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

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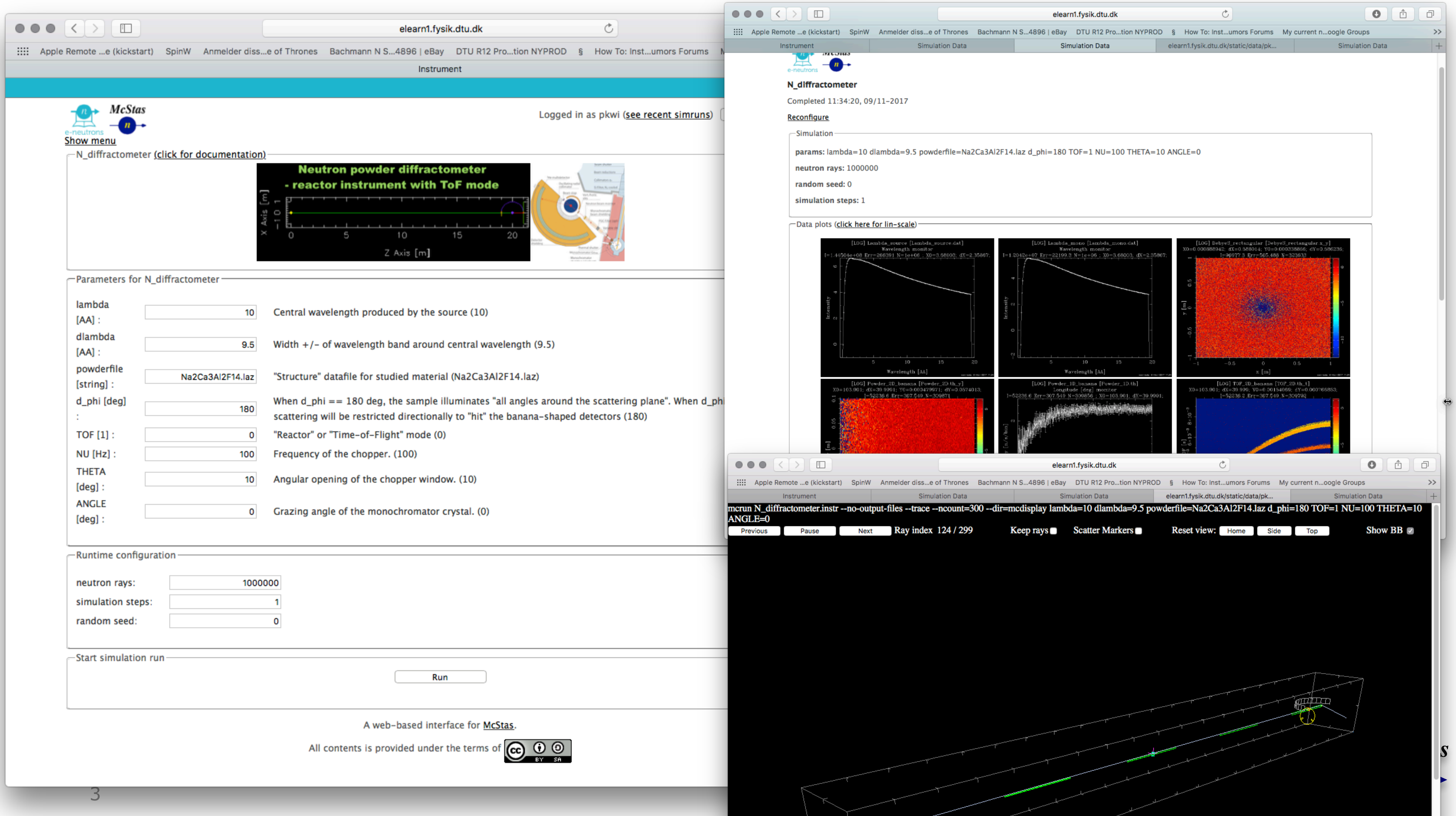
McXtrace McStas

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

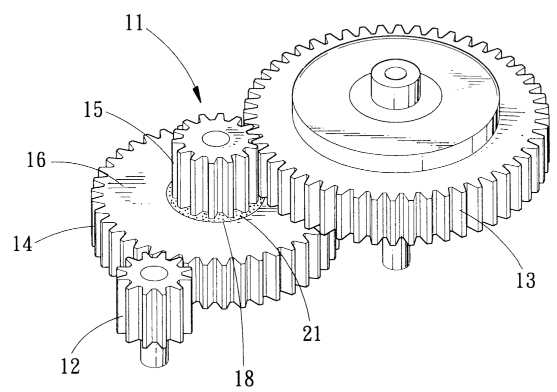
McStas & McXtrace

- In some sense you already "know" these codes… They are what you have been running in the elearn1 "simulator"

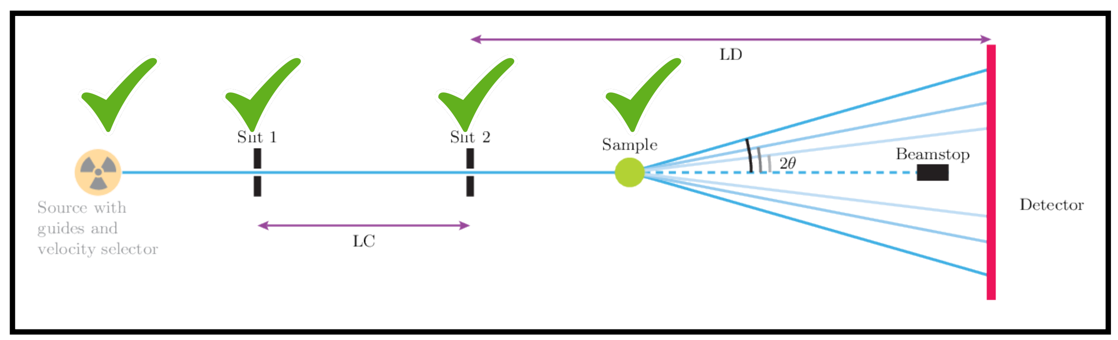


Purpose of today's activities

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



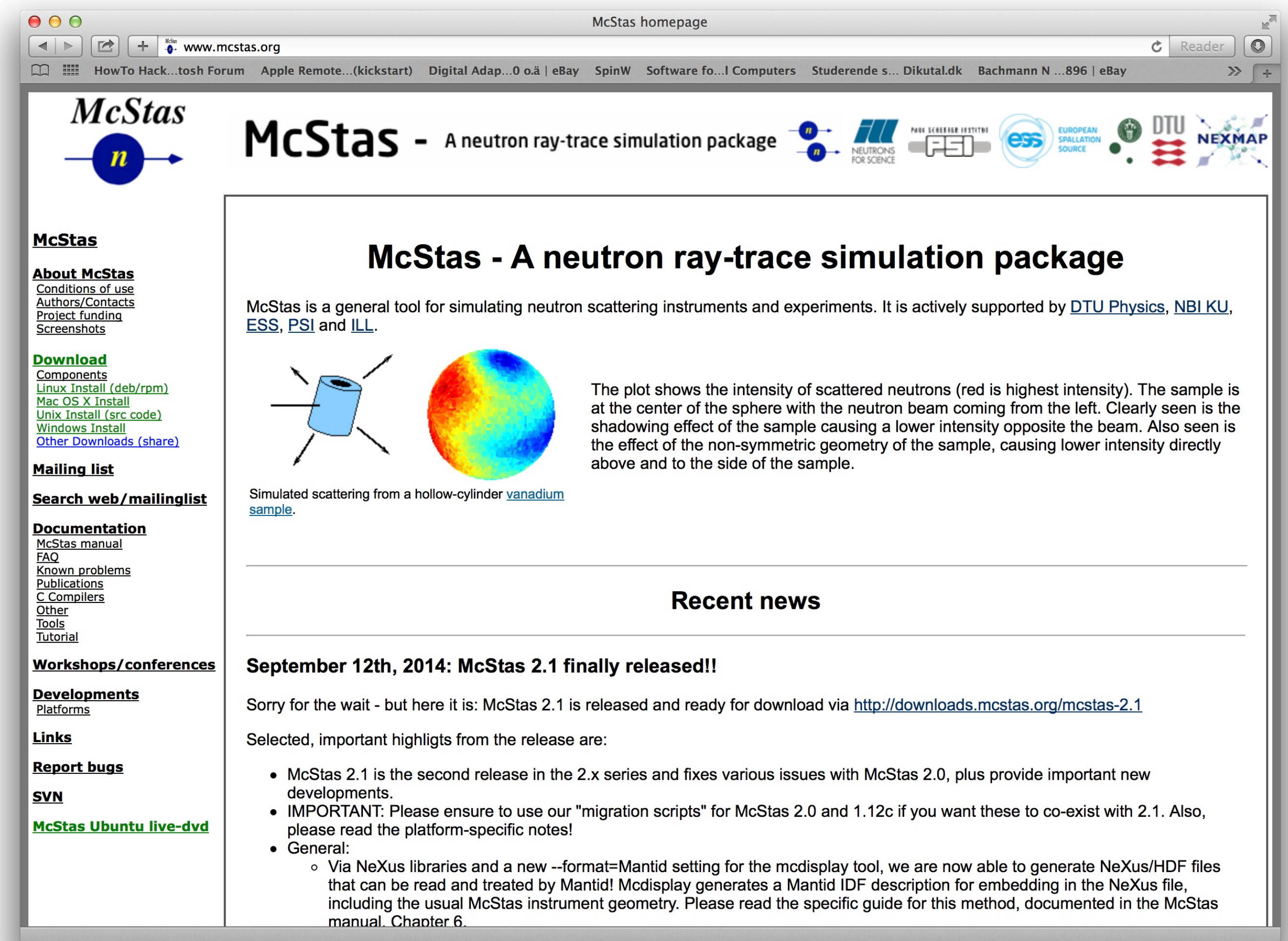
- Produce an instrument model



McStas Introduction

- Flexible, general simulation utility for neutron scattering experiments.
- Original design for **M**onte **c**arlo **S**imulation of **t**riple **a**xis **s**pectrometers
- 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

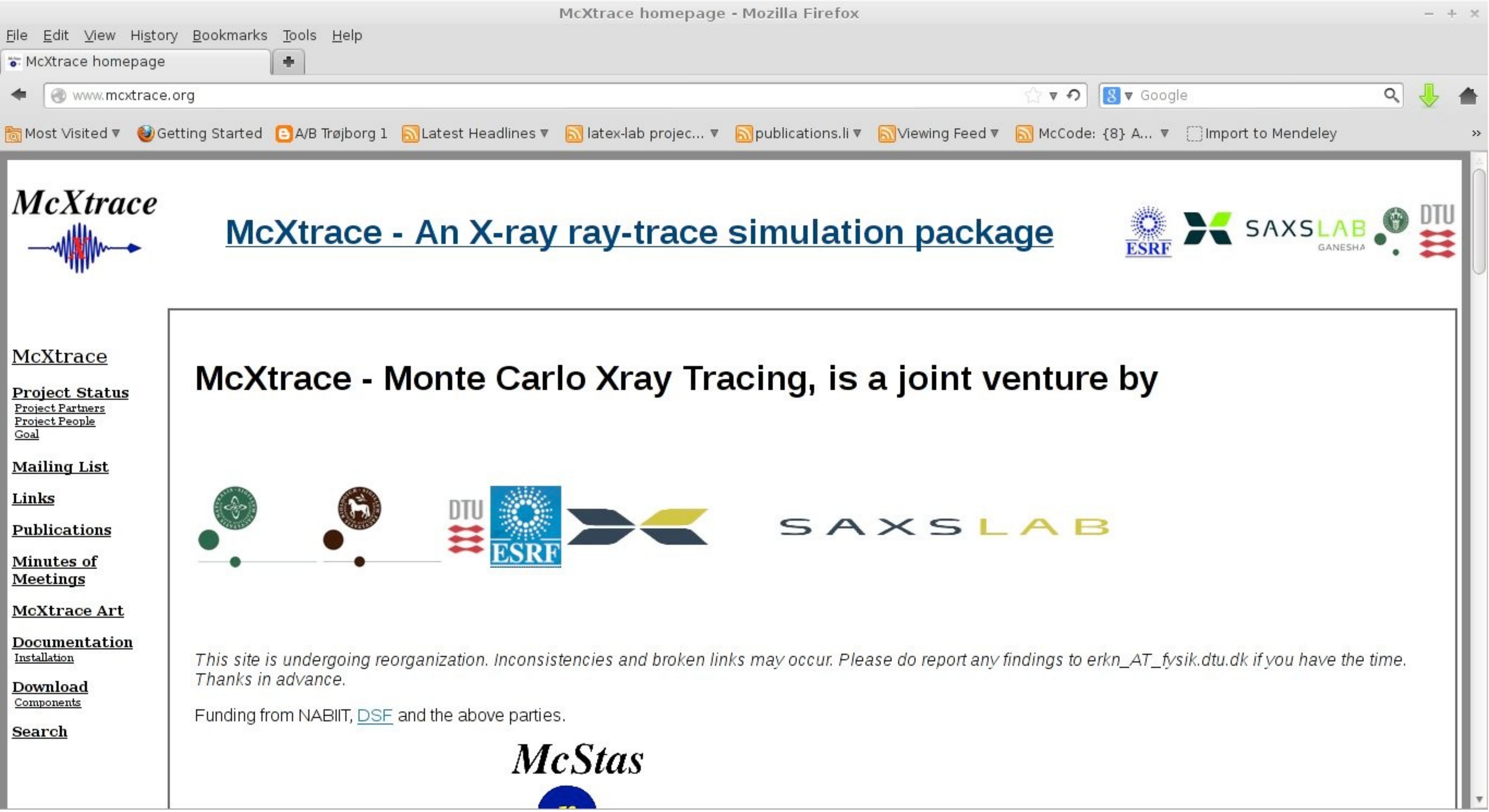
GNU GPL
license
Open Source



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

mcstas-users@mcstas.org mailinglist

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



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)

