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McStas Simulation Tools for Neutron Focusing Optics and Virtual Experiments

Agenda

- McStas general intro
- Reflectivity-models in McStas
- Overview of available focusing options in McStas
- Conclusions

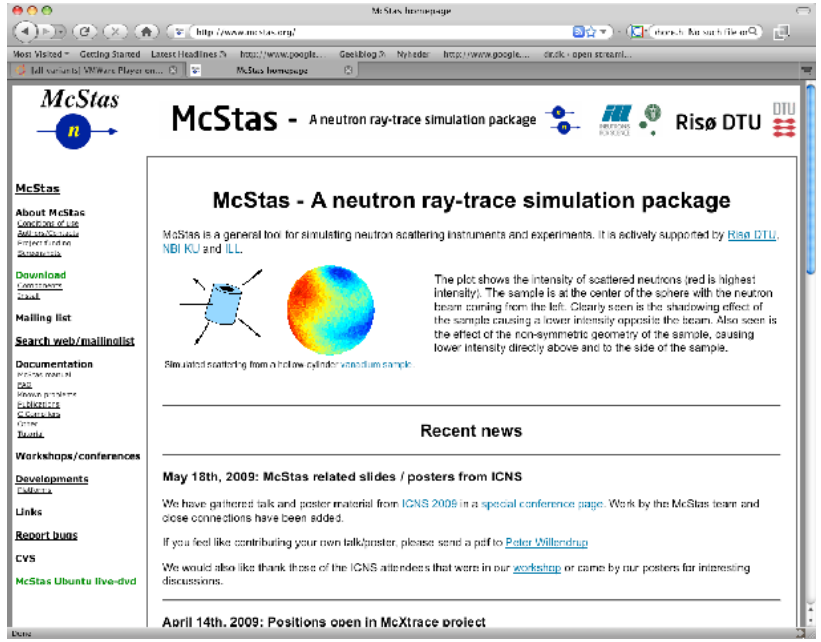
McStas Introduction

GNU GPL license

Open Source

- 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 DMSC
- V. 1.0 by K Nielsen & K Lefmann (1998) RISØ
  (work initiated in 1997, 25 year project anniversary, 2023 anniversary release)
- Small, dedicated team, many contributions from users, students

Celebrating 25th anniversary!

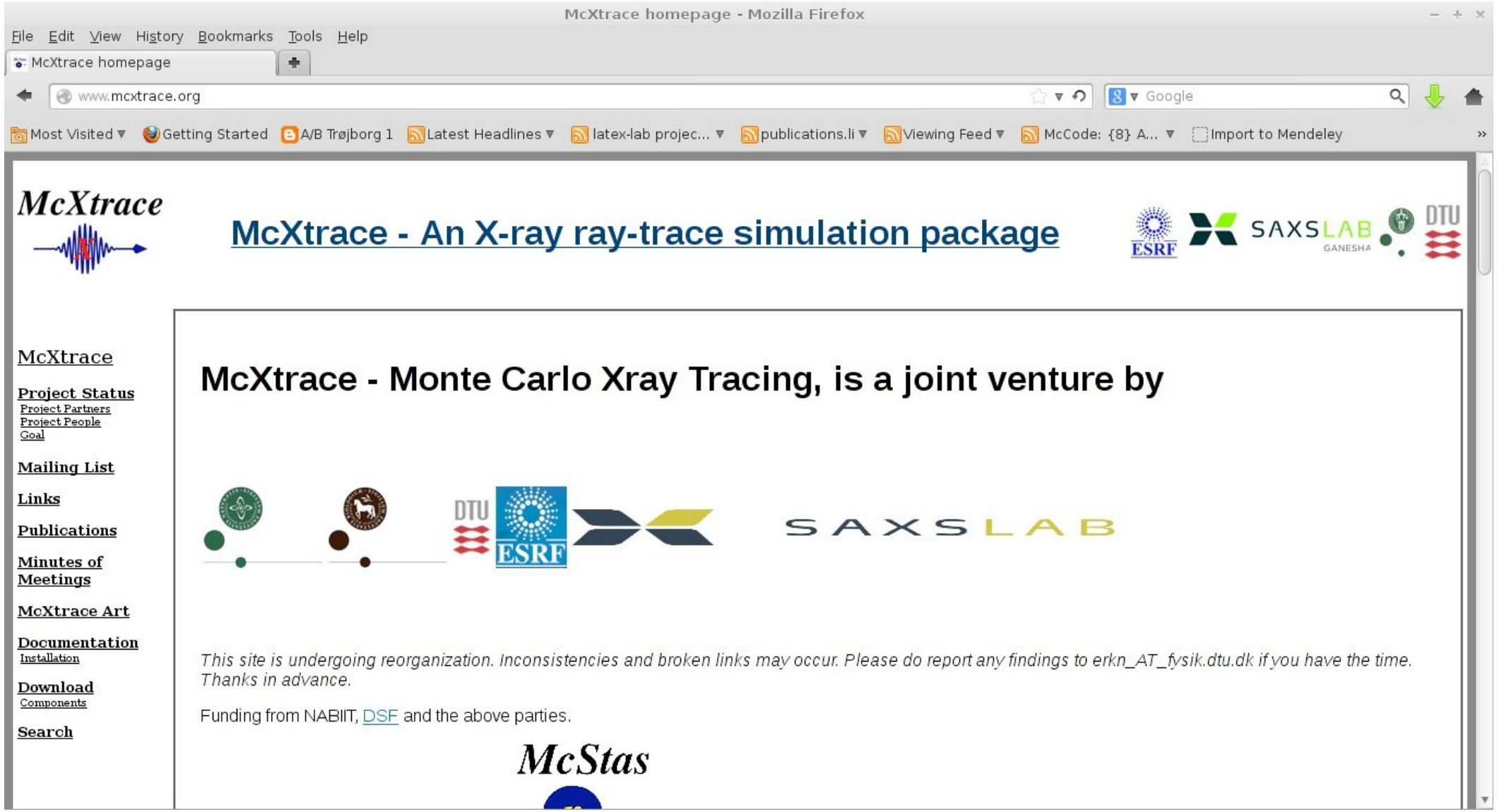


Project website at

http://www.mcstas.org

mcstas-users@mcstas.org mailinglist

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



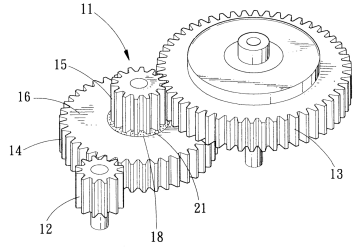
https://www.mcxtrace.org

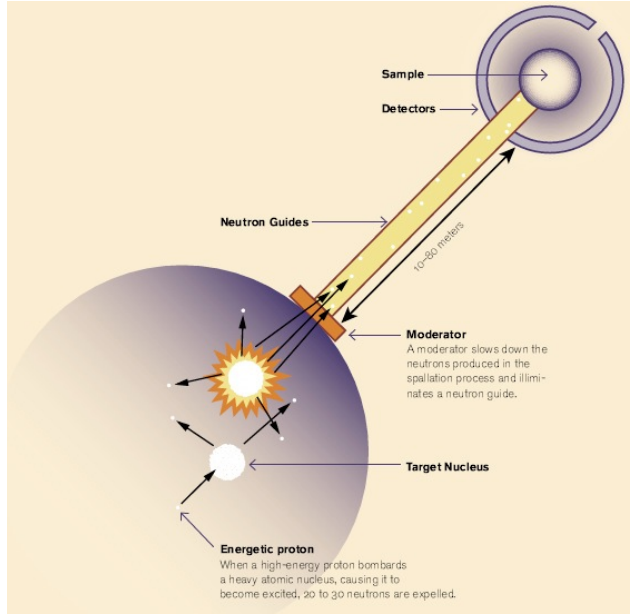
McStas overview

- Portable code (Unix/Linux/Mac/Windoze)
  - Ran on everything from iPhone to 1000+ node cluster!
- 'Component' files (~200) inserted from library
  - Sources
  - Optics
  - Samples
  - Monitors
  - If needed, write your own comps
- DSL + ISO-C code generator (LeX+Yacc grammar)
- Simple Instrument language → Code generation → ISO C
- “Components” describe physics

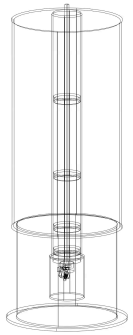
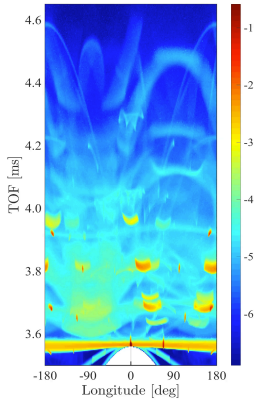
CPU’s

+ NVIDIA GPU’s



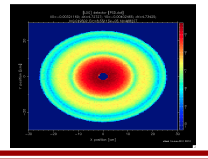
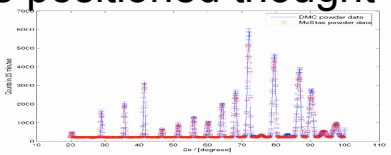


eutron instruments

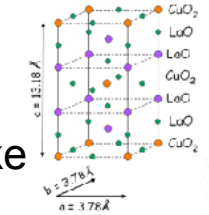
Union (M. Bertelsen) is a framework for complex assemblies of materials, e.g. sample env.

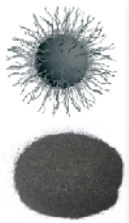
Detectors are “monitors” in McStas. Mostly they act as “perfect probes” and can be positioned thought your instrument gathering 1D/2D/ event lists…

The sample:

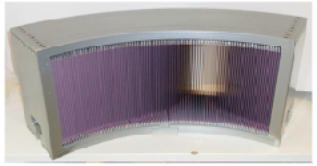
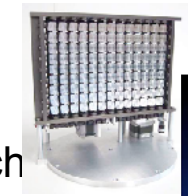
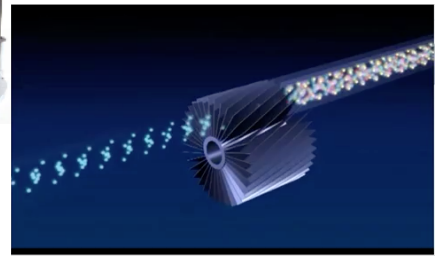
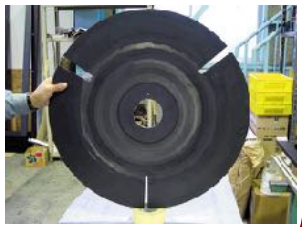
Crystalline, powders, liquids, micelles, structures to image, inelastic features like phonons…






Neutron optics include things like:

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

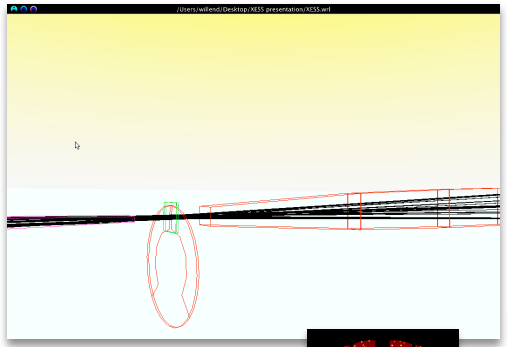






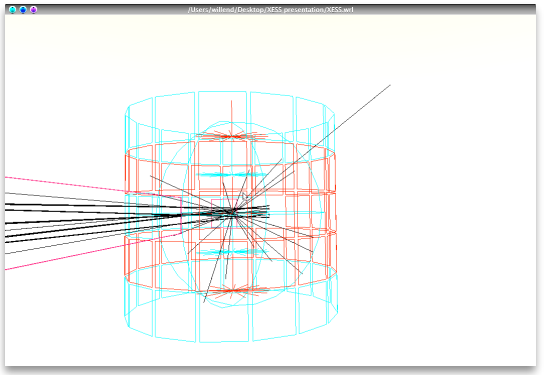
In McStas the moderator is the “source”

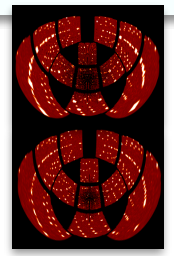
What is McStas used for?

