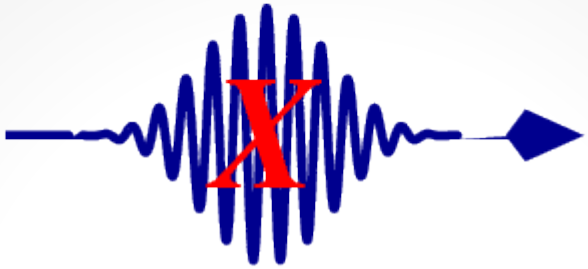
McXtrace



McXtrace - an overview

Powered by McStas technology

McXtrace

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Andrea Prodi [4]
Jana Baltser [2]
Søren Schmidt [1]
Martin Meedom [1]
Henning Friis Poulsen [1]
Manuel Sanchez del Rio [4]
Claudio Ferrero [4]
Karsten Joensen [5]
Kell Mortensen [3]
Søren Kynde [3]
Martin Petersen [3]
Robert Feidenhans'l [2]
Kim Lefmann [2]
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McXtrace

NaBiIT

Strategisk Forskningsråd

DTU

SAXSLAB

User base


Kort
Trafik
Canada
United States
México (Mexico)
North Atlantic Ocean
South Pacific Ocean
South Atlantic Ocean
Indian Ocean
Suomi (Finland)
Россия (Russia)
Polska (Poland)
Україна (Ukraine)
Казахстан (Kazakhstan)
Монгол Улс (Mongolia)
España (Spain)
Italia (Italy)
Türkiye (Turkey)
中国 (China)
日本 (Japan)
대한민국 (South Korea)
العراق (Iraq)
ایران (Iran)
افغانستان (Afghanistan)
پاکستان (Pakistan)
India
ประเทศไทย (Thailand)
الجزائر (Algeria)
ليبيا (Libya)
مصر (Egypt)
السعودية (Saudi Arabia)
Mali
Niger
Tchad (Chad)
السودان (Sudan)
Nigeria
ኢትዮጵያ (Ethiopia)
Kenya
DR Congo
Tanzania
Angola
Namibia
Botswana
South Africa
Madagasikara (Madagascar)
Indonesia
Papua New Guinea
Australia
New Zealand
Venezuela
Colombia
Perú (Peru)
Brasil (Brazil)
Bolivia
Chile
Argentina
2000 mil
2000 km
Billedmateriale ©2012 NASA, TerraMetrics, Kortdata ©2012 MapLink, Tele Atlas -

Features of releases

Beta:

a. First package build of McXtrace Linux and Windows XP
b. 2 Example beamlines
c. Few components

1.0:

a. Optimized packaging, Linux, Windows7, XP and Mac OSX
b. Time-propagation
c. Phase-propagation, wavefront reconstruction experimental
d. Sample models
e. Monochromator crystal (Perfect_crystal)

1.1_pre:

a. Linux, Windows 7, XP, Mac OSX, FreeBSD
b. Optimized grammar
c. Chopper model
d. Faster data file searching
e. Lots more components
f. More Sample models
g. OFF-support - anyshape options enabled
h. Roughness in lenses
i. Shadow interfaces

Component history - 2009

McXtrace

Sources
- Source_pt
- Source_flat
- Source_div

Optics
- Arm
- Lens_simple
- Mirror_curved
- Slit

Monitors
- E_monitor
- L_monitor
- PSD_monitor
- PSD_monitor_4PI

Misc
- Progress_bar

Samples

Component history - 2012

McXtrace

Sources
- Source_pt
- Source_lab
- Source_gaussian
- Source_flat
- Source_div

Optics
- Arm
- Beamstop
- Chopper_simple
- Filter
- Lens_kinoform
- Lens_parab
- Lens_parab_Cyl
- Lens_simple
- Mirror_curved
- Mirror_elliptic
- Mirror_parabolic
- Multilayer_elliptic
- Slit
- Slit_N
- Twin_KB_ML

Monitors
- E_monitor
- EPSD_monitor
- L_monitor
- Monitor
- Monitor_nD
- PreMonitor_nD
- PSD_monitor
- PSD_monitor_4PI
- PSD_monitor_coh
- W_psd_monitor

Misc
- Progress_bar
- Shadow_input
- Shadow_output

Samples
- Single_crystal
- Saxs_spheres
- PowderN
- Perfect_crystal
- Absorption_sample
- SAXS-samples
- Molecule_2state

Component history - 2013?

McXtrace

Sources
- Source_pt
- Source_lab
- Source_gaussian
- Source_flat
- Source_div
- Source_SPECTRA

Optics
- Arm
- Beamstop
- Chopper_simple
- Filter
- Lens_kinoform
- Lens_parab
- Lens_parab_Cyl
- Lens_simple
- Mirror_curved
- Mirror_elliptic
- Mirror_parabolic
- Multilayer_elliptic
- Slit
- Slit_N
- Twin_KB_ML
- Zone_plate
- Grating

Monitors
- E_monitor
- EPSD_monitor
- L_monitor
- Monitor
- Monitor_nD
- PreMonitor_nD
- PSD_monitor
- PSD_monitor_4PI
- PSD_monitor_coh
- W_psd_monitor

Misc
- Progress_bar
- Shadow_input
- Shadow_output
- SRW_input
- SRW_output

Samples
- Single_crystal
- Saxs_spheres
- PowderN
- Perfect_crystal
- Absorption_sample
- SAXS-samples
- Molecule_2state
- Isotropic_Sqw

McStas / McXtrace inheritance

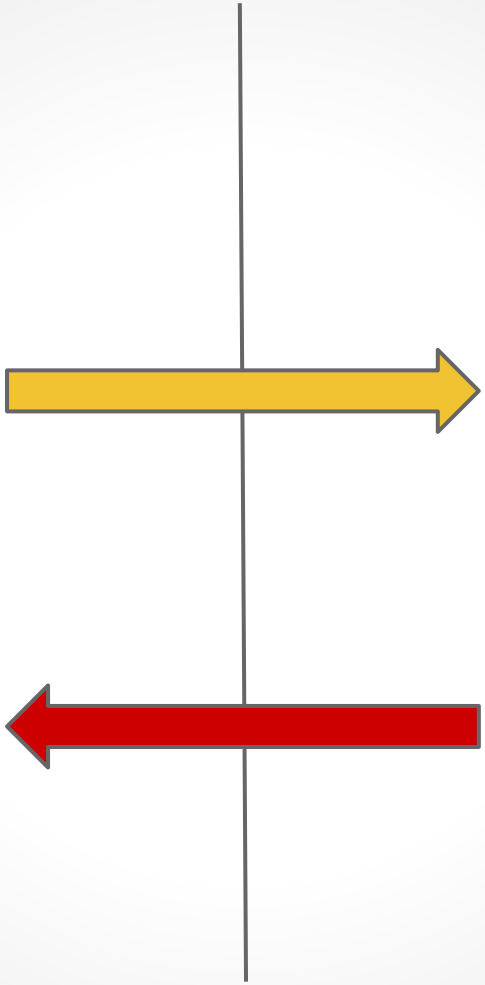
McStas

Geometry engine

Fast runtime library

Monitor models

Crystal sample models



McXtrace

Binary datafile searching

Perfect crystal model

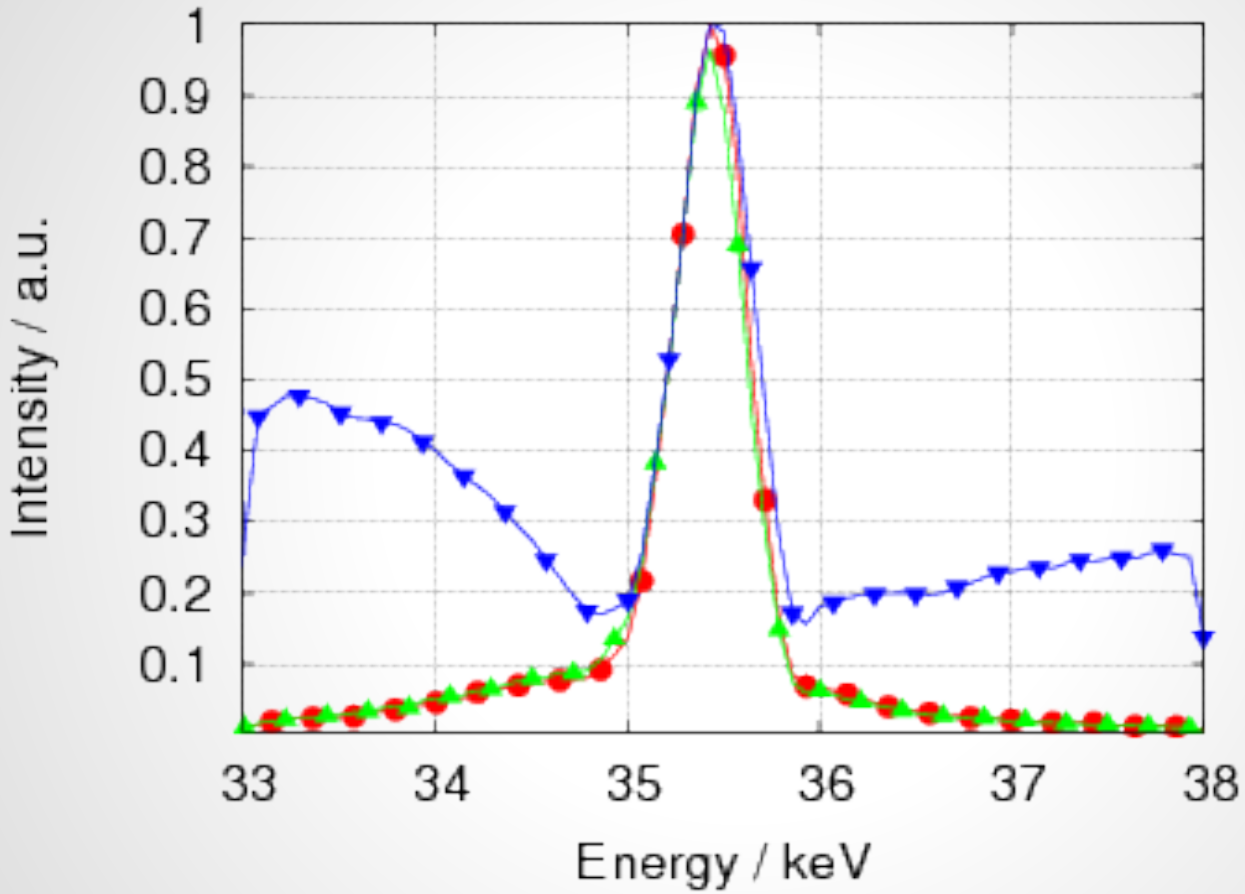
Phase handling (?)