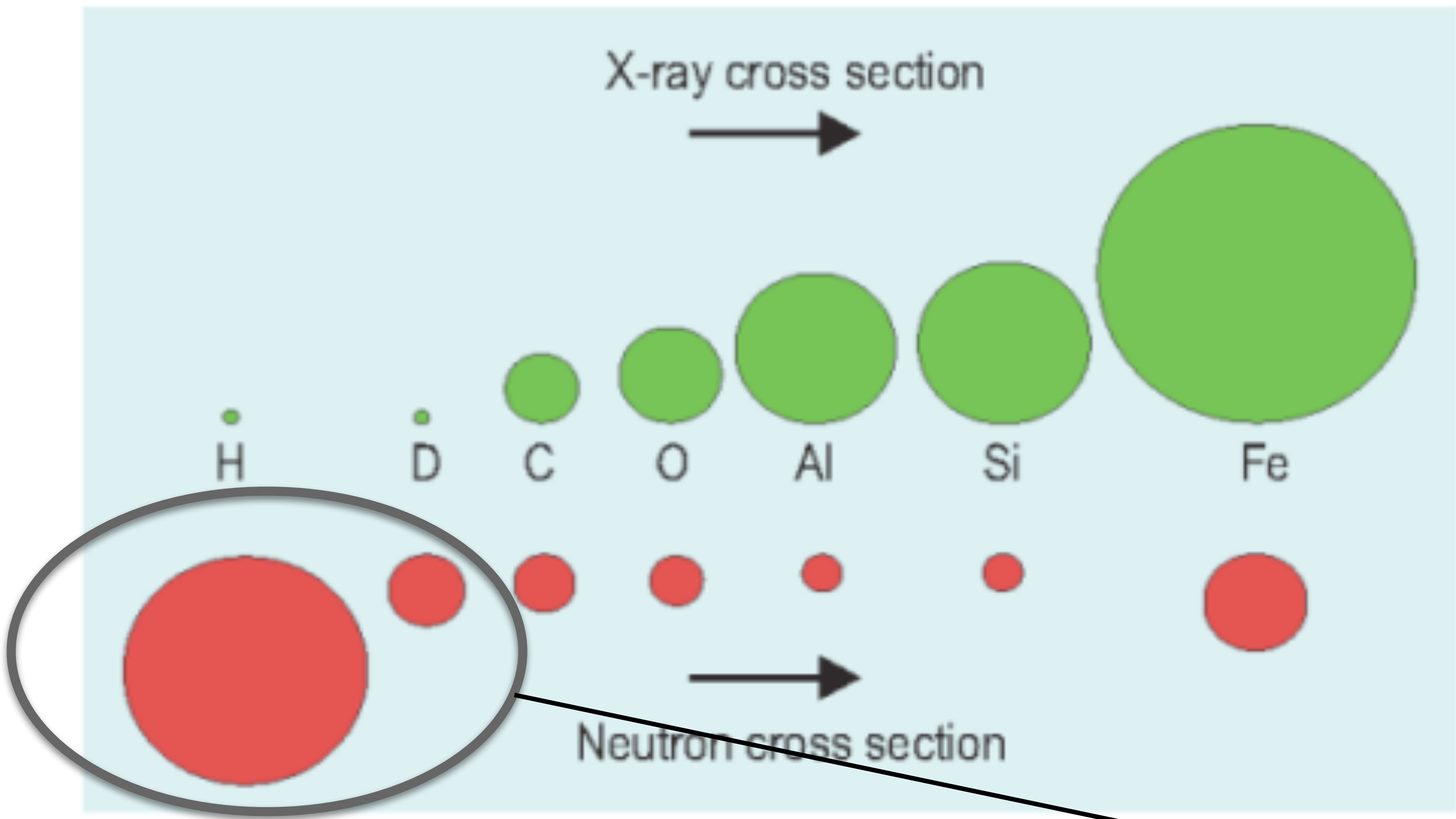
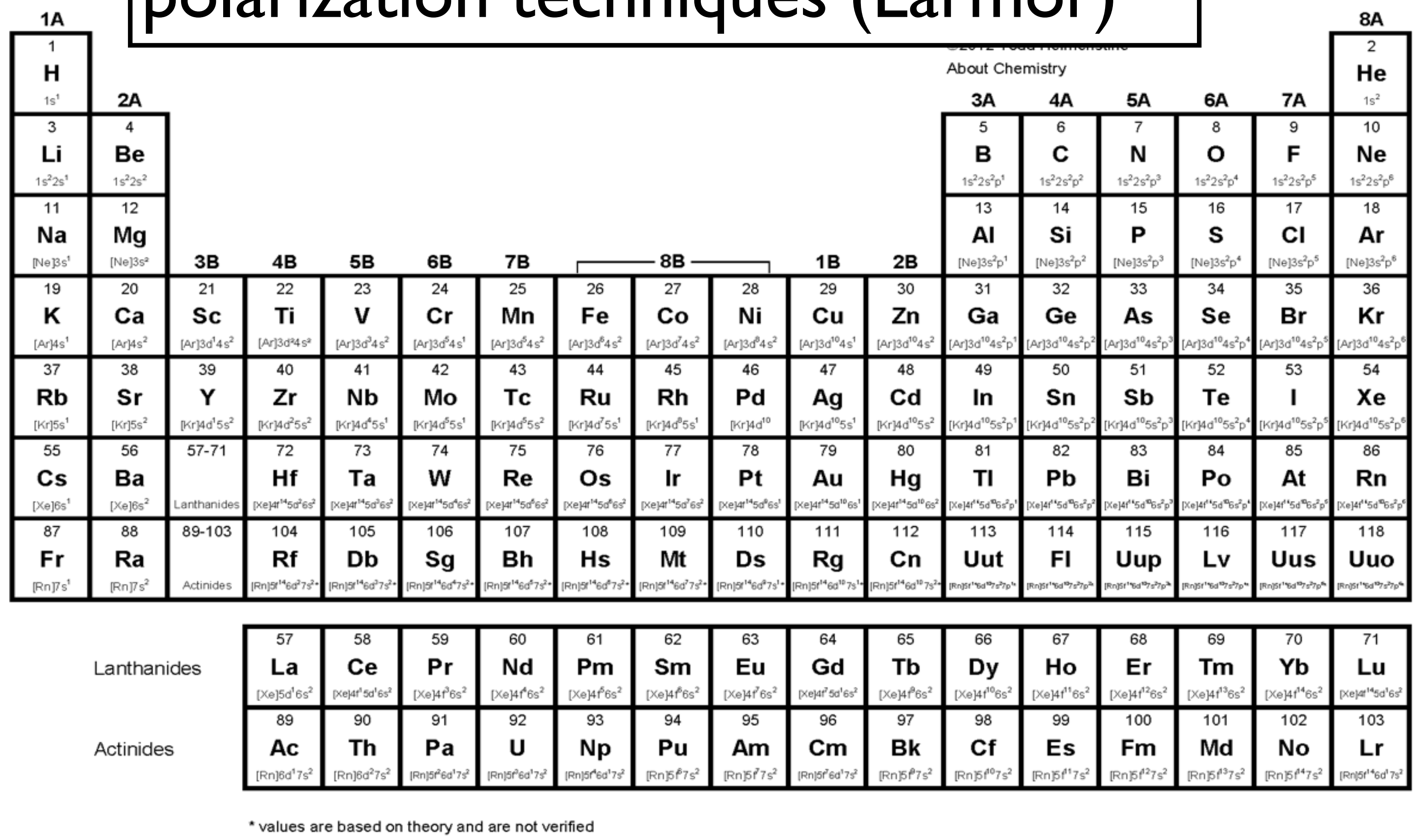


Fig. 2. Neutron and x-ray scattering cross-sections compared. Note that neutrons penetrate through Al much better than x rays do, yet are strongly scattered by hydrogen.



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

- Result: Two very different response/contrasts

DTU Fysik
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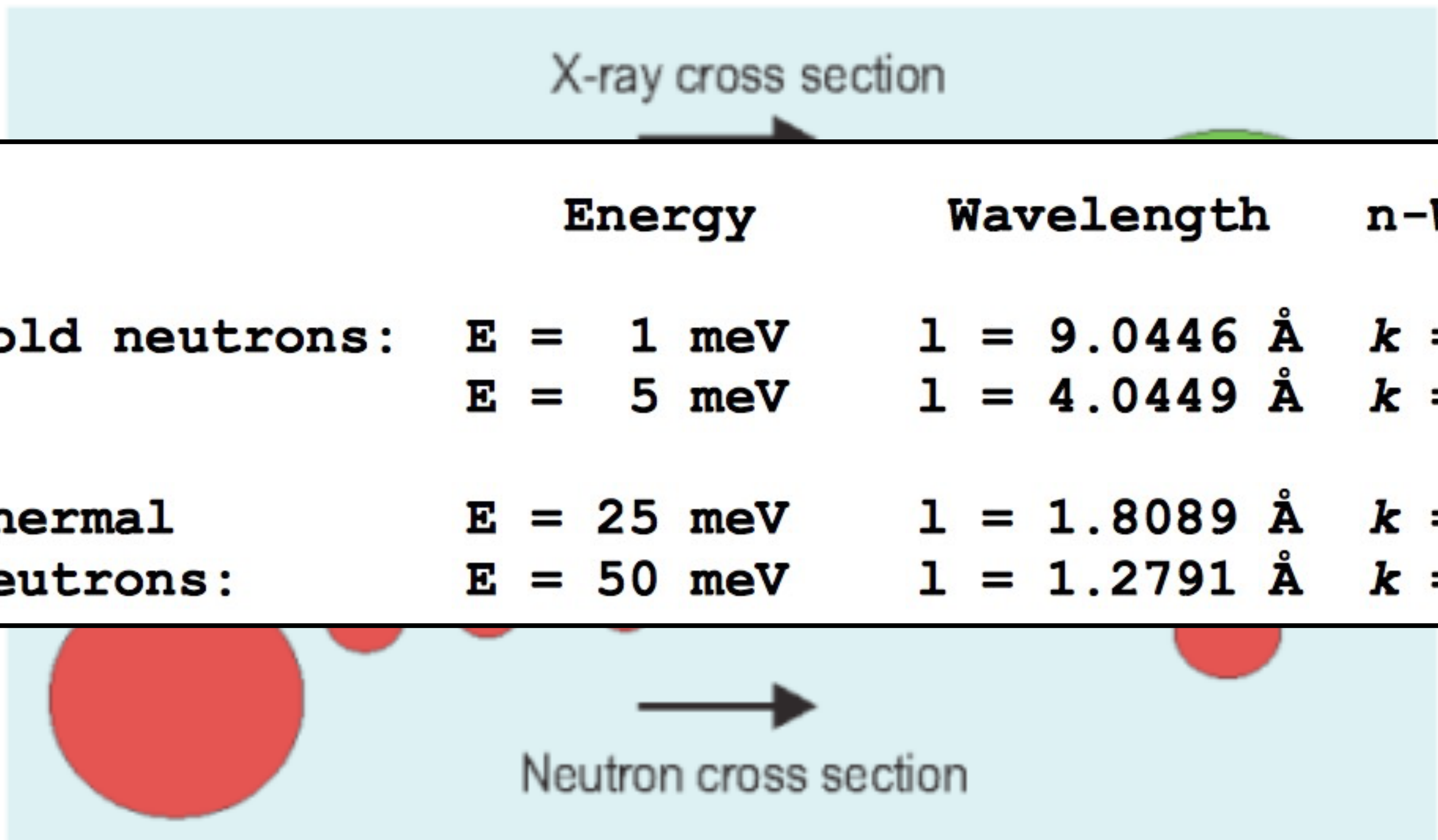
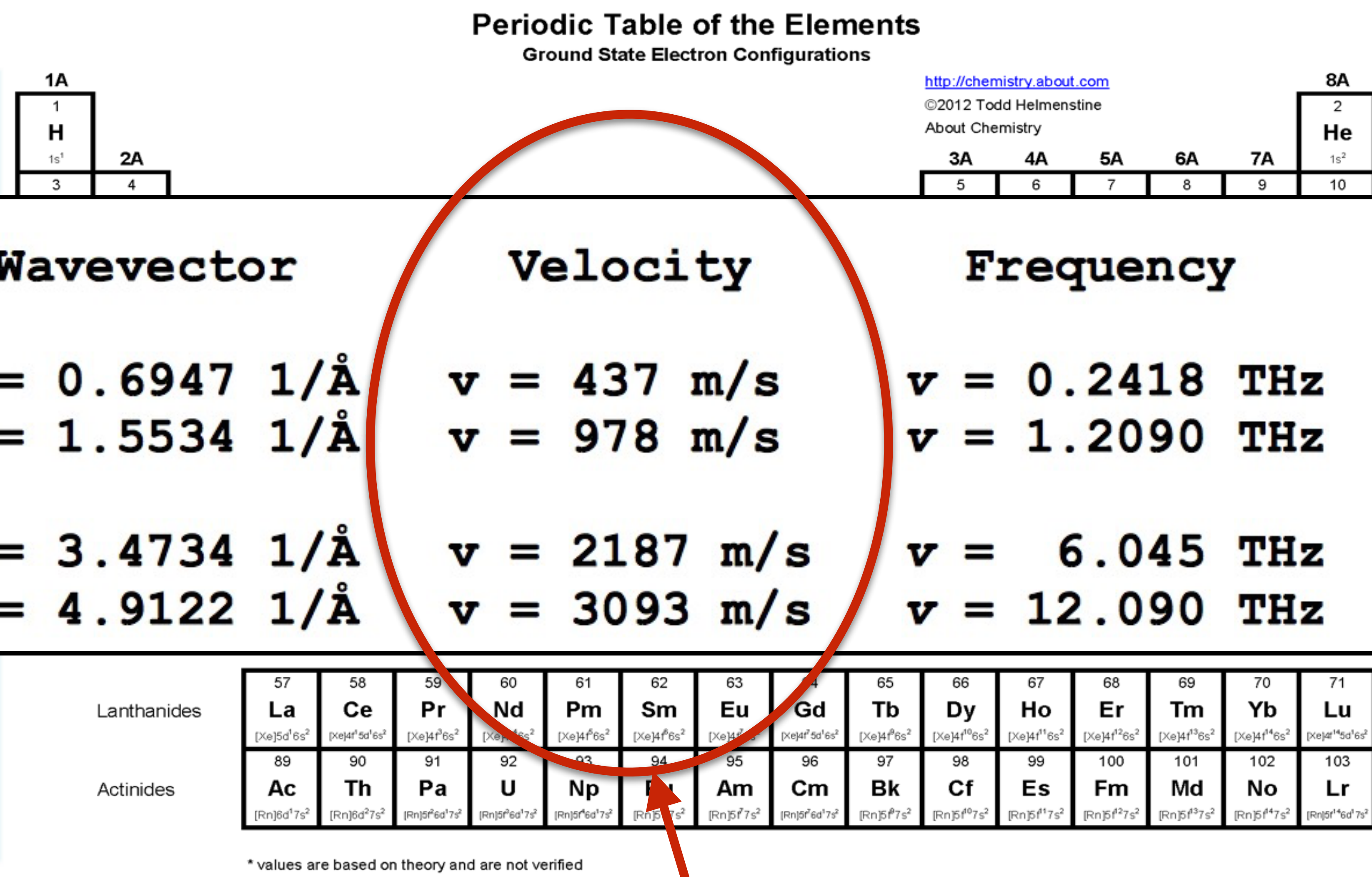
Both neutrons and X-rays interact with atoms

- 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.





	Energy	Wavelength	n-Wavevector	Velocity	Frequency
cold neutrons:	E = 1 meV	l = 9.0446 Å	k = 0.6947 1/Å	v = 437 m/s	v = 0.2418 THz
	E = 5 meV	l = 4.0449 Å	k = 1.5534 1/Å	v = 978 m/s	v = 1.2090 THz
thermal neutrons:	E = 25 meV	l = 1.8089 Å	k = 3.4734 1/Å	v = 2187 m/s	v = 6.045 THz
	E = 50 meV	l = 1.2791 Å	k = 4.9122 1/Å	v = 3093 m/s	v = 12.090 THz

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

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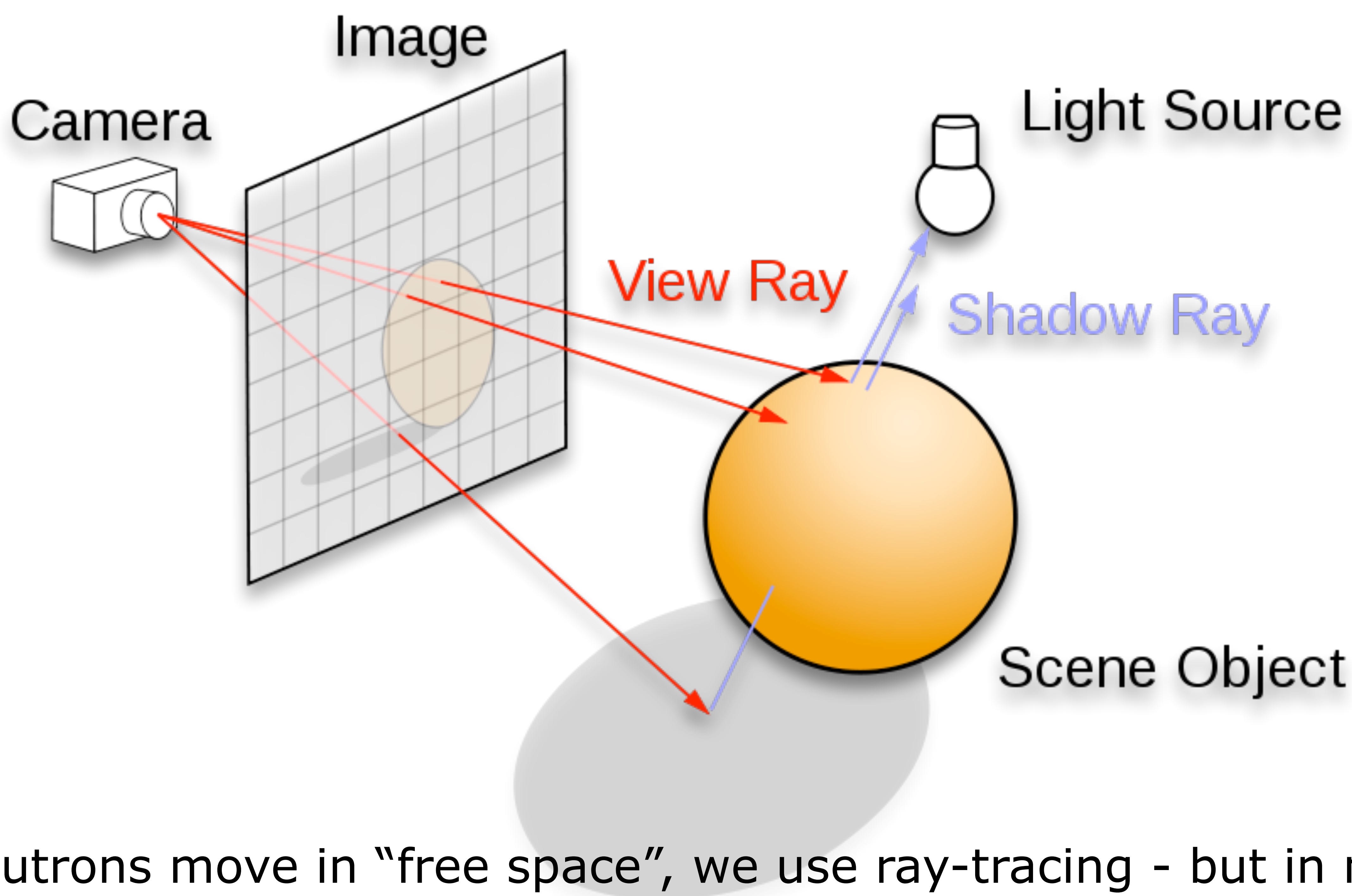
Monte Carlo techniques

