McXtrace

"McXtrace: a Monte Carlo software package for simulating X-ray optics, beamlines and experiments", *Journal of Applied Crystallography*, vol. 46, part 3, June 2013

Powered by McStas technology

Outline

- People/Funding etc.
- McXtrace at a glance
- Examples by McXtrace
- Details of a beamline simulation (Max II 811)

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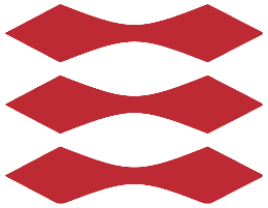
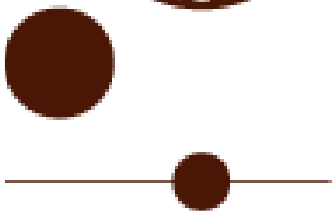
NaBiIT

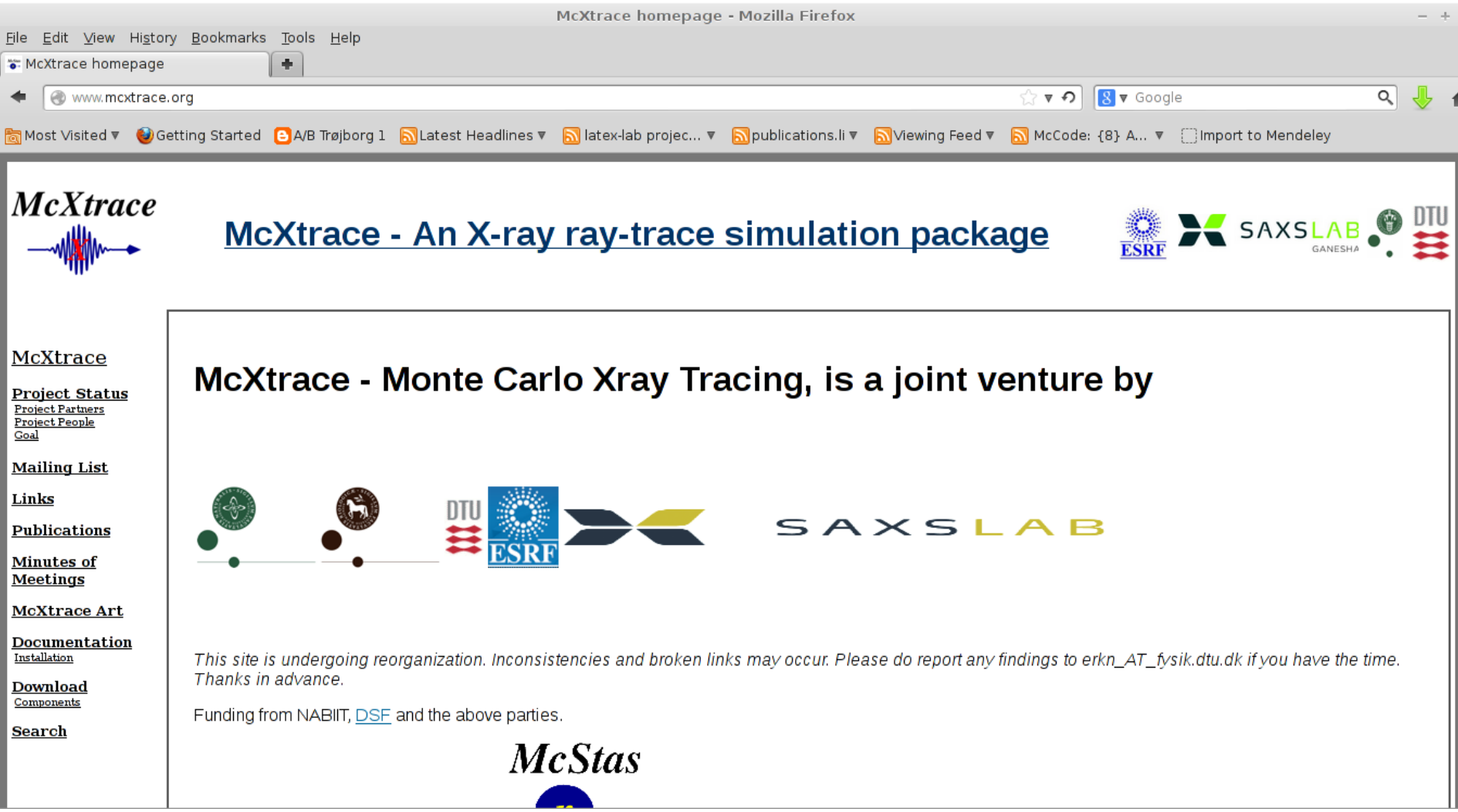
Strategisk Forskningsråd

DTU





SAXSLAB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McXtrace - An X-ray ray-trace simulation package
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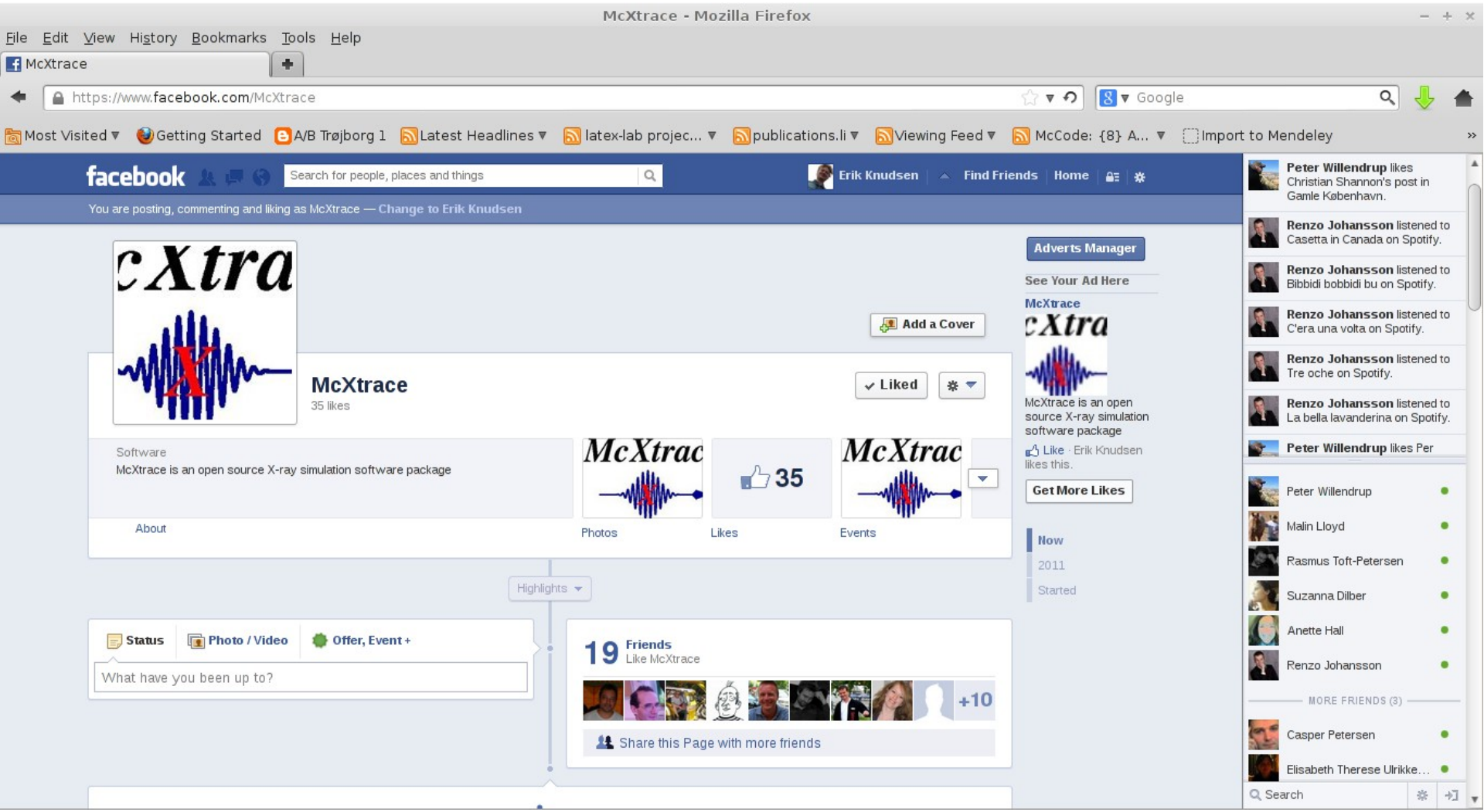
McXtrace - Monte Carlo Xray Tracing, is a joint venture by
DTU
ESRF
SAXSLAB
This site is undergoing reorganization. Inconsistencies and broken links may occur. Please do report any findings to erkn_AT_fysik.dtu.dk if you have the time. Thanks in advance.
Funding from NABIIT, DSF and the above parties.
McStas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South Africa
Venezuela
Colombia
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Brasil (Brazil)
Bolivia
Chile
Argentina
2000 mil
2000 km
Billedmateriale ©2012 NASA, TerraMetrics, Kortdata ©2012 MapLink, Tele Atlas -

McXtrace History

- 1998 McStas 1.0
- 2009 McXtrace project start
  - 2009 McXtrace beta
- 2011 McXtrace 1.0
- 2013 McXtrace 1.1

Feature History

Beta:

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

1.0:

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

1.1:

i. Linux, Windows 7, XP, Mac OSX, FreeBSD
j. Optimized grammar
k. Chopper model
l. Faster data file searching
m. Lots more components
n. More Sample models
o. OFF-support - anyshape options enabled
p. Roughness in lenses
q. Shadow interfaces

McXtrace buzzwords

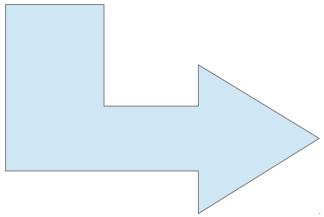
- Built on proven base of McStas for neutron ray tracing
  K. Lefmann and K. Nielsen, Neutron News 10, 20, (1999).
- Release 1.1
- Portable code (Unix/Linux/Mac/Windows, 32 and 64 bit support)
  Has run on all from iPhone to 1000+ node clusters

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

- GPL-license
- DSL / Compiler Technology.
  Using Lex & Yacc
- Modular Open Structure.
  Components/devices written in structured ISO-c automatically fits in the system
- Dependencies: c-compiler (perl/tk for gui).
- Permanent staff at DTU Physics maintaining the code

The McXtrace Way

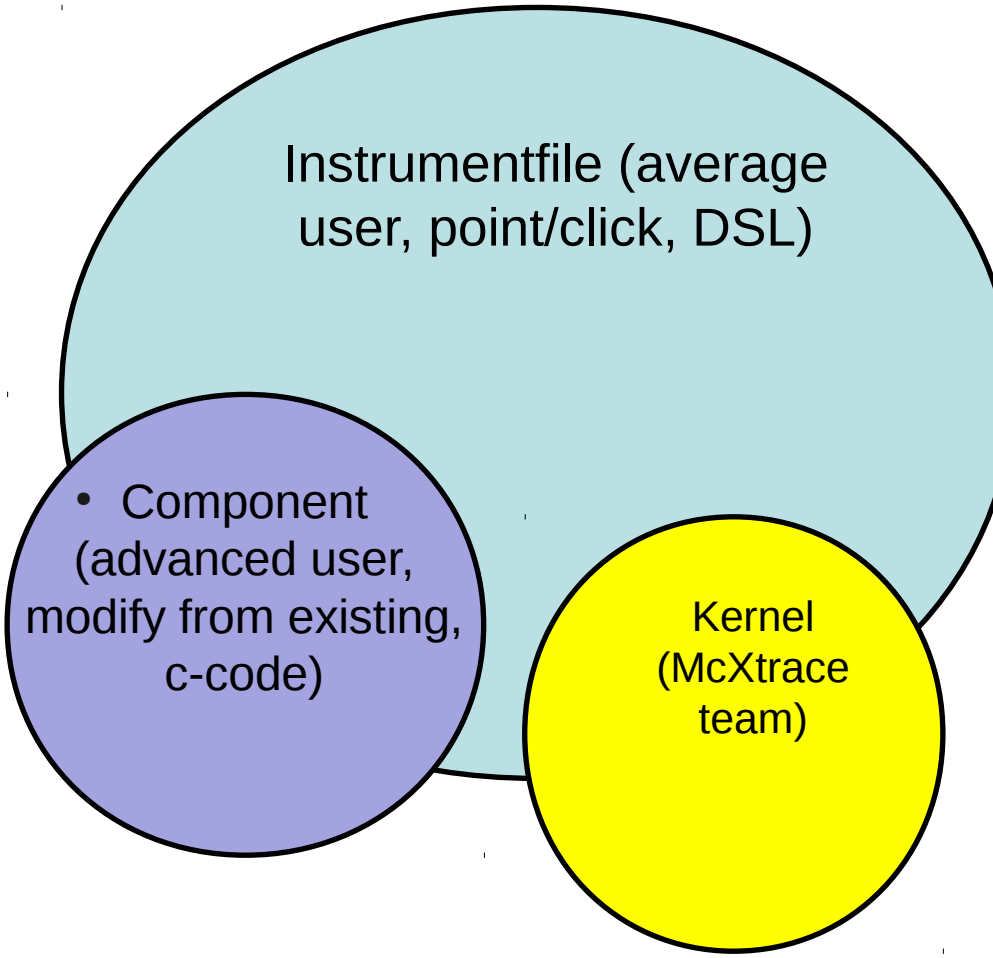
1. Describe your beamline in the McXtrace language (In a text file).
2. Automatically convert beamline into ANSI c
3. Compile
4. Run



1. Optimized for your platform
2. Only includes what you use

Levels of Code

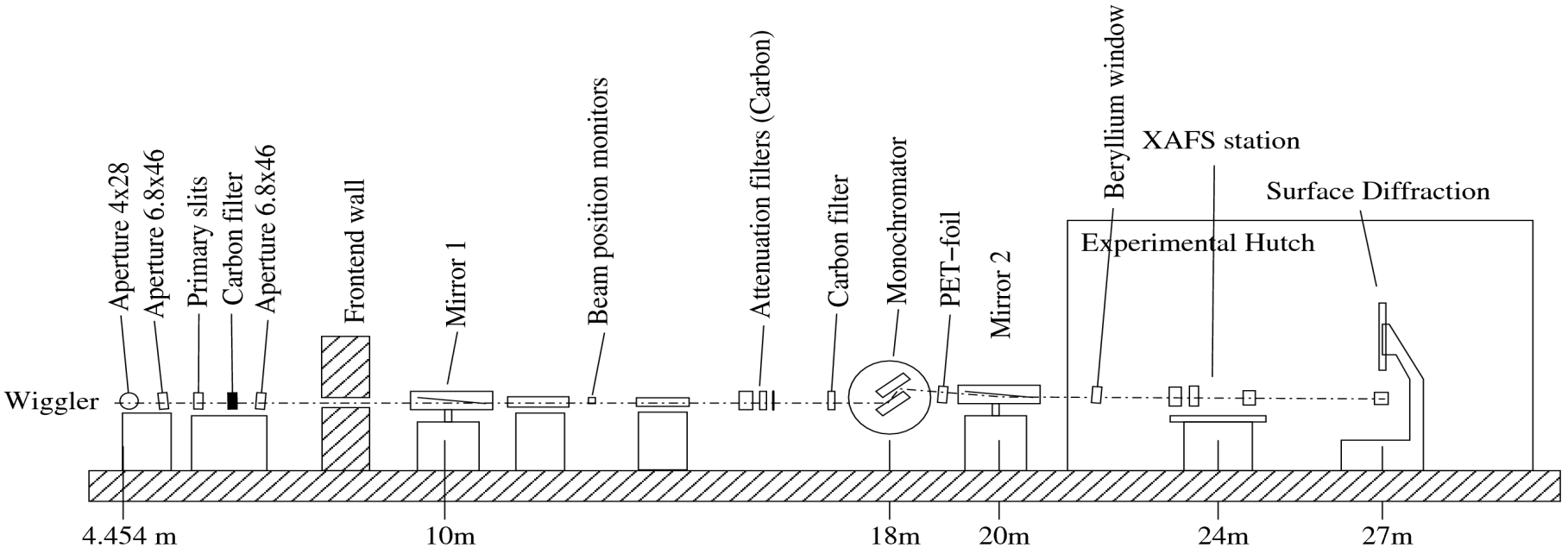
- Instrument file – all users
  - existing examples
  - user written – GUI assisted
- Component files – some users
  - Short pieces of code
  - Easy to modify from existing
- Kernel code – McXtrace developers
  - Propagation routines
  - Intersections
- Generated ISO-C code – “no” users
  - Assembled by code generation
  - Very low overhead of unneeded code
  - Includes runtime libs that comps rely on (propagation etc.)