McXtrace

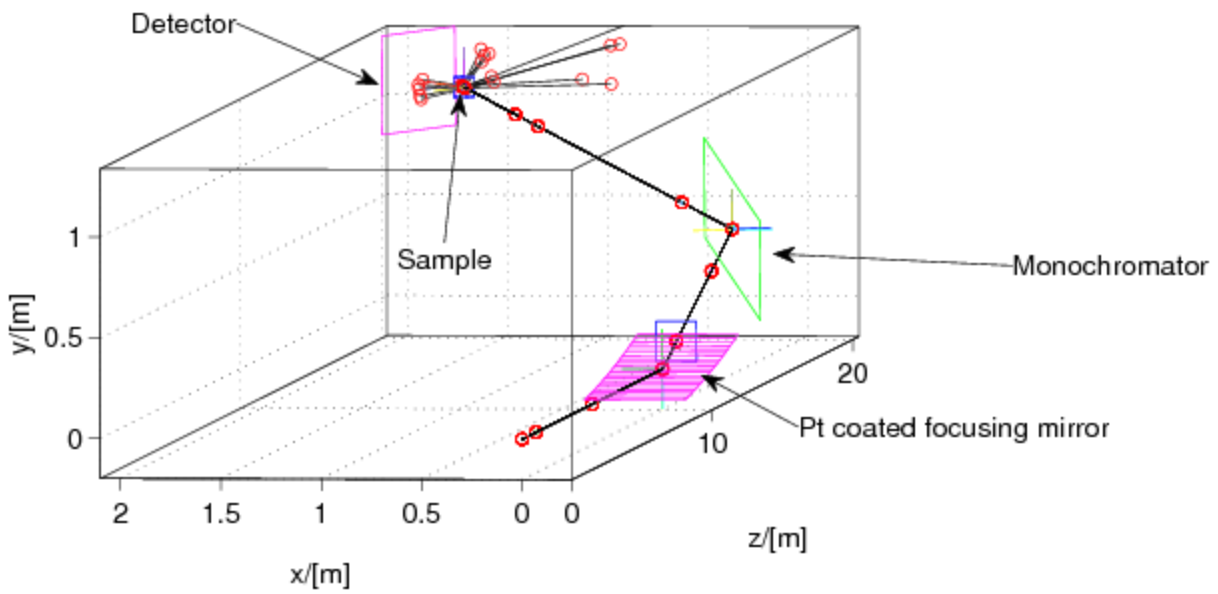
ID11 - Pink beam monochromator experimental setup

McXtrace

ID11 - Pink beam monochromator

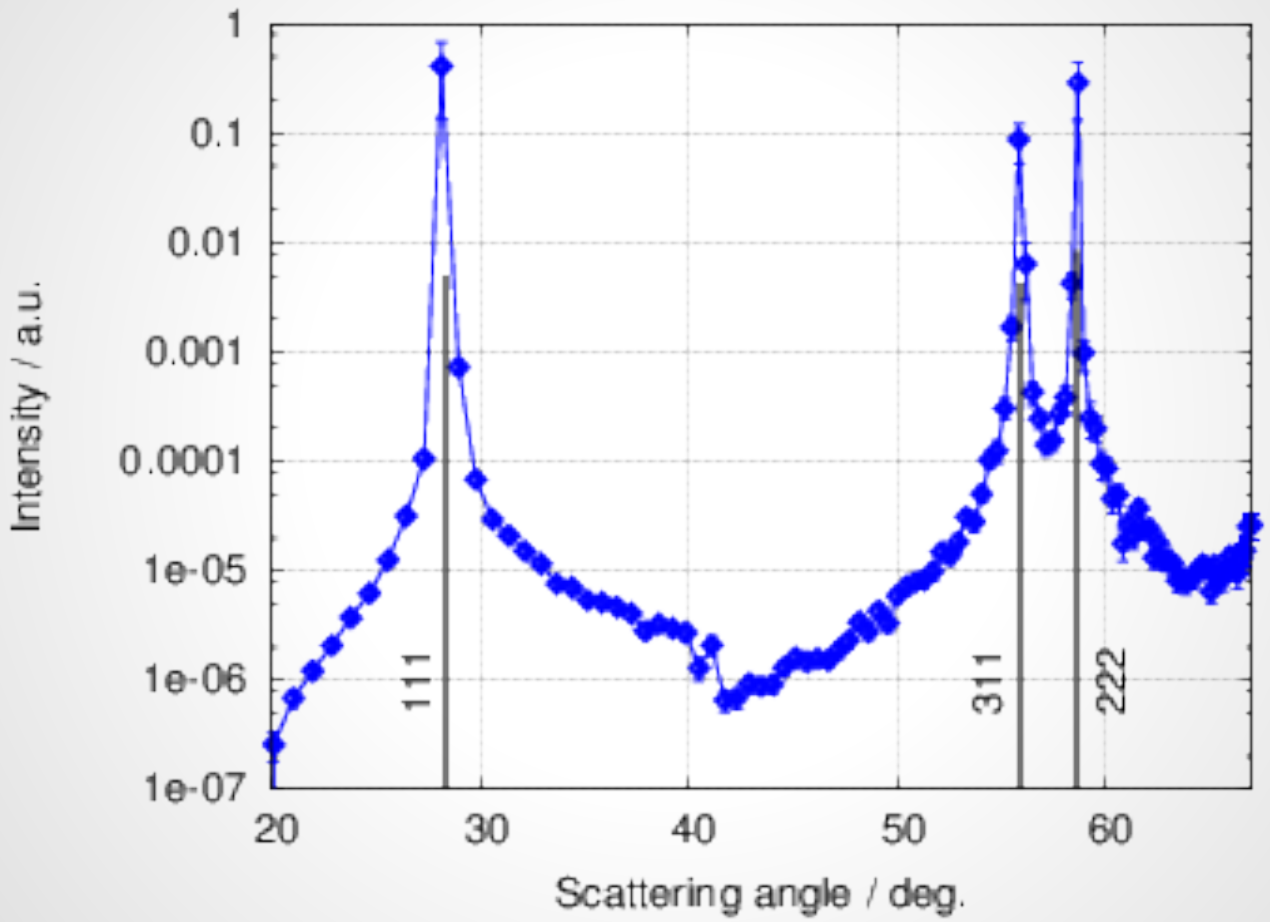


Max 711


Detector
Sample
Monochromator
Pt coated focusing mirror
y/[m]
1
0.5
0
x/[m]
2
1.5
1
0.5
0
0
z/[m]
10
20

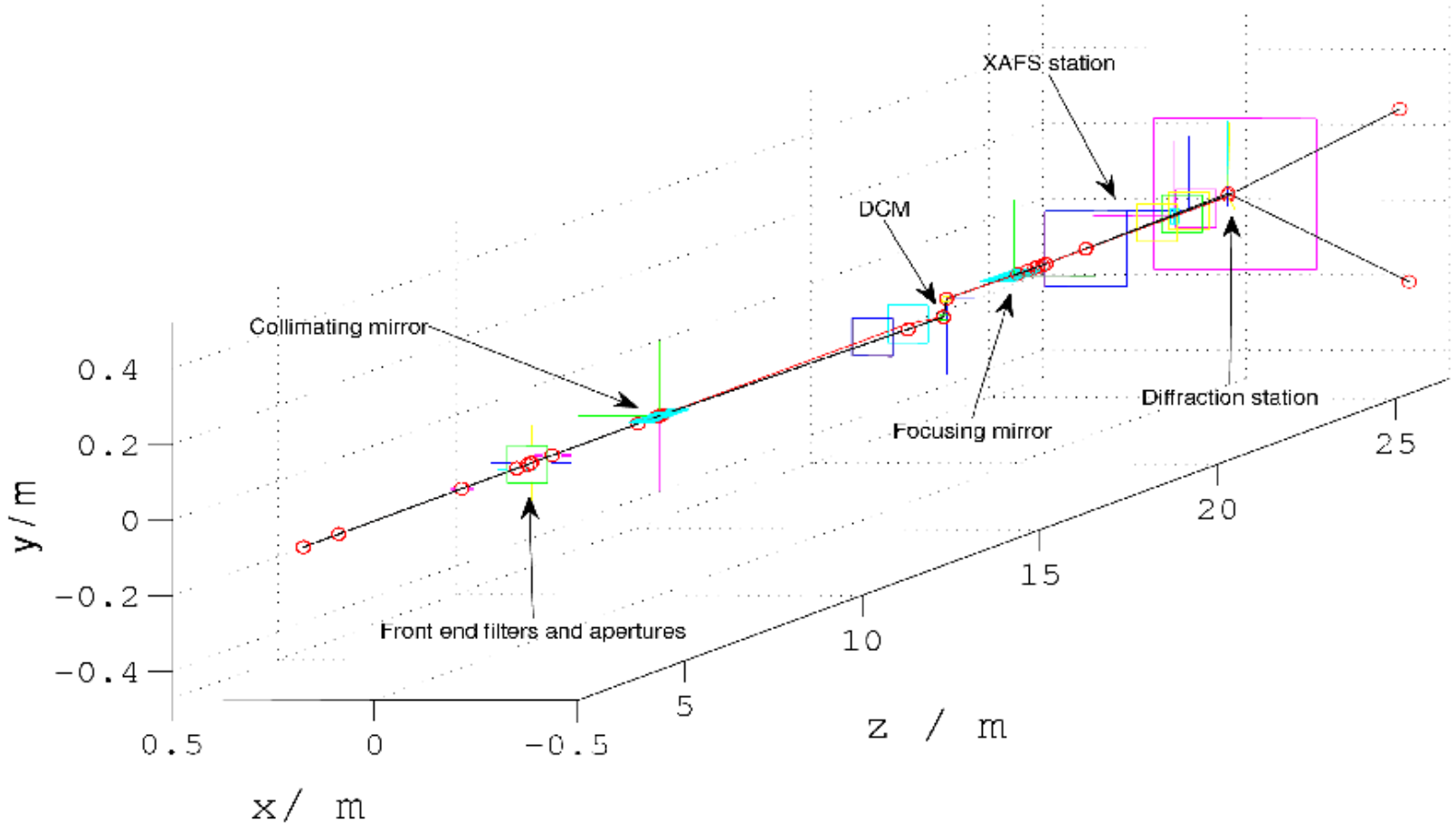
McXtrace

Max 711 Powder Diffraction Signal at virtual detector



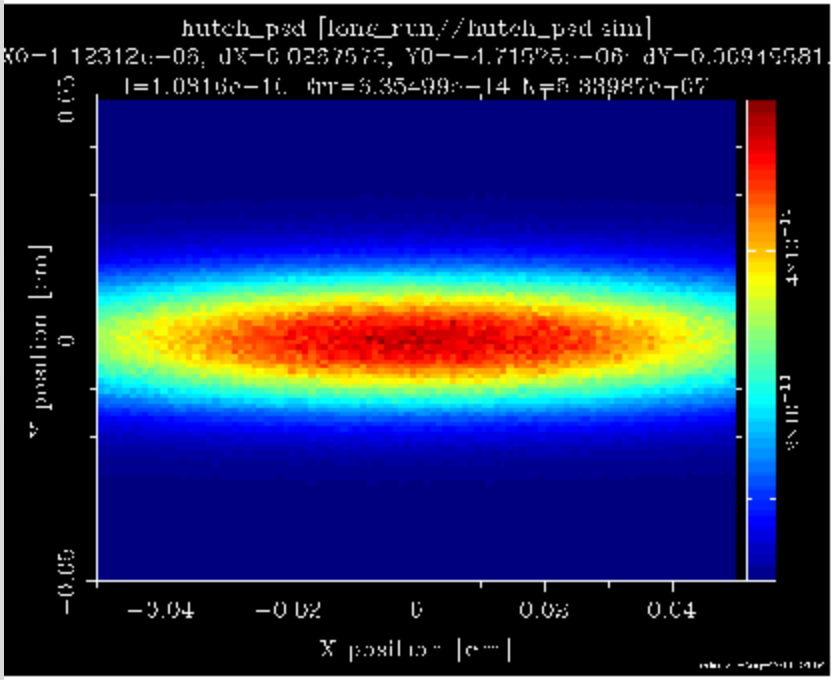
Max 811 surface diffraction and XAFS beamline