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

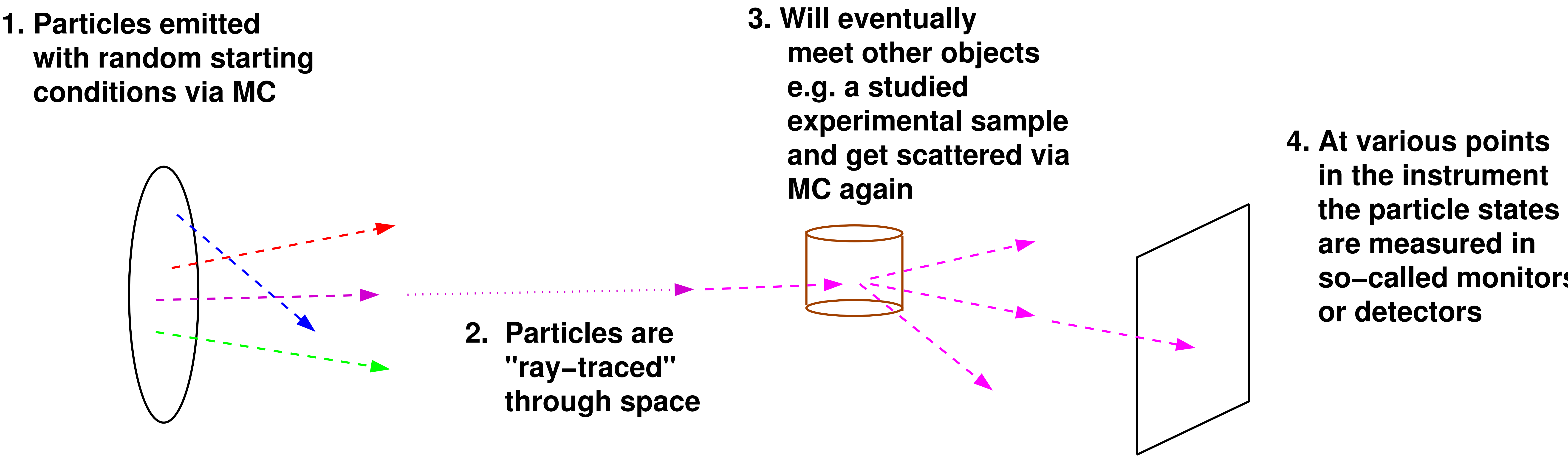
- Notable fathers: John v. Neumann Stanislav Ulam Nicholas Metropolis
- Named “Monte Carlo” after Ulam’s fathers frequent visits to the Monte Carlo casino in Las Vegas
- Initially “implemented” by letting large numbers of women use tabularized random numbers and hand calculators for individual particle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

Ray-tracing methods



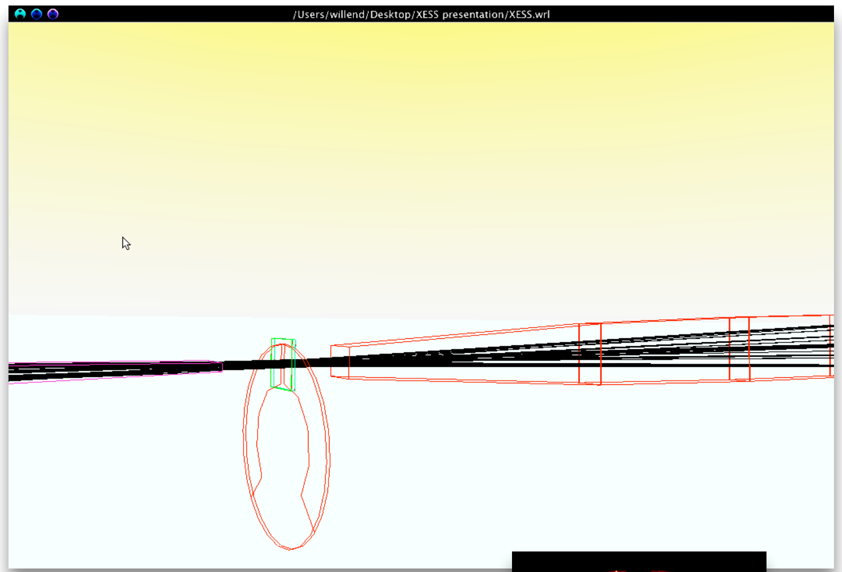
- When neutrons move in “free space”, we use ray-tracing - but in most cases in direction source -> detector
- Of course parabolas rather than straight lines are uses to implement gravity

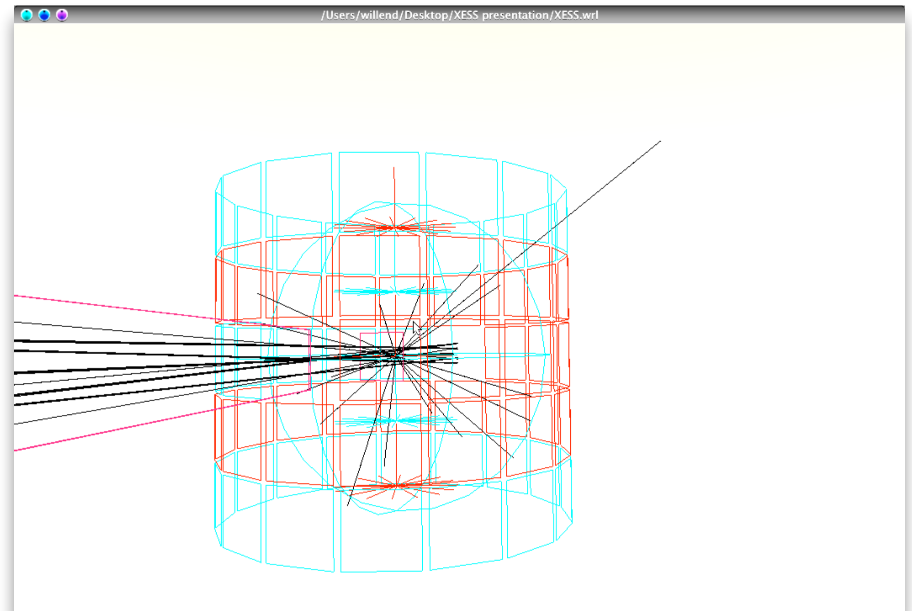
Overall picture: *Monte Carlo Ray-Tracing*



- 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

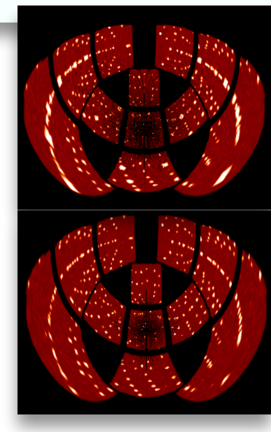
What are the codes used for?

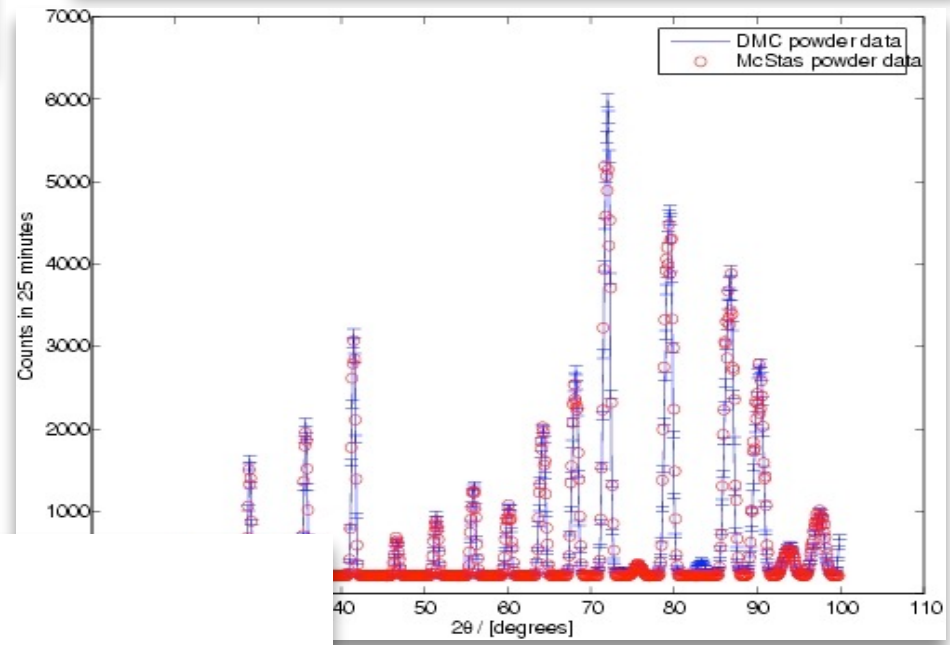


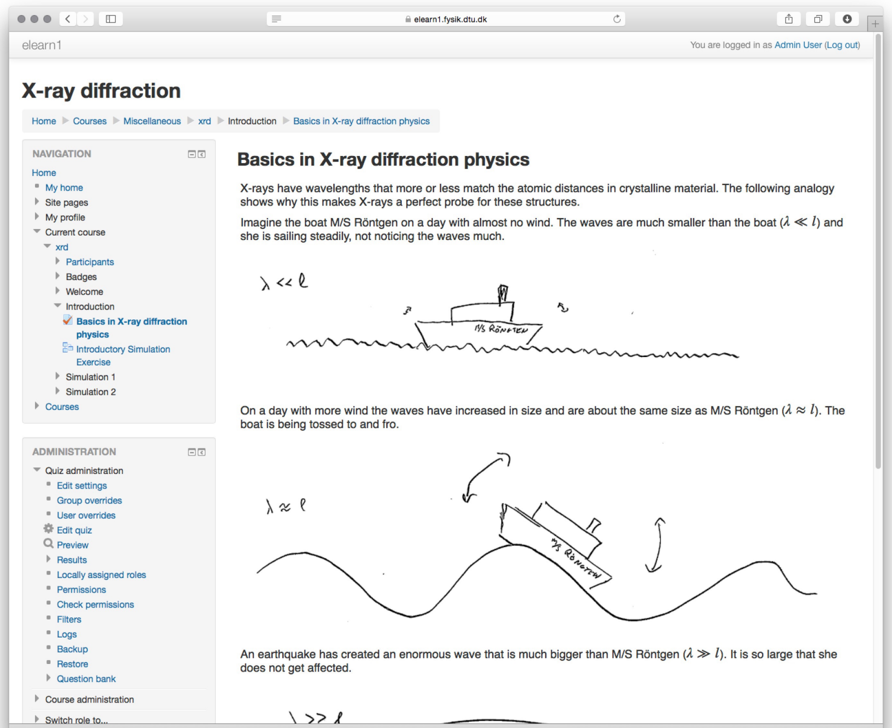


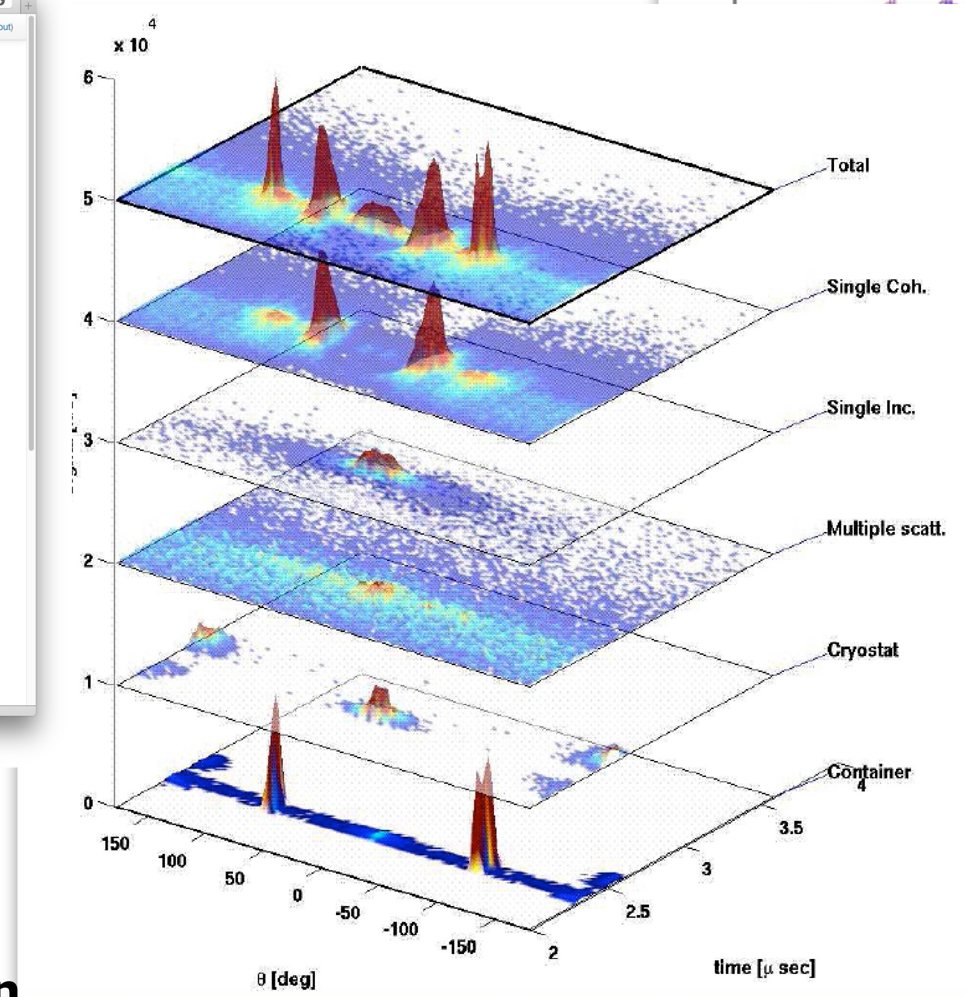
- Instrumentation
- Virtual experiments
- Data analysis
- Teaching

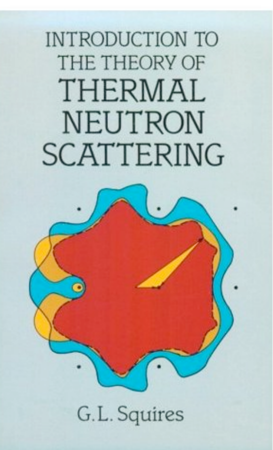
(KU, DTU)