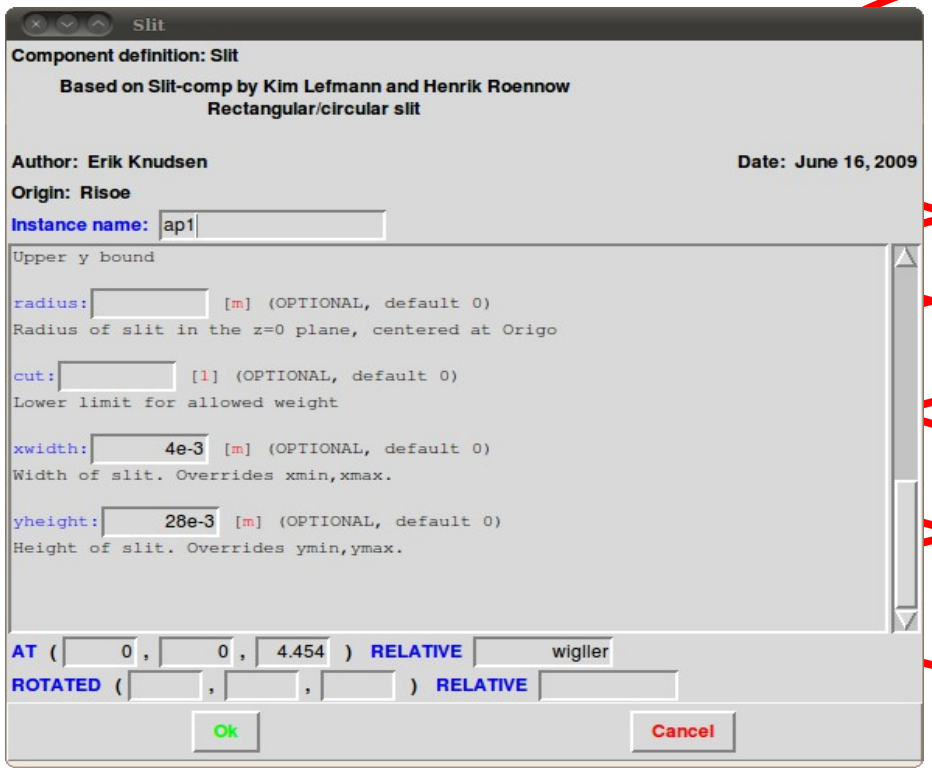
Beamline Description / Instrument File

- Instrument file

  Written by all users

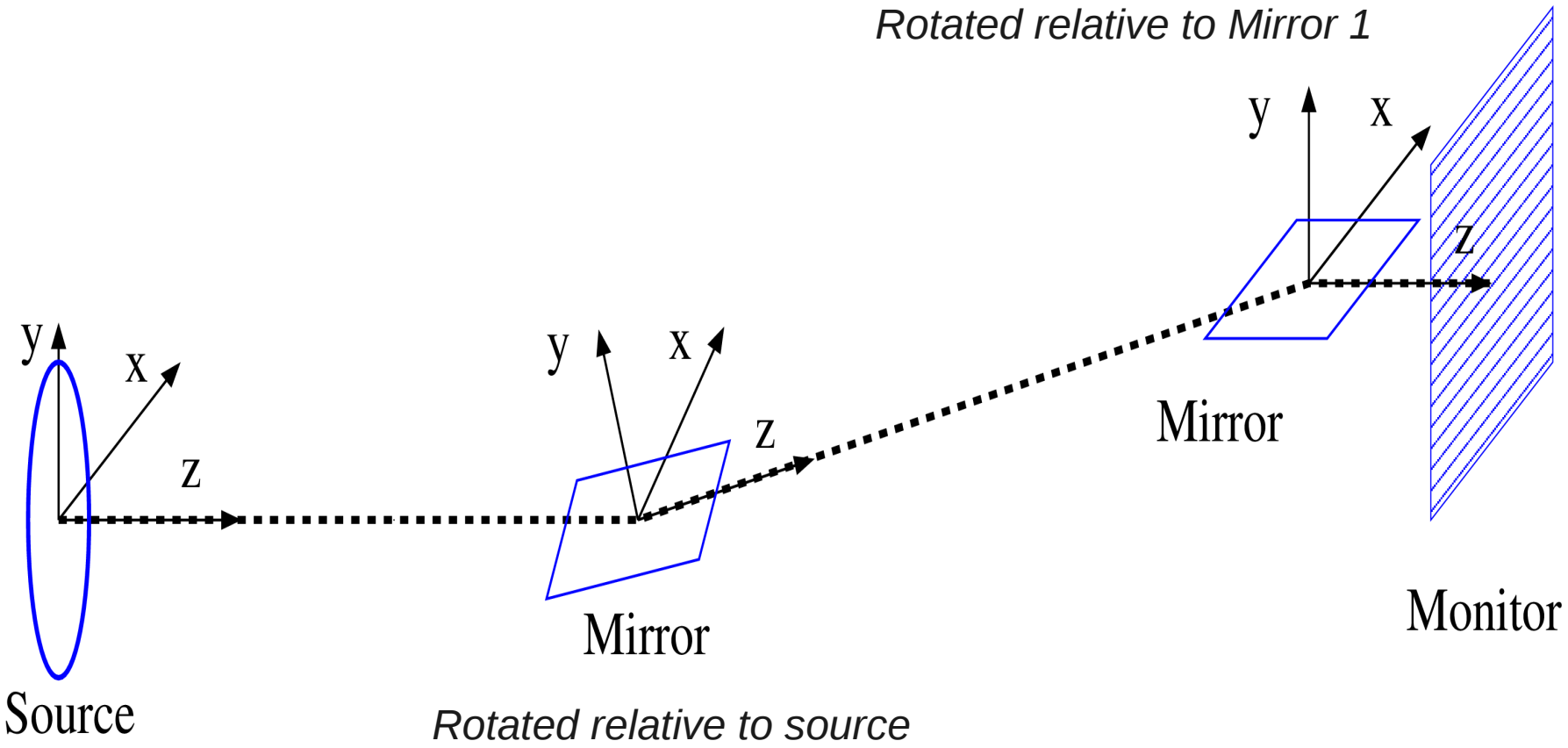


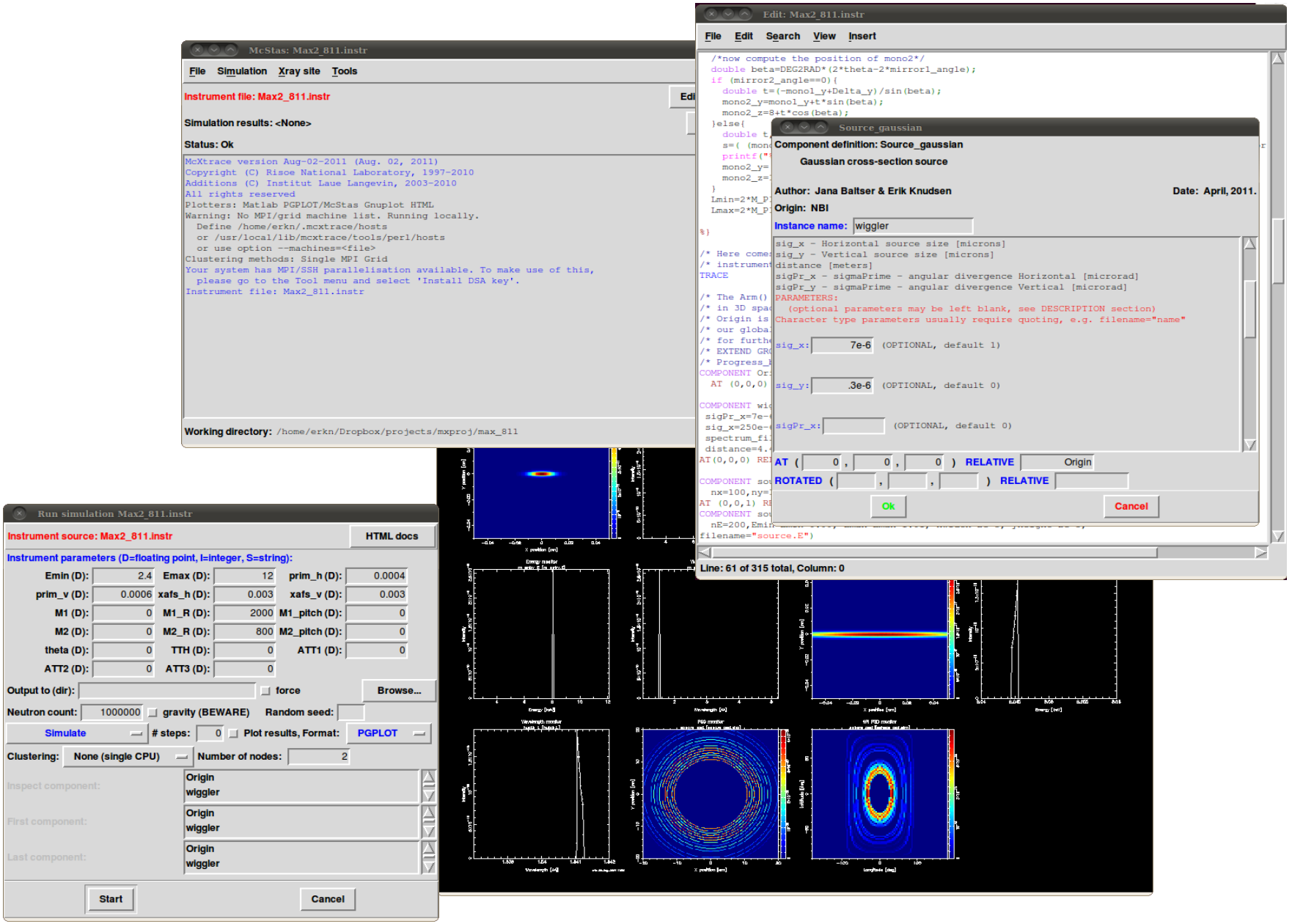
Beamline Description



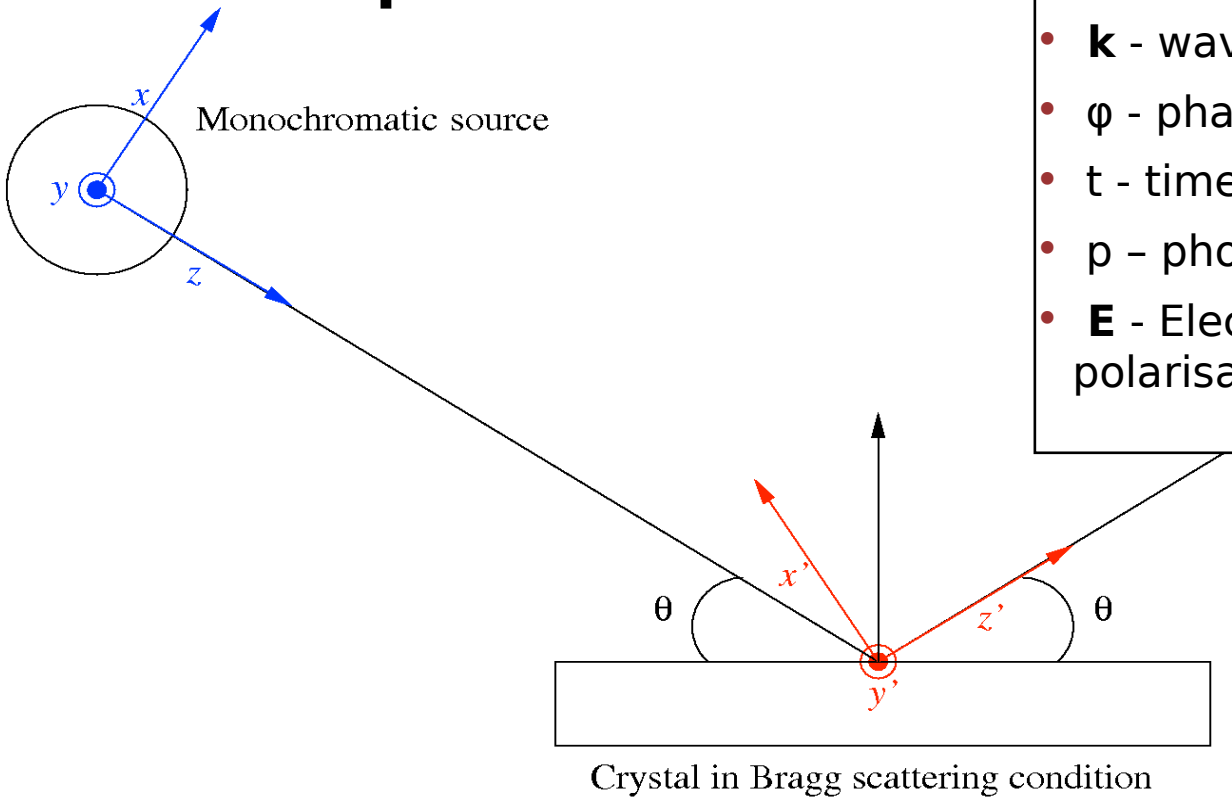

```
123 /* Here comes the TRACE section, where the actual      */
124 /* instrument is defined as a sequence of components.  */
125 TRACE
126 []
127 /* The Arm() class component defines reference points and orientations  */
128 /* in 3D space. Every component instance must have a unique name. Here, */
129 /* Origin is used. This Arm() component is set to define the origin of  */
130 /* our global coordinate system (AT (0,0,0) ABSOLUTE). It may be used   */
131 /* for further RELATIVE reference, Other useful keywords are : ROTATED  */
132 /* EXTEND GROUP PREVIOUS. Also think about adding a neutron source !    */
133 /* Progress_bar is an Arm displaying simulation progress.              */
134 COMPONENT Origin = Progress_bar()
135   AT (0,0,0) ABSOLUTE
136
137 COMPONENT wiggler = Source_gaussian(
138  sigPr_x=7e-6*FWHM2RMS, sigPr_y=0.3e-6*FWHM2RMS,
139  sig_x=250e-6*FWHM2RMS, sig_y=50e-6*FWHM2RMS,
140  spectrum_file="characteristics.dc0",E0=(Emin+Emax)/2.0,dE=(Emax-Emin)/2.0,
141  distance=4.454,dlambda=0)
142 AT(0,0,0) RELATIVE Origin
143
144 COMPONENT source_psd=PSD_monitor(
145   nx=100,ny=100,xwidth=1e-3,yheight=1e-3,filename="source.psd")
146 AT (0,0,1) RELATIVE wiggler
147 COMPONENT source_E=E_monitor(
148   nE=200,Emin=Emin*0.99, Emax=Emax*1.01, xwidth=2e-3, yheight=2e-3,
149 filename="source.E")
150 AT (0,0,1e-9) RELATIVE PREVIOUS
151 COMPONENT source_L=L_monitor(
152   nL=200,Lmin=Lmin*0.99, Lmax=Lmax*1.01, xwidth=2e-3, yheight=2e-3,
153 filename="source.L")
154 AT (0,0,1e-9) RELATIVE PREVIOUS
155
156 COMPONENT ap1 = Slit(
157   yheight=4e-3, xwidth=28e-3)
158 AT(0,0,4.454) RELATIVE wiggler
159
160 COMPONENT ap2 = Slit(
161   yheight=6.8e-3,xwidth=46e-3)
162 AT(0,0,ap2_L) RELATIVE wiggler
```

McXtrace positioning scheme




McStas: Max2_811.instr
File Simulation Xray site Tools
Instrument file: Max2_811.instr
Simulation results: <None>
Status: Ok
McXtrace version Aug-02-2011 (Aug. 02, 2011)
Copyright (C) Risoe National Laboratory, 1997-2010
Additions (C) Institut Laue Langevin, 2003-2010
All rights reserved
Plotters: Matlab PGPLOT/McStas Gnuplot HTML