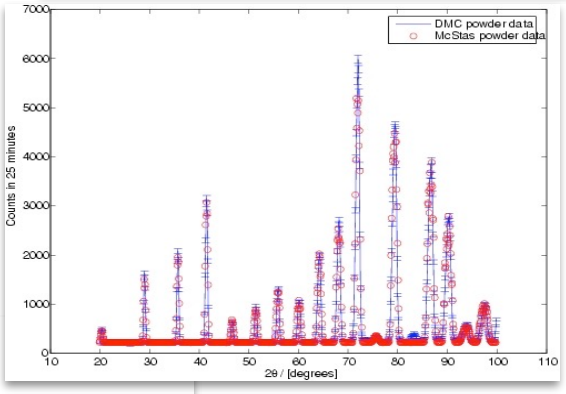
- Instrumentation
- Virtual experiments
- Data analysis
- Teaching

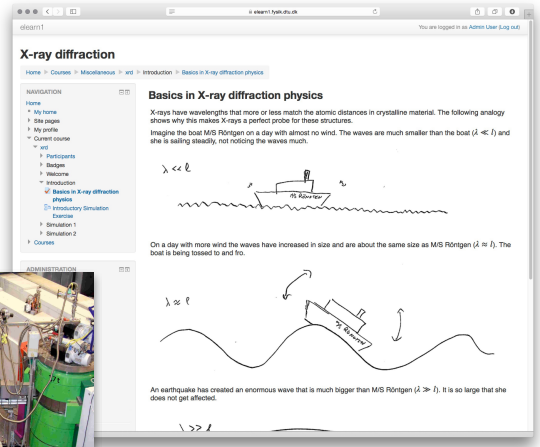
(KU, DTU)

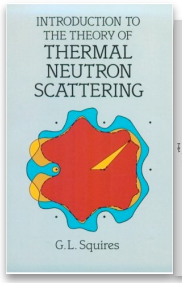


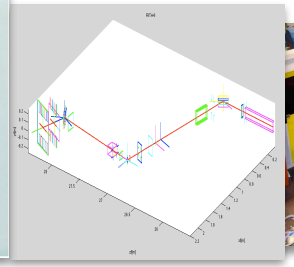


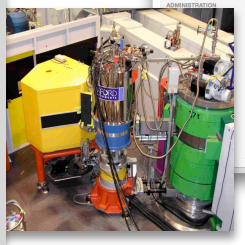


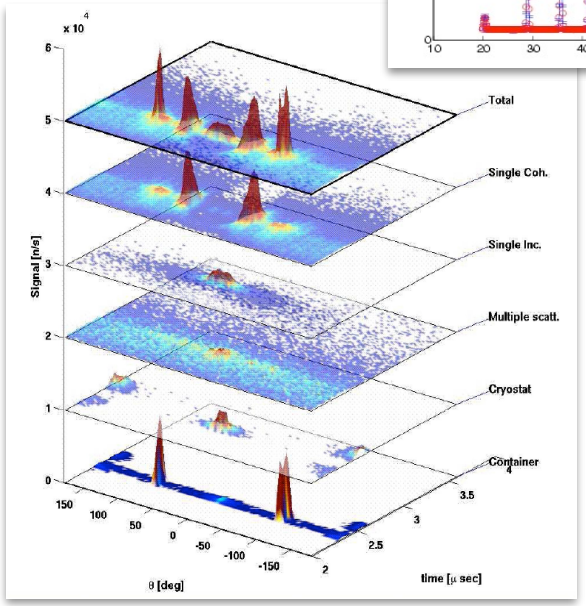




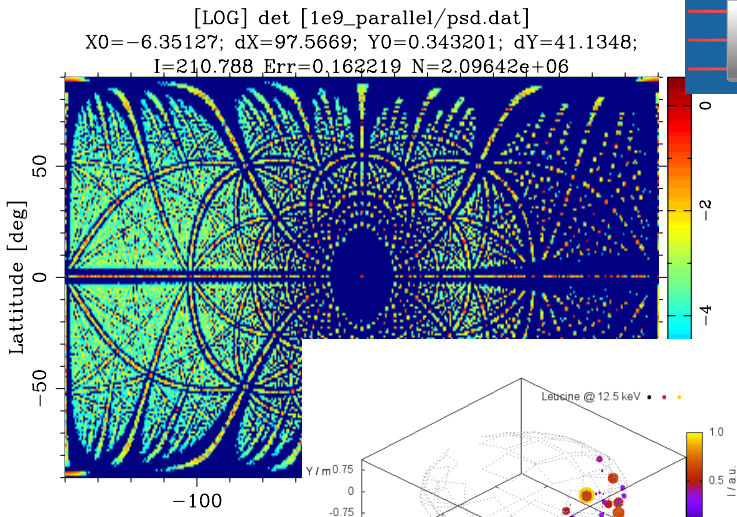


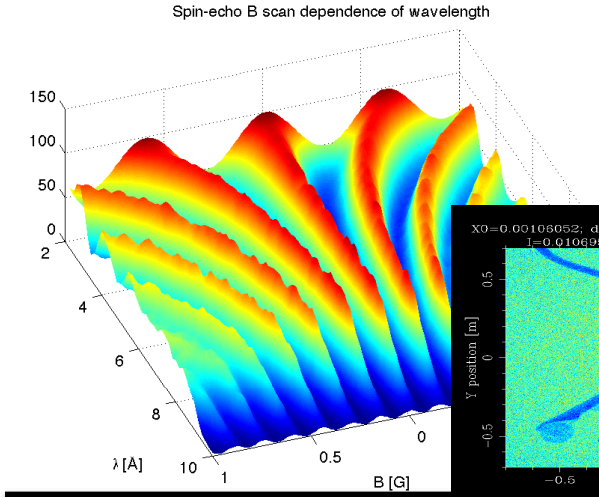


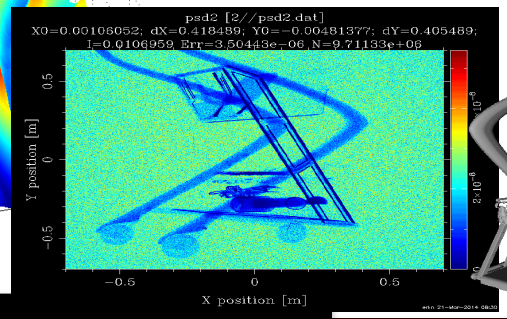


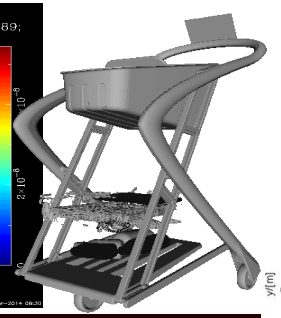


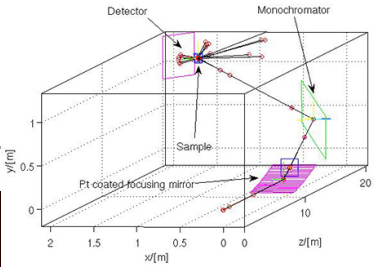
Example suite - instruments:
247 McStas
63 McXtrace