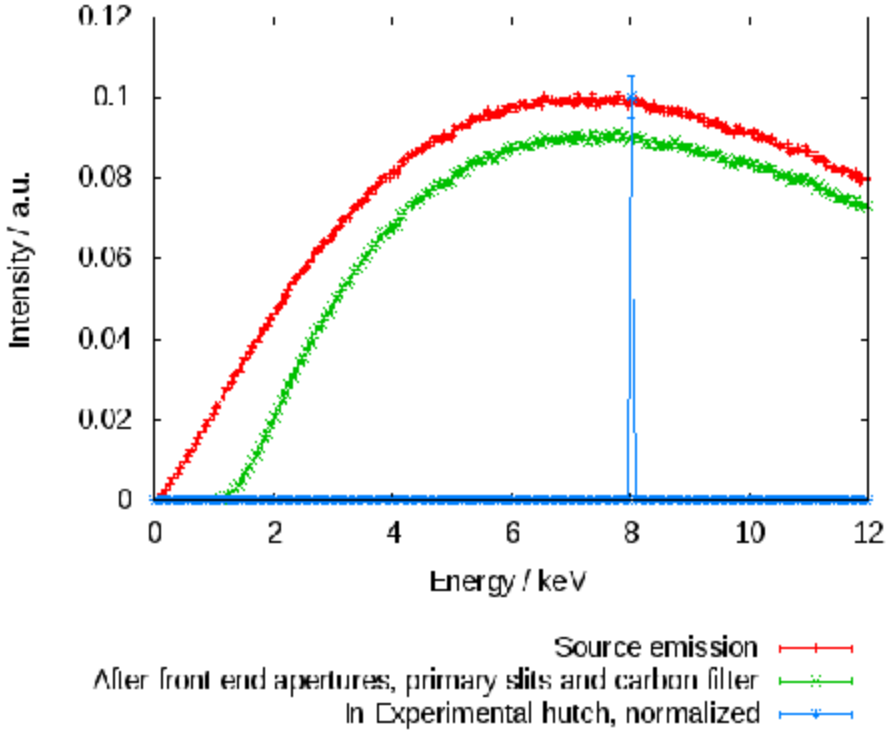
McXtrace



Max 811 surface diffraction and XAFS beamline

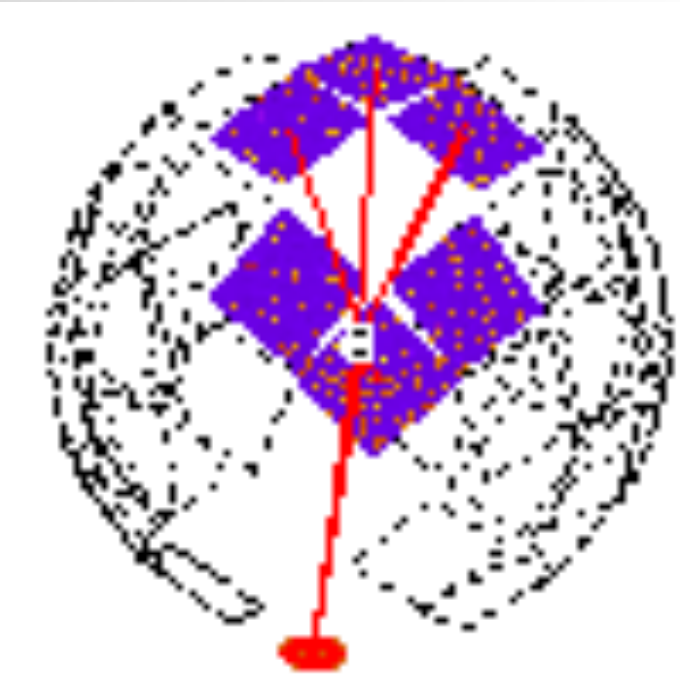
- Unslit Spatial beam distribution

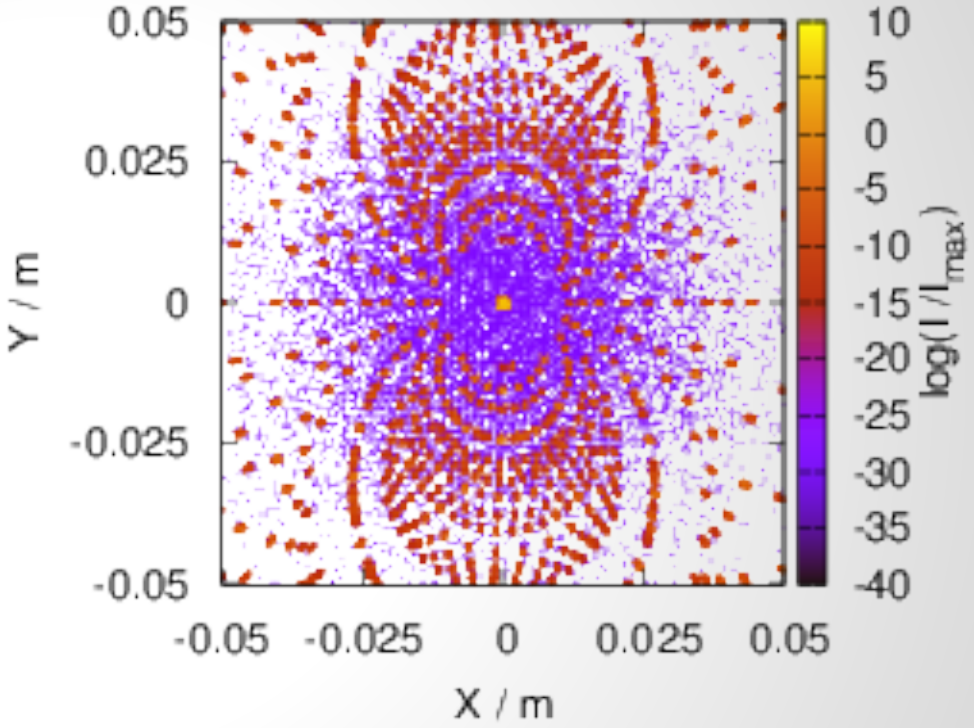




Reported flux on sample: [2000...20000] photons /s
Simulated flux on sample: 20080 photons / s