Warning: No MPI/grid machine list. Running locally.
Define /home/erkn/.mcxtrace/hosts
or /usr/local/lib/mcxtrace/tools/perl/hosts
or use option --machines=<file>
Clustering methods: Single MPI Grid
Your system has MPI/SSH parallelisation available. To make use of this,
please go to the Tool menu and select 'Install DSA key'.
Instrument file: Max2_811.instr
Working directory: /home/erkn/Dropbox/projects/mxproj/max_811
Edit: Max2_811.instr
File Edit Search View Insert
/*now compute the position of mono2*/
double beta=DEG2RAD*(2*theta-2*mirror1_angle);
if (mirror2_angle==0){
double t=(-mono1_y+Delta_y)/sin(beta);
mono2_y=mono1_y+t*sin(beta);
mono2_z=8+t*cos(beta);
}else{
Source_gaussian
Component definition: Source_gaussian
Gaussian cross-section source
Author: Jana Baltser & Erik Knudsen
Date: April, 2011.
Origin: NBI
Instance name: wiggler
sig_x - Horizontal source size [microns]
sig_y - Vertical source size [microns]
distance [meters]
sigPr_x - sigmaPrime - angular divergence Horizontal [microrad]
sigPr_y - sigmaPrime - angular divergence Vertical [microrad]
PARAMETERS:
(optional parameters may be left blank, see DESCRIPTION section)
Character type parameters usually require quoting, e.g. filename="name"
sig_x: 7e-6 (OPTIONAL, default 1)
sig_y: .3e-6 (OPTIONAL, default 0)
sigPr_x: (OPTIONAL, default 0)
AT (0 , 0 , 0) RELATIVE Origin
ROTATED (, ,) RELATIVE
Ok
Cancel
filename="source.E")
Line: 61 of 315 total, Column: 0
Run simulation Max2_811.instr
Instrument source: Max2_811.instr
HTML docs
Instrument parameters (D=floating point, I=integer, S=string):
Emin (D): 2.4
Emax (D): 12
prim_h (D): 0.0004
prim_v (D): 0.0006
xafs_h (D): 0.003
xafs_v (D): 0.003
M1 (D): 0
M1_R (D): 2000
M1_pitch (D): 0
M2 (D): 0
M2_R (D): 800
M2_pitch (D): 0
theta (D): 0
TTH (D): 0
ATT1 (D): 0
ATT2 (D): 0
ATT3 (D): 0
Output to (dir):
force
Browse...
Neutron count: 1000000
gravity (BEWARE)
Random seed:
Simulate
steps: 0
Plot results, Format: PGPLOT
Clustering: None (single CPU)
Number of nodes: 2
Inspect component:
Origin
wiggler
First component:
Origin
wiggler
Last component:
Origin
wiggler
Start
Cancel

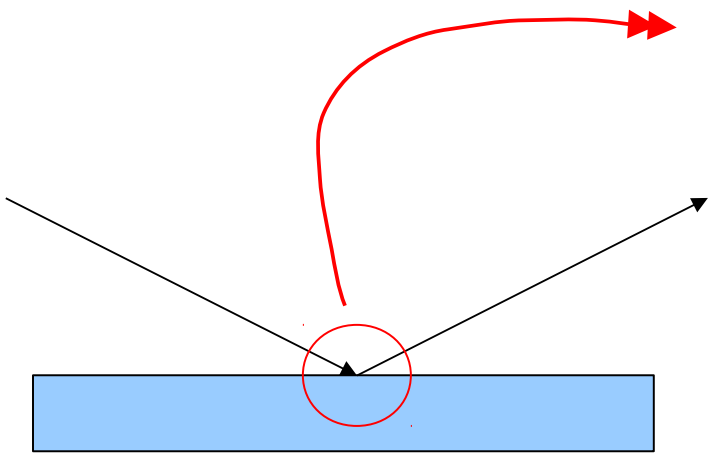
McXtrace photon model



- Photon ray/package:
- (**r**,**k**,φ,t,p,**E**)
- **r** - spatial coordinates
- **k** - wave vector
- φ - phase
- t - time
- p – photon weight package
- **E** - Electrical field polarisation