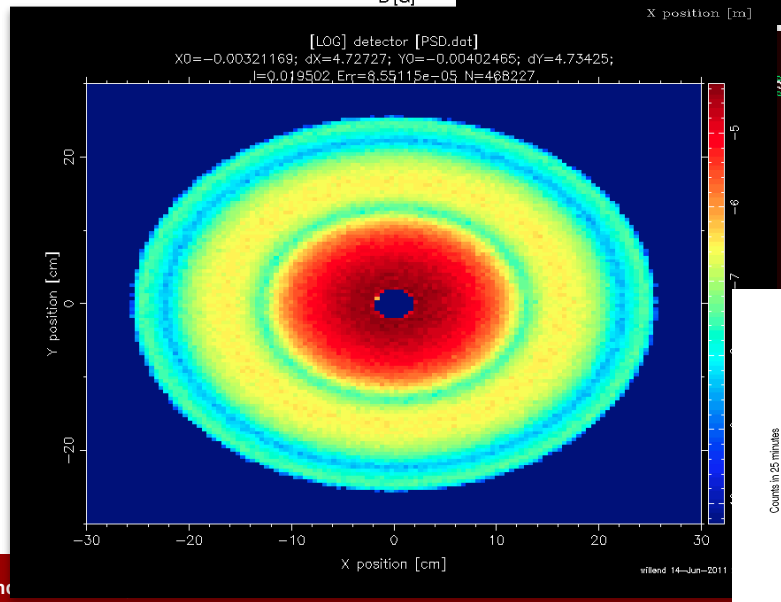


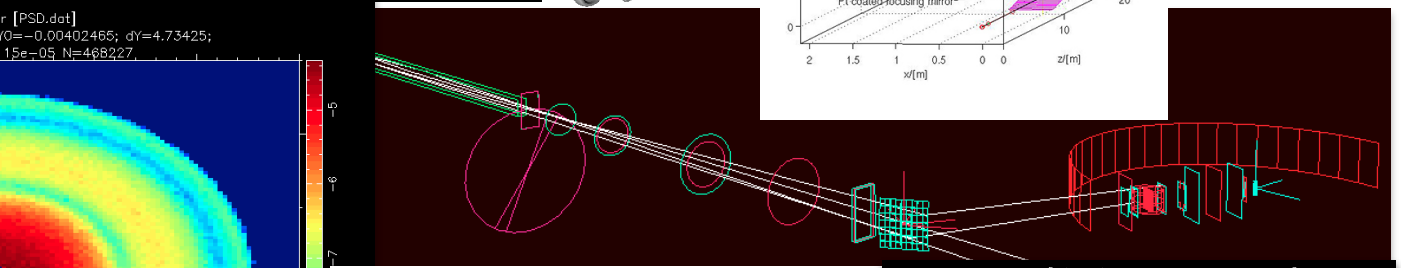


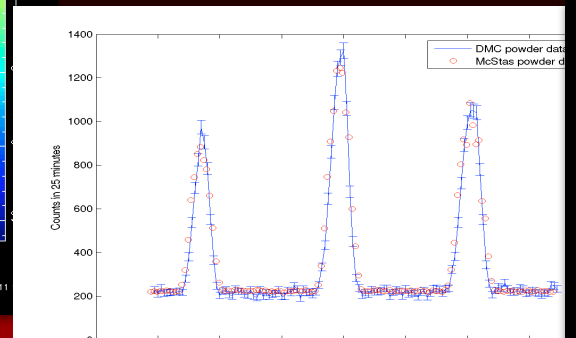


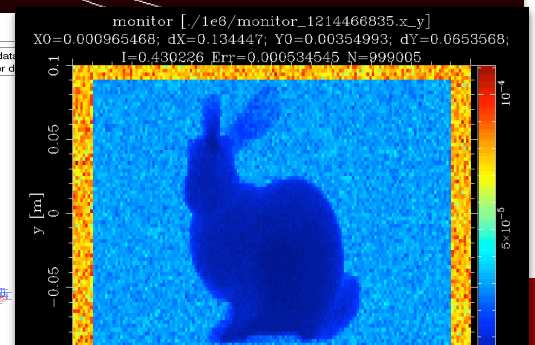




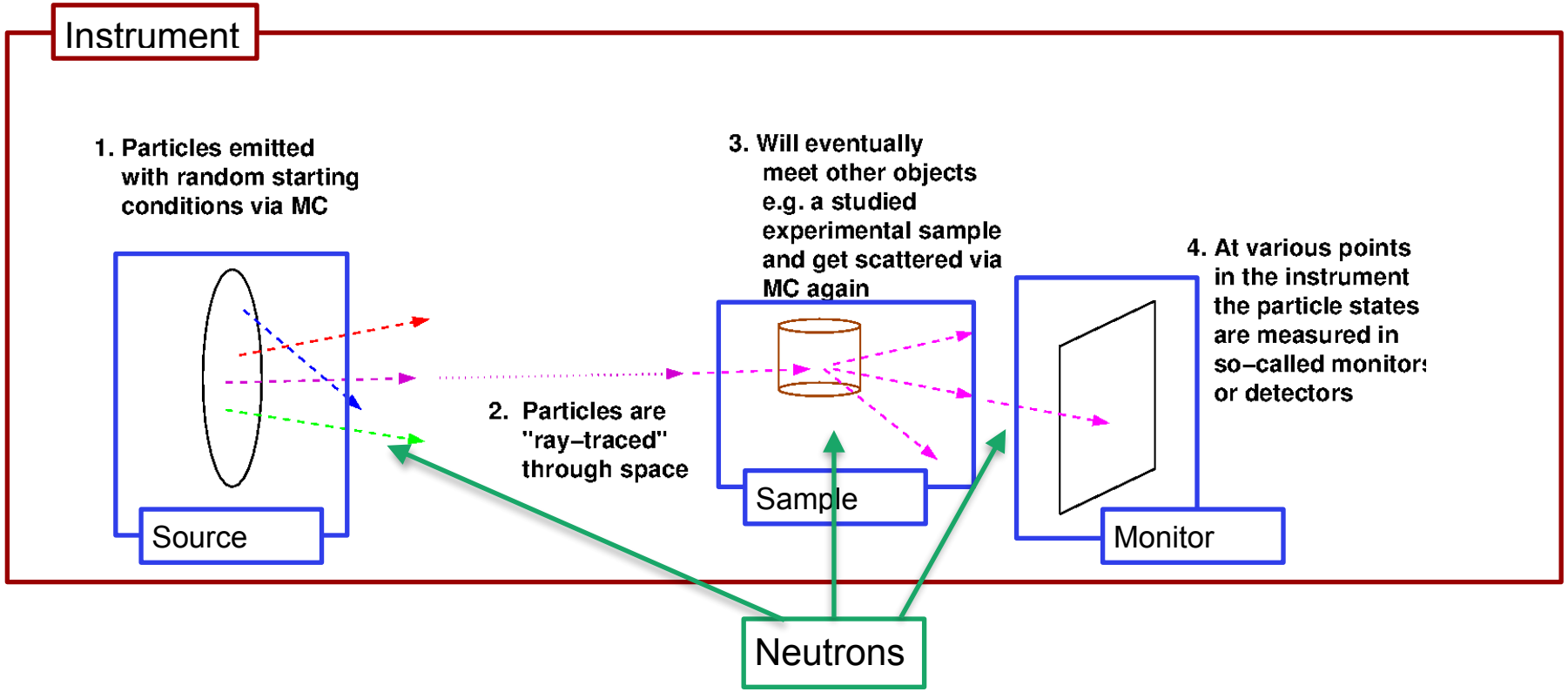


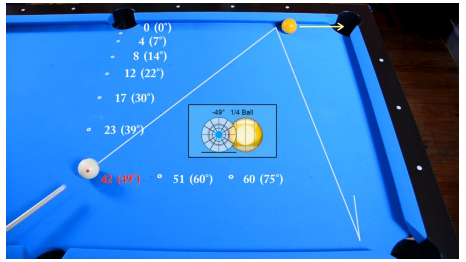




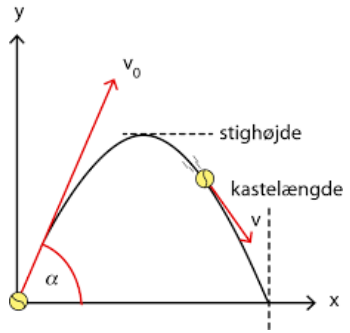


In the big picture, McStas is this…





Classical Newtonian mechanics (independent, particles though…)

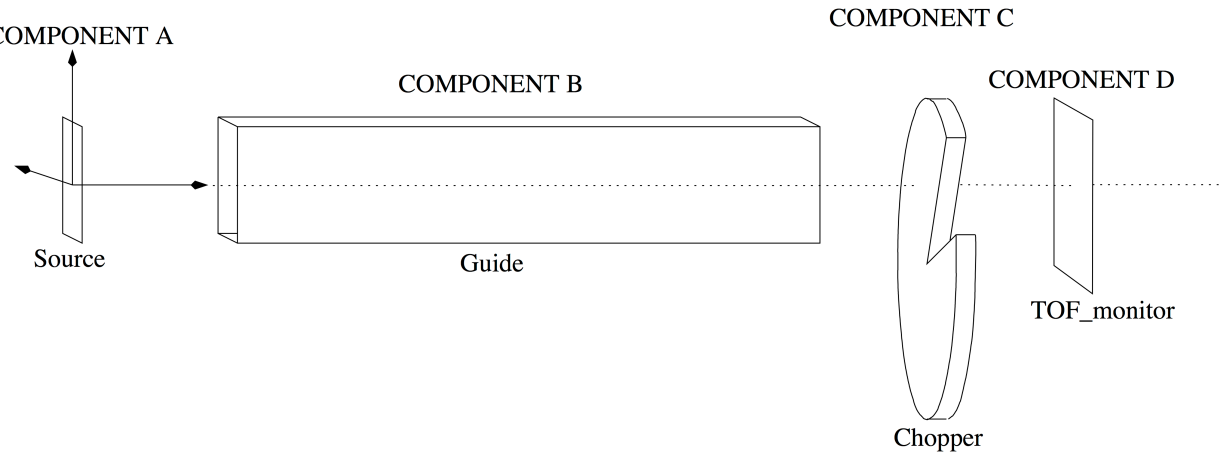


The instrument defines our “lab coordinate system”

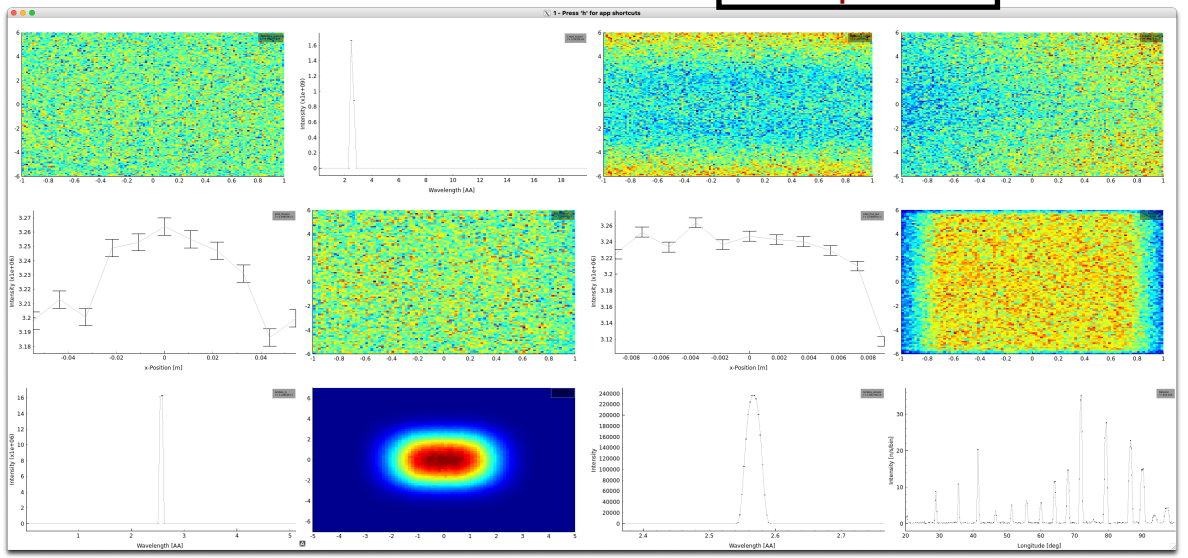
The components define devices or features available in our instrument - they have different function

Neutron particles are passed on from one component to the next, changing state under way

INSTRUMENT



5. Output data



The "tool layer" consists of programs manipulated by the McStas user:

mcgui, graphical user interface	**mcplot, visualize histogram outp.**	**mcdisplay, visualize instrument**

mcgui is used to assemble an instrument file, which is taken over by the McStas system

```
DEFINE INSTRUMENT Example(Param1=1, string Param2="two", ...)

COMPONENT A = Source(Parameters...)
AT (0, 0, 0) ABSOLUTE

COMPONENT B = Guide(Parameters...)
AT (0, 0, 1) RELATIVE A

COMPONENT C = DiskChopper(Parameters...)
AT (0, 0, 1) RELATIVE B

COMPONENT D = TOF_monitor(Parameters, filename="Tof.dat")
AT (0, 0, Param1) RELATIVE PREVIOUS
```