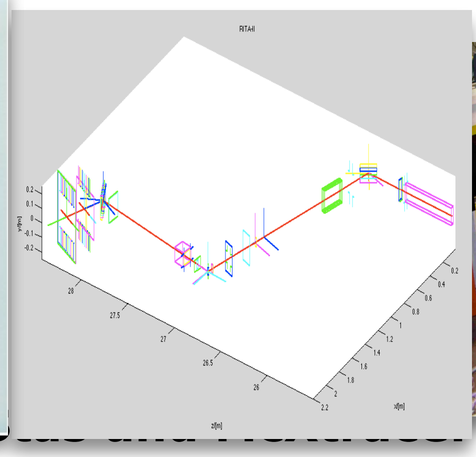


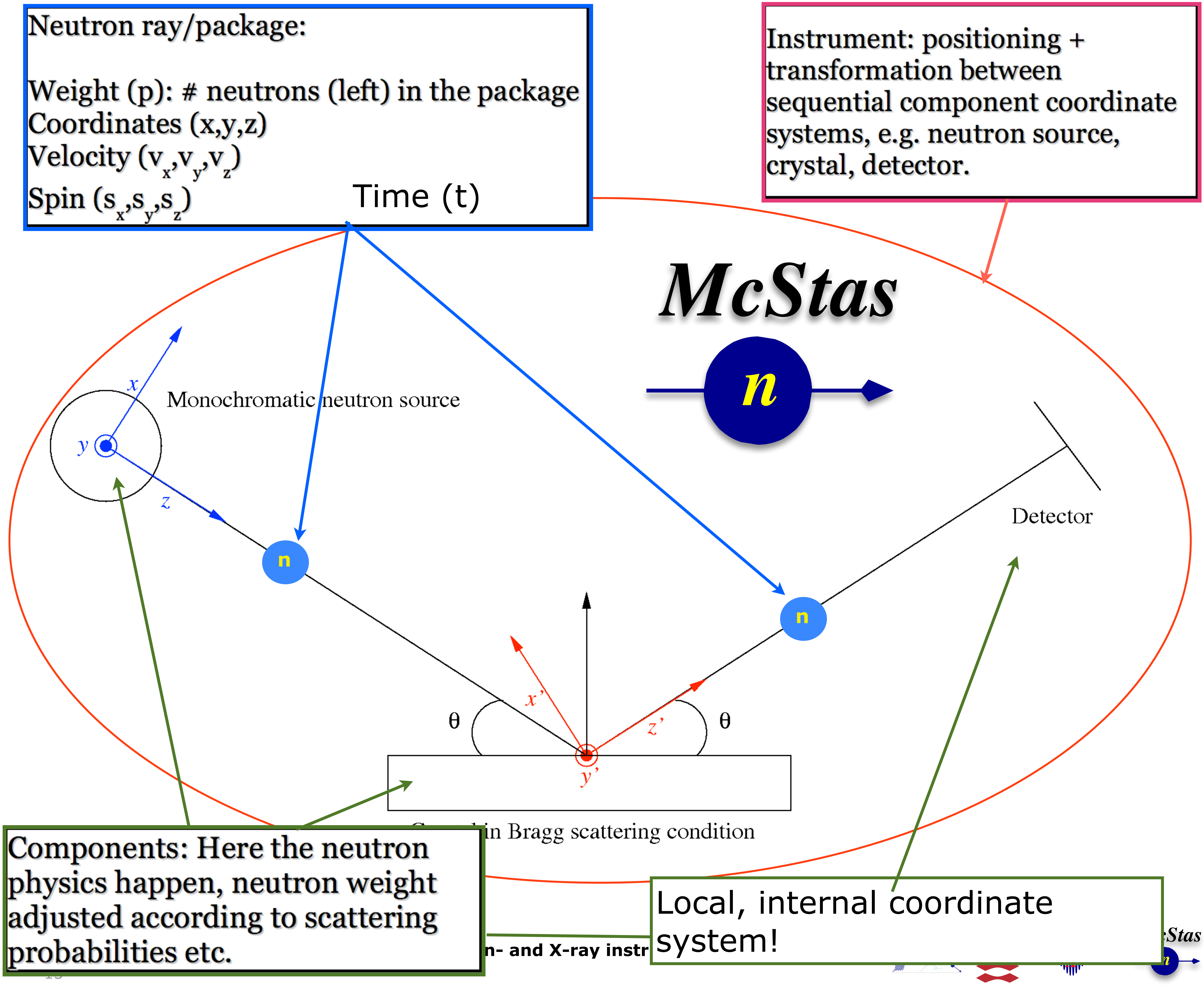








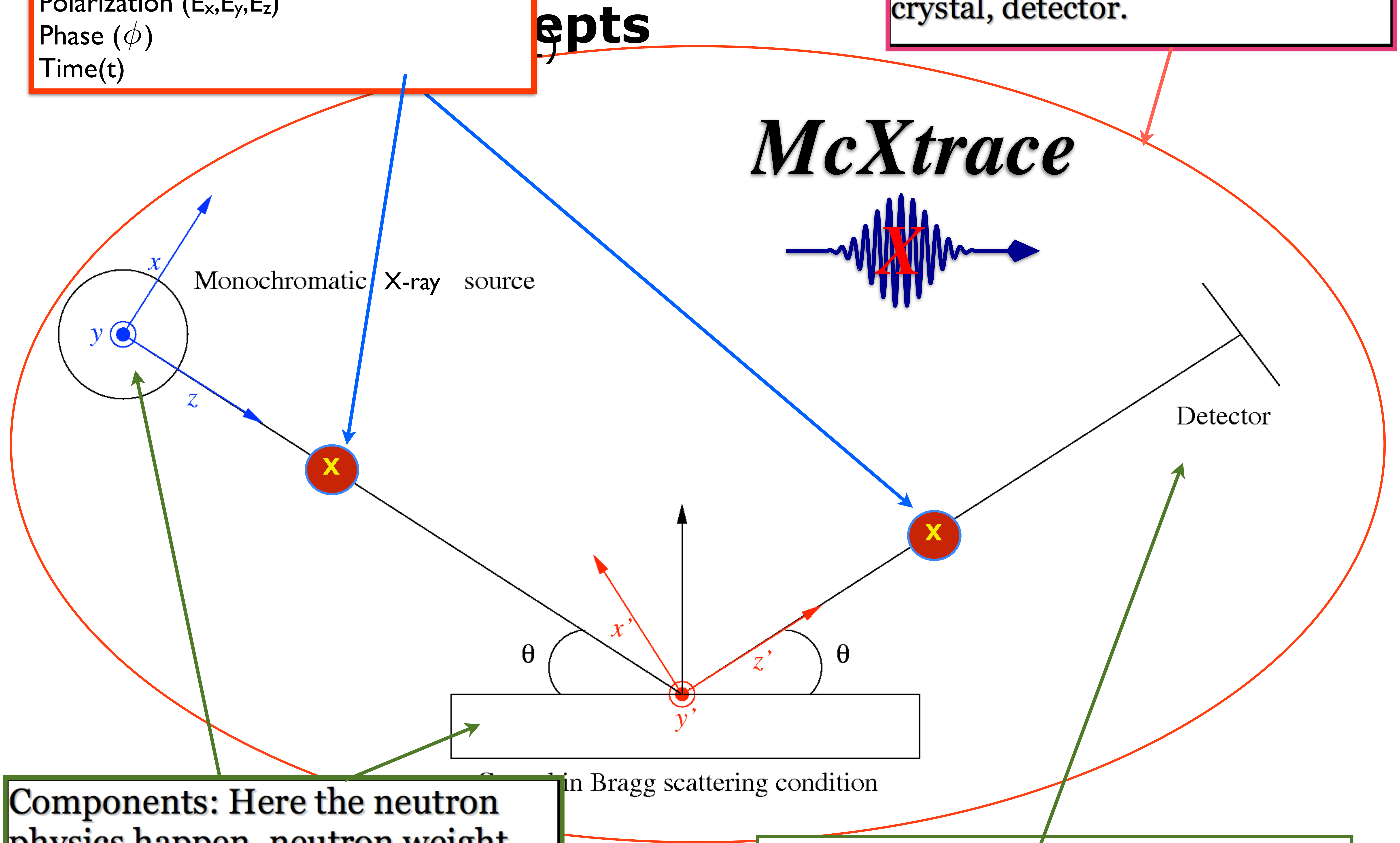



Neutron ray/package:
Weight (p): # neutrons (left) in the package
Coordinates (x,y,z)
Velocity (v_x,v_y,v_z)
Spin (s_x,s_y,s_z)
Time (t)
Instrument: positioning + transformation between sequential component coordinate systems, e.g. neutron source, crystal, detector.
McStas
n
x
y
z
Monochromatic neutron source
n
n
Detector
x'
z'
y'
θ
θ
in Bragg scattering condition
Components: Here the neutron physics happen, neutron weight adjusted according to scattering probabilities etc.
Local, internal coordinate system!

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.



Components: Here the neutron physics happen, neutron weight adjusted according to scattering probabilities etc.

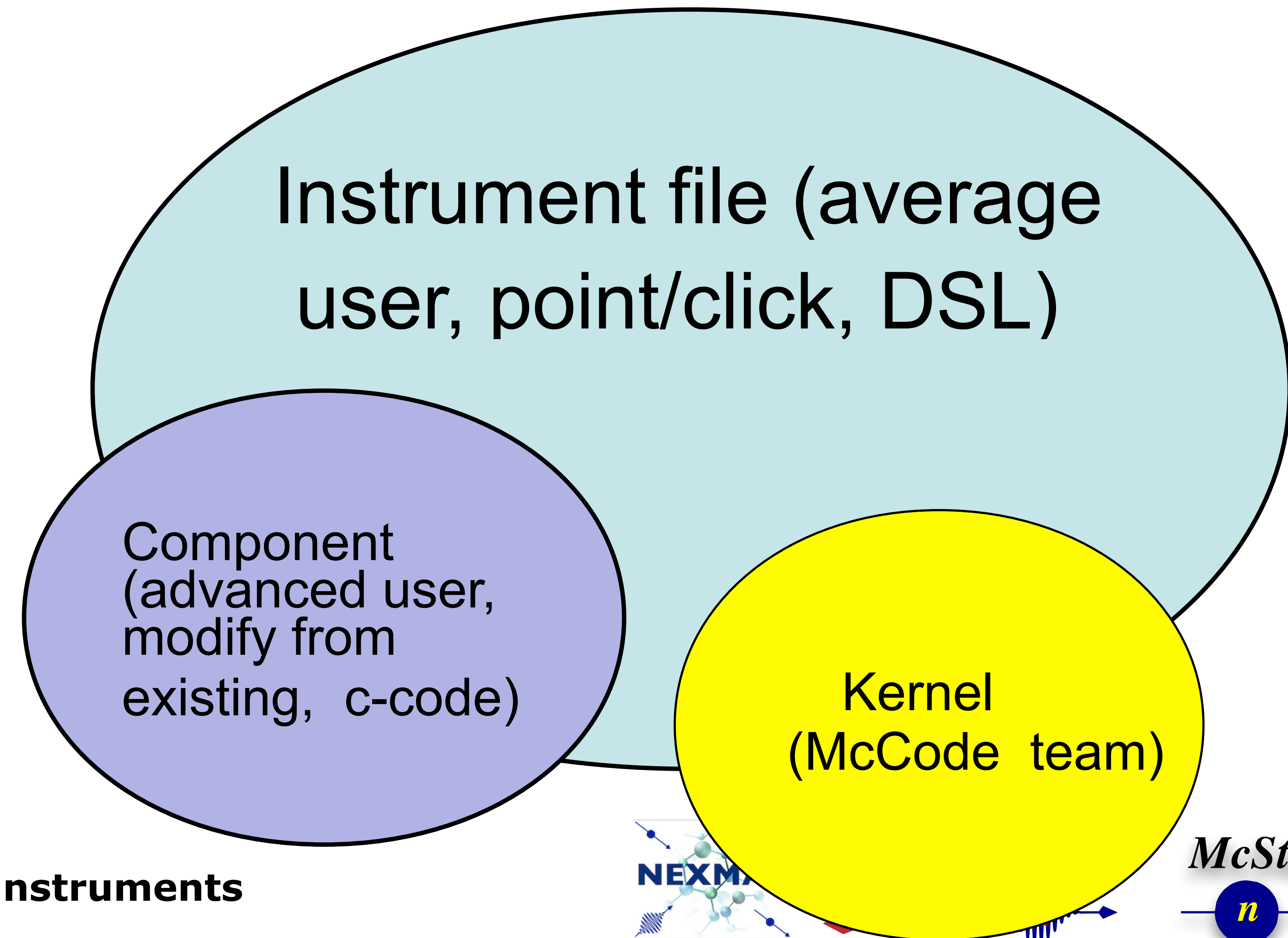
Local, internal coordinate system!

McStas/McXtrace tech overview

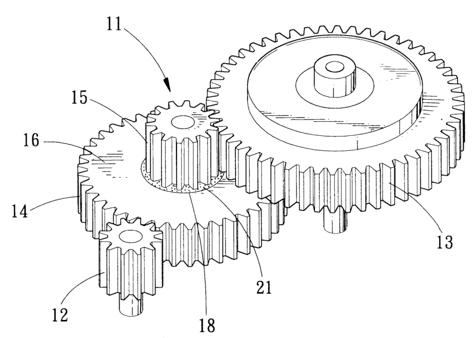
- Portable code (Unix/Linux/Mac/Windoze)

- 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

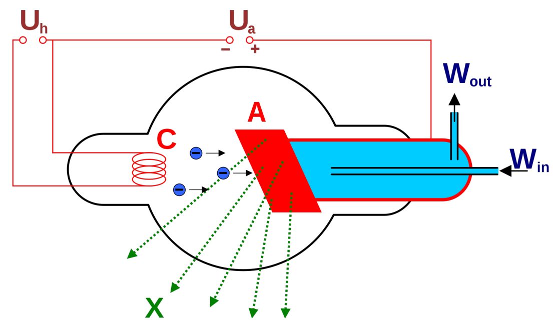


- DSL + ISO-C code gen.

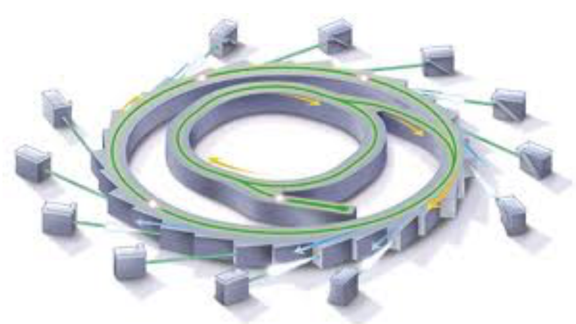


Sources - 1

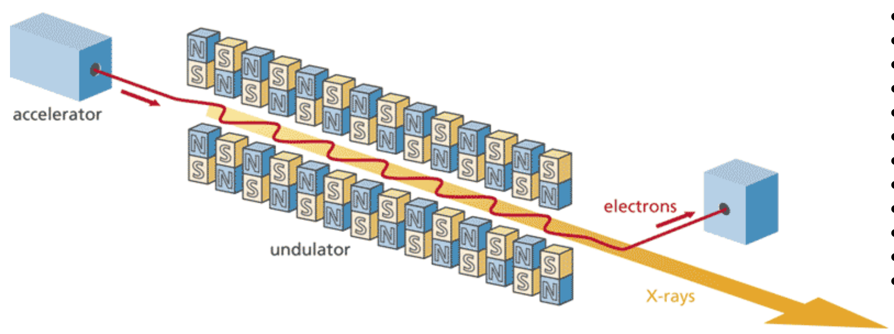
- **X-ray sources**
  - Lab equipment
    - X-ray tube
    - Rotating anode
    - Liquid jet anode



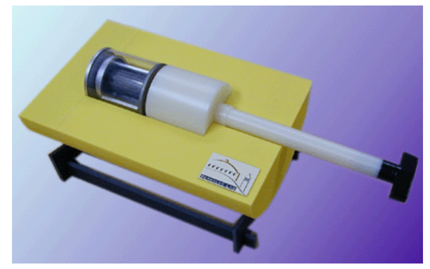
  - Synchrotron
    - Bending magnet
    - Wiggler
    - Undulator



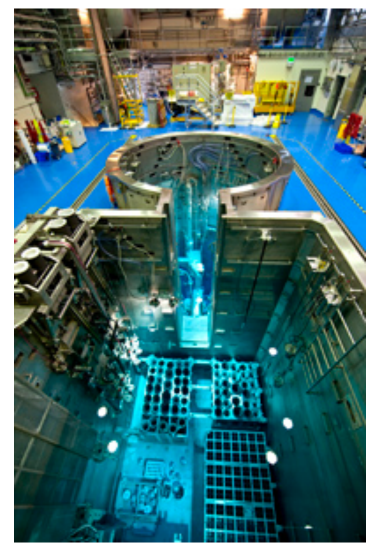
  - XFEL
    - SASE (very long undulator)



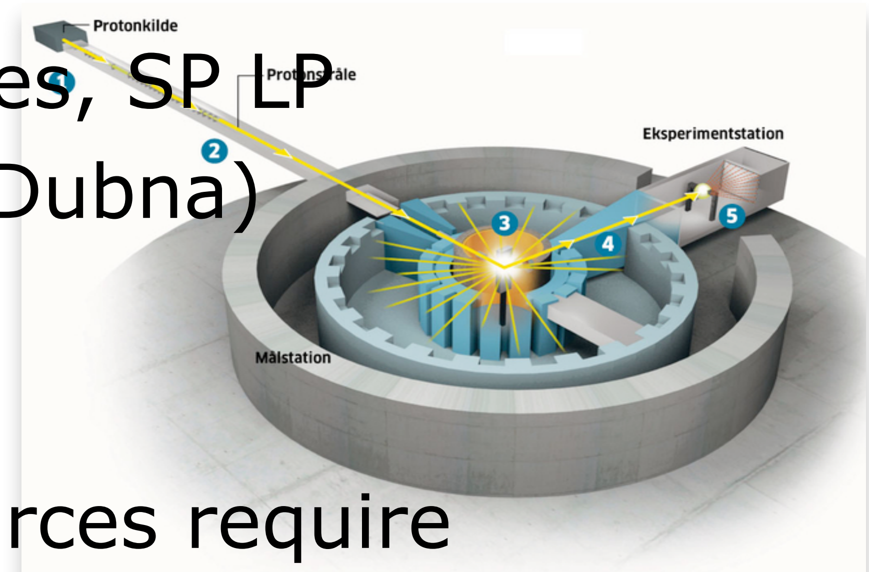
- **Neutron sources**
  - Lab equipment
    - Radioisotope-based
    - CANS (Compact accellerator based)