Component Internals

Written by expert users and developers
Where photons interact with beamline objects ->
Where physics happen
Structured ISO-C



```
90    /*correction for only solving in xz-plane*/
91    dl*=sqrt(scalar_prod(kx,ky,kz,kx,ky,kz)/scalar_prod(kx,0,kz,kx,0,kz));
92
93    PROP_DL(dl);
94    alpha=asin(z/radius);
95    if (length<radius*alpha){
96      ABSORB;
97      //restore_xray(&x,&y,&z,&kx,&ky,&kz,&phi,&Ex,&Ey,&Ez,&p);
98    }else{
99      SCATTER;
100     /*reflection*/
101     nx=radius-x;
102     nz=-z;
103     n=sqrt(nx*nx+nz*nz);
104     nx/=n;
105     nz/=n;
106
107     s=scalar_prod(kx,0,kz,nx,0,nz);
108     kx=kx-2*s*nx;
109     kz=kz-2*s*nz;
110
111
112     if (prmsp && !R0){
113       /*compute reflectivity from material data*/
```

Component history - 2009

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

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

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

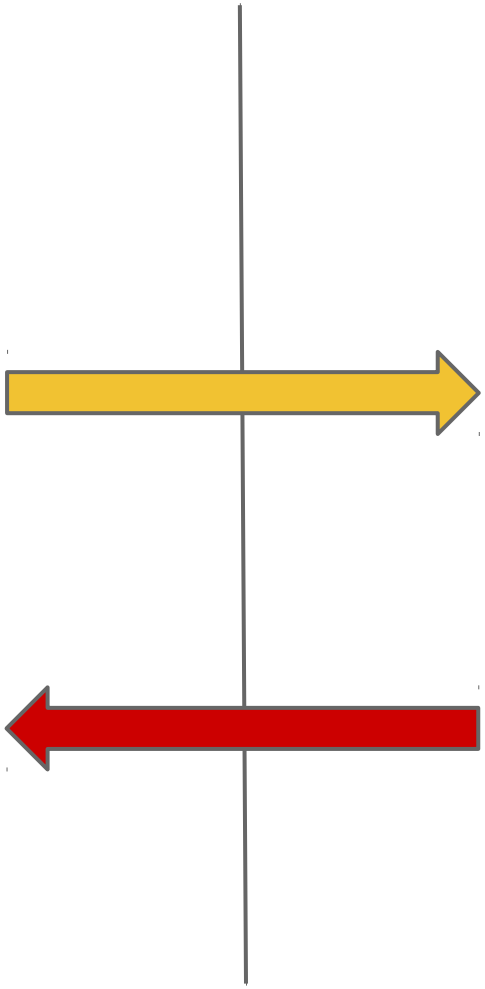
McStas

Geometry engine

Fast runtime library

Monitor models

Crystal sample models



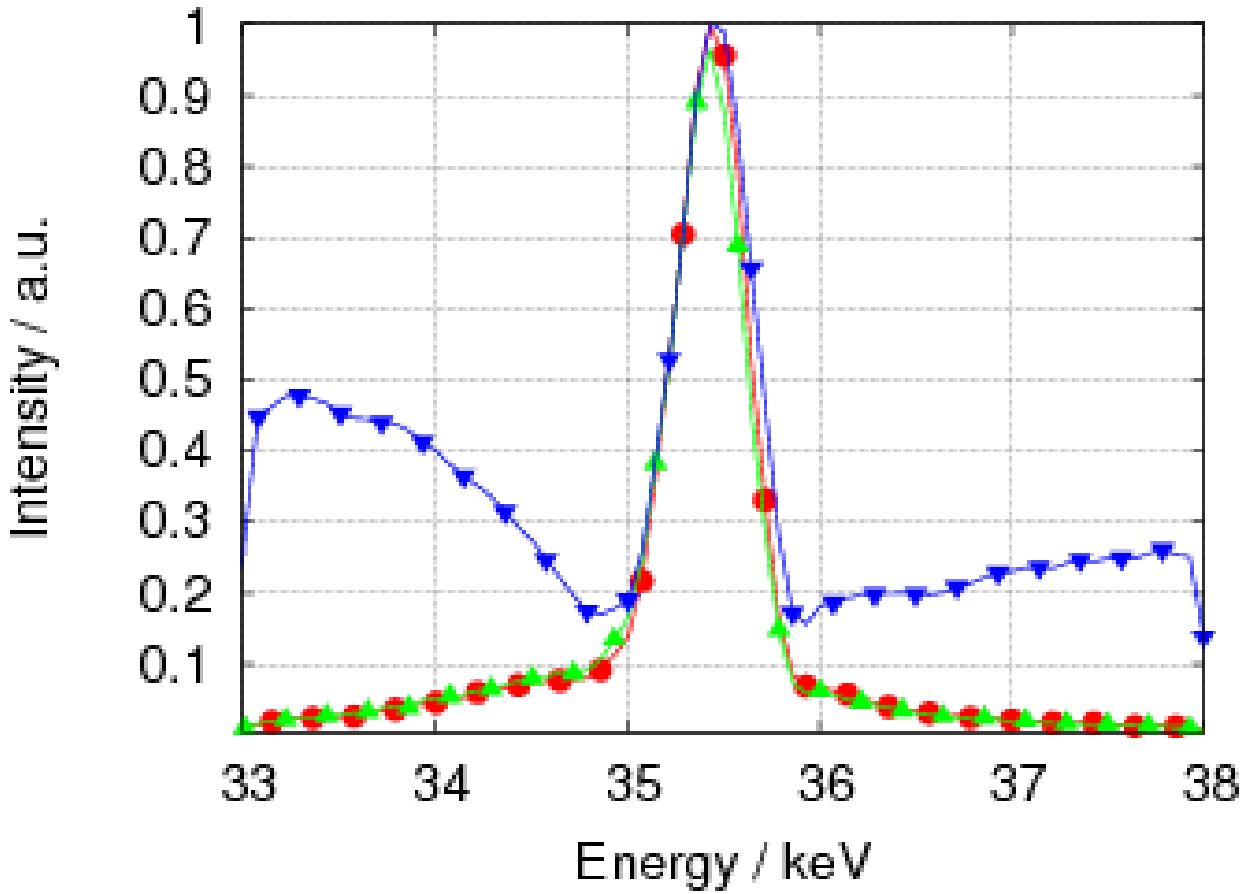
McXtrace

Binary datafile searching

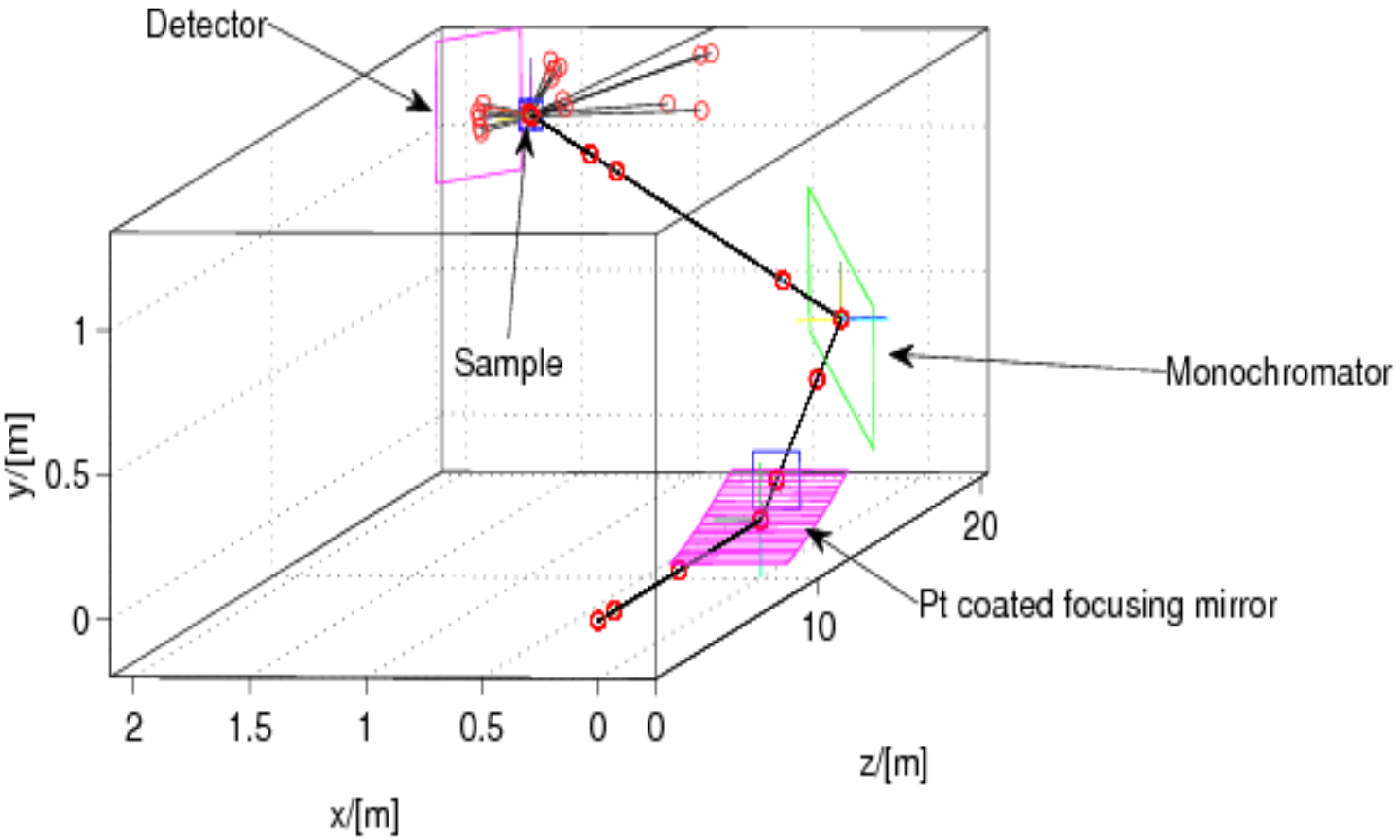
Perfect crystal model

Phase handling (?)