1. Instrument code

"Instrument file"

Source.comp – c–code

Guide.comp – c–code

DiskChopper.comp – c–code

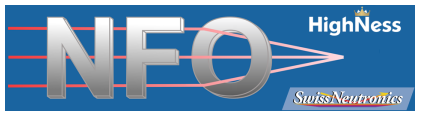
TOF_monitor.comp – c–code

Component library

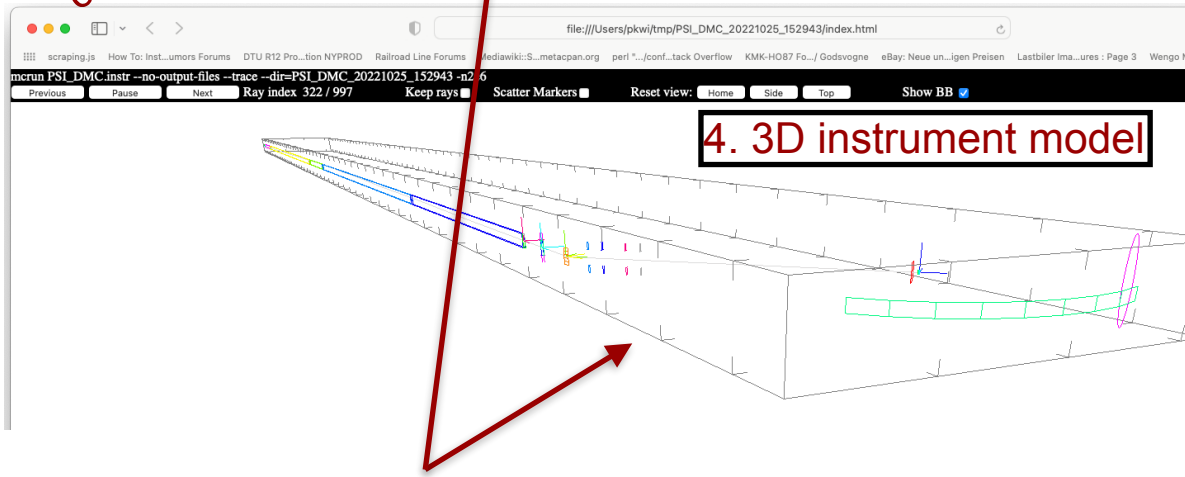
Random numbers	I/O	Physical consts.

"Kernel and runtime c–code"

\+ 2. Component codes



McStas



4. 3D instrument model

The McStas system generates an "ISO C file" and an executable from instrument file and c–codes

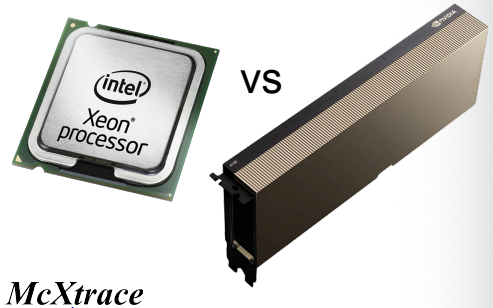
The simulation executable produces data output which can be visualized using the mcplot and mcdisplay tools

= 3. C-code and binary

Maximum performance indication on NVIDIA A100 (Ampere)

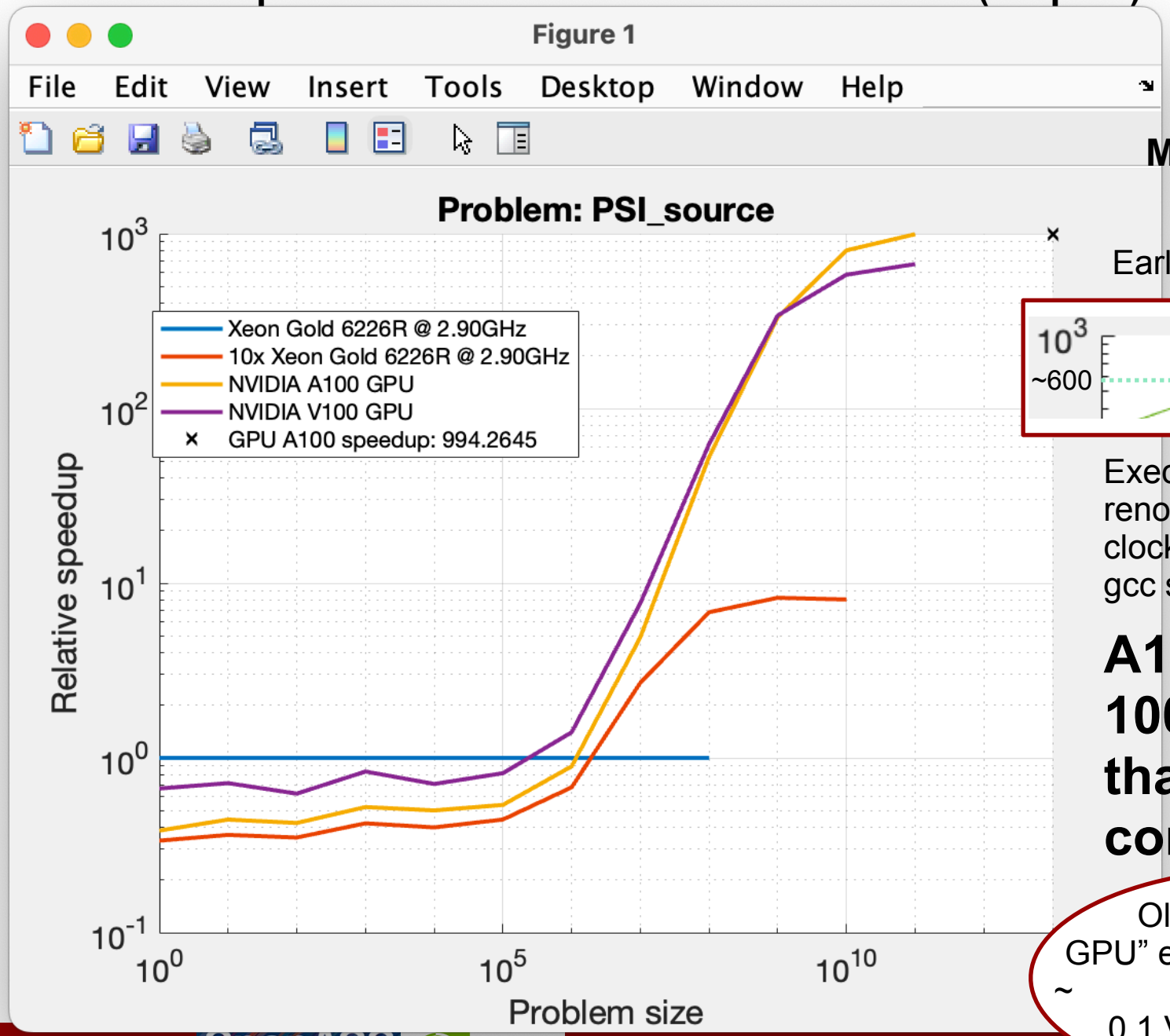
Idealised instrument with source and monitor only - i.e. without any use of the ABSORB macro.

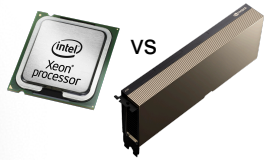
(Good indication of maximal speedup achievable.)



McXtrace

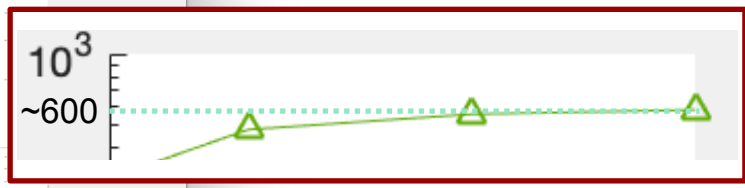
McStas





Maximal speedup: ~1000

Earlier dataset from V100 ~600



Execution speedups renormalised to wall-clock of single-core gcc standard simulation,

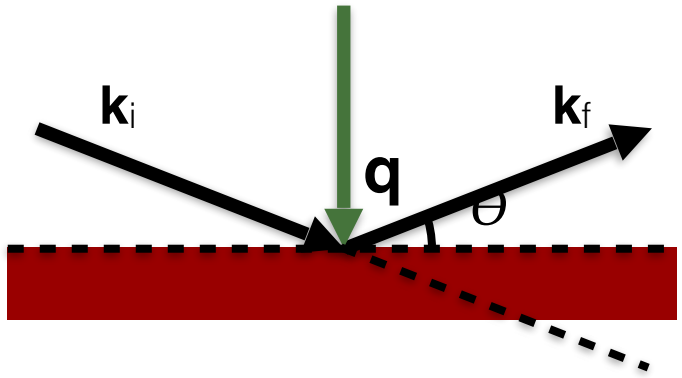
A100 run can be ~ 1000 times faster than a single-core CPU run

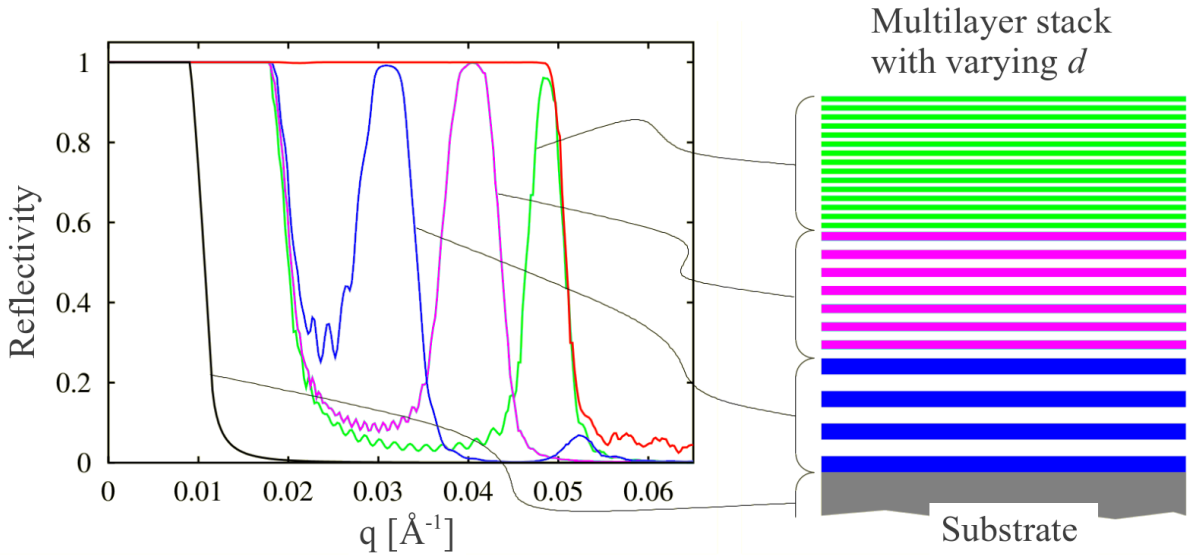
Older "Gamer-GPU" e.g. GeForce 1030 is ~ 0.1 V100 or 0.05 A100