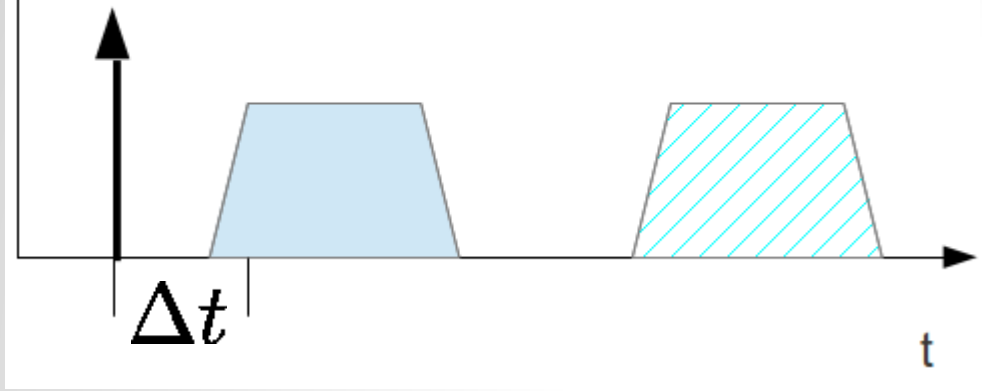
Neutron style Laue camera

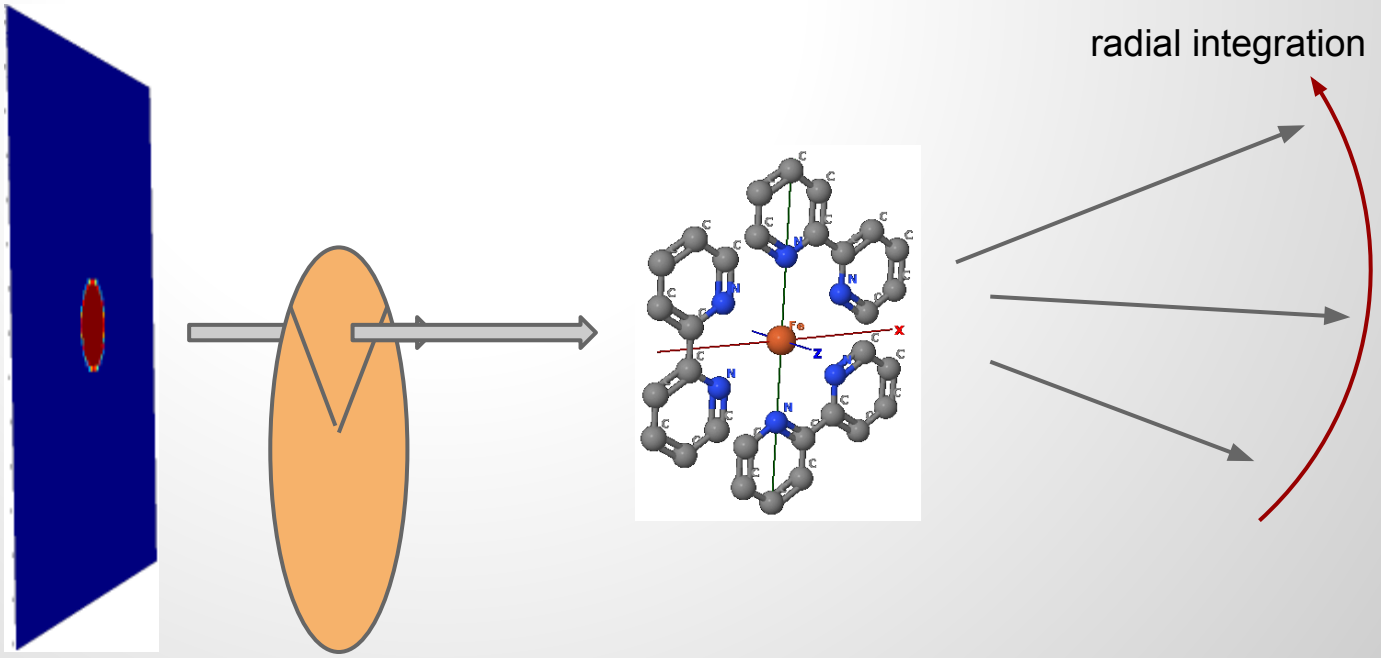




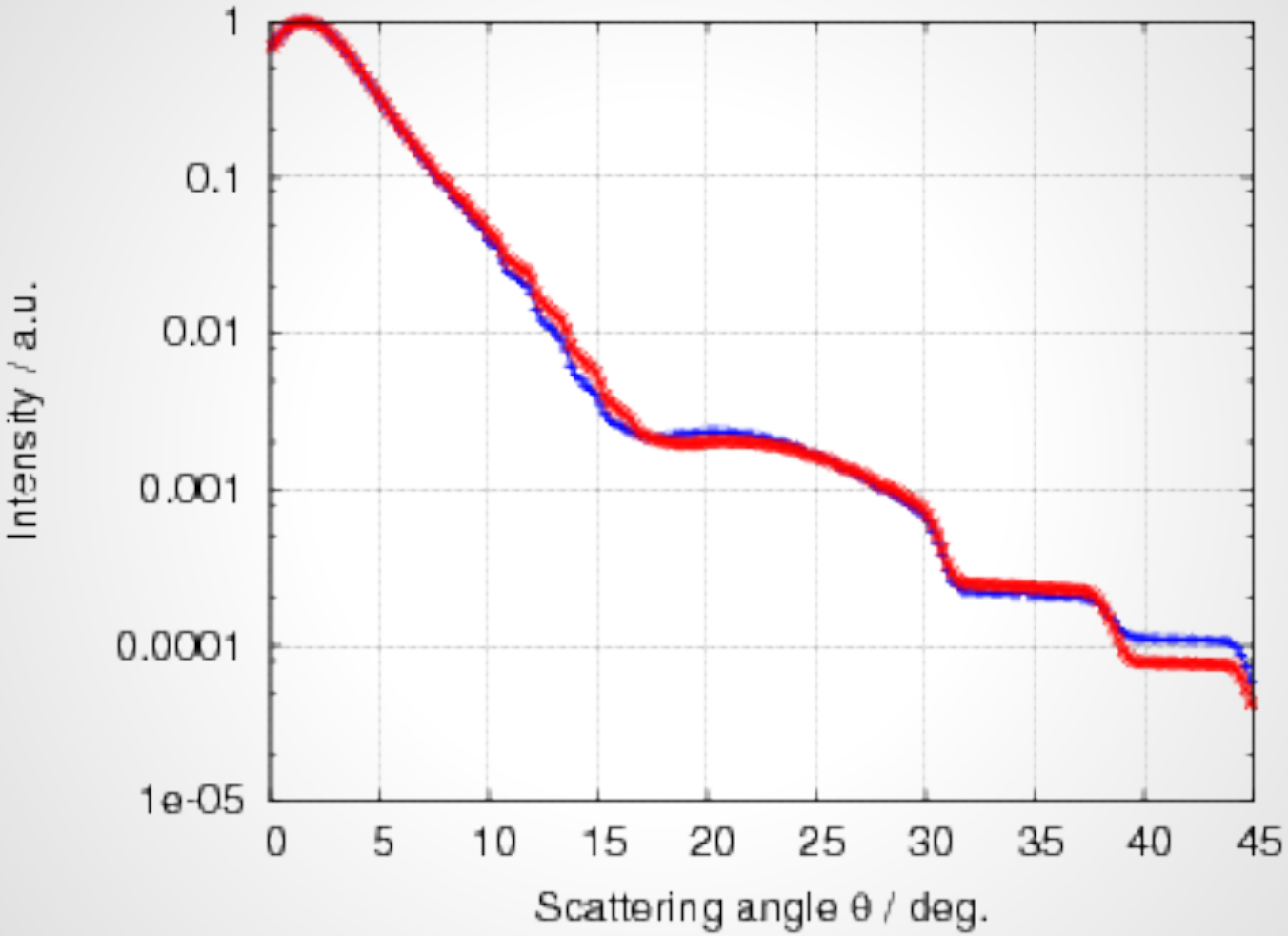
Time resolved studies

$$\text{PHOTON\_STATE}=(x, y, z, k_x, k_y, k_z, t, \varphi, E_x, E_y, E_z, p)$$

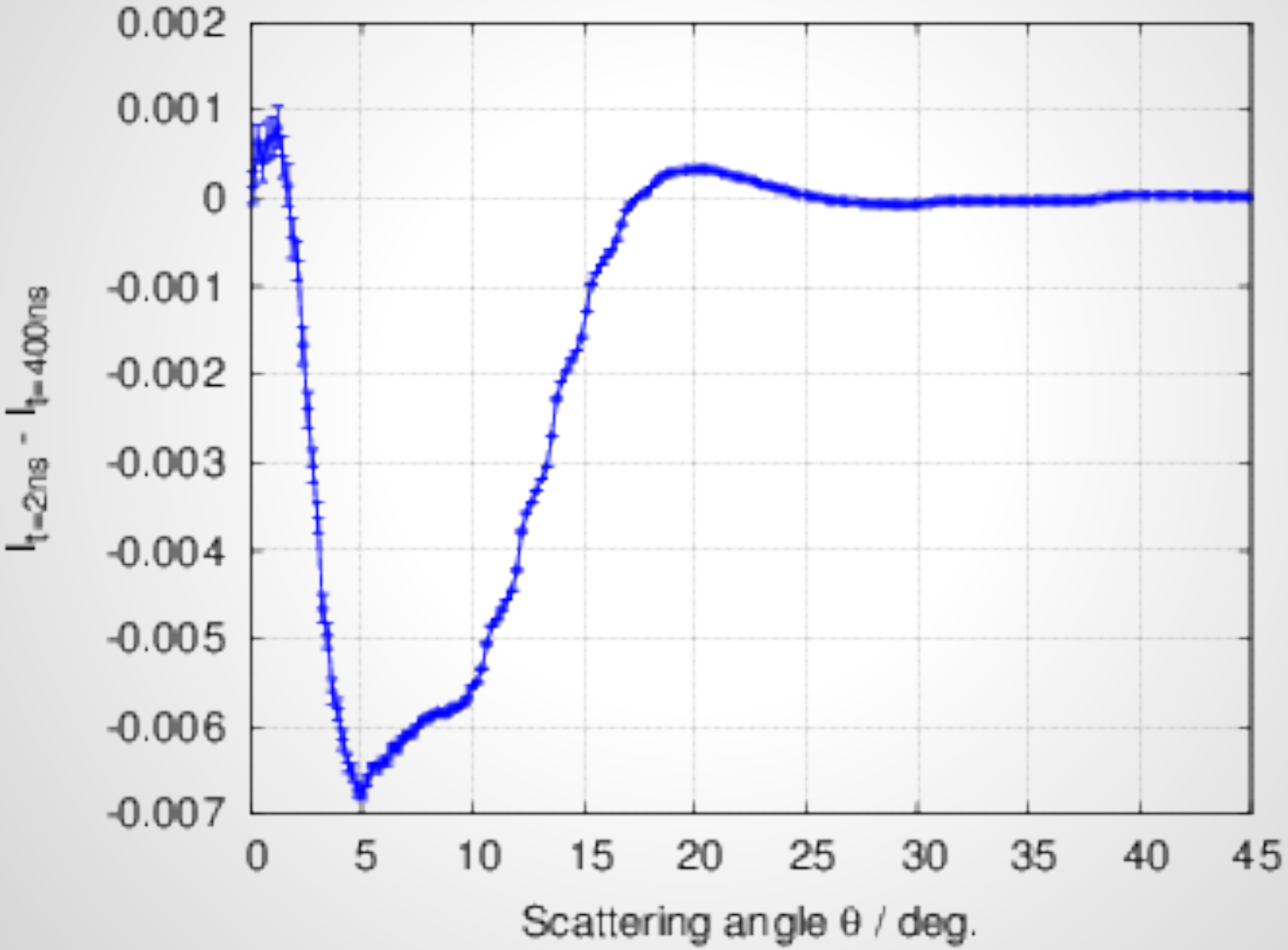




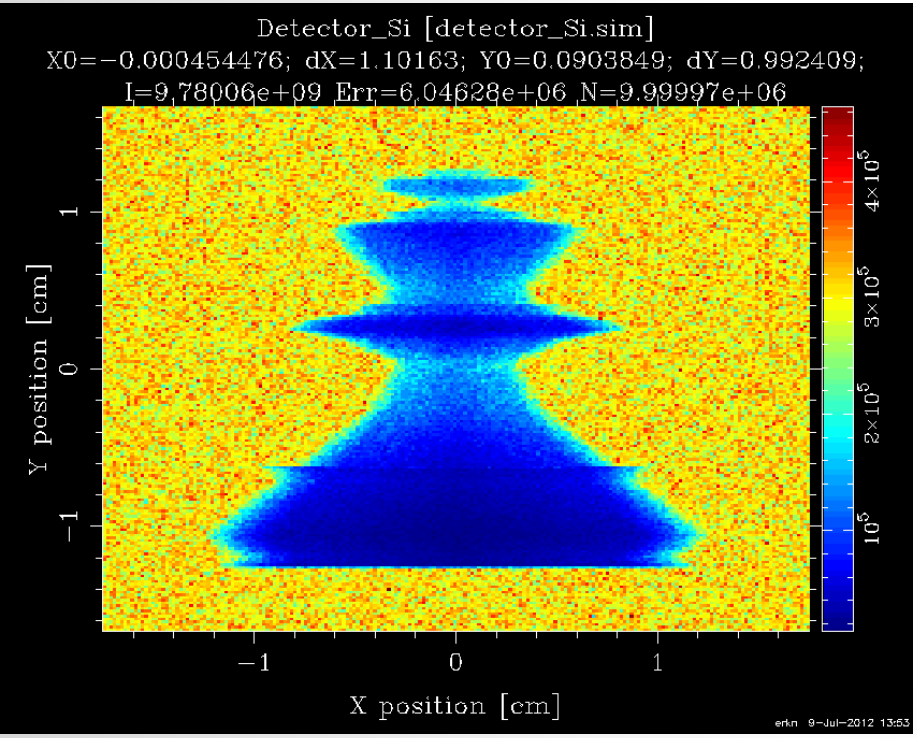
Time resolved studies

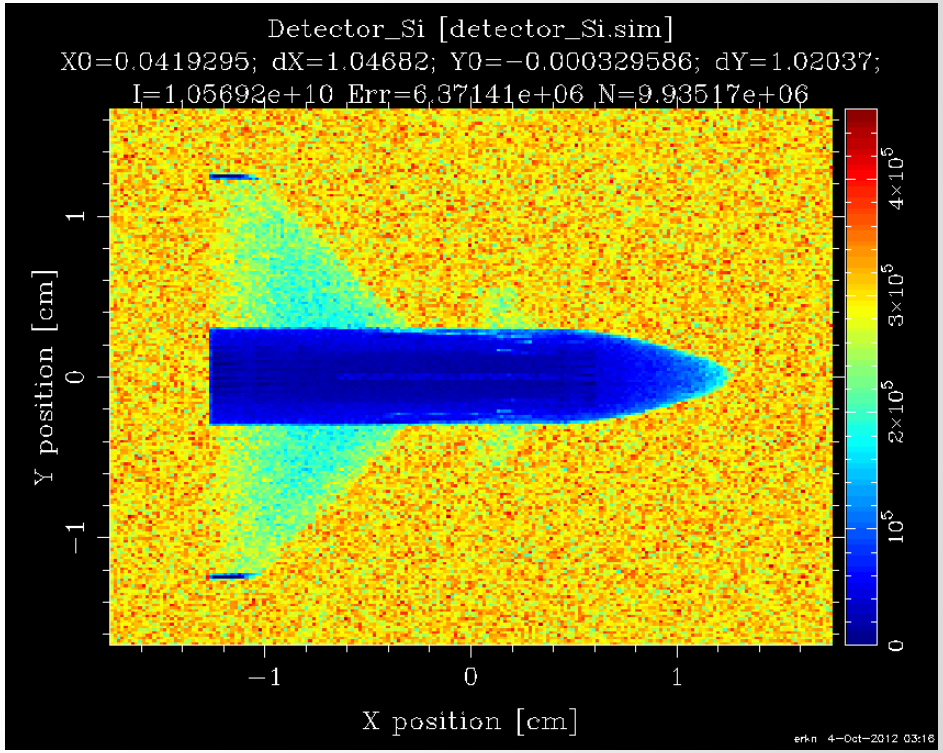


Time resolved studies

