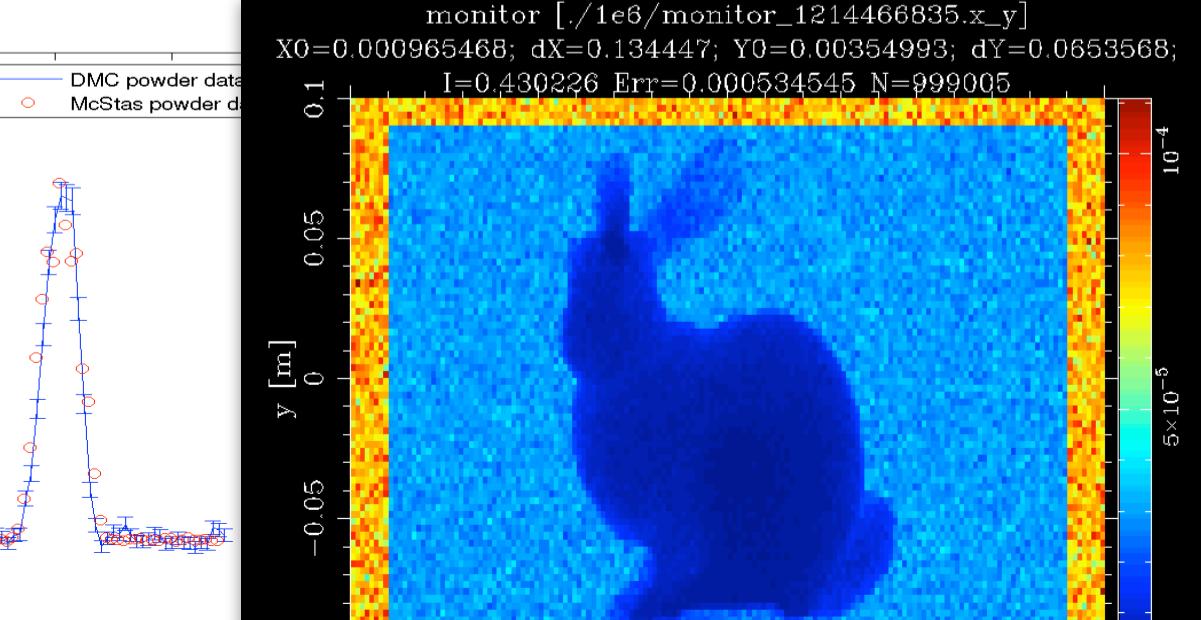
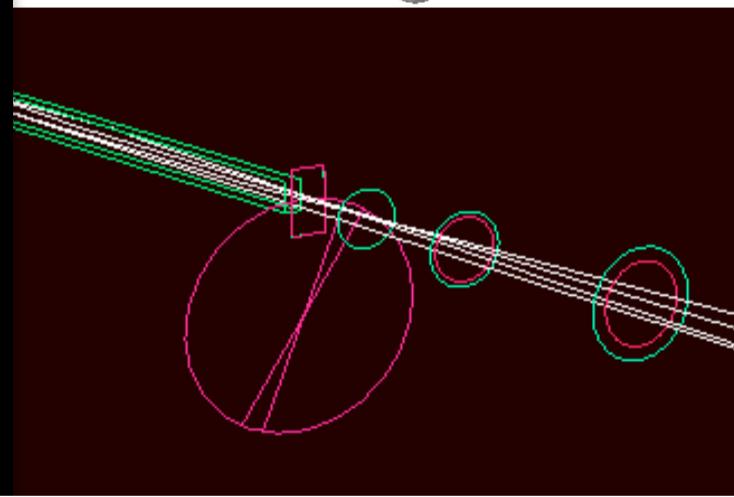
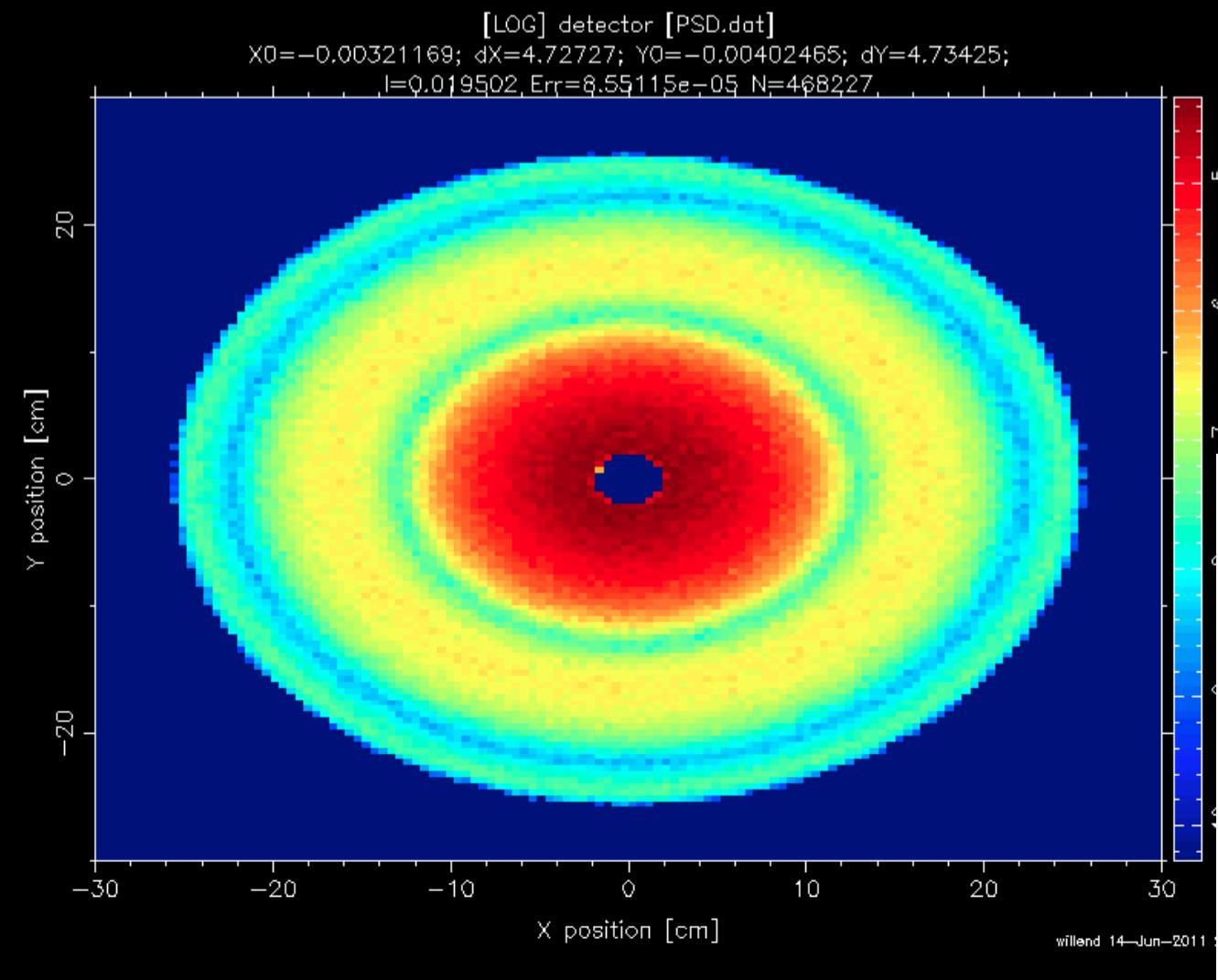
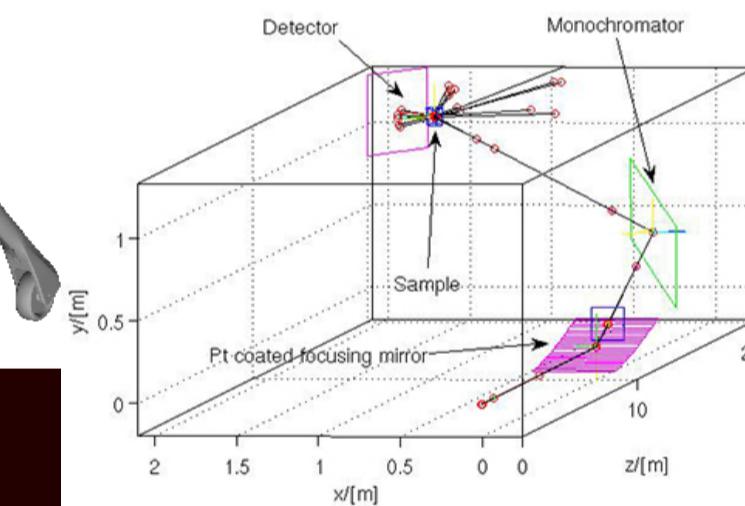