Neutron optics in McStas, Reflectivity curves

- Reflectivity, super mirror, reflectivity curve

$$m = \frac{\theta_{mirror}}{\theta_{Ni}}$$





Reflectivity curves in McStas

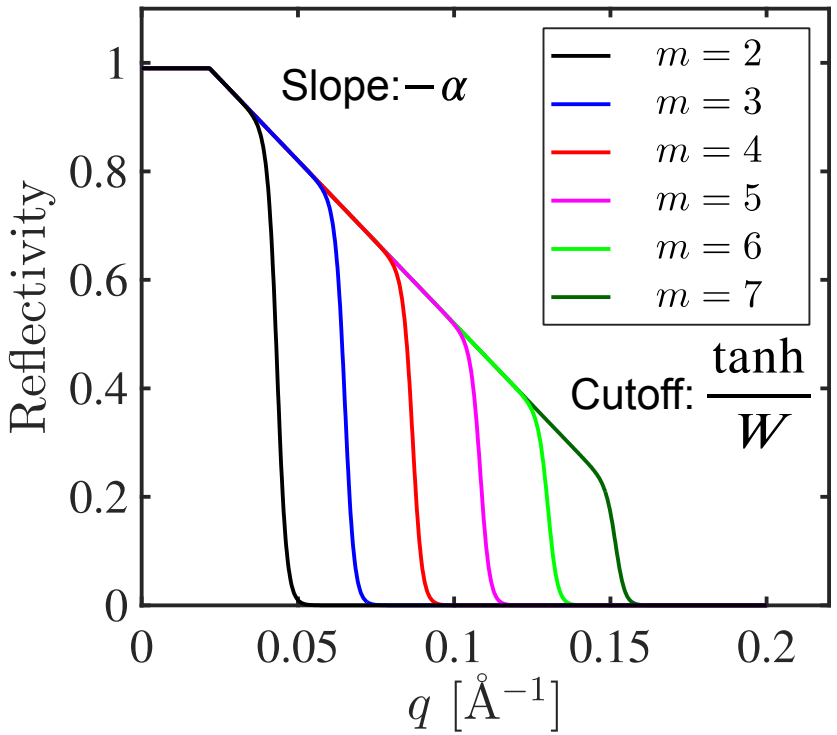
(defined in $MCSTAS/share/ref-lib.h/c)

Most components also take an I(q) input-file.

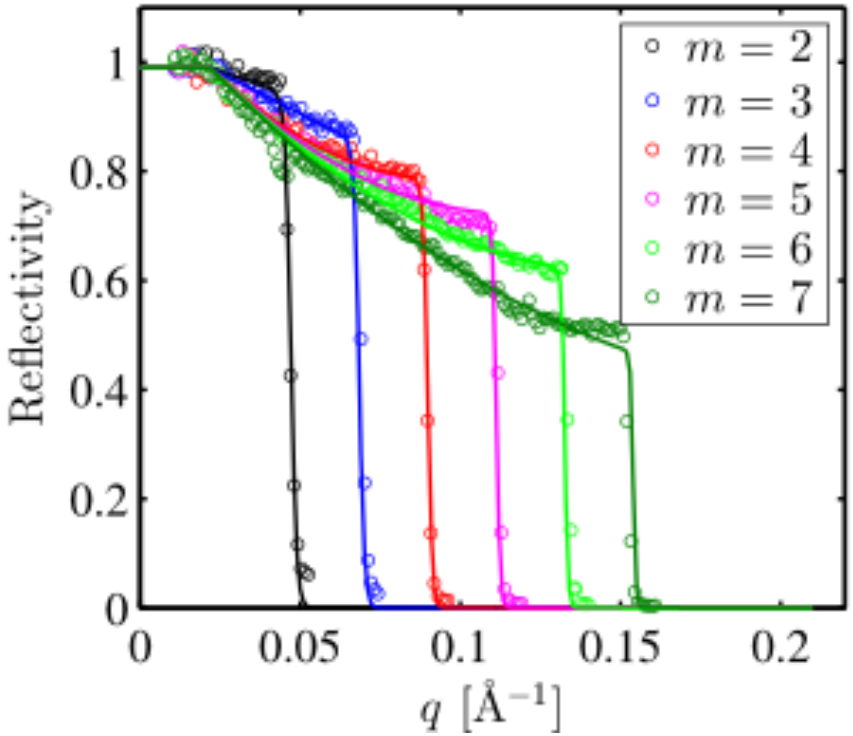
$MCSTAS/data contains examples, including .txt from Klaus Lieutenant (FZJ) for major vendors.

$$R(q) = \begin{cases} R_0 & \text{if } q < q_c \\ R_0(1 - \tanh((q - mq_c)/W))(1 - \alpha(q - q_c))/2 & \text{otherwise} \end{cases}$$

McStas standard model



McStas fitted model (aka. “Henrik Jacobsen”)



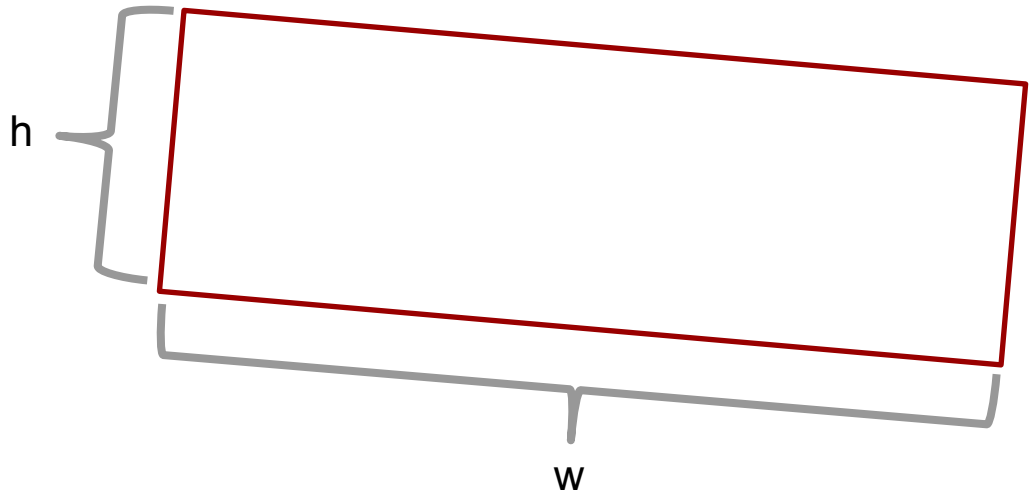
α = 0
W = 0

Only m matters

Better mirrors available today

Single-mirror components

- Mirror (simple, flat mirror)
- Mirror_Elliptic (S. Desert)
- Mirror_Parabolic (S. Desert)



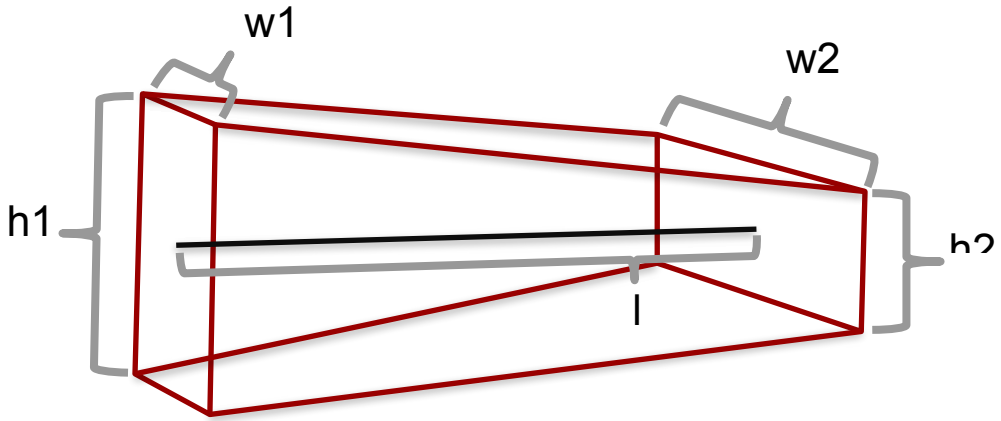
- Mirror_Curved_Bispectral (H. Jacobsen)
- Mirror_Elliptic_Bispectral (H. Jacobsen)

- Various polarising mirrors…

Black == “McStas system”, Red == “contribution”

Assorted (tapered) guides

- **Guide.comp** (uniform reflectivity, also from file), derivates:
  - Guide_m (reflectivity pr. face)
  - Guide_wavy (waviness model, reflectivity pr. face)
    - Guide_channeled (subdivided vertically, v/h reflectivity,)
    - Guide_multichannel (idem, semi-transparent blades, bispectral beam-extraction, J. Šaroun, NPI)
- Guide_tapering (tapered + elliptic, parabolic, “cross-section list from file”, U. Filges PSI)
- **Guide_gravity** (**gravitational** propagation, subdivided vertically, reflectivity pr. face)
- Various curved and polarising guides…



Black == “McStas system”, Red == “contribution”

Ballistic / parabolic / elliptical guides

```
c Guide_tapering.comp
c i = 0 - 199 segments
c h1(i)     h2(i)   w1(i)    w2(i)
0.120000 0.119850 0.020000 0.020000
0.119850 0.119700 0.020000 0.020000
0.119700 0.119550 0.020000 0.020000
0.119550 0.119400 0.020000 0.020000
0.119400 0.119250 0.020000 0.020000
0.119250 0.119100 0.020000 0.020000
...
```