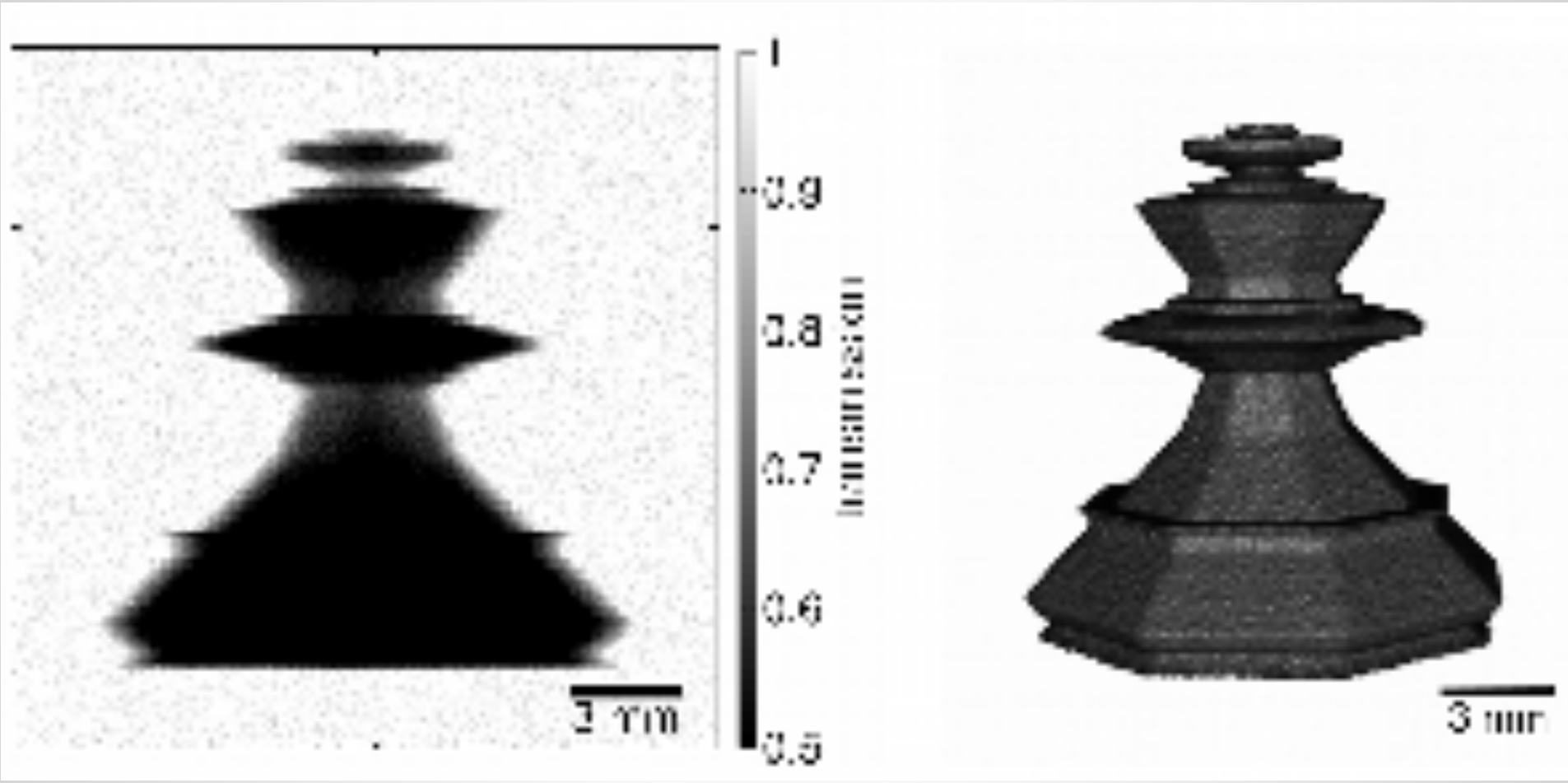


Anyshape Tomography

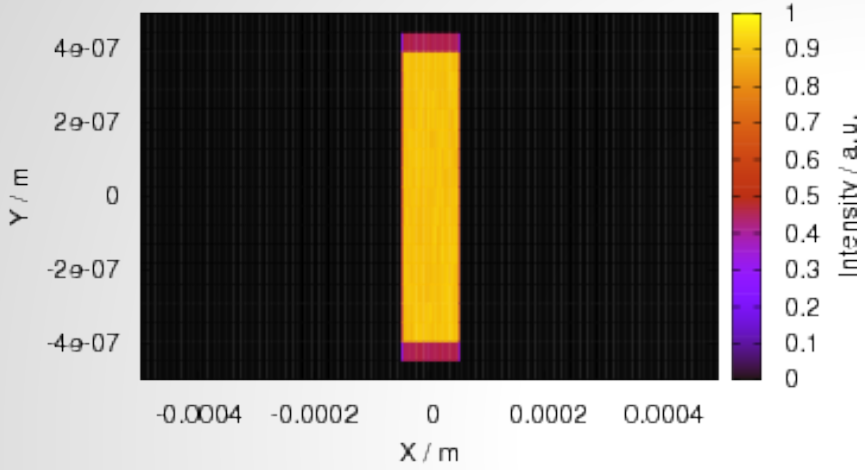


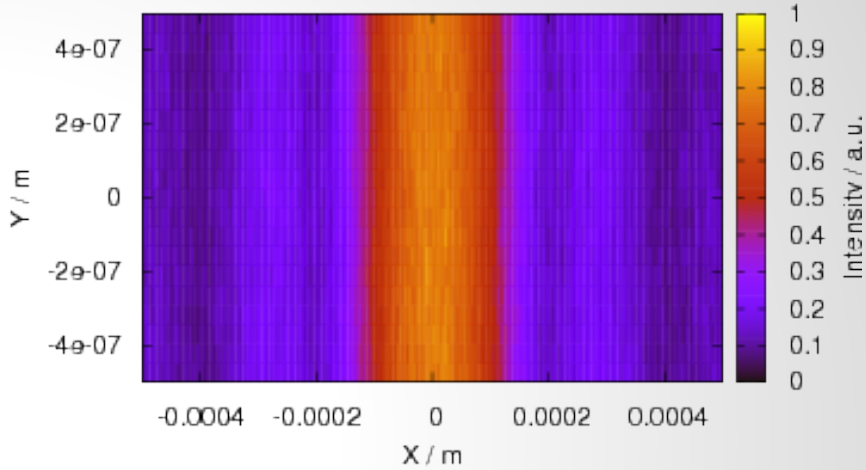


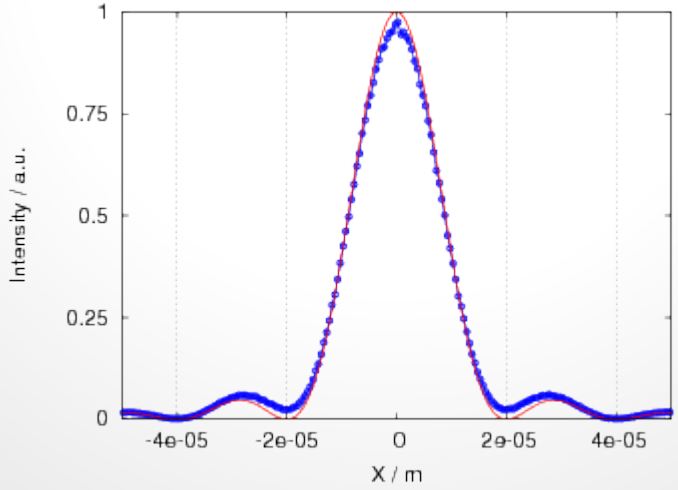
Anyshape Tomography



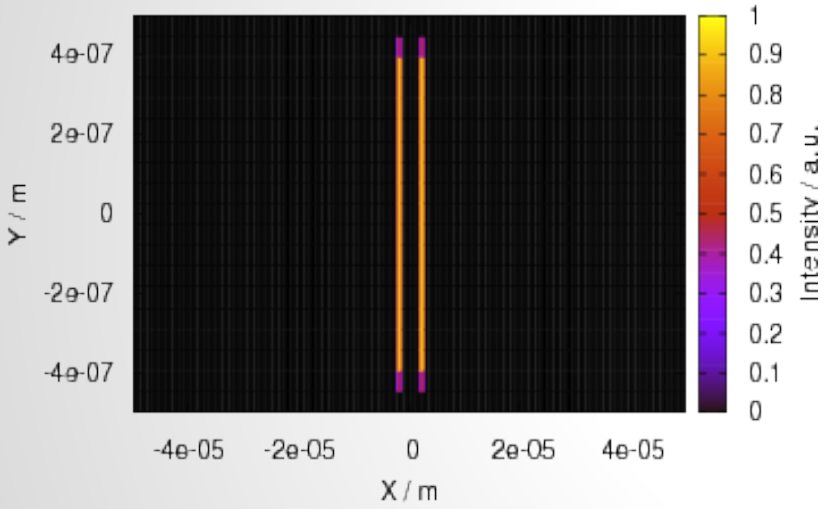
Single Slit

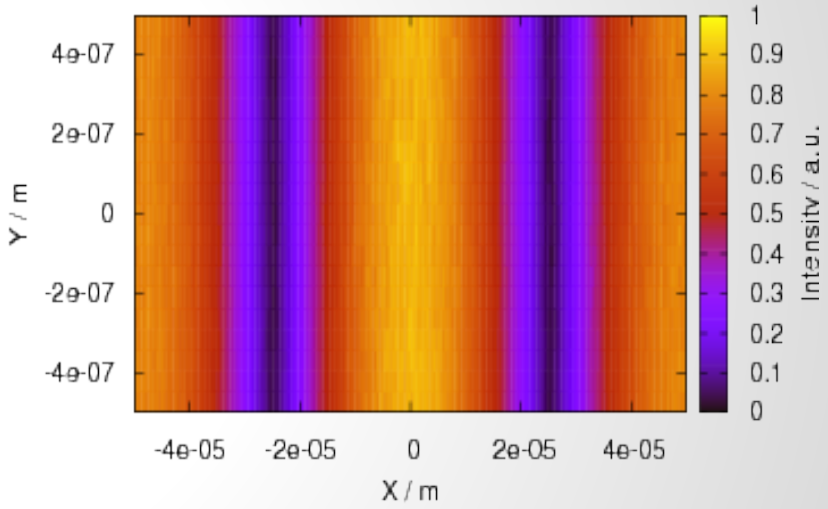

4e-07
2e-07
0
-2e-07
-4e-07
Y / m
-0.0004
-0.0002
0
0.0002
0.0004
X / m
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Intensity / a.u.


4e-07