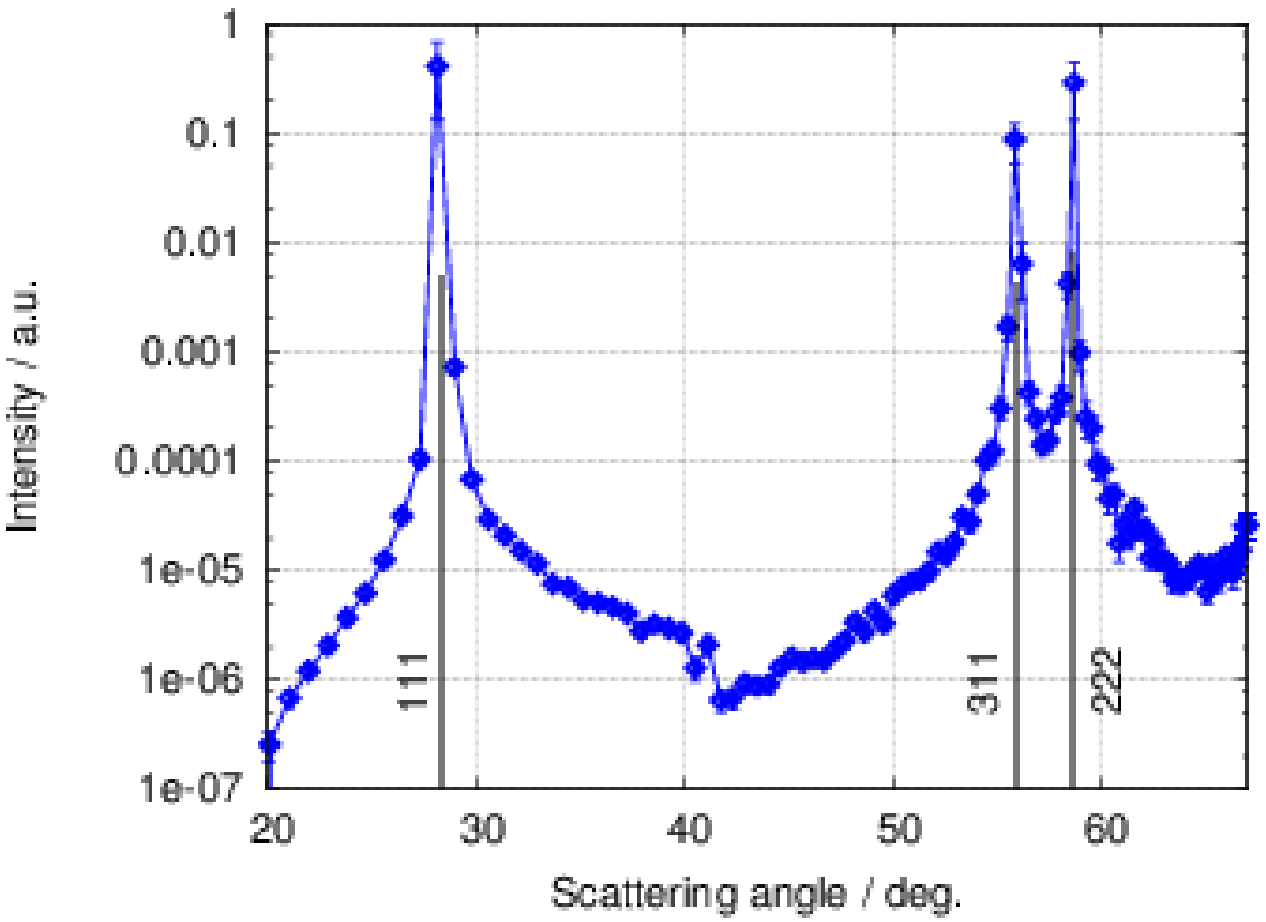
ID11 pink beam monochromator



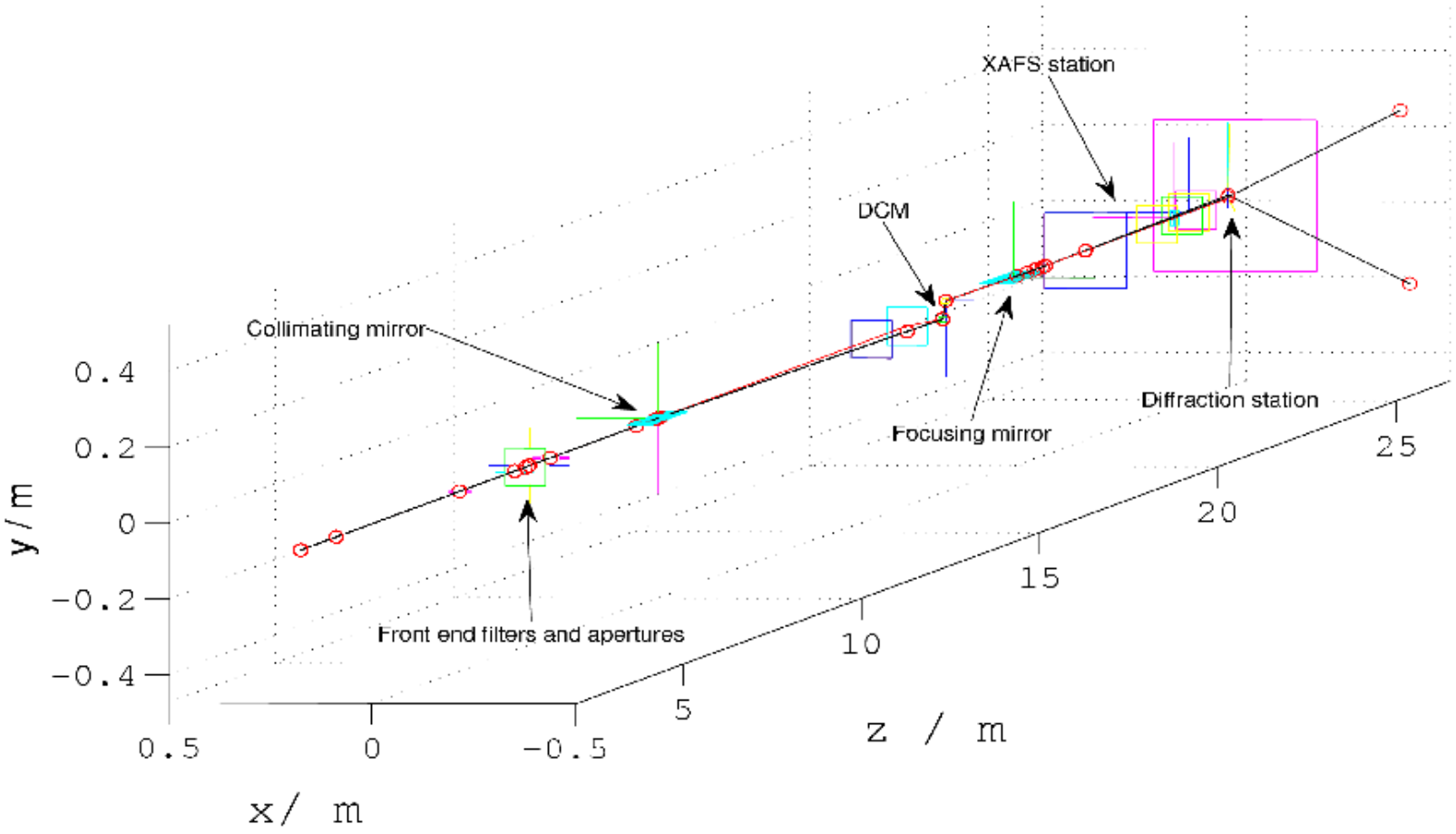
Max II 711 Powder Diffraction



Max II 711 Powder Diffraction Si-crystal

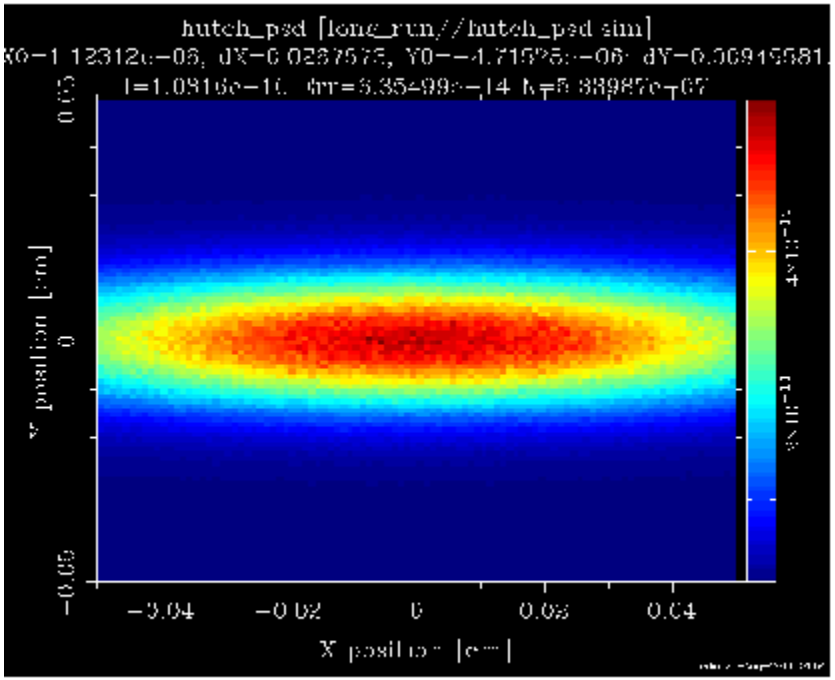


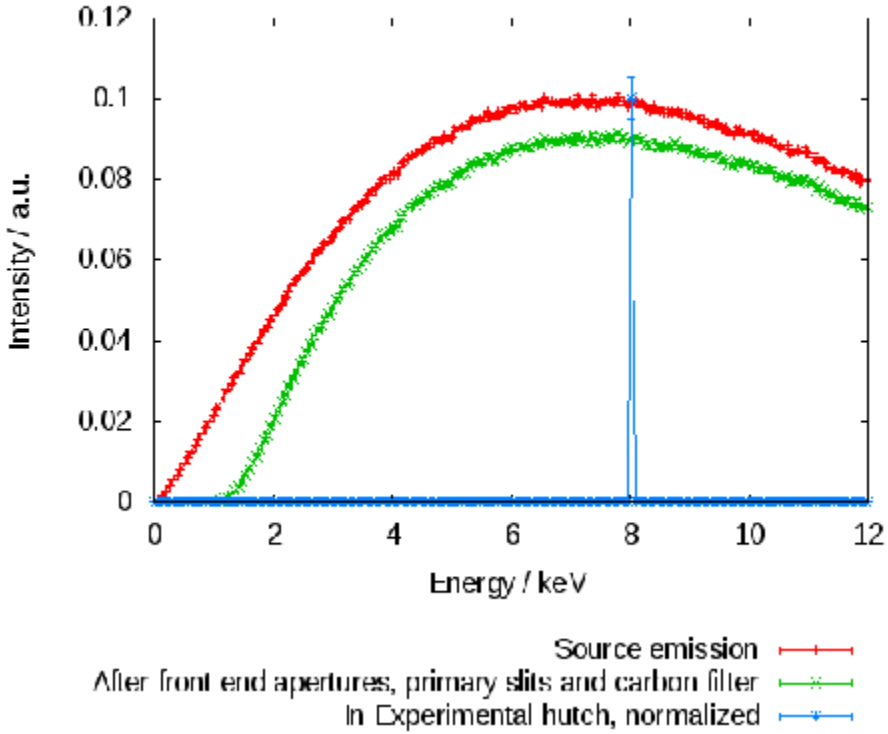