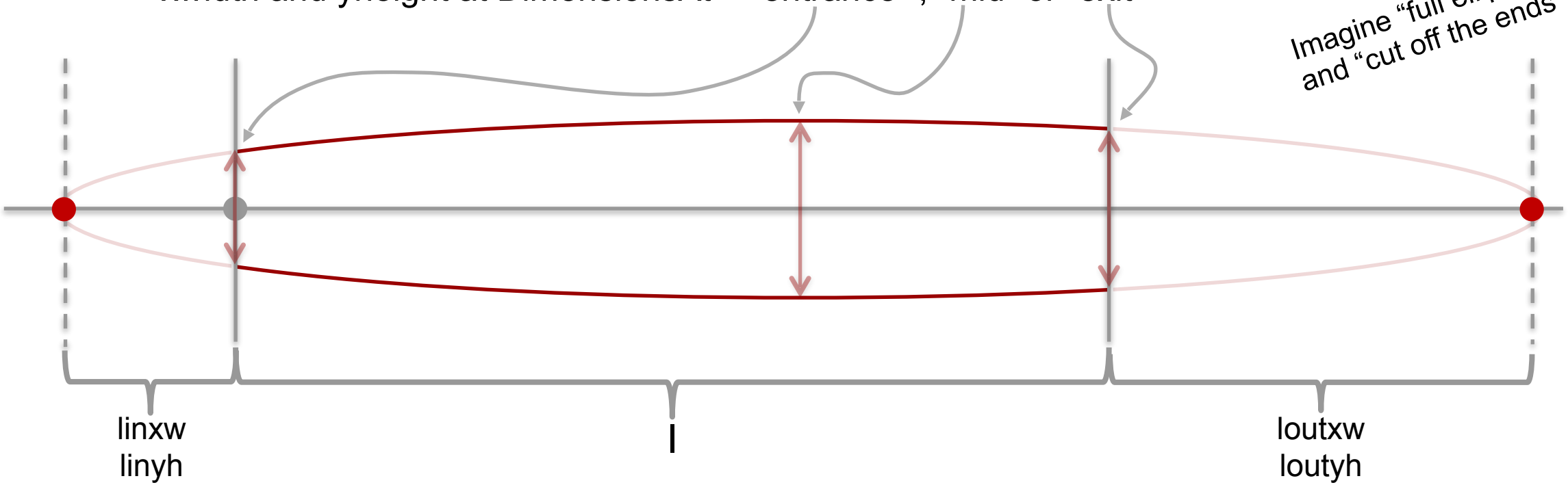
- Guide_tapering, as mentioned in previous slide, geometry from file-input

- Guide_four_side, “rich-interface” combine geometries as you like, T. Panzner PSI

Black == “McStas system”
Red == “contribution”

- **Elliptic_guide_gravity**
  - Useful for elliptic and parabolic guide geometries, focusing, ballistic, coating distribution, …

    xwidth and yheight at DimensionsAt = ”entrance” , ”mid” or ”exit”

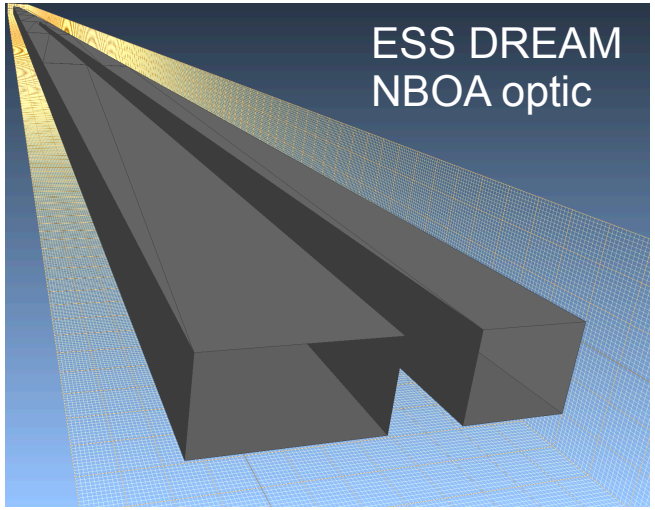


OFF-geometry focusing optics

Vertices-faces model, also used elsewhere in McStas for “free-form” surface-definition

- Guide_anyshape (uniform coating)

- Guide_anyshape_r (coating “pr. face”, P. Link, G. Mangiapia, MLZ)




```
OFF
# This is an Object File Format (geomview) to describe a 1 m^3 cube
# nb points, nb faces, void
8 4 0
# List 8 points coordinates
0.025 -0.025 0
-0.025 0.025 0
-0.025 -0.025 1.0
-0.025 -0.025 0
0.025 -0.025 1.0
0.025 0.025 0
0.025 0.025 1.0
-0.025 0.025 1.0
# List six faces, all squared
4 0 5 6 4
4 1 5 6 7
4 3 0 4 2
4 3 1 7 2
```

```
OFF
# This is an Object File Format (geomview) to describe a 1 m^3 cube
# nb points, nb faces, void.
# Reflectivity m=1 has been assigned to the faces for use with
# Guide_anyshape_r.
8 4 0
# List 8 points coordinates
0.025 -0.025 0
-0.025 0.025 0
-0.025 -0.025 1.0
-0.025 -0.025 0
0.025 -0.025 1.0
0.025 0.025 0
0.025 0.025 1.0
-0.025 0.025 1.0
# List six faces, all squared with reflectivity 1, alpha and W 0.003
4 0 5 6 4 1.0 6.07 0.003
4 1 5 6 7 1.0 6.07 0.003
4 3 0 4 2 1.0 6.07 0.003
4 3 1 7 2 1.0 6.07 0.003
```

Black == “McStas system”, Red == “contribution”

Wolter optics

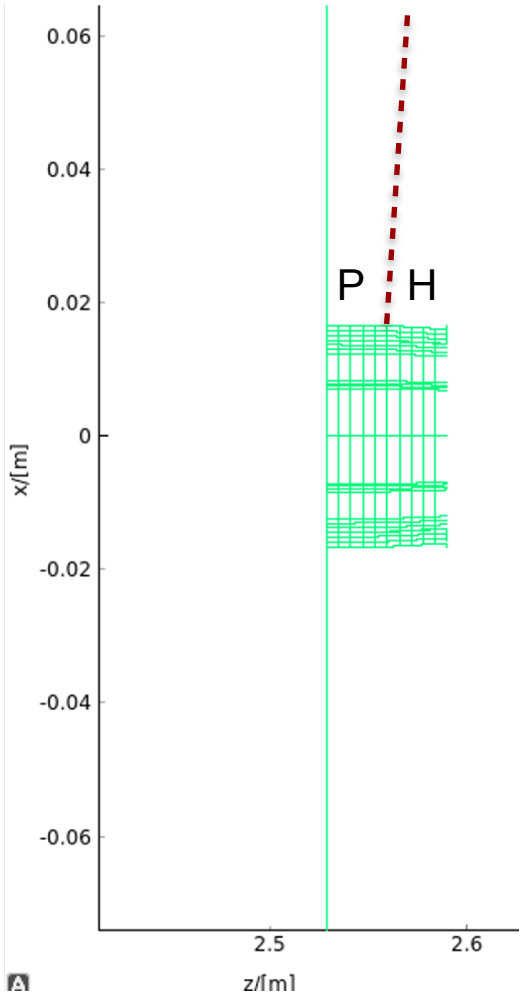
- Via "ConicTracer" lib. from B. Khaykovich MIT, new contrib. McStas
  - 3 Wolter-1 variants included in current McStas releases:
    - Conics_PP
    - Conics_EH
    - Conics_PH

- These aim to provide a simplified McStas-oriented interface for the very flexible/general conic.h library

Input parameters

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

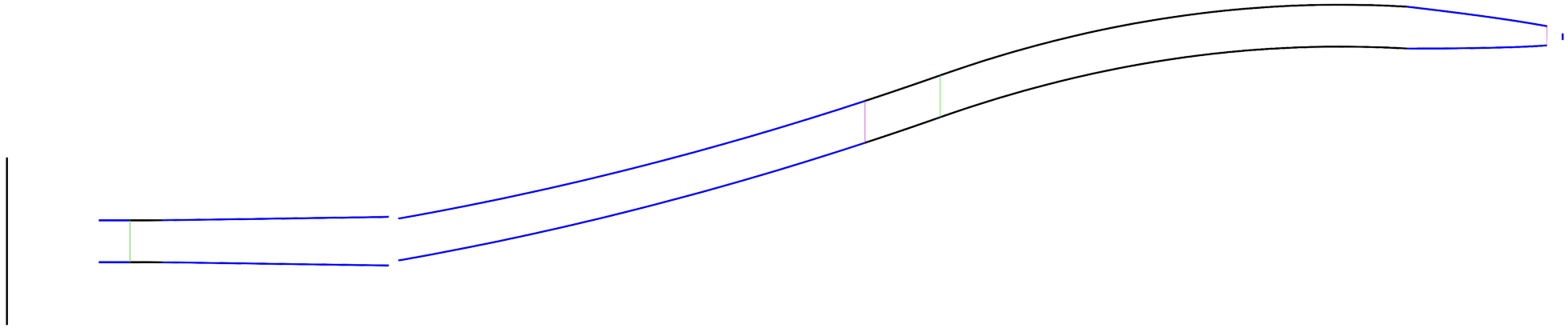
Name	Unit	Description	Default	CompInstanceName
rmin	m	Midoptic plane radius of innermost mirror pair.	0.325	
rmax	m	Midoptic plane radius of outermost mirror pair.	0.615	
focal_length	m	Focal length of the mirror pairs.	10.070	
lp	m	Paraboloid mirror length.	0.84	
lh	m	Hyperboloid mirror length.	0.84	
nshells	1	Number of nested shells to expect	4	
m	1	Critical angle of mirrors as multiples of Ni.	1	
mirr_thick	m	Thickness of mirror shell surfaces - NOT YET IMPLEMENTED	0	
disk		Flag. If nonzero, insert a disk to block the central area within the innermost mirror.	1	
R0	1	Reflectivity at Low angles for reflectivity curve approximation	0.99	
Qc	AA-1	Critical scattering vector	0.021	
W	AA-1	Width of supermirror cut-off	0.003	
alpha	AA	Slope of reflectivity for reflectivity curve approximation	6.07	
transmit	1	Fraction of statistics to assign to transmitted beam - NOT YET IMPLEMENTED	0	



- Basic focusing functionality is there, but substrate/transmission physics needs implementation

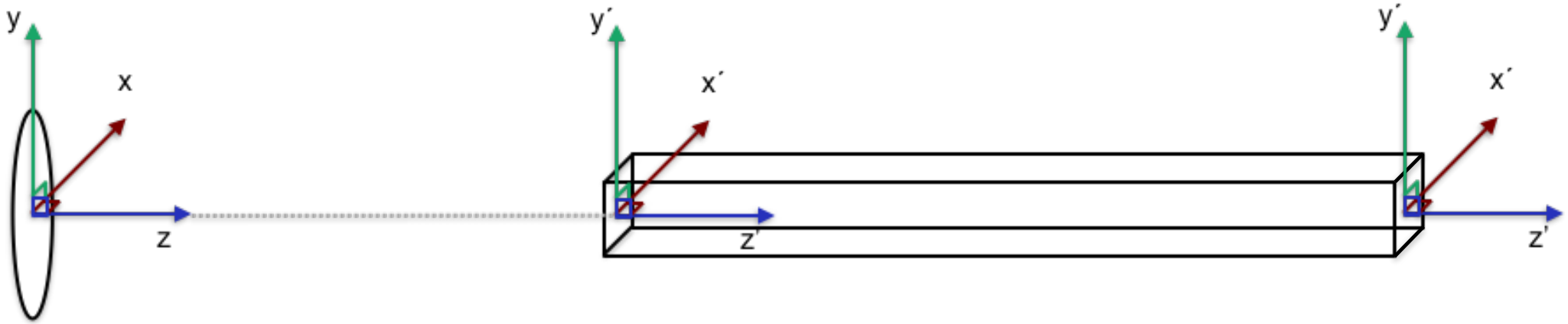
Full neutron guide transports often composed of several component types