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



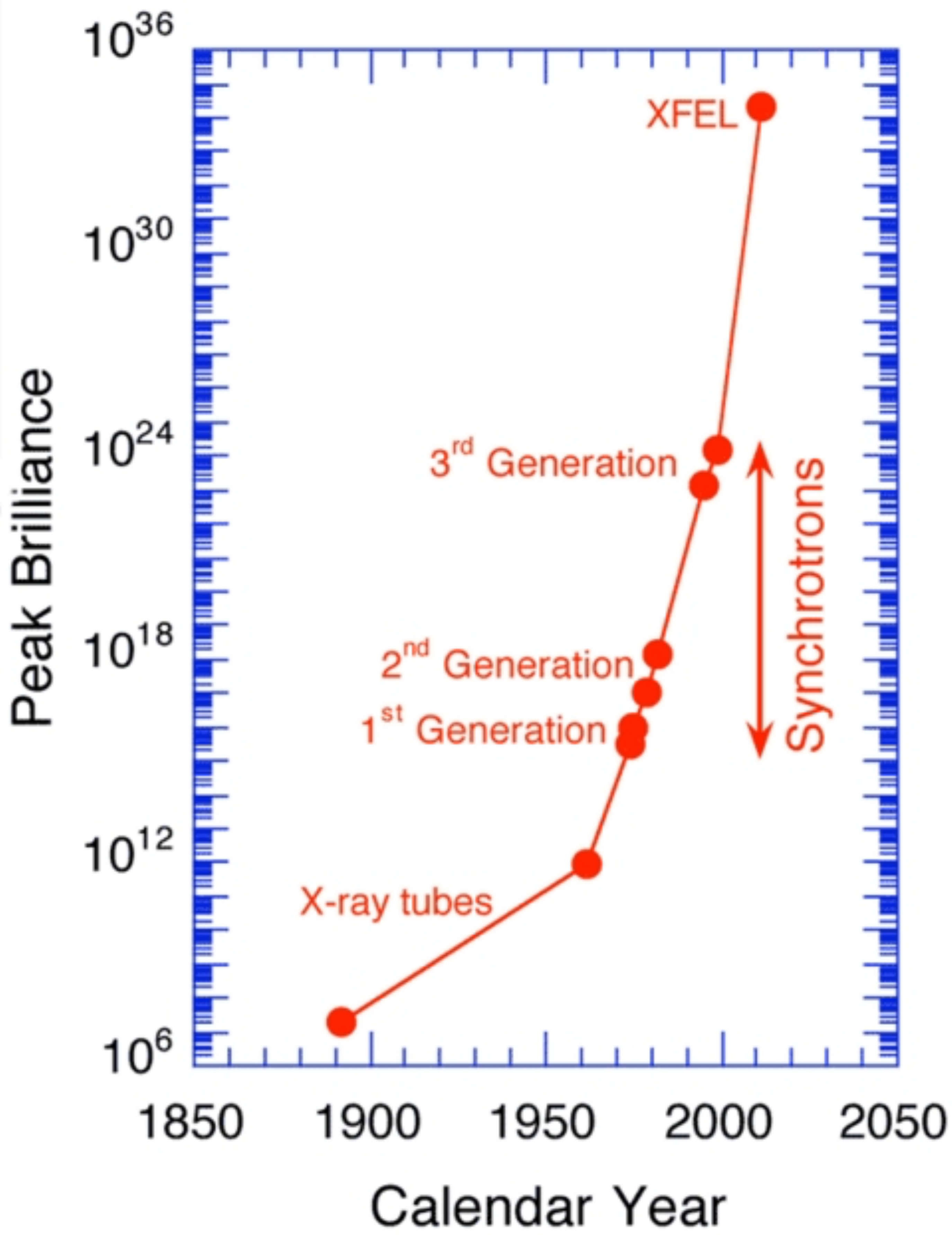
  - Pulsed sources
    - Spallation sources, SP LP
    - Pulsed reactor (Dubna)



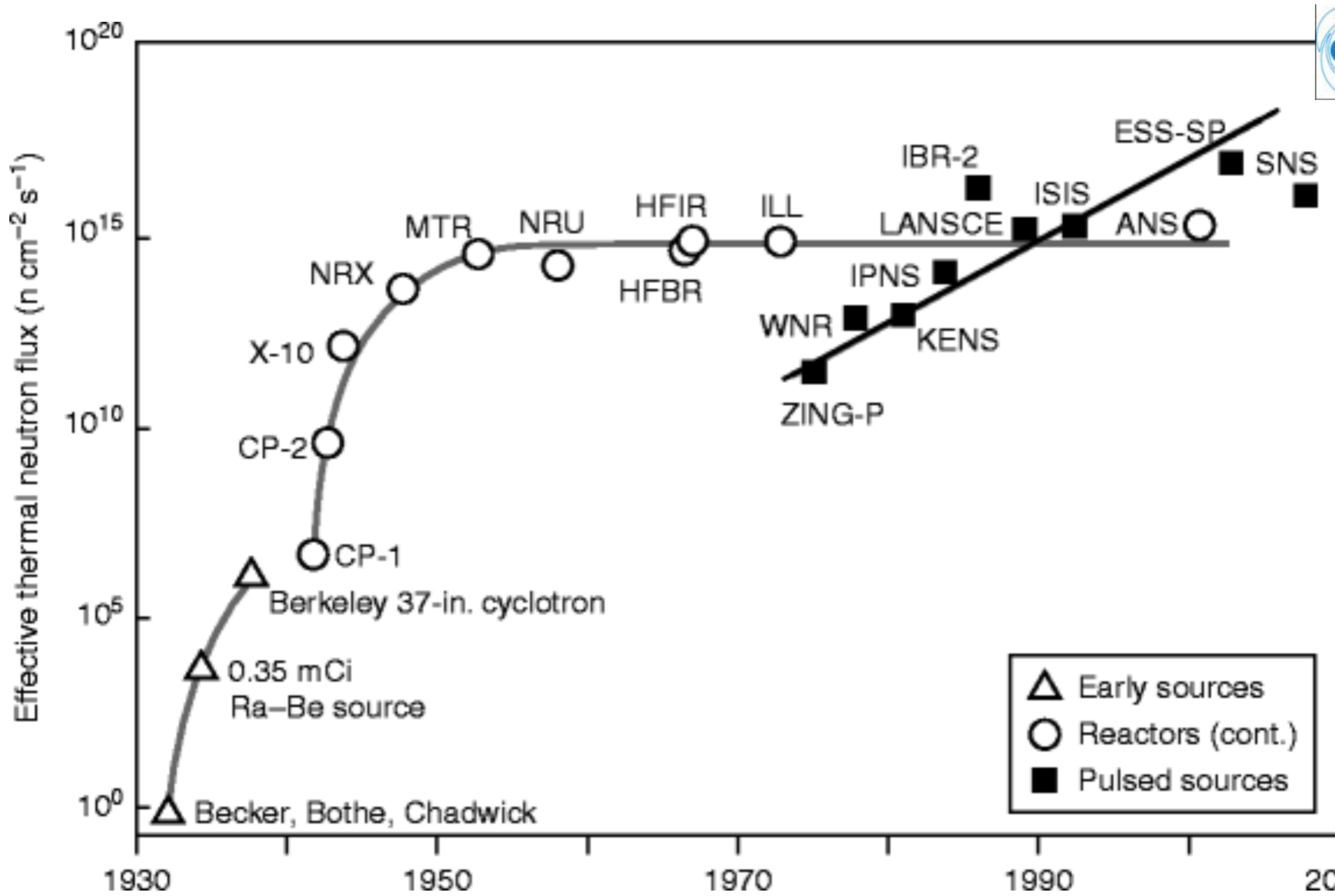
  - Most neutron sources require moderation of the neutron energy