Max II 811, surface diffraction and XAFS beamline



Max II 811, surface diffraction and XAFS beamline

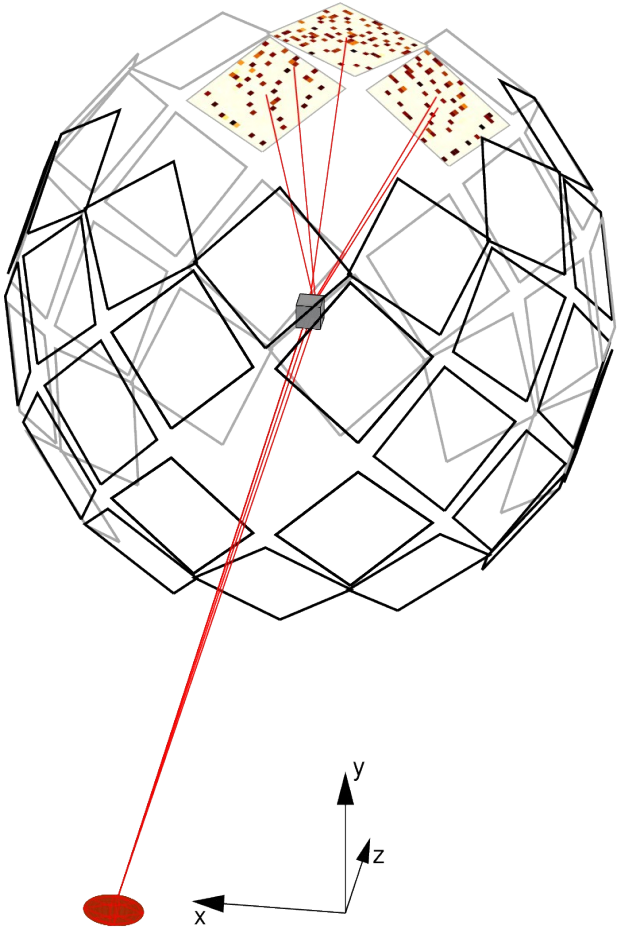
- Unslit Spatial beam distribution

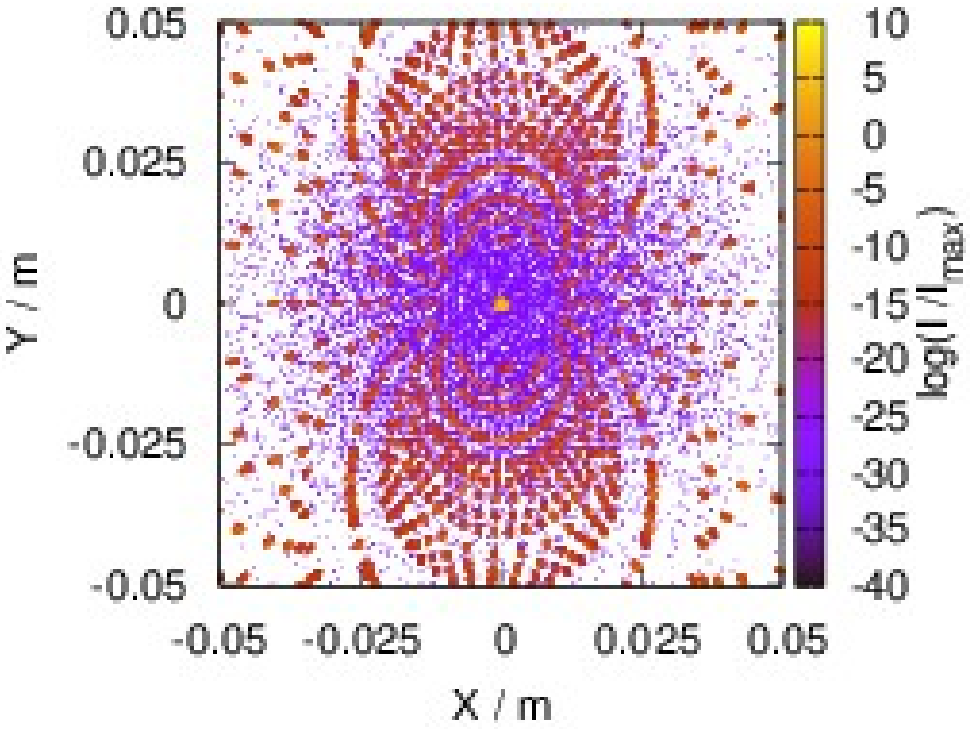




Reported flux on sample: [2000...20000] photons /s
Simulated flux on sample: 20080 photons / s