- Here is an example from guide_bot (M. Bertelsen, ESS) with a chopper pit, s-curved bending section and focusing trumpet…



Guide placement in McStas

- The center is the front of the guide element
- Tip: Insert a guide at the end of the guide



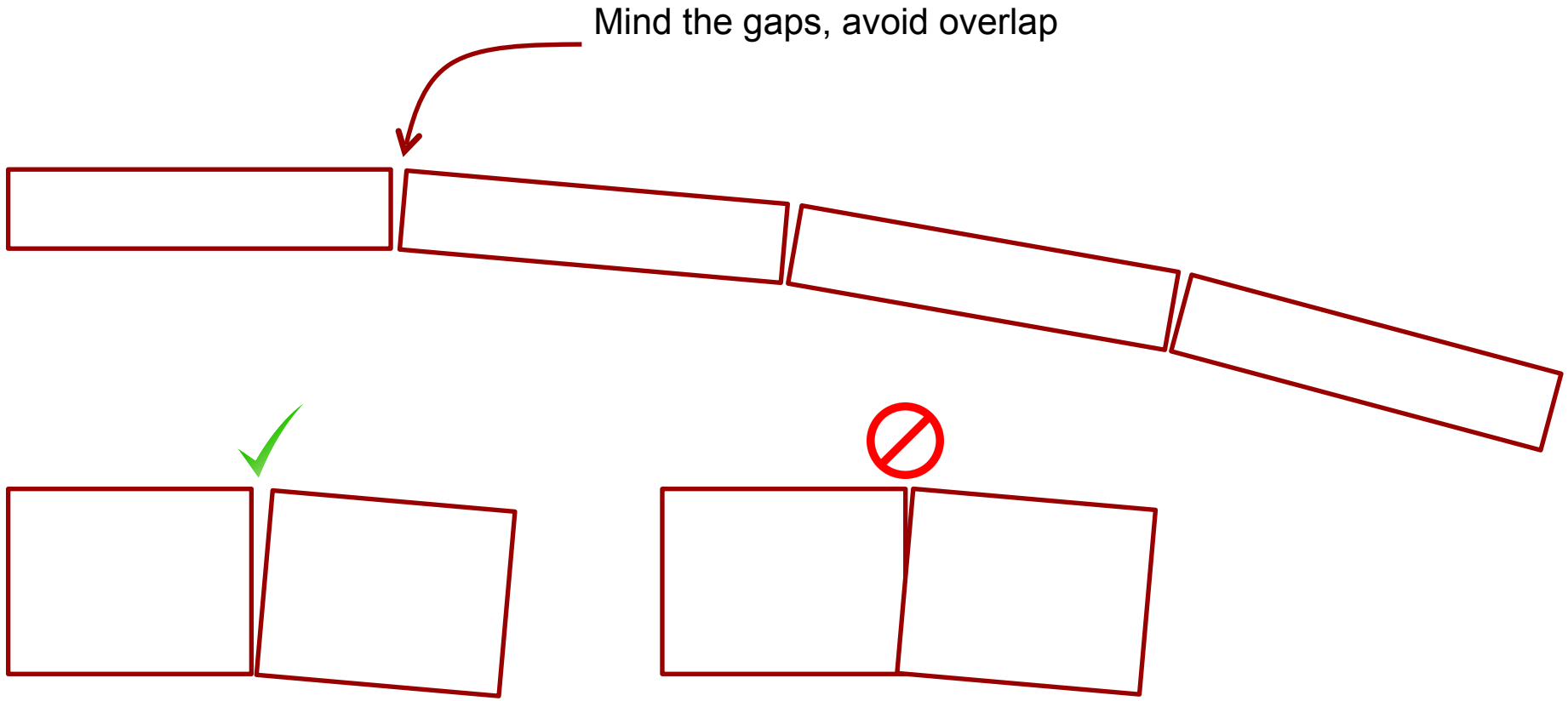
COMPONENT Source
AT (0,0,0) ABSOLUTE

COMPONENT Guide(length=A)
AT (0,0,2) RELATIVE Source

COMPONENT Arm
AT (0,0,A) RELATIVE Guide

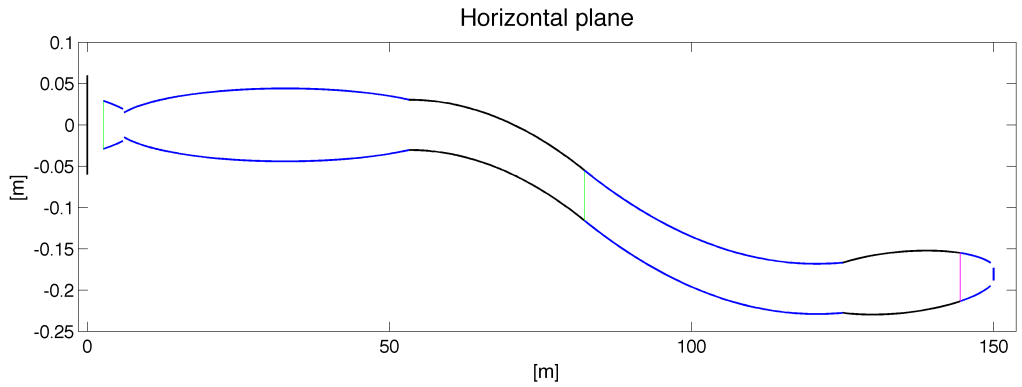
Breaking line of sight

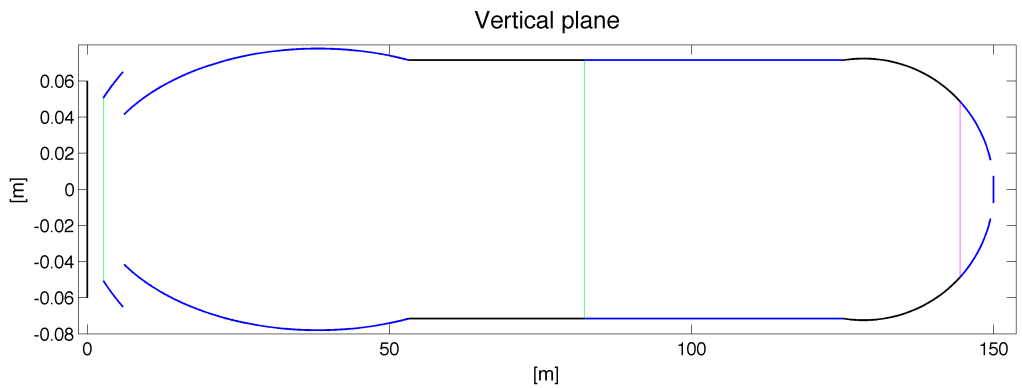
- Bender / Guide_curved component or many straight sections

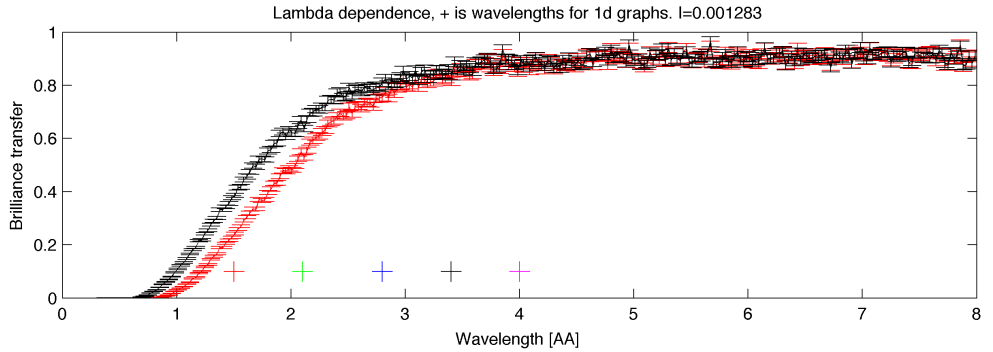


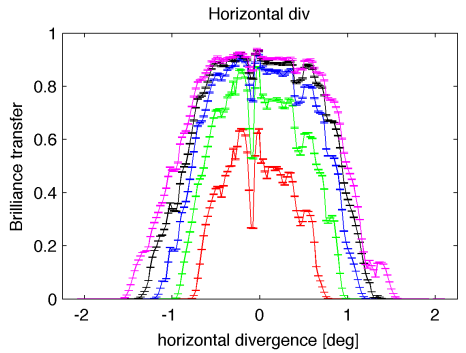
Guide optimization

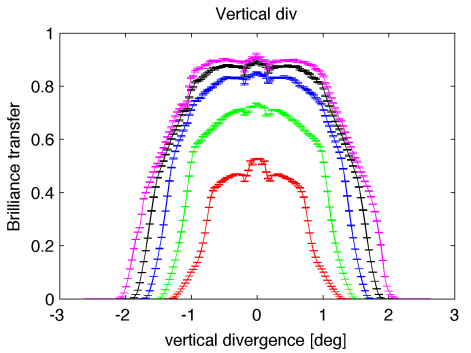
- Optimization result from MATLAB guide_bot
- Python **guide_bot** available

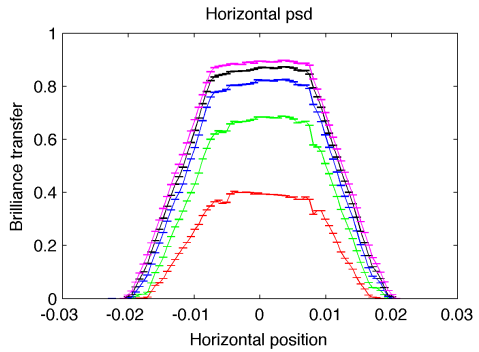


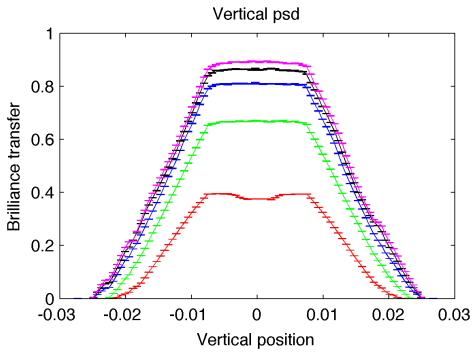












M. Bertelsen, ESS

Guide optimization

- Optimization results from python guide_bot
- **pip install guide_bot --upgrade**

```
In [13]: results.plot_any_monitor()
```

Data source

monitor: divergence_2D

run_name: large_wavelength_band

moderator: Moderator

Scanned sample parameters

height 0.03 [m]

max_wavel... 6.0 [AA]