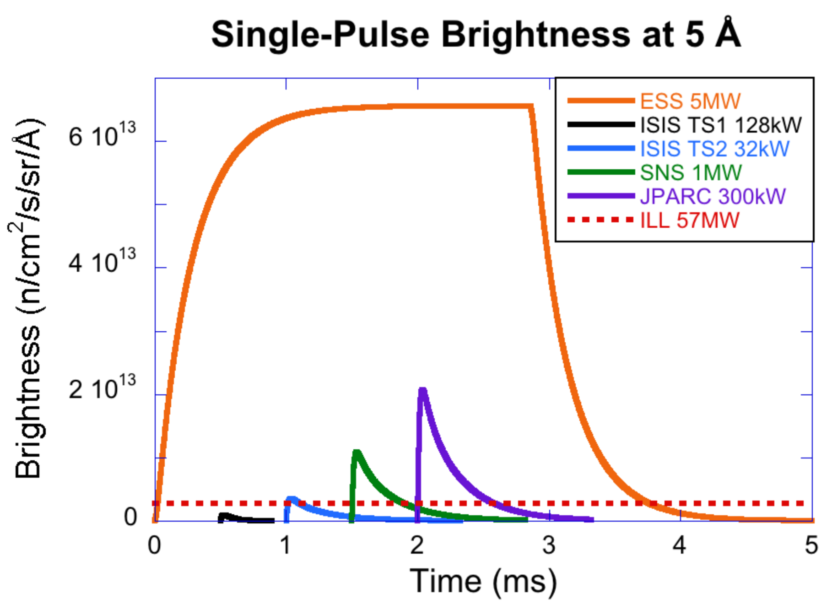
Sources - 2

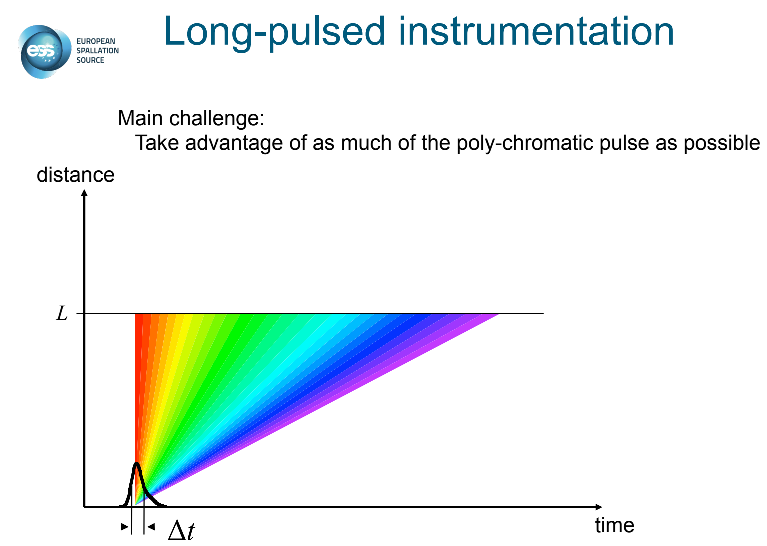
- X-ray sources



- Neutron sources



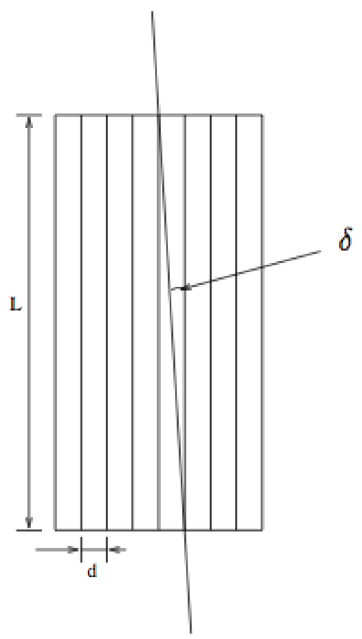


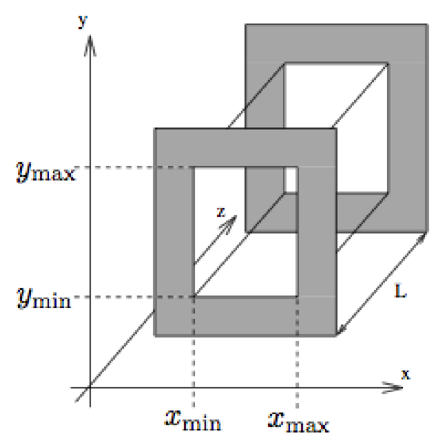


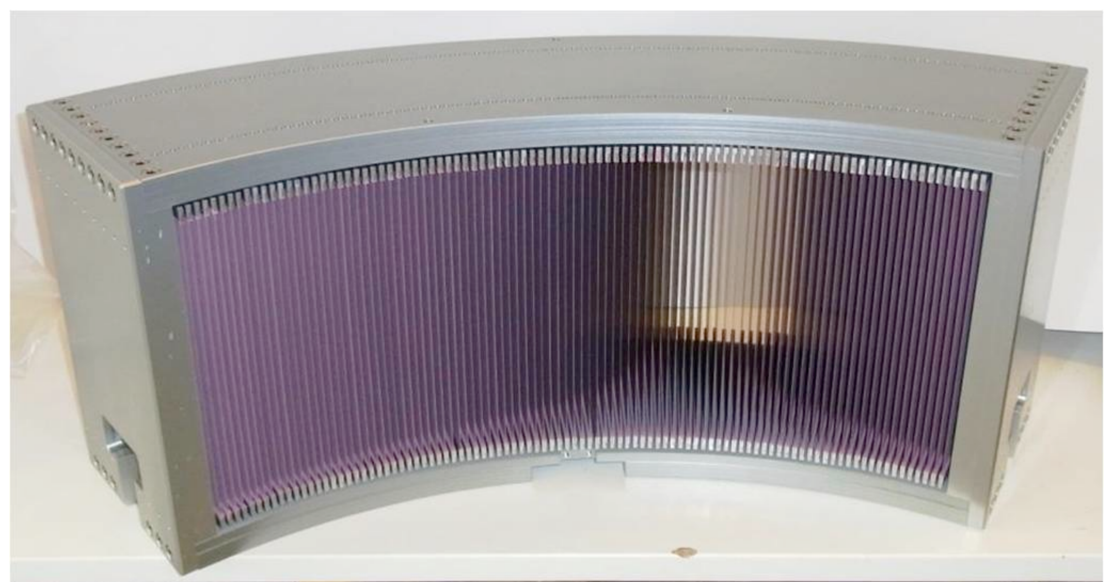
Spatial / directional beam adjustment

- **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

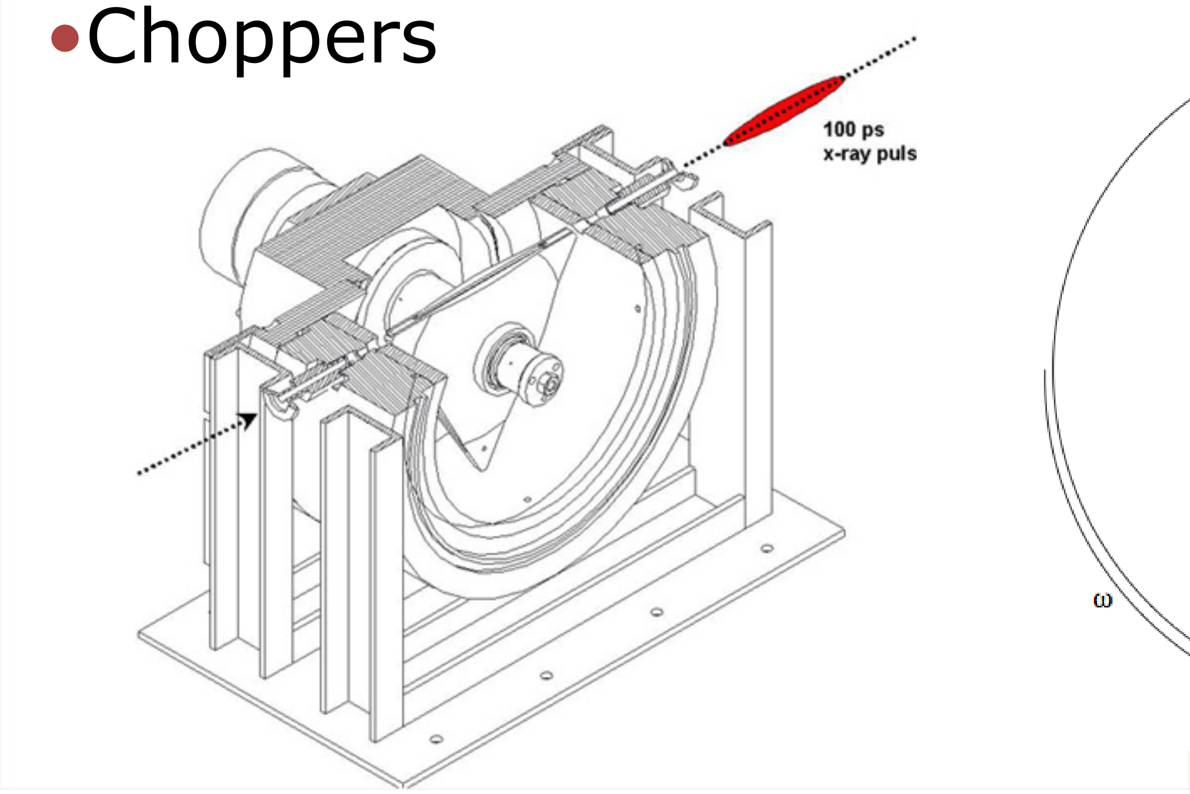


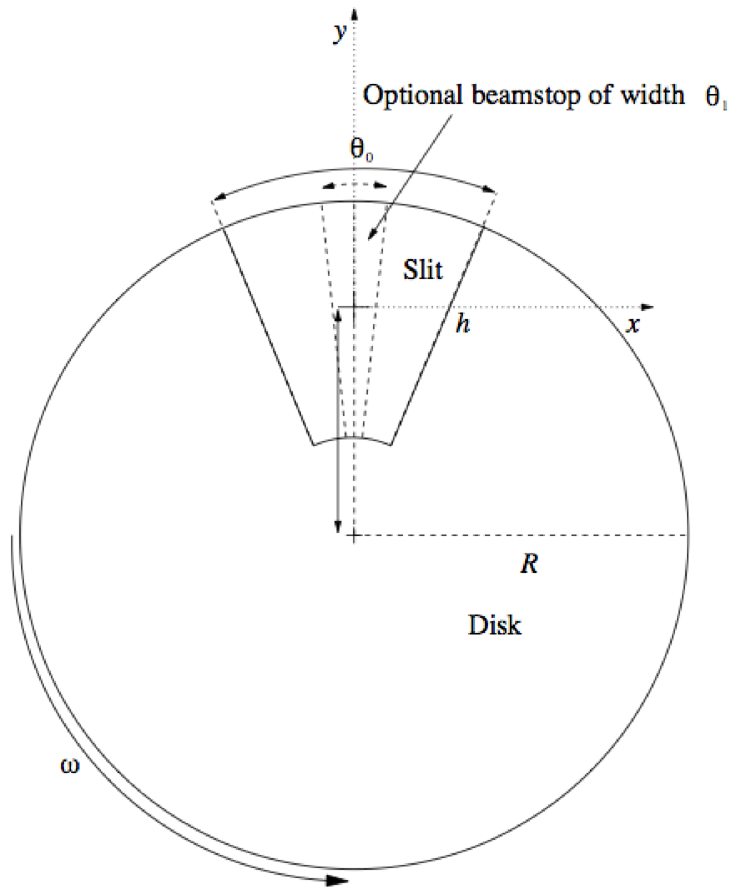


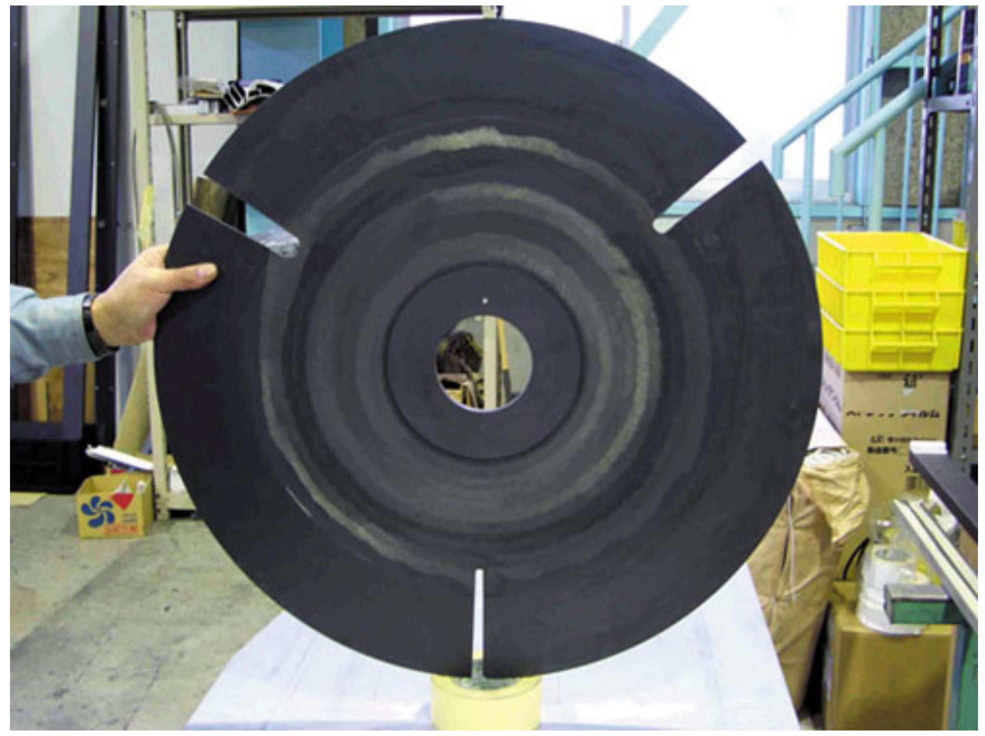


Temporal beam adjustment, rotating optics

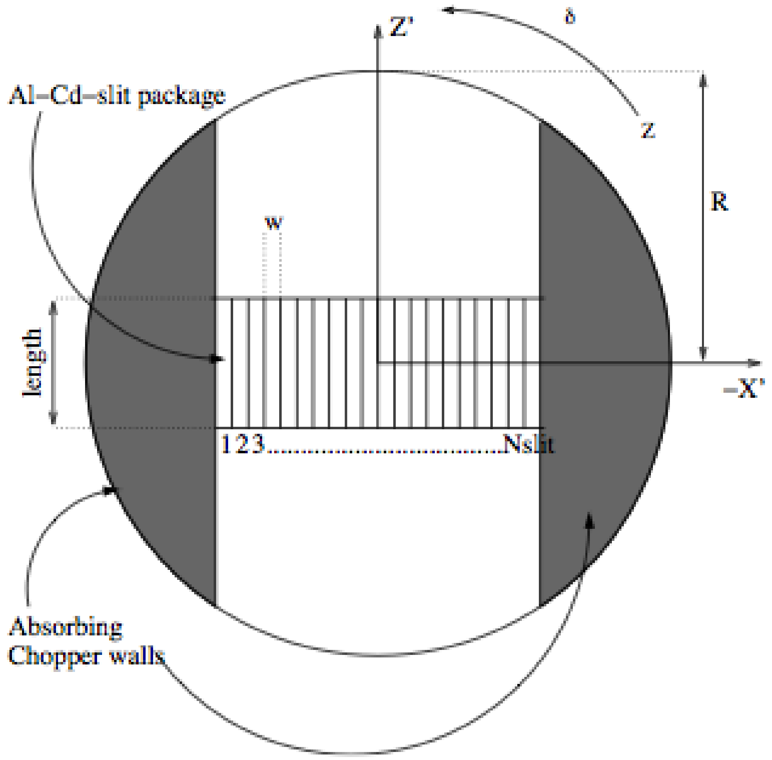
- **X-ray and neutrons**
  - Choppers

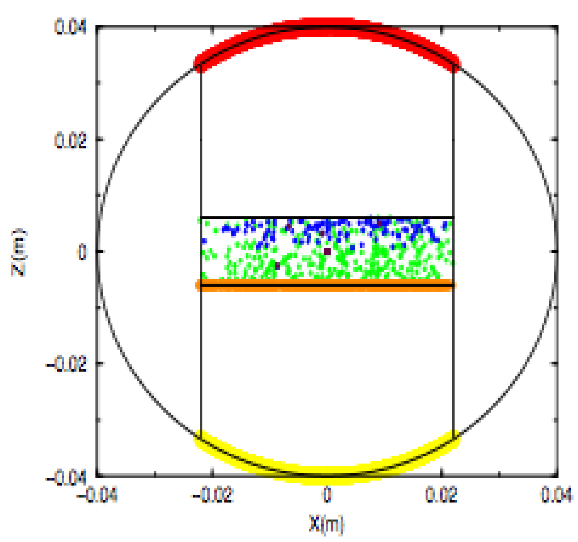






- **Neutrons only - monochromating rotating optics**
  - Fermi-chopper "rotating collimator"



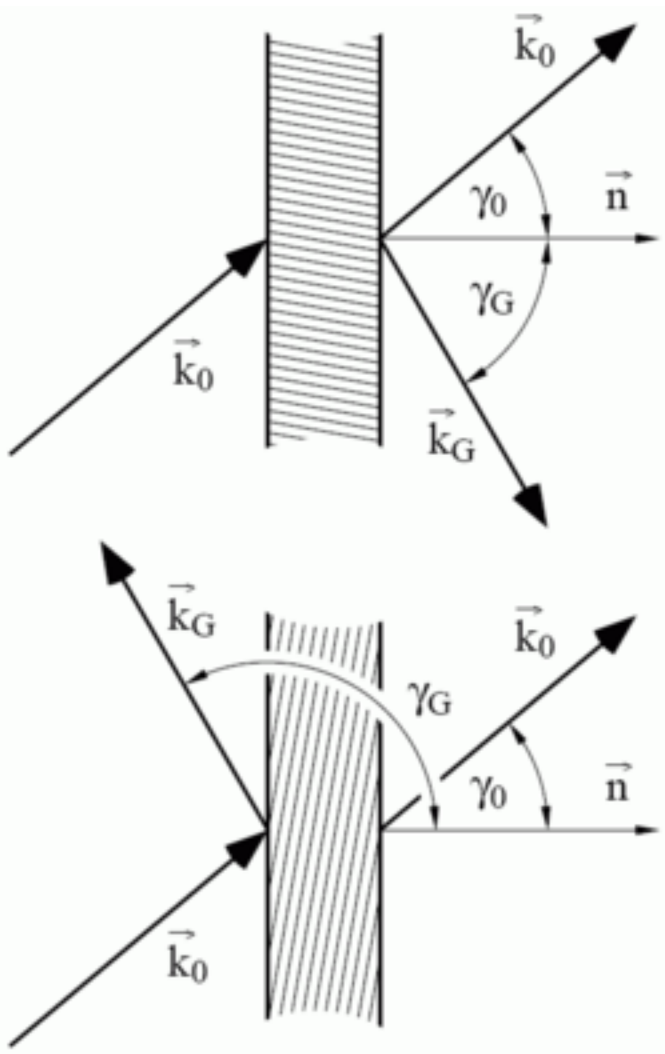


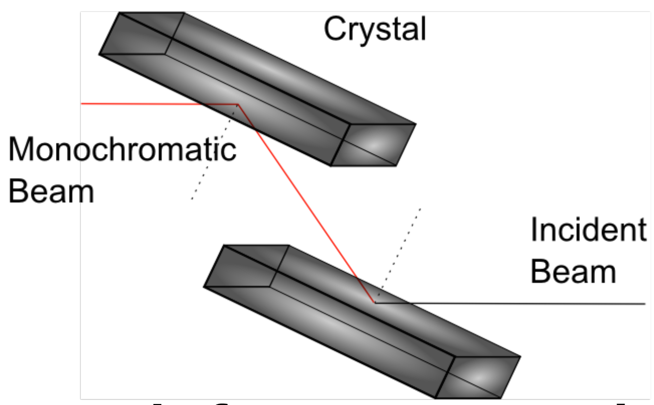
Velocity-selector

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

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

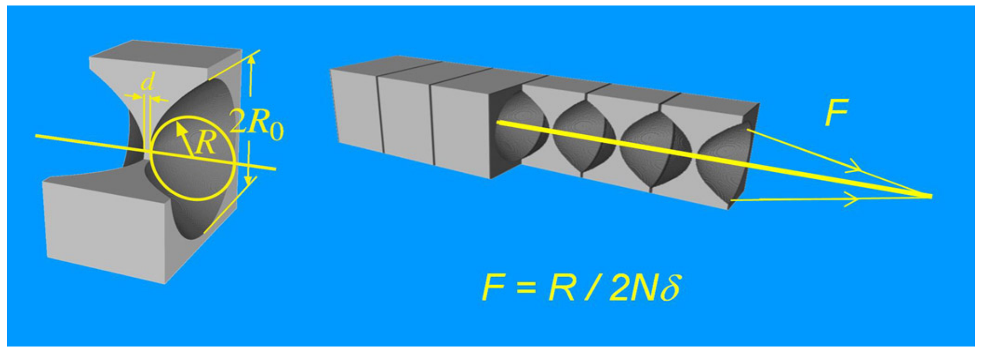




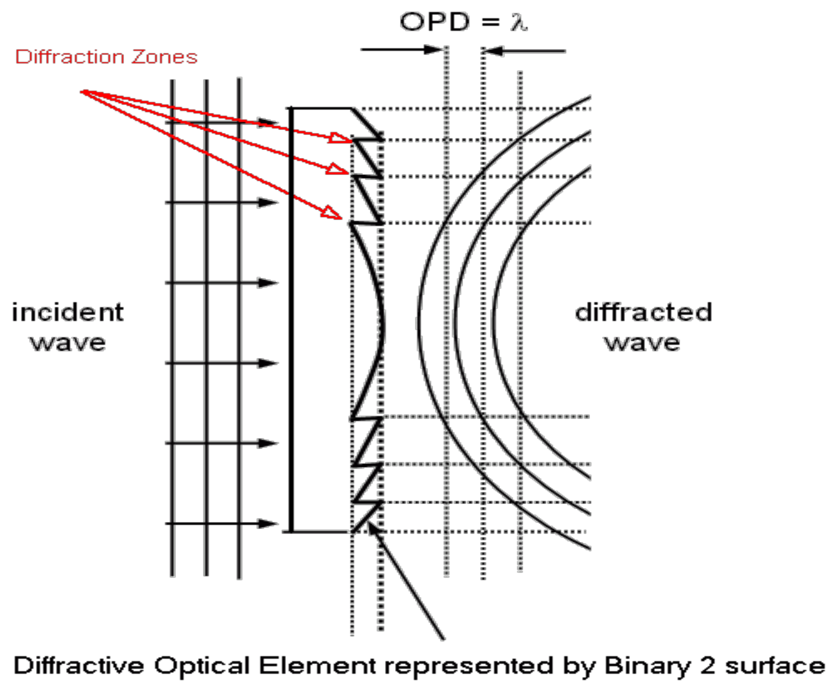
- **Neutron** $\frac{\delta\lambda}{\lambda} \approx 3\%$
  - Typically high-mosaicity (pyrolytic graphite, deformated Cu, Ge, …)
  - Often focusing, multi-crystal
  - Typically Bragg geometry (reflection)
  - Creates medium divergence monochromatic beams

Refractive optics

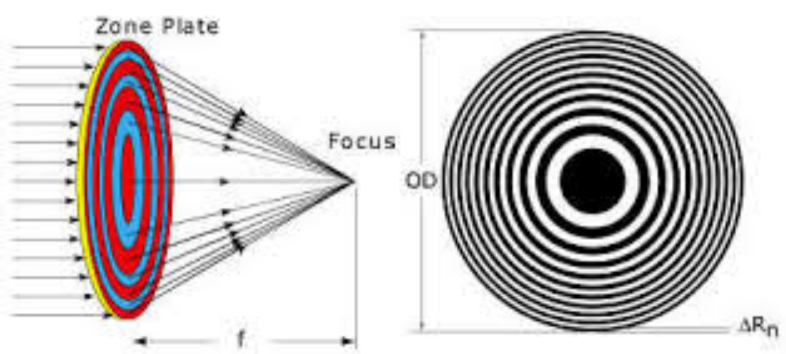
- **X-ray**
  - Refractive lenses (CRLs)