2e-07
0
-2e-07
-4e-07
Y / m
-0.0004
-0.0002
0
0.0002
0.0004
X / m
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Intensity / a.u.


1
0.75
0.5
0.25
0
Intensity / a.u.
-4e-05
-2e-05
0
2e-05
4e-05
X / m

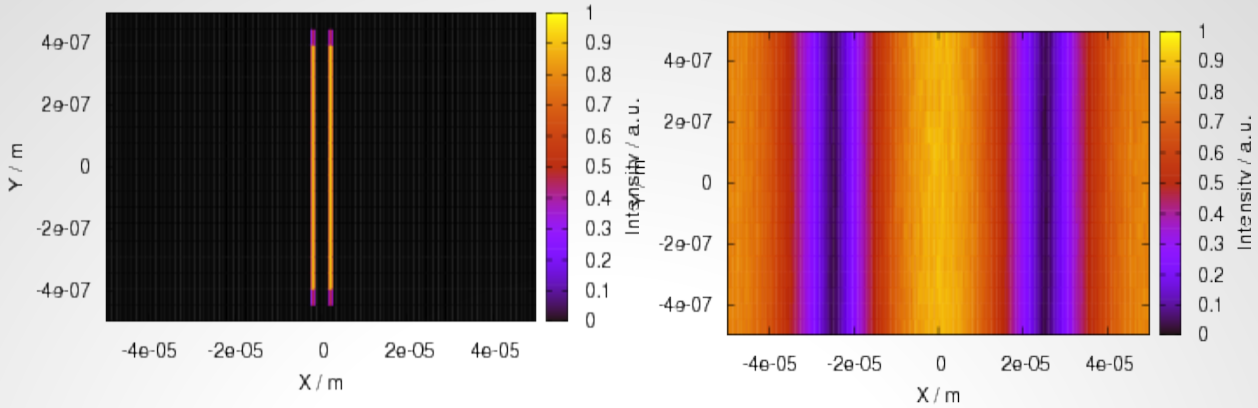
Double Slit

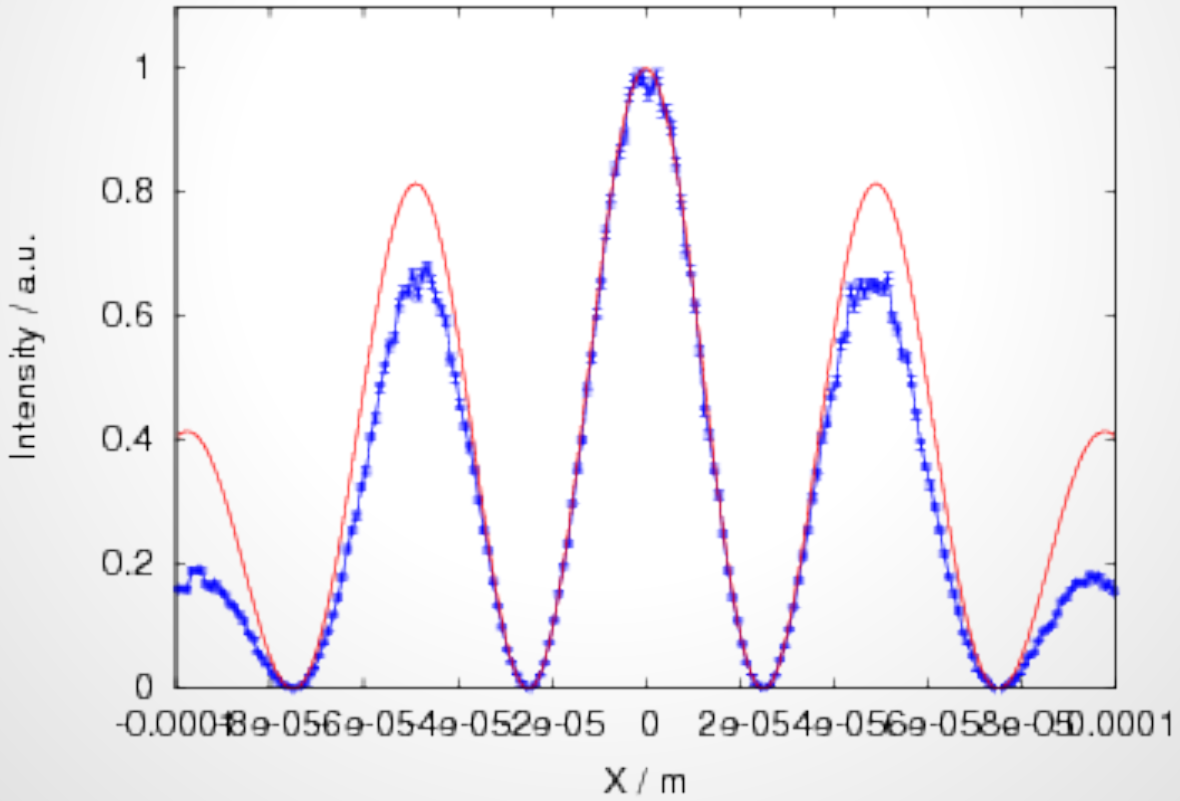

4e-07
2e-07
0
-2e-07
-4e-07
Y / m
-4e-05
-2e-05
0
2e-05
4e-05
X / m
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Intensity / a.u.