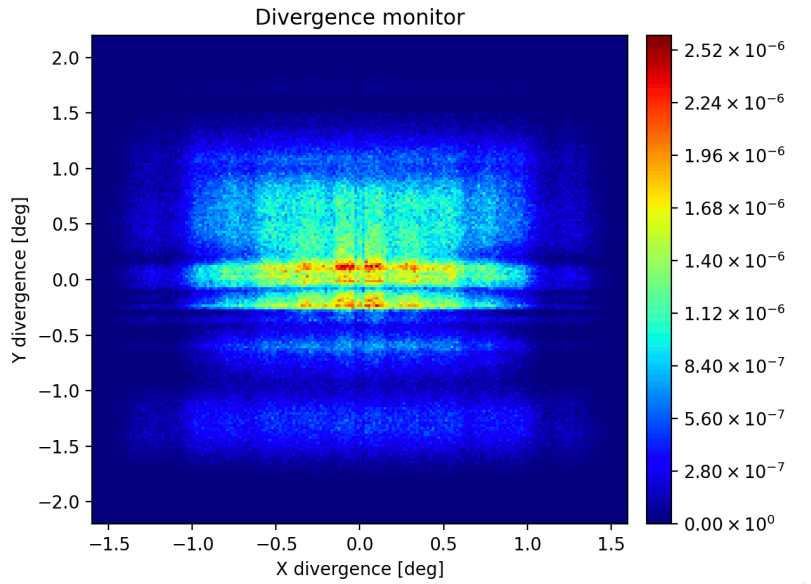
Scanned moderator parameters

height 0.05 [m]

Guide selection

- Guide_SGS
- Guide_EGE
- Guide_SCS
- Guide_E

Figure 4




```
In [11]: results.plot_guide()
```

Data source

moderator: Moderator

Scanned sample parameters

height 0.02 [m]

max_wavel... 3.0 [AA]

Scanned moderator parameters

height 0.03 [m]

Guide selection

- Guide_SGS
- Guide_EGE
- Guide_SCS
- Guide_E

Fom slider

Worst 7549 Best

Figure 1

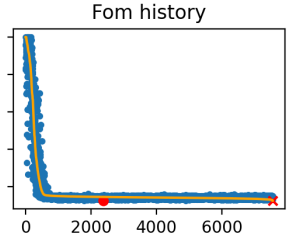
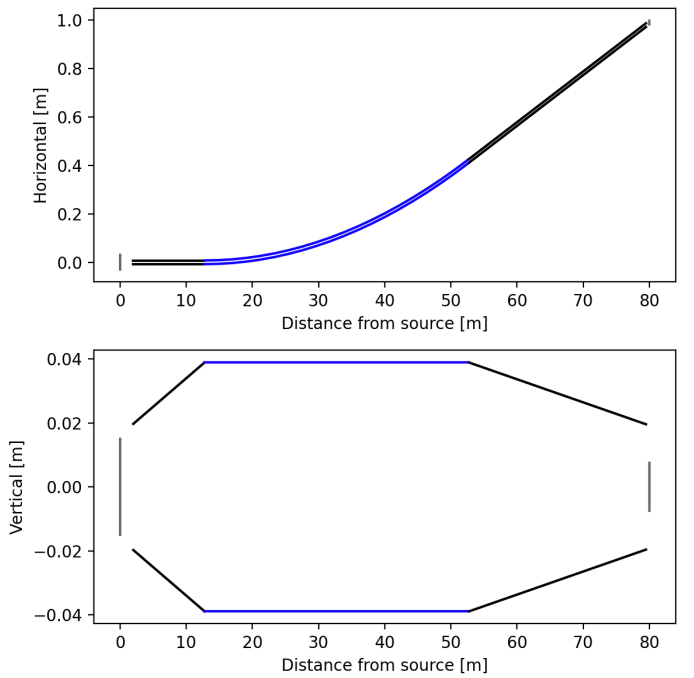


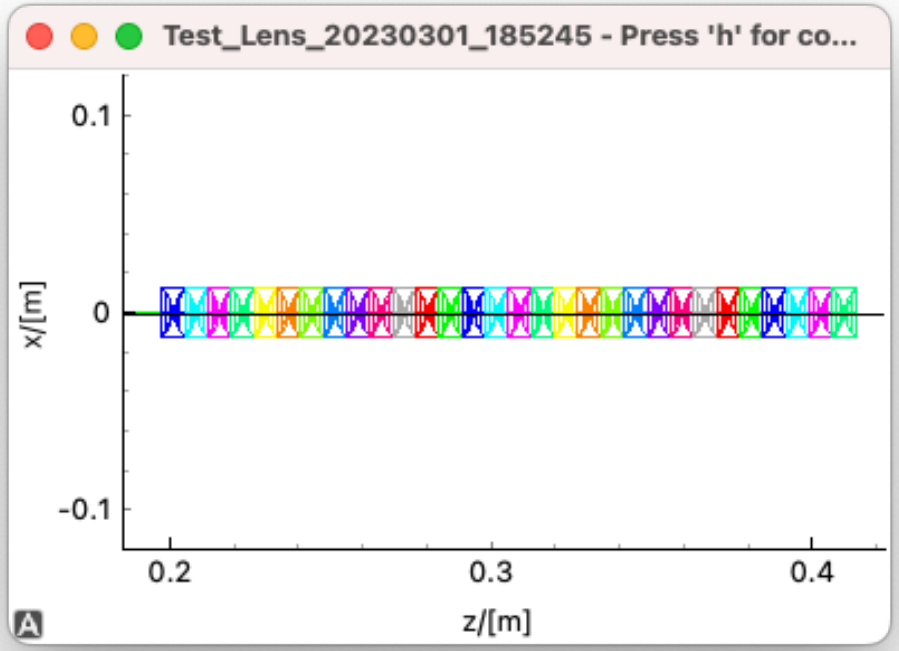
Figure 2

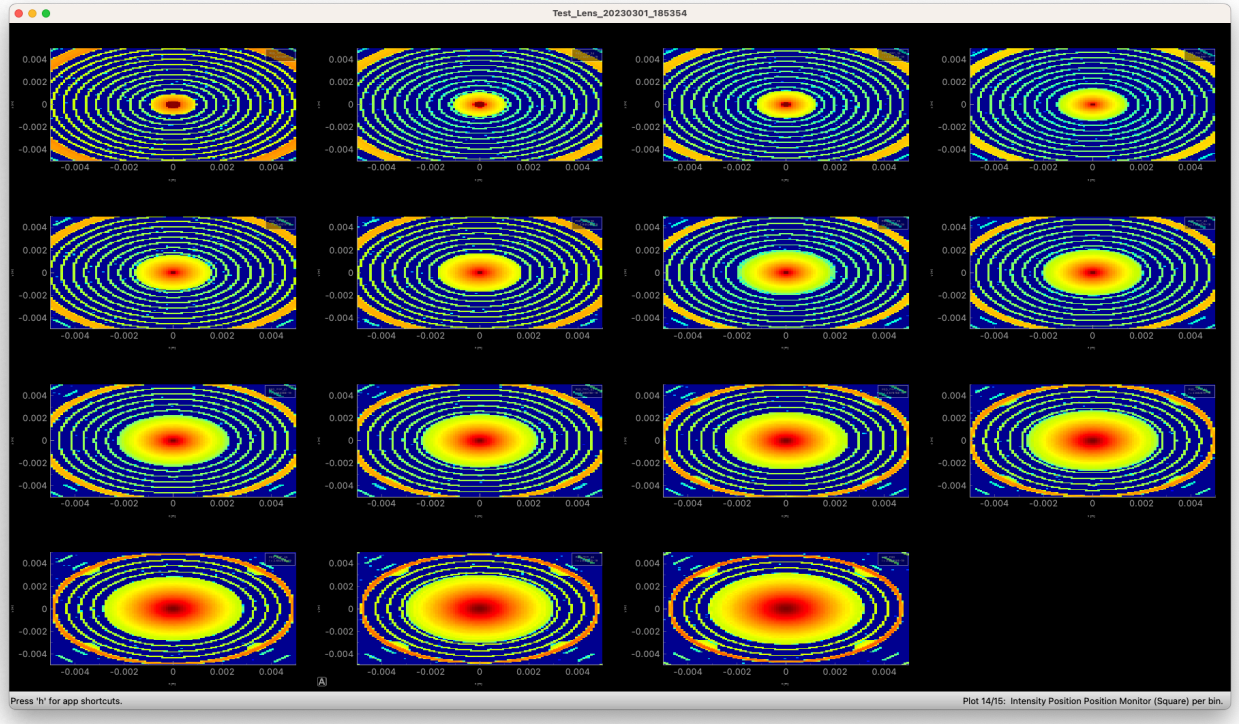


M. Bertelsen, ESS

Refractive optics

- Refraction-oriented components, can be used e.g. for prisms and lenses, CRL assemblies
  - Refractor (Simple std. geometries, OFF-geometry)
  - Lens (Spherical, planar, parabolic, OFF-geometry, C. Monzat ILL et al.)
  - Lens_simple (Parabolic, spherical, H. Frielinghaus FZJ)





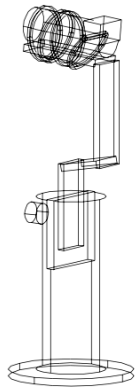
Black == “McStas system”, Red == “contribution”

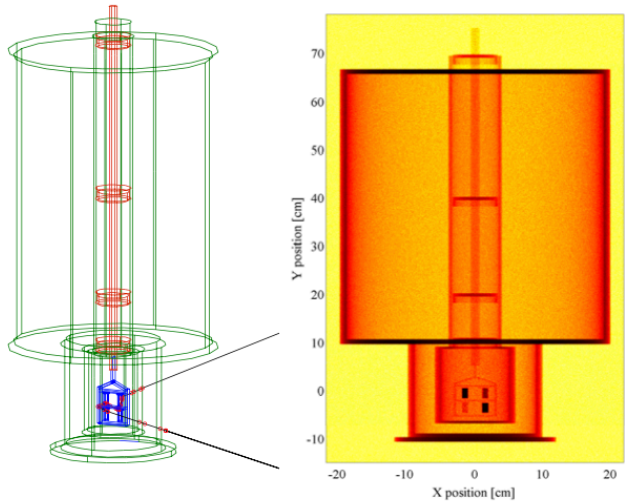
Forthcoming developments

- A PSI-DTU-ESS collaboration recently started:
  Zhanwen Ma (PSI) workforce to bring reflectivity and refraction to the Union subsystem

  - To enable modelling of advanced sample environments with embedded optics

  - To allow multi-phase samples where refractive effects and e.g. propagation-base phase contrast may be studied





HighNESS is funded by the European Framework for Research and Innovation Horizon 2020, under grant agreement 951782

Conclusions

- McStas is a widely adapted and trusted simulation platform for neutron optics, neutron scattering instruments
- Widely portable
- Large suite of components and instruments included
- Recent and upcoming highlights in focusing optics include
  - Wolter optics (B. Khaykovich) added during HighNESS
  - New project to add reflectivity and refraction to Union