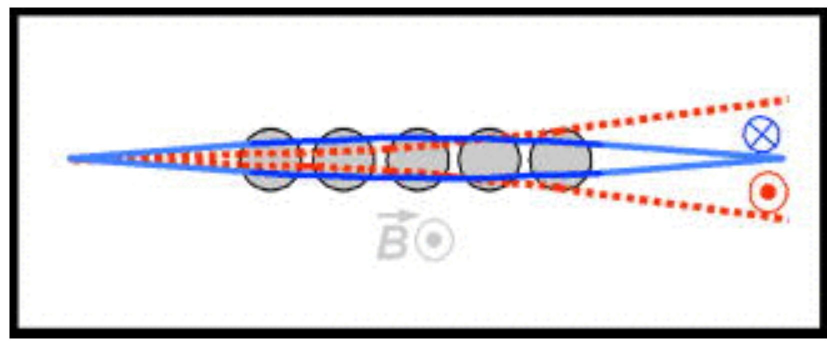
Kinoform Lens



Fresnel Zone Plates

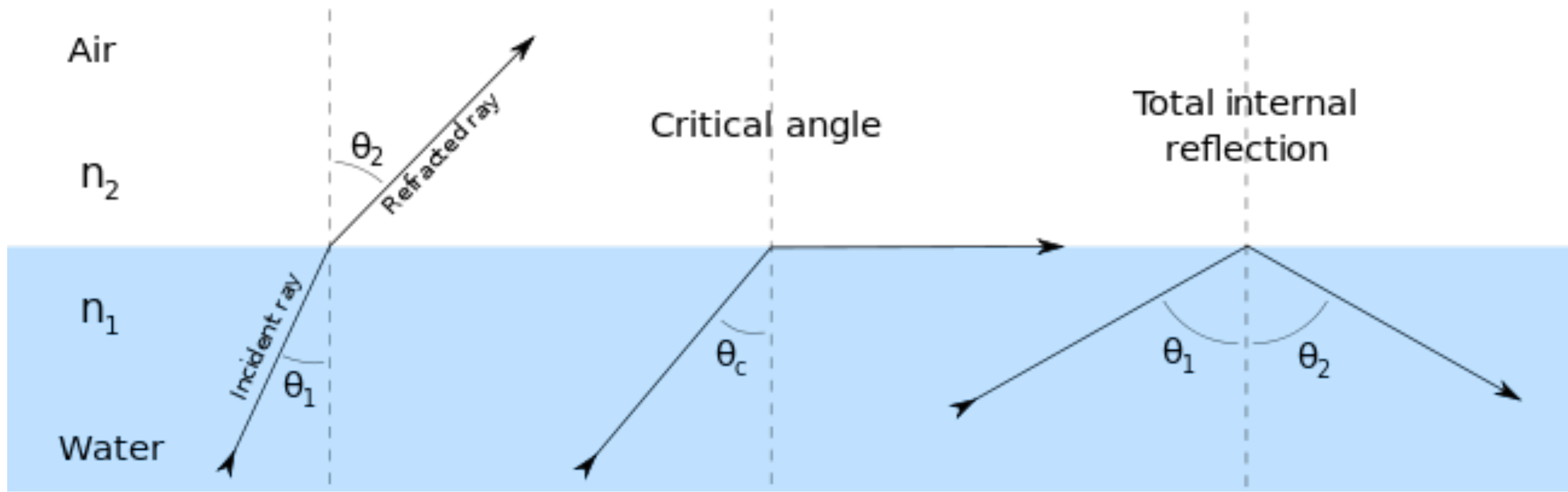


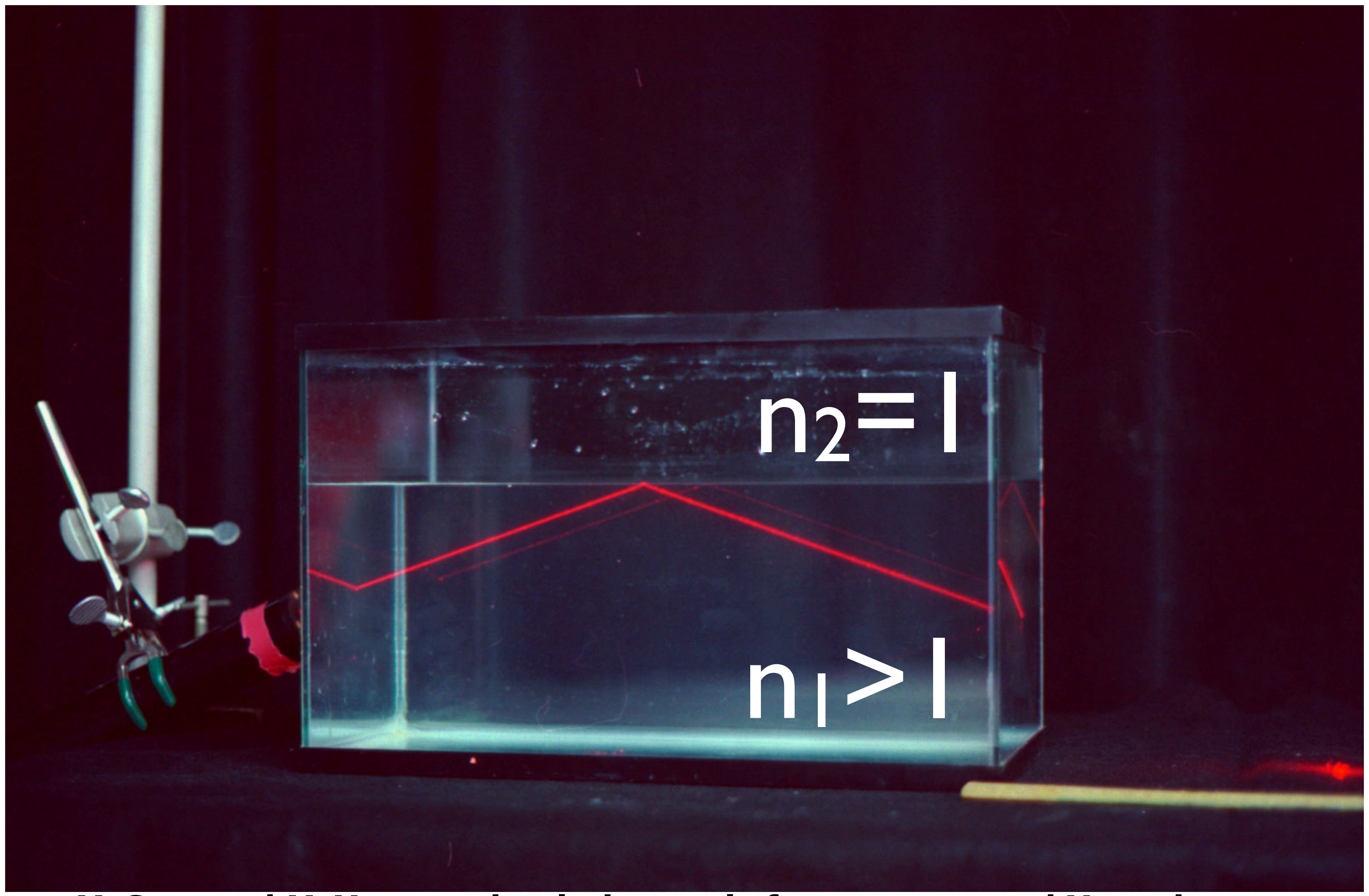
- **Neutron**
  - Refractive Lenses (CRLs)
  - Magnetic Materials (focusing e.g. “spin-up”)



Refractive optics, total reflection - a reminder

Visible light





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

Absorption term

Refraction term

Refractive optics

- **X-ray**
  - Refractive index < 1

- **Neutron**
  - Refractive Index < 1 for b>1

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

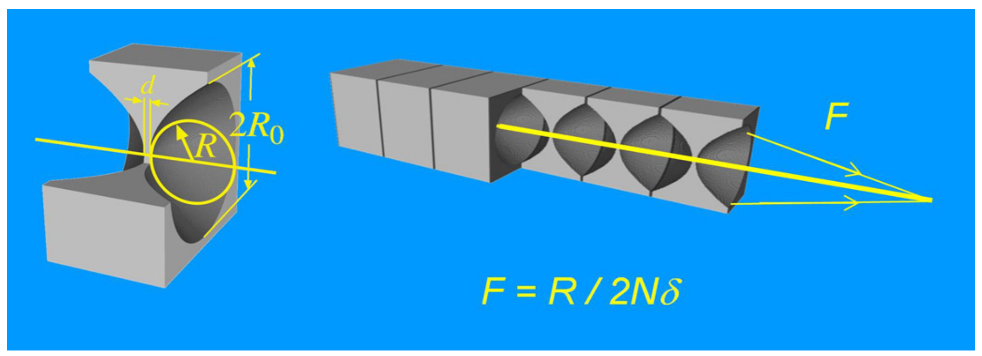
$$n = 1 - \delta + i\beta$$

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

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

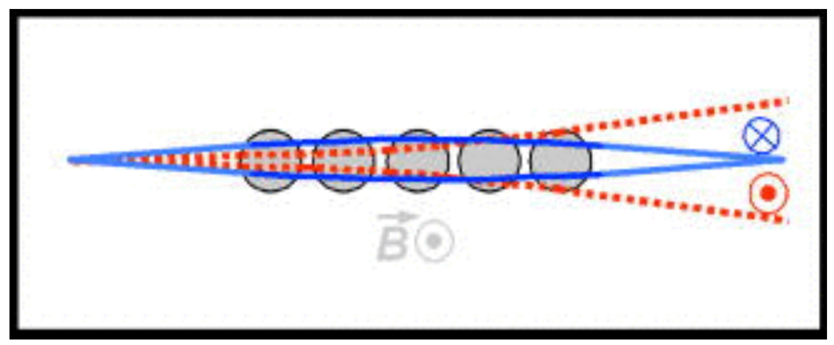
Low Z materials with low absorption. Be, Al.

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



High b materials with low absorption. Mg_2F

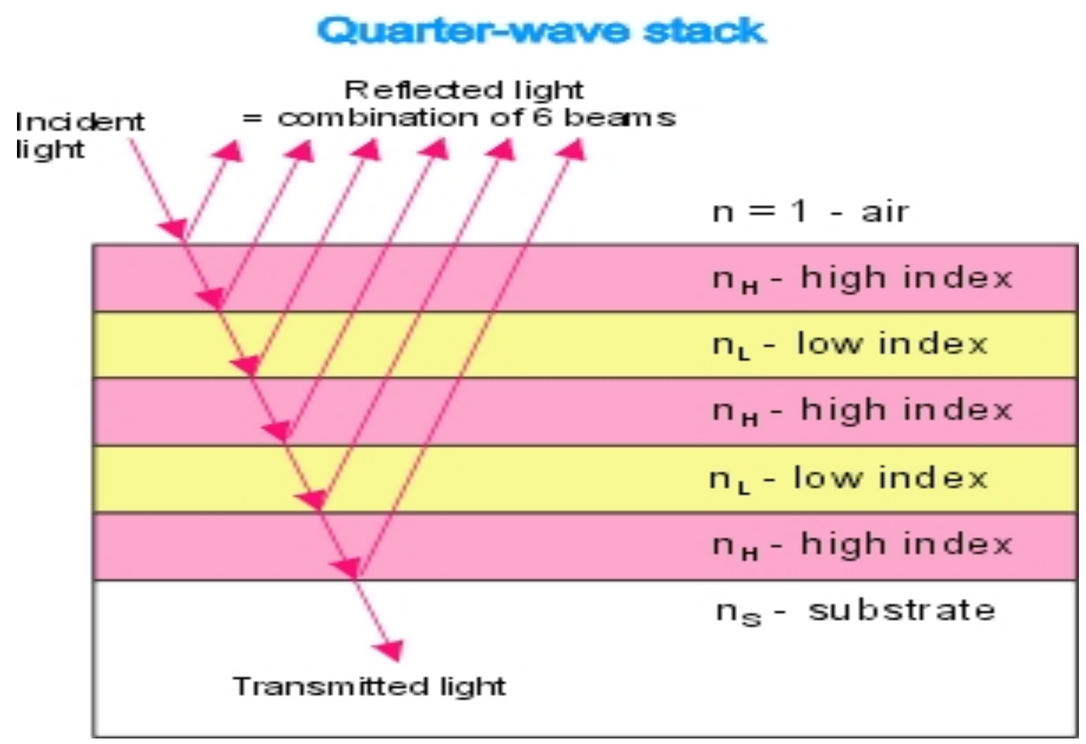
With neutrons, Lens effect from magnetism is small, hence "CRL"



Multilayers

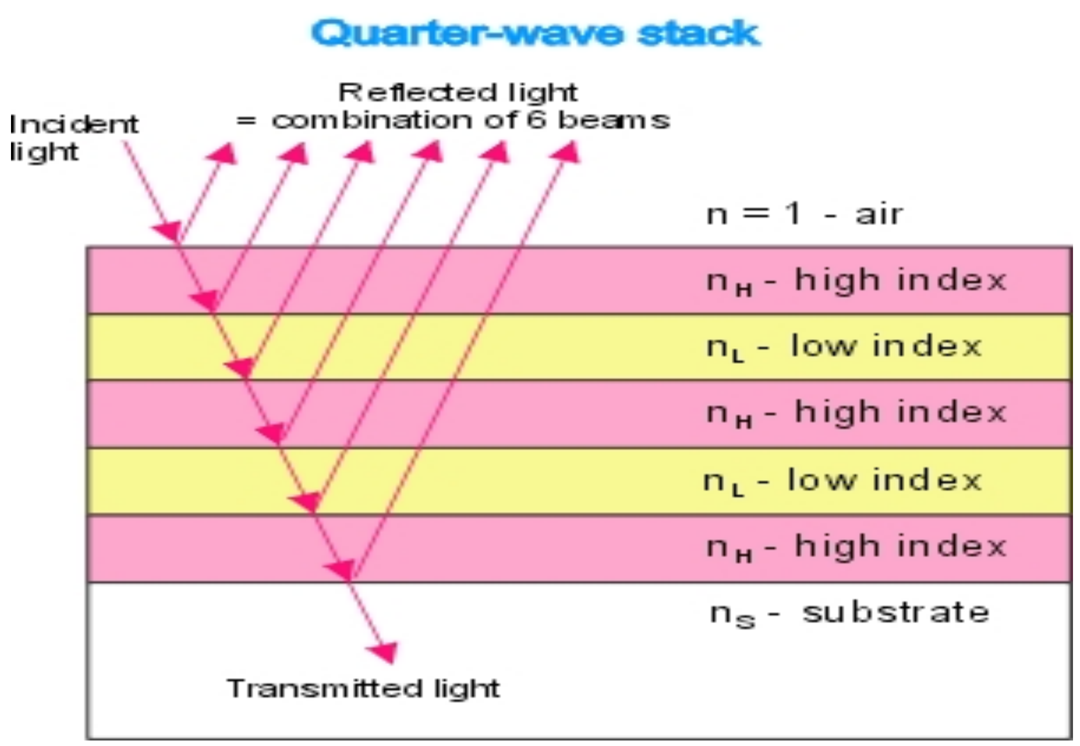
- **X-ray and neutrons**

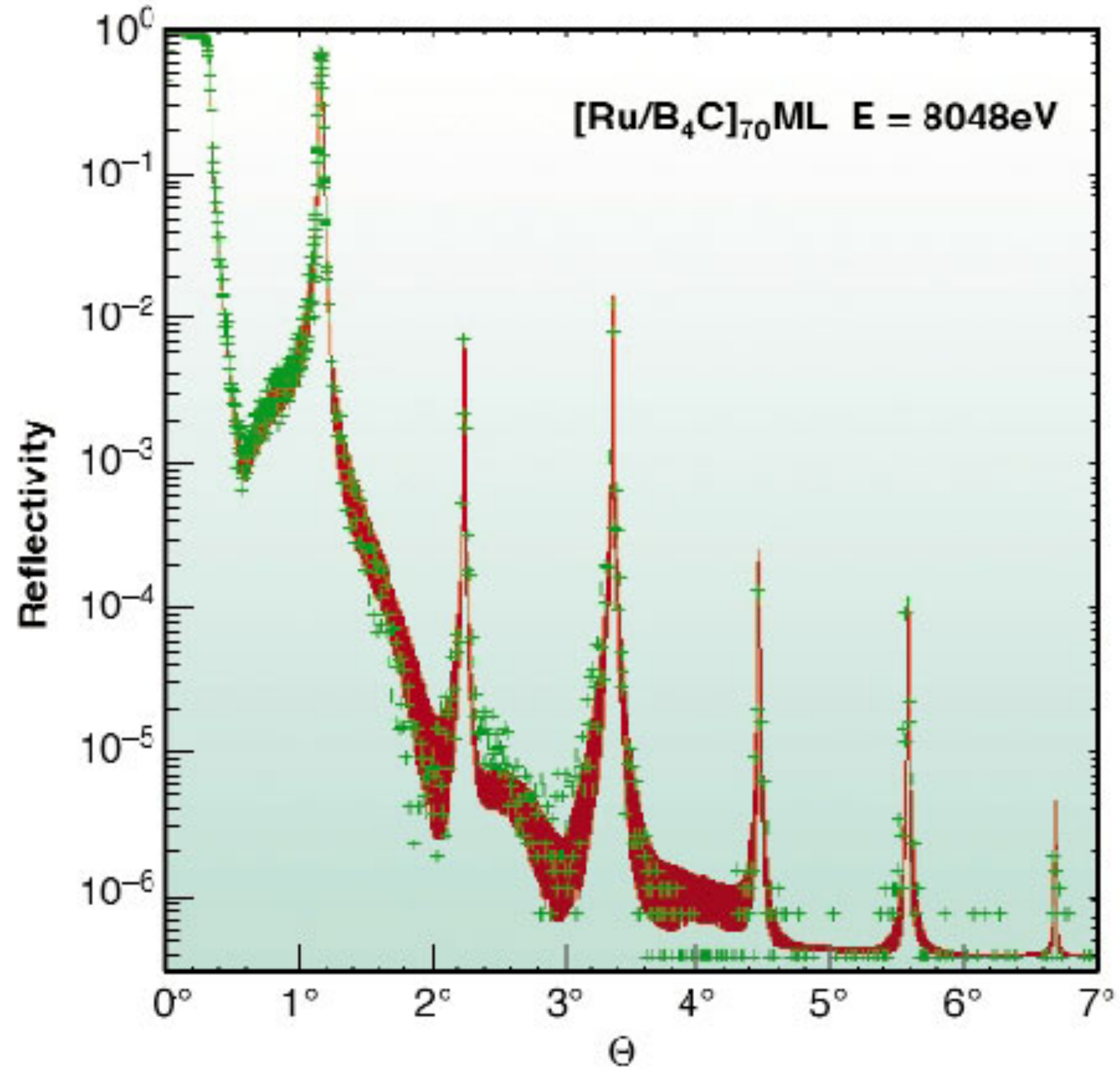
Playing with phase of partial ray reflected from a given layer in the structure