4e-07
2e-07
0
-2e-07
-4e-07
Y / m
-4e-05
-2e-05
0
2e-05
4e-05
X / m
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Intensity / a.u.

McXtrace

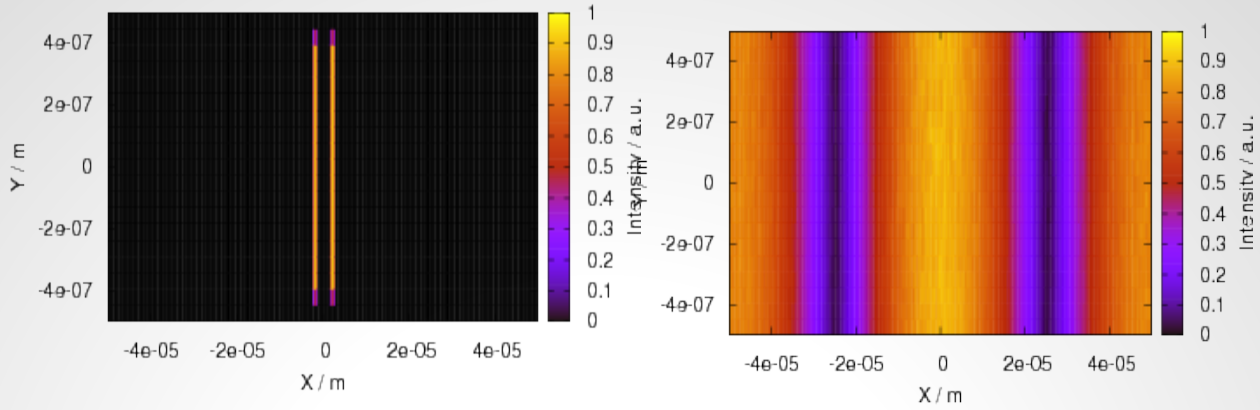
Double Slit

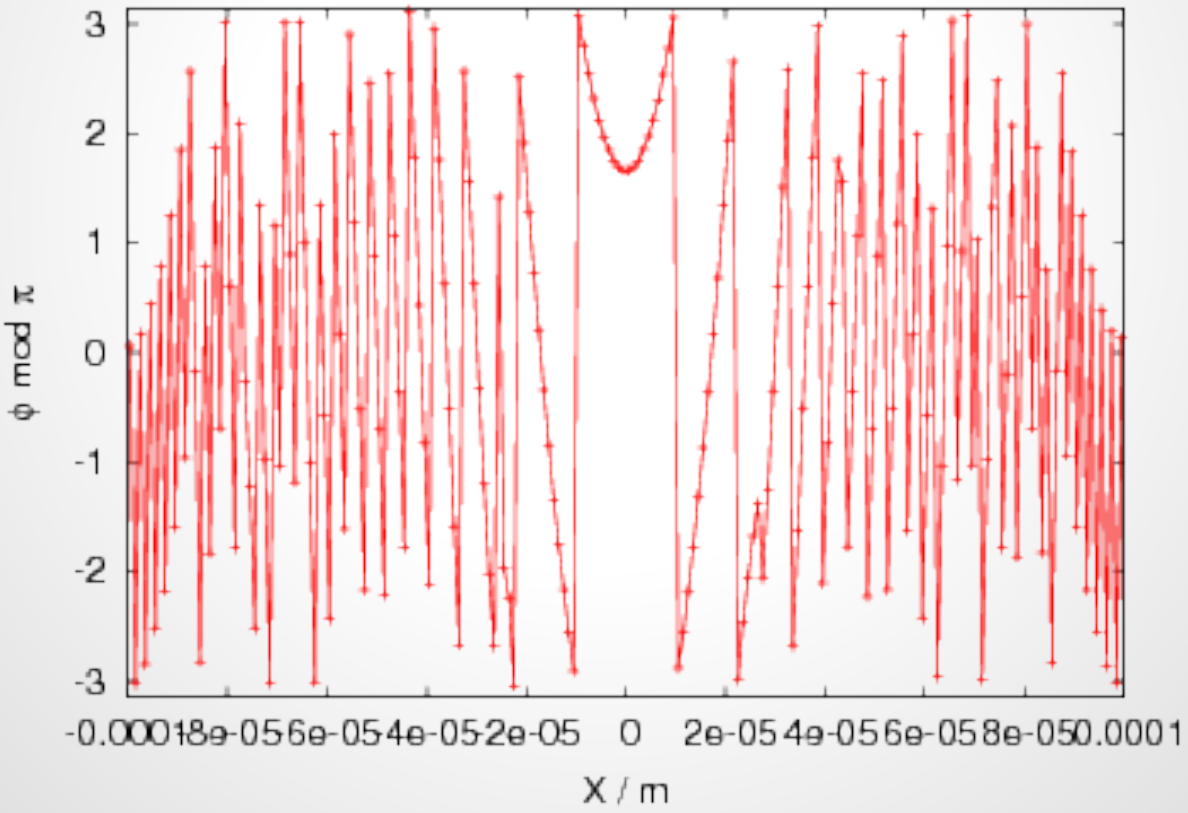




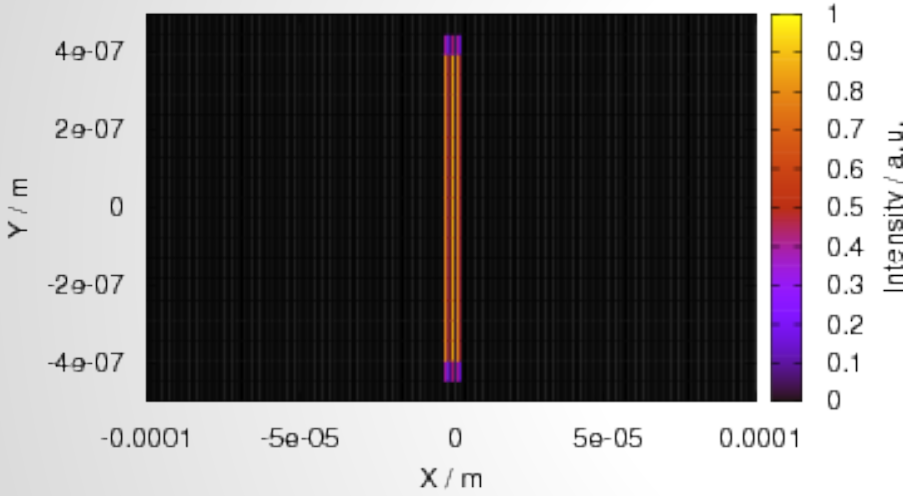
McXtrace

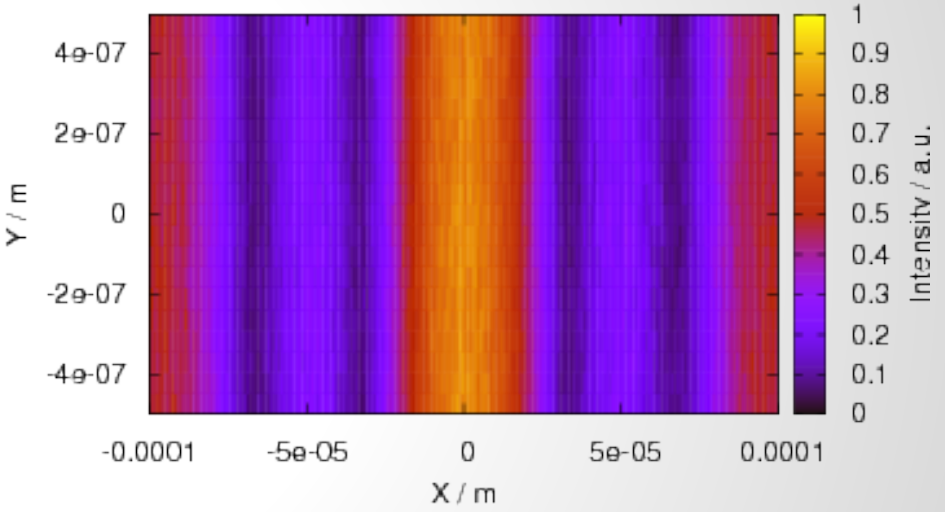
Double Slit

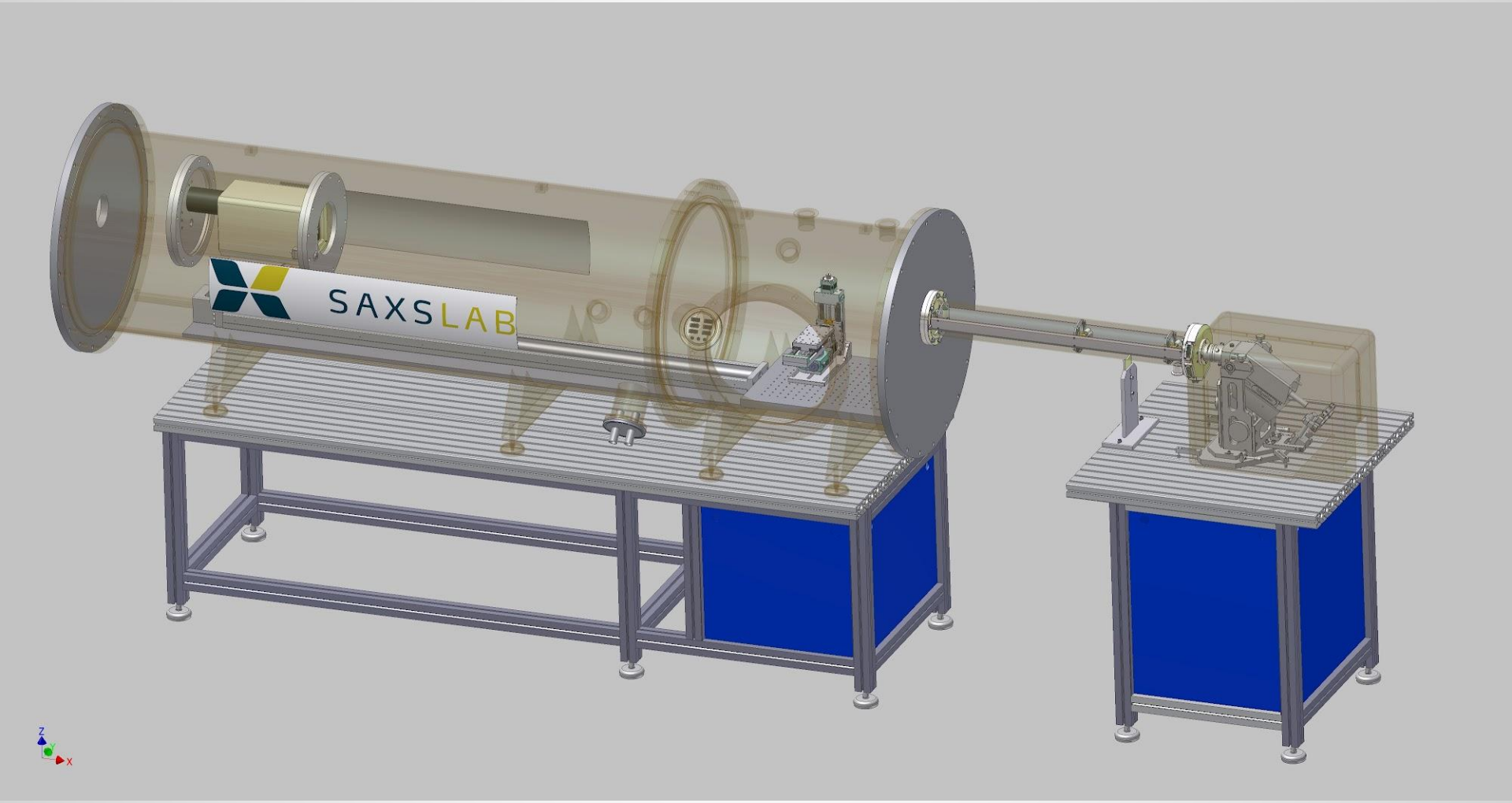


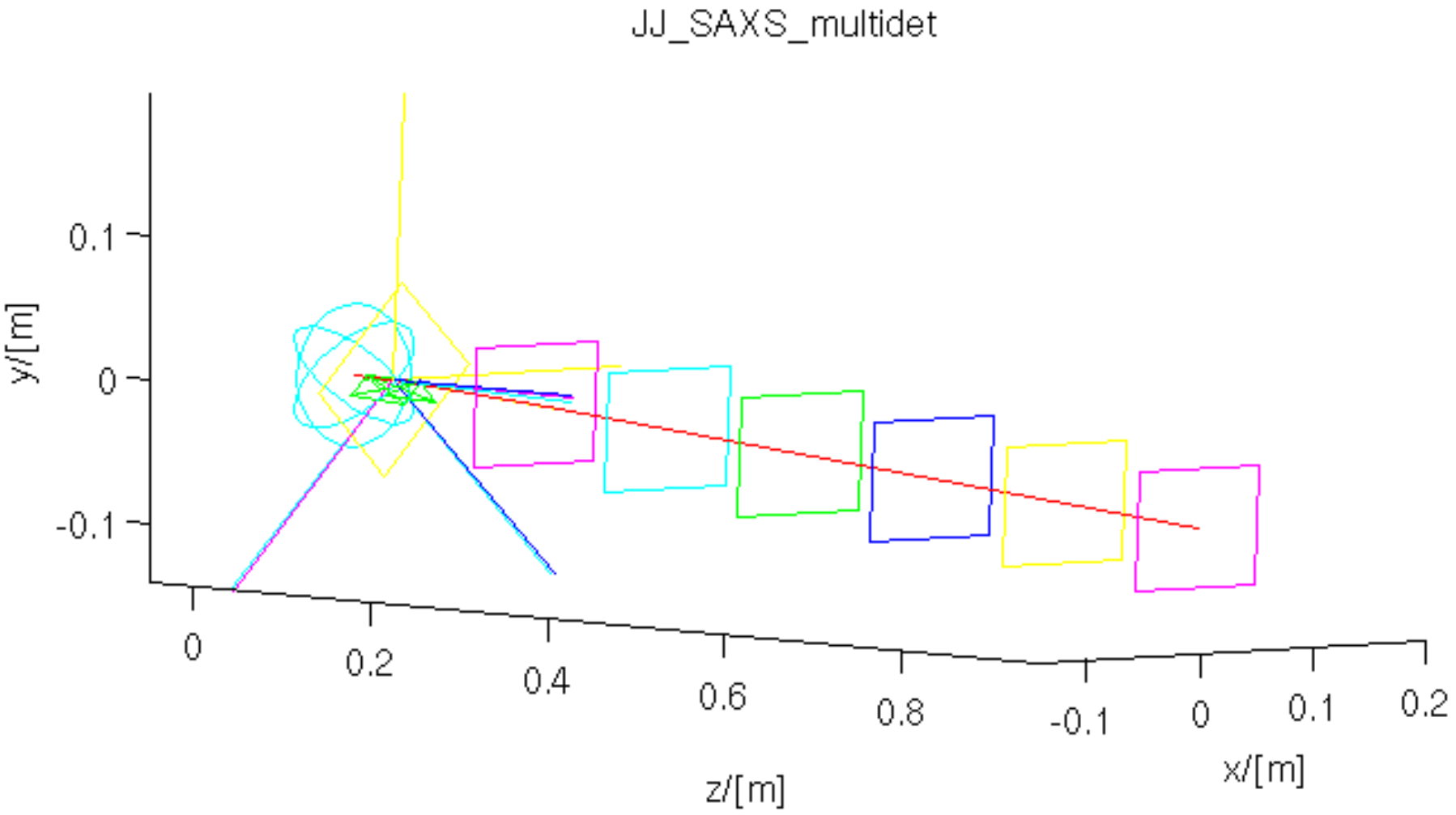


Triple Slit

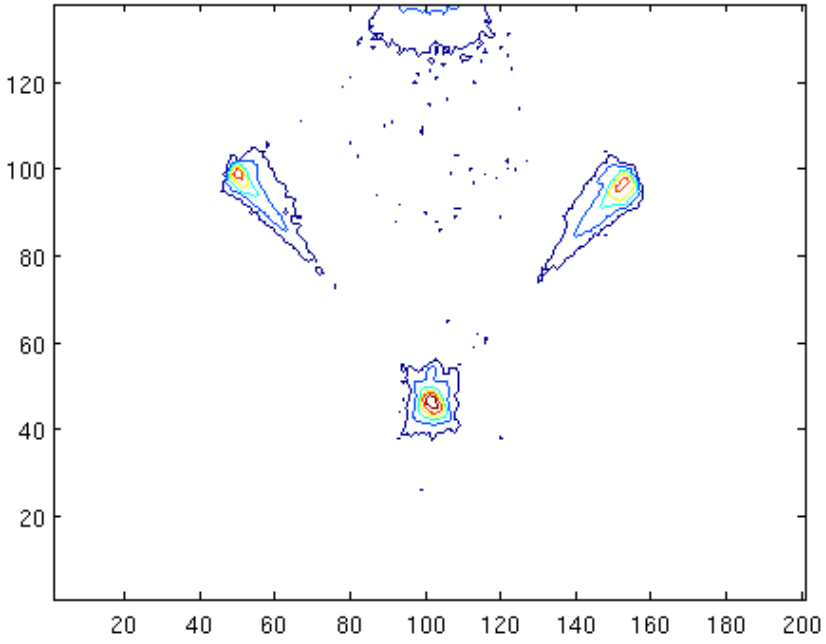

4e-07
2e-07
0
-2e-07
-4e-07
Y / m
-0.0001
-5e-05
0
5e-05
0.0001
X / m
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Intensity / a.u.

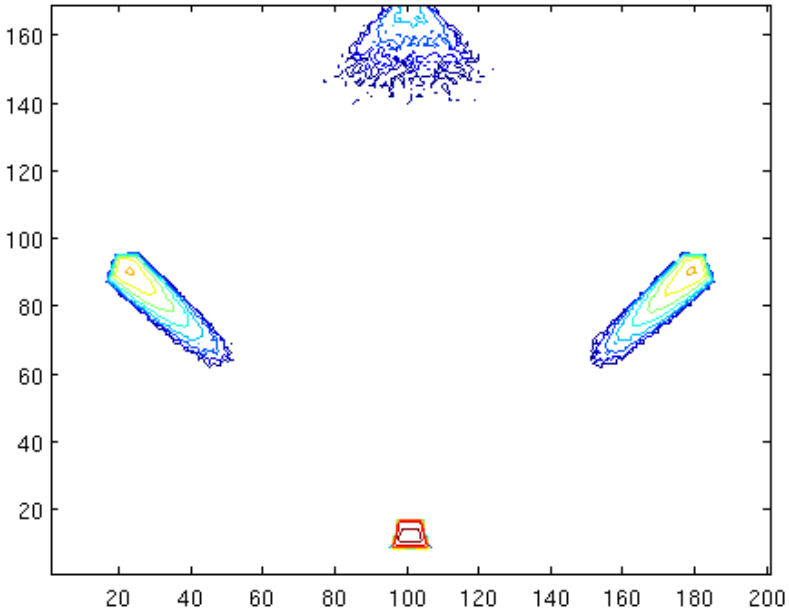

4e-07
2e-07
0
-2e-07
-4e-07
Y / m
-0.0001
-5e-05
0
5e-05
0.0001
X / m
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Intensity / a.u.


SAXSLAB
Z
X


JJ_SAXS_multidet
0.1
0
-0.1
y/[m]
0
0.2
0.4
0.6
0.8
z/[m]
-0.1
0
0.1
0.2
x/[m]