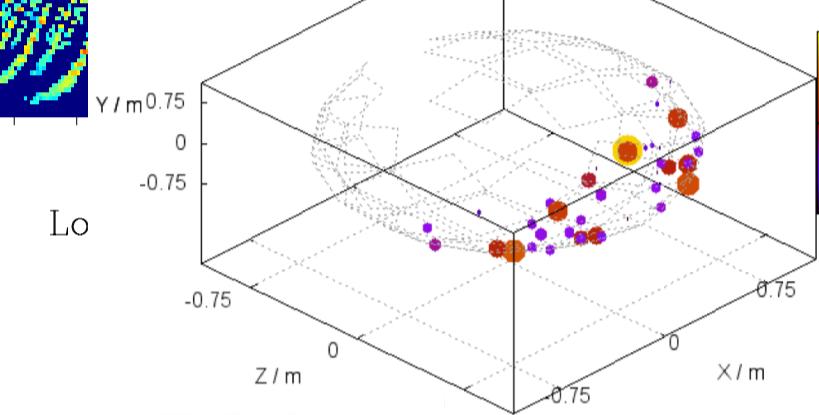
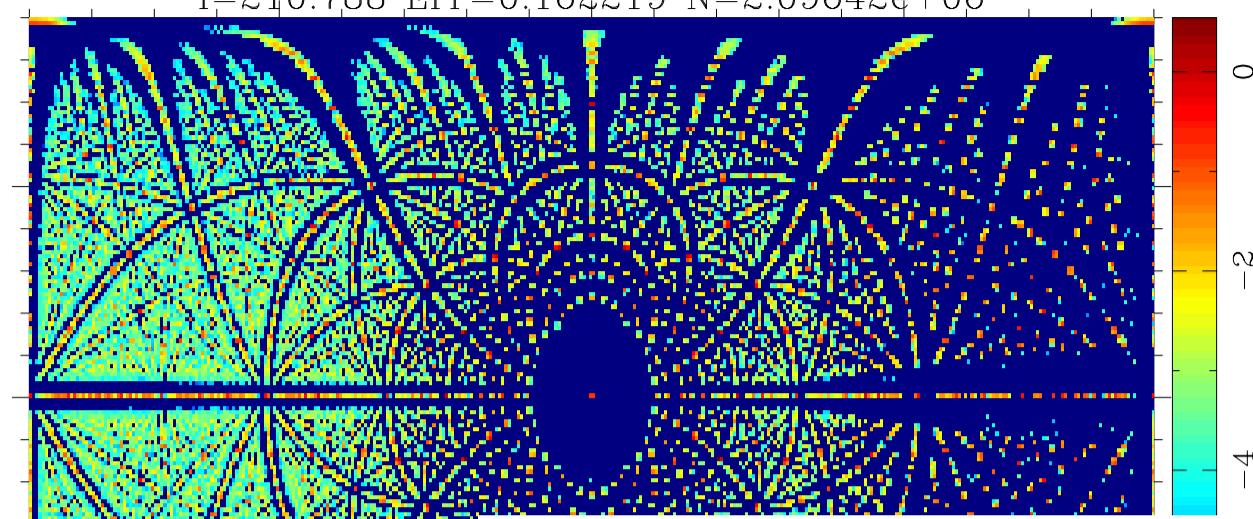
Example suite - instruments: 247 McStas 63 McXtrace

Spin-echo B scan dependence of wavelength



[LOG] det [1e9_parallel/psd.dat]
 $X_0=-6.35127; dX=97.5669; Y_0=0.343201; dY=41.1348;$

$I=210.788; Err=0.162219; N=2.09642e+06$





Questions?