Multilayers

- **X-rays:**

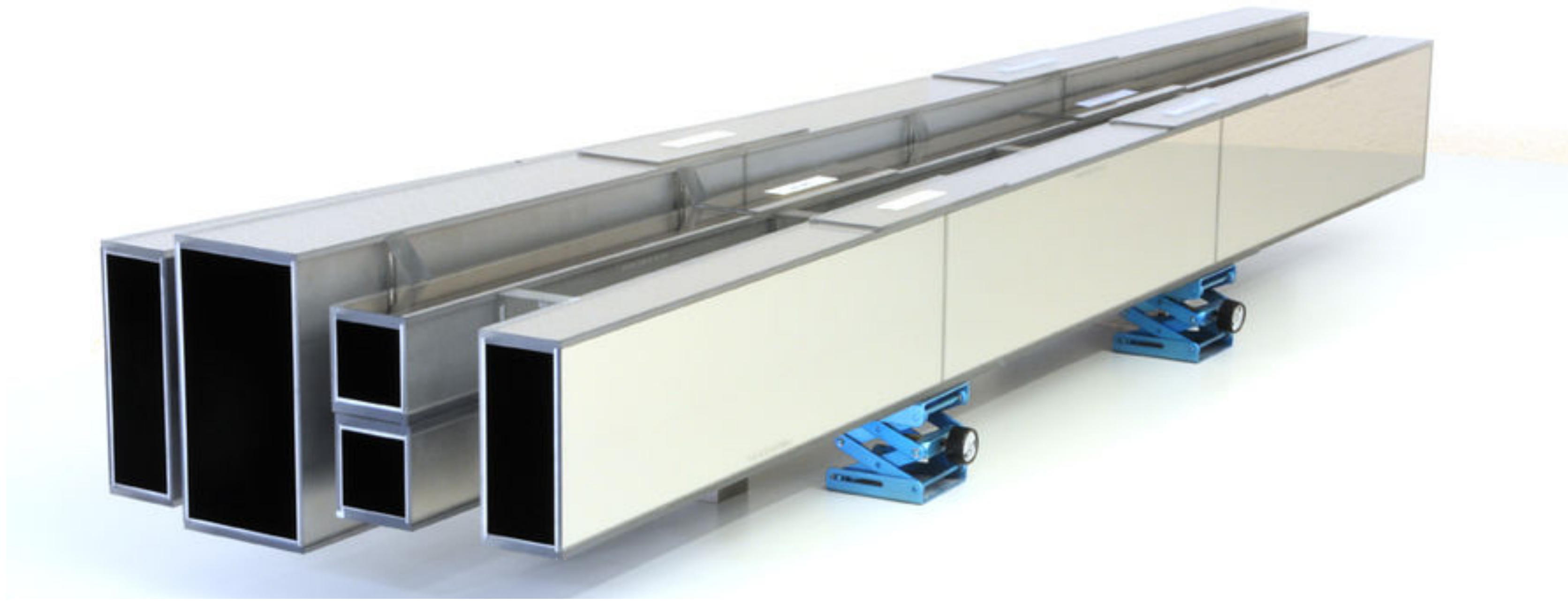




Superstructure often used as "monochromator" - also in focusing geometry

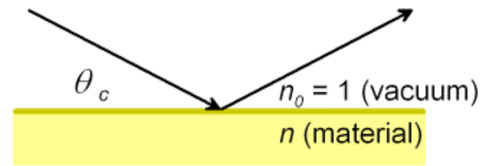
- When used as monochromator, use one of the first "side peaks" on the reflectivity curve

Multilayers



- **Neutrons:**

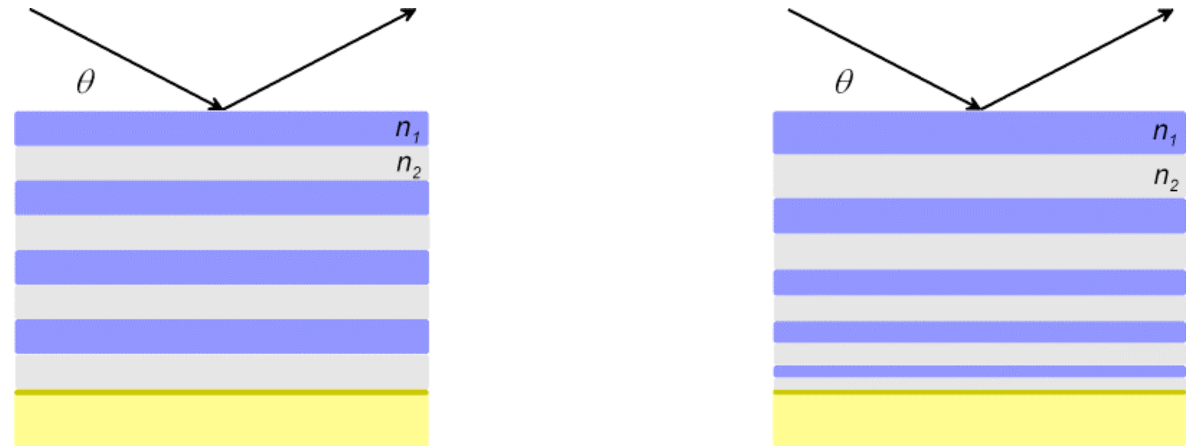
single mirror



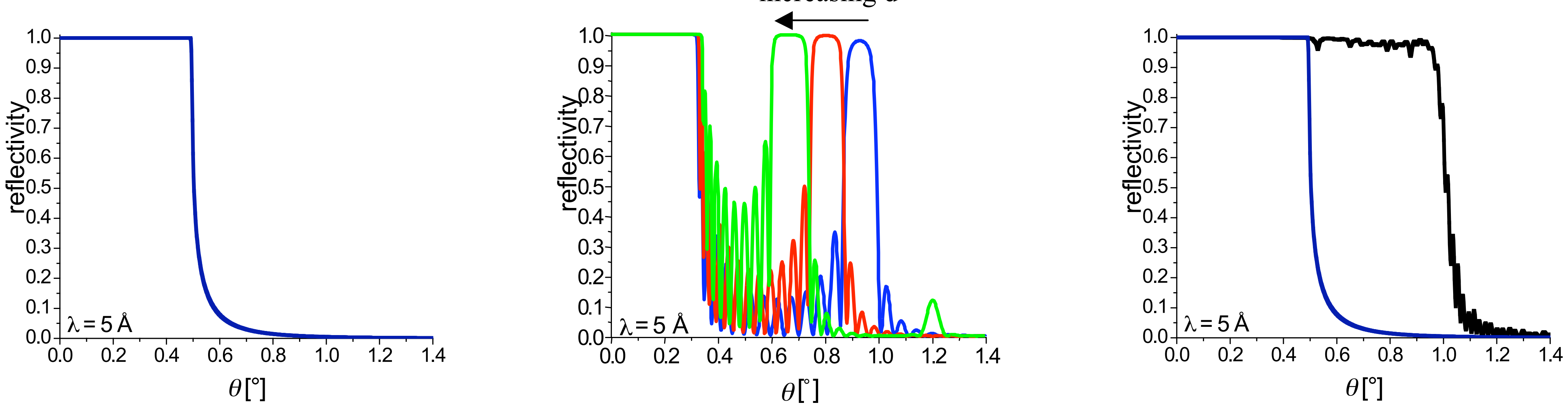
- refractive index n < 1
- total external reflection
  e.g. Ni θ_c = 0.1 °/Å

multilayer

supermirror



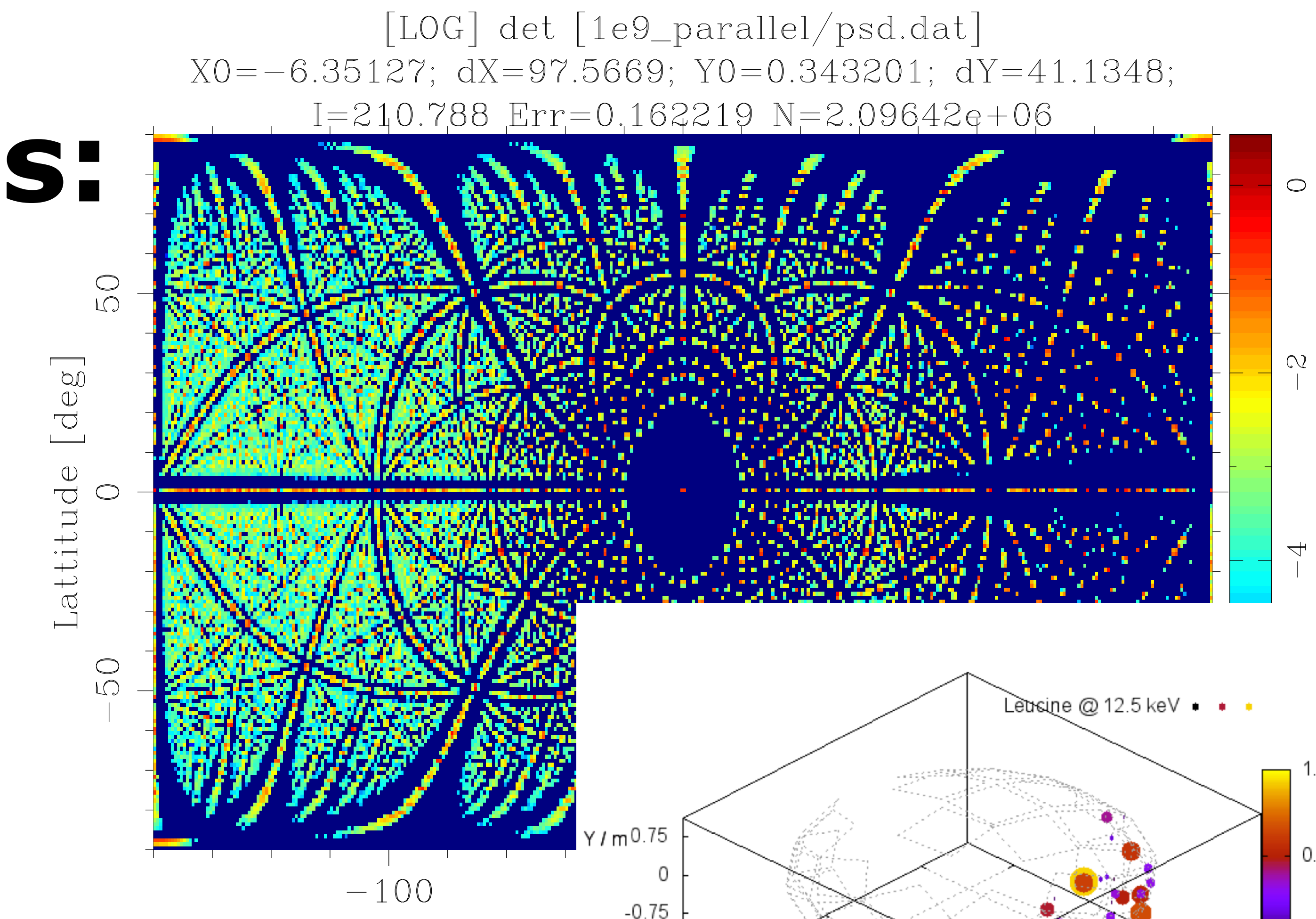
$$\lambda = 2nd\sin\theta$$

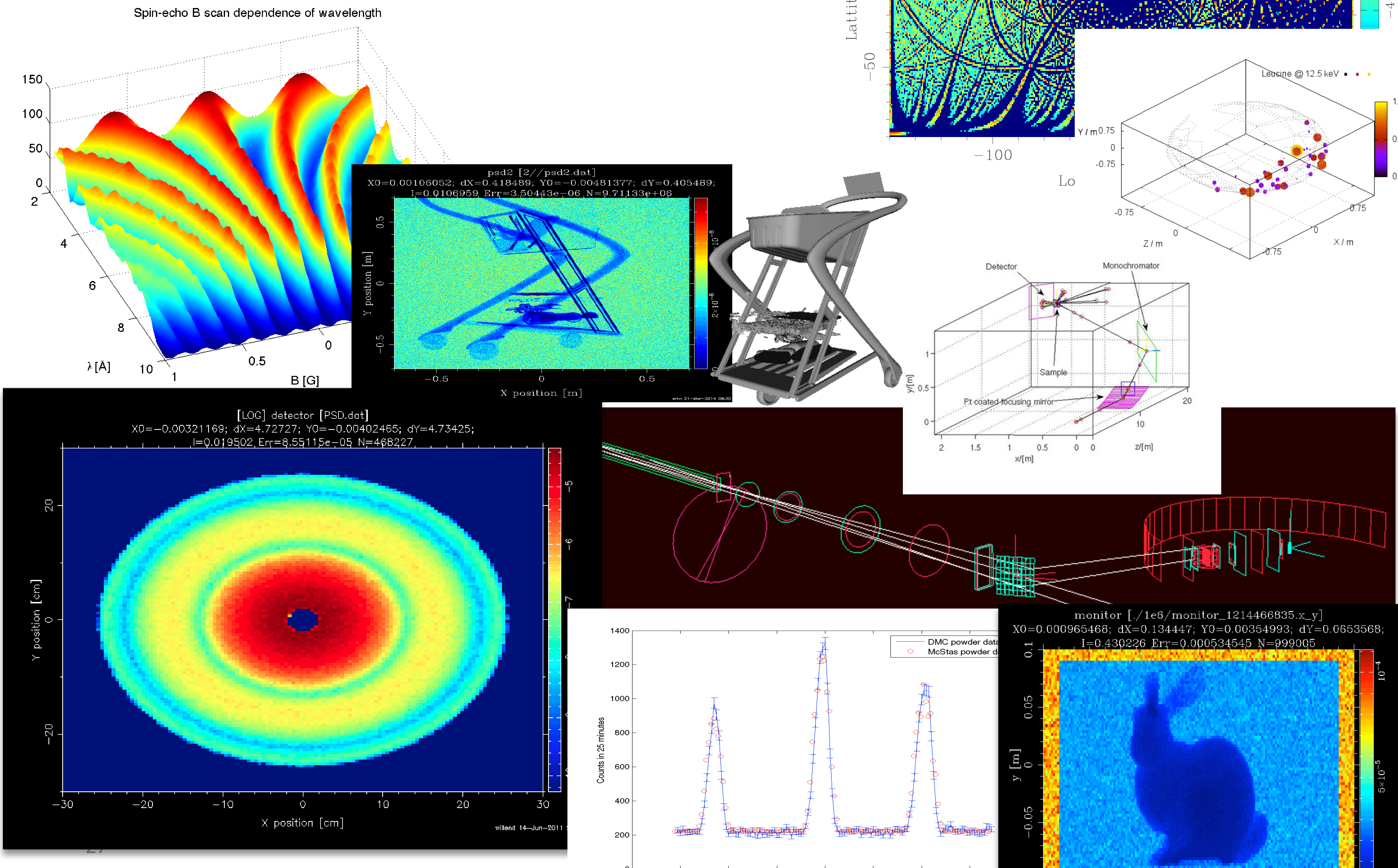


Superstructure "extends" the total-reflection range in Q by "Bragg peaks"

- 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





Questions?