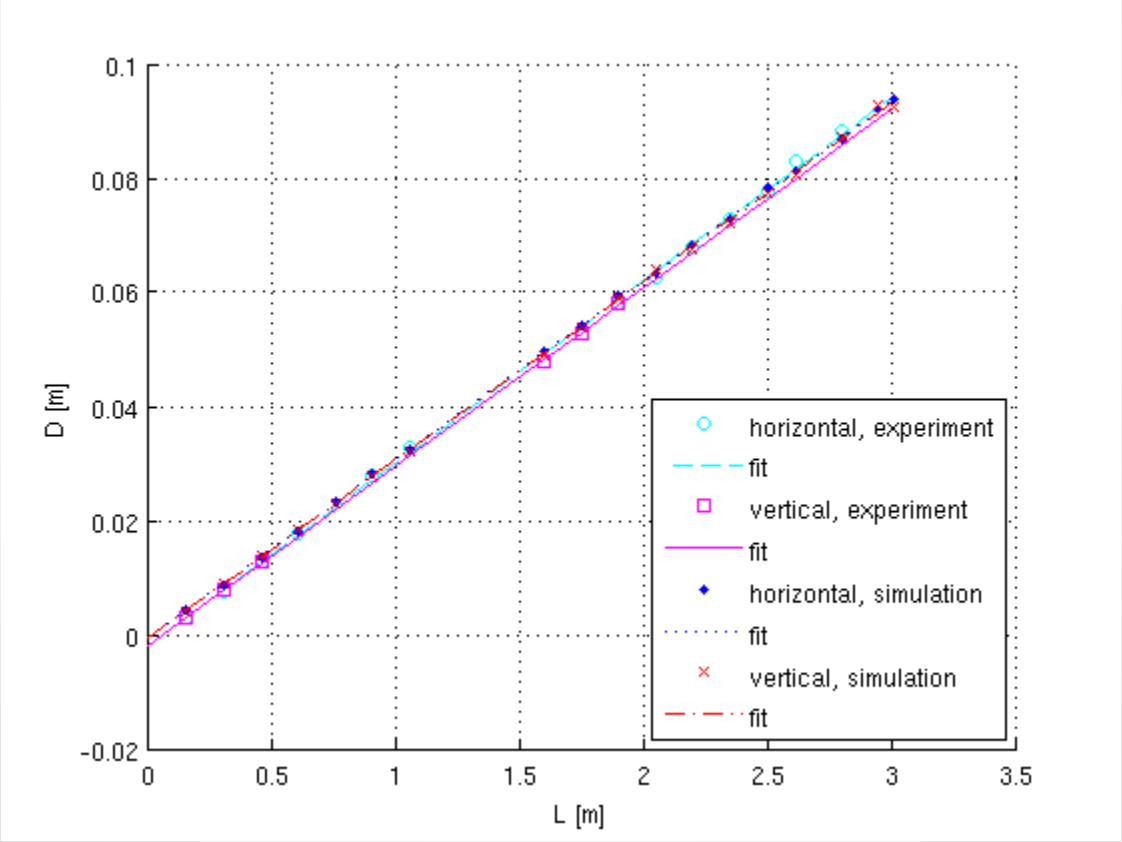
Test Data


120
100
80
60
40
20
20 40 60 80 100 120 140 160 180 200

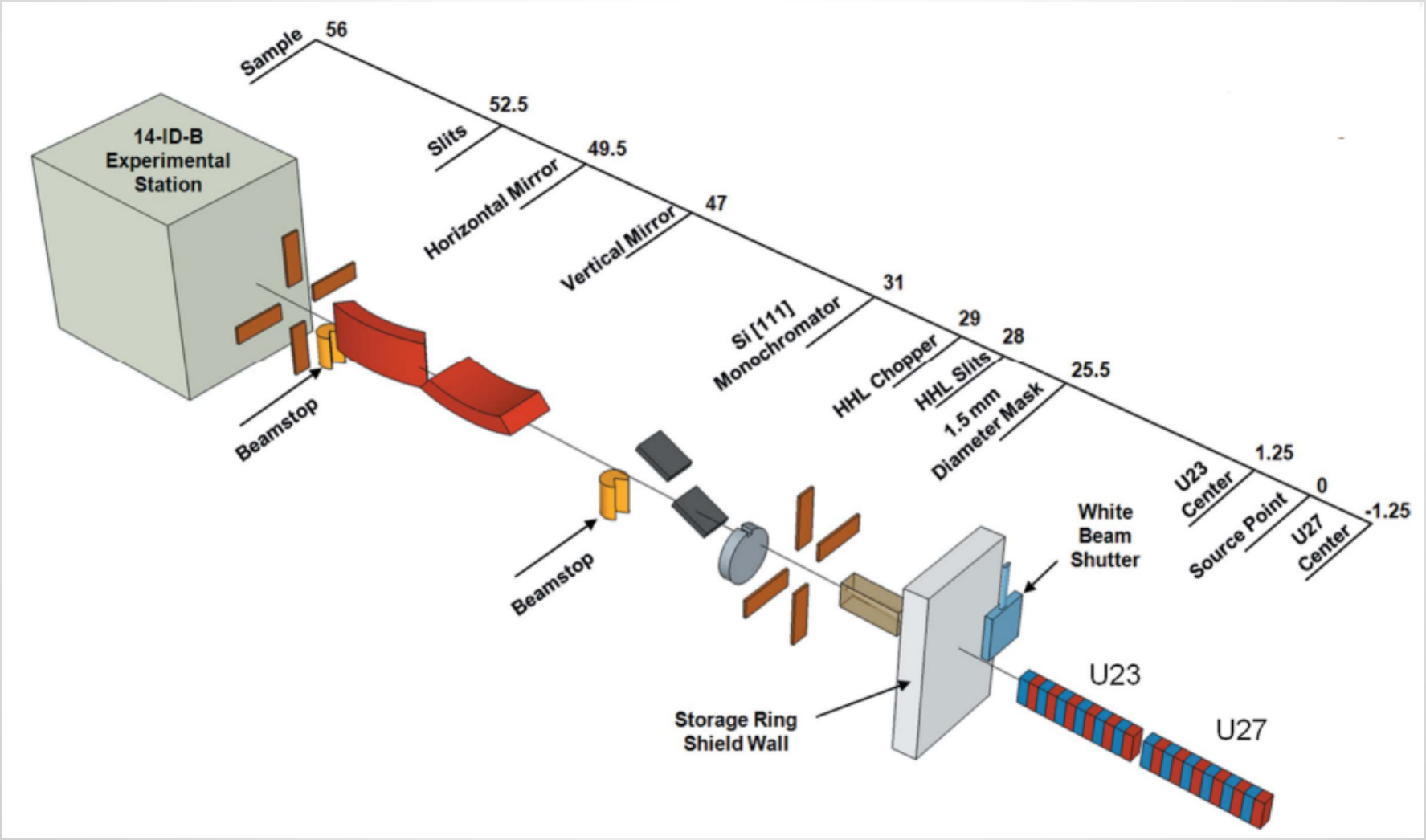

160
140
120
100
80
60
40
20
20 40 60 80 100 120 140 160 180 200

Why different

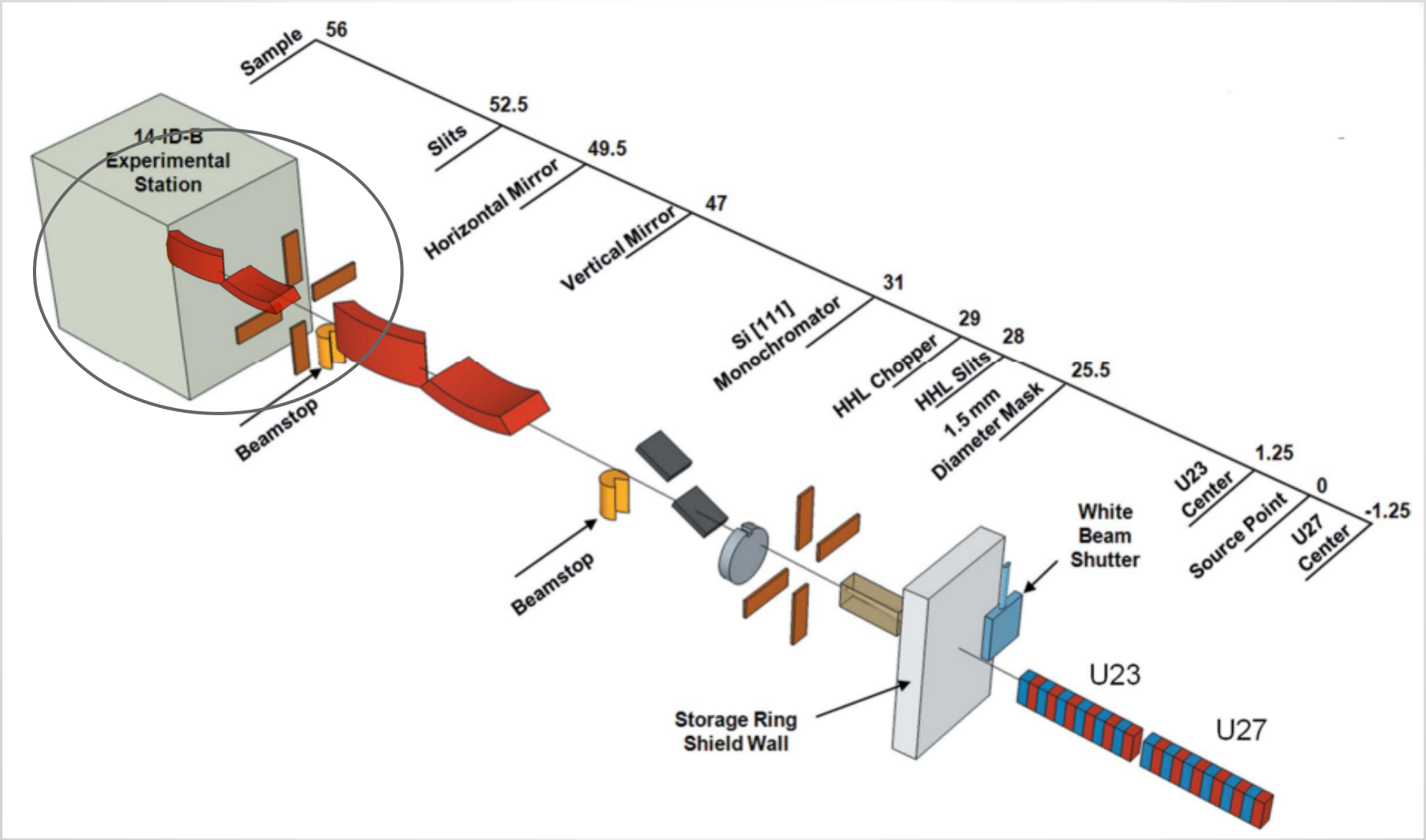
Add an *offset* slit after Side-by-Side KB-mirror



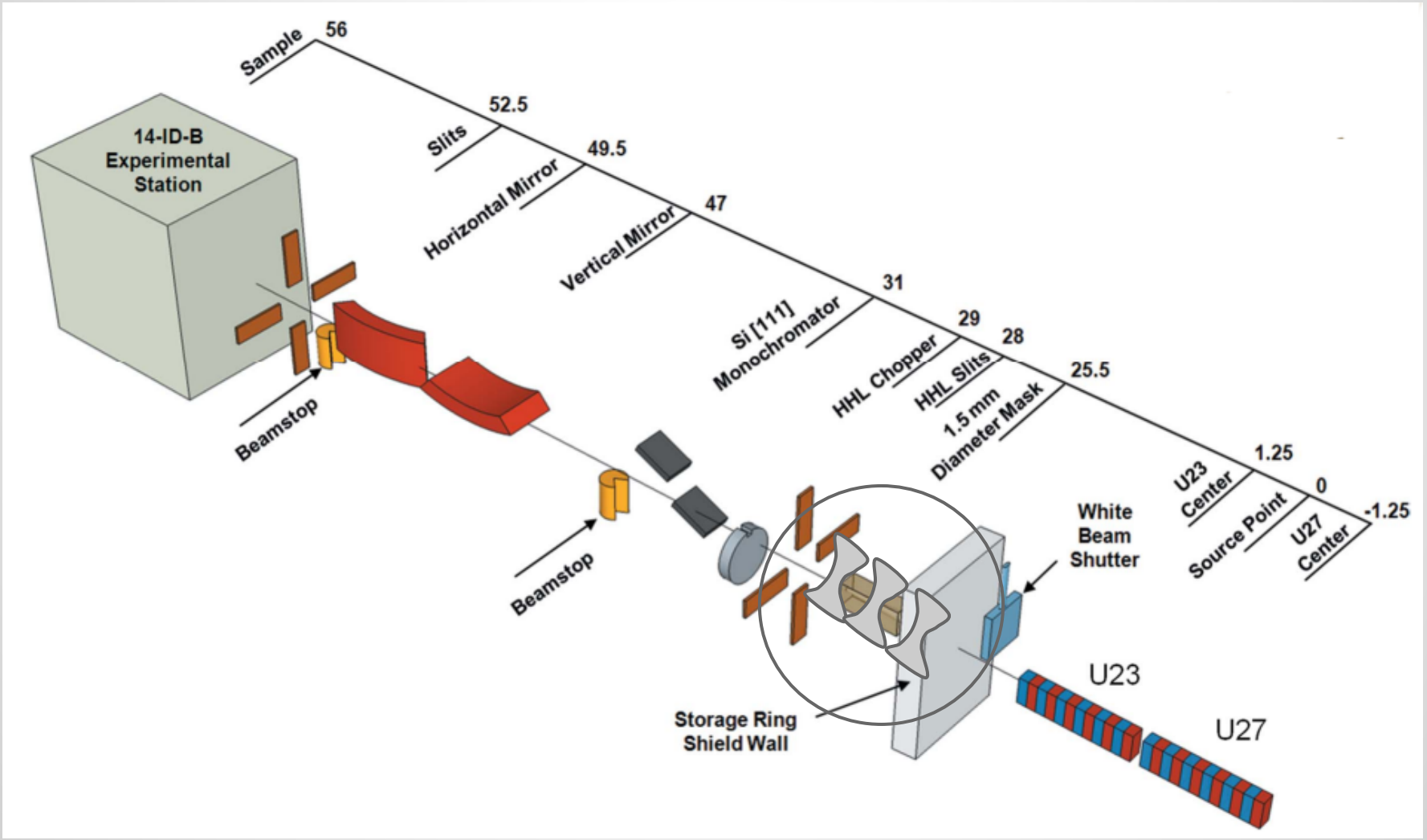
APS ID14 BioCARS



APS ID14 high focus option 1



APS ID14 high focus option 2



1 or 2? simulations can show

- KB-mirrors definitely work
  - but are expensive
  - not easy to align

- upstream CRLs could work - less experience in the community
  - fairly cheap
  - monochromatic-ish
  - quite simple to align (transfocators)

McXtrace

TODO 2012

- Update Manual
- Finish setting up ESRF ID9b
  - skeleton exists
- Prove slit-scatter with crystal sample
- Revamp website
- Publish manual POD (amazon?)
- Consolidate reflectivity models
- Partial Coherence Work
- Finish (a) SPECTRA and (b)SRW interfaces
- Allow python/ruby components?
- McXtrace under ROOT/cling?