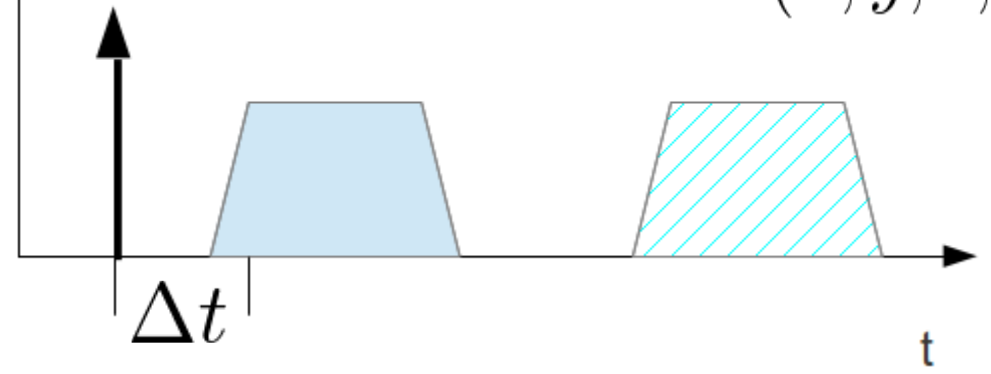
Laue Camera

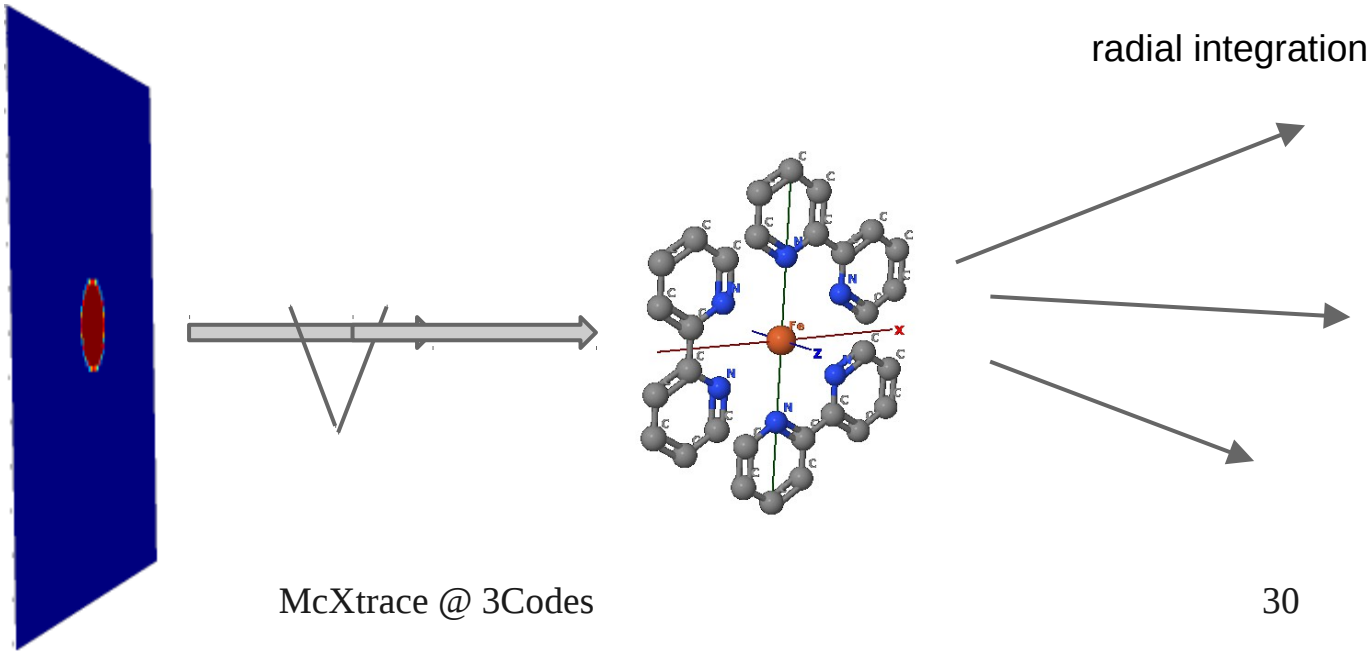

y
z
x


0.05
0.025
0
-0.025
-0.05
Y / m
-0.05
-0.025
0
0.025
0.05
X / m
10
5
0
-5
-10
-15
-20
-25
-30
-35
-40
log(I / I_max)

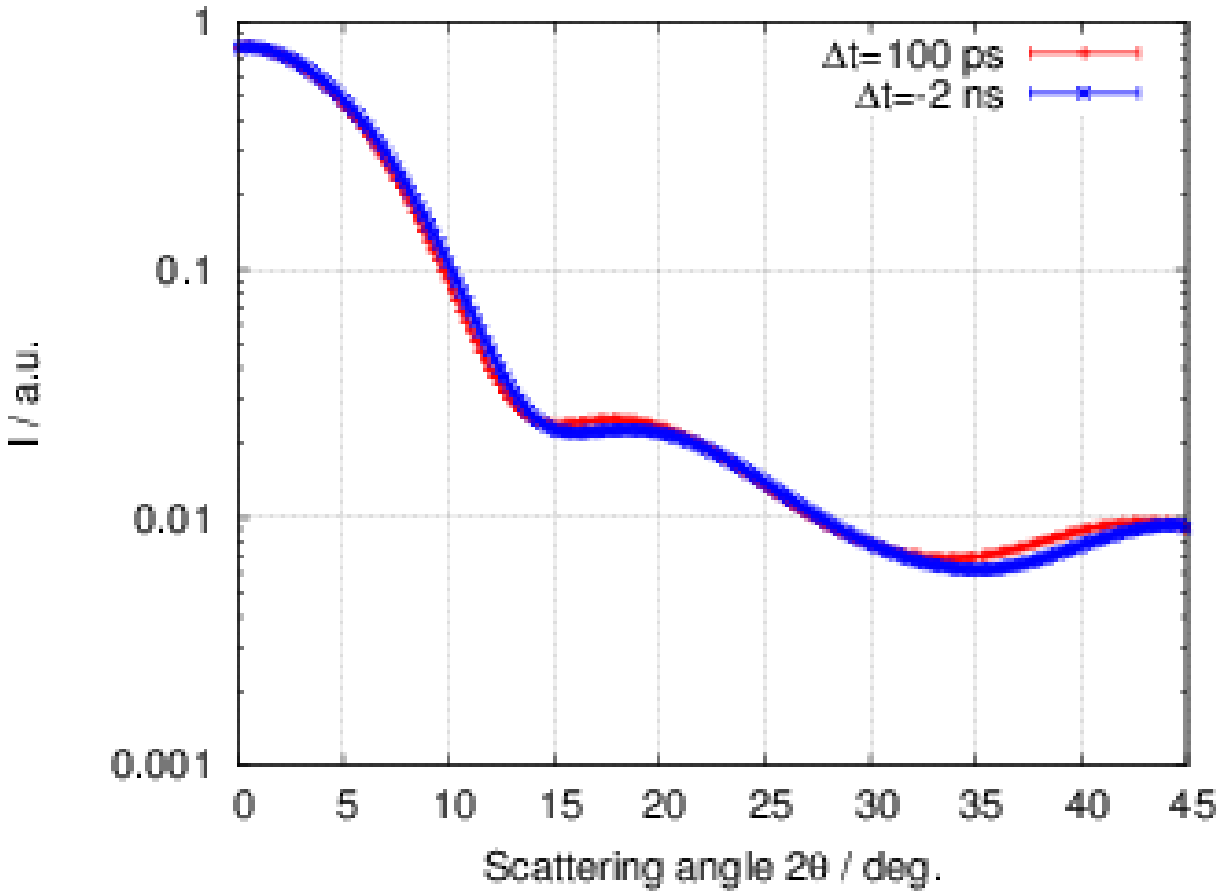
Time resolved scattering, Pump & Probe

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

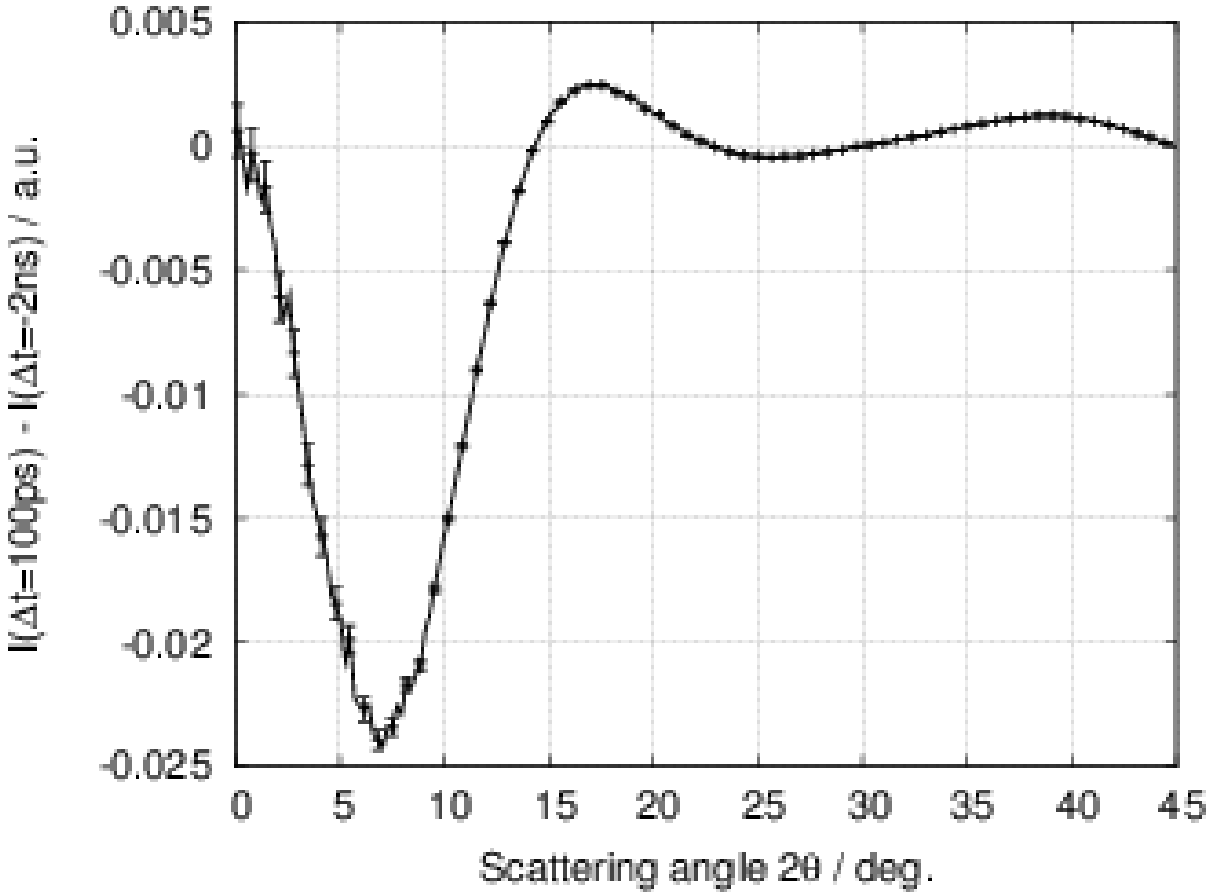




Time resolved scattering, Fe (2,2' bpy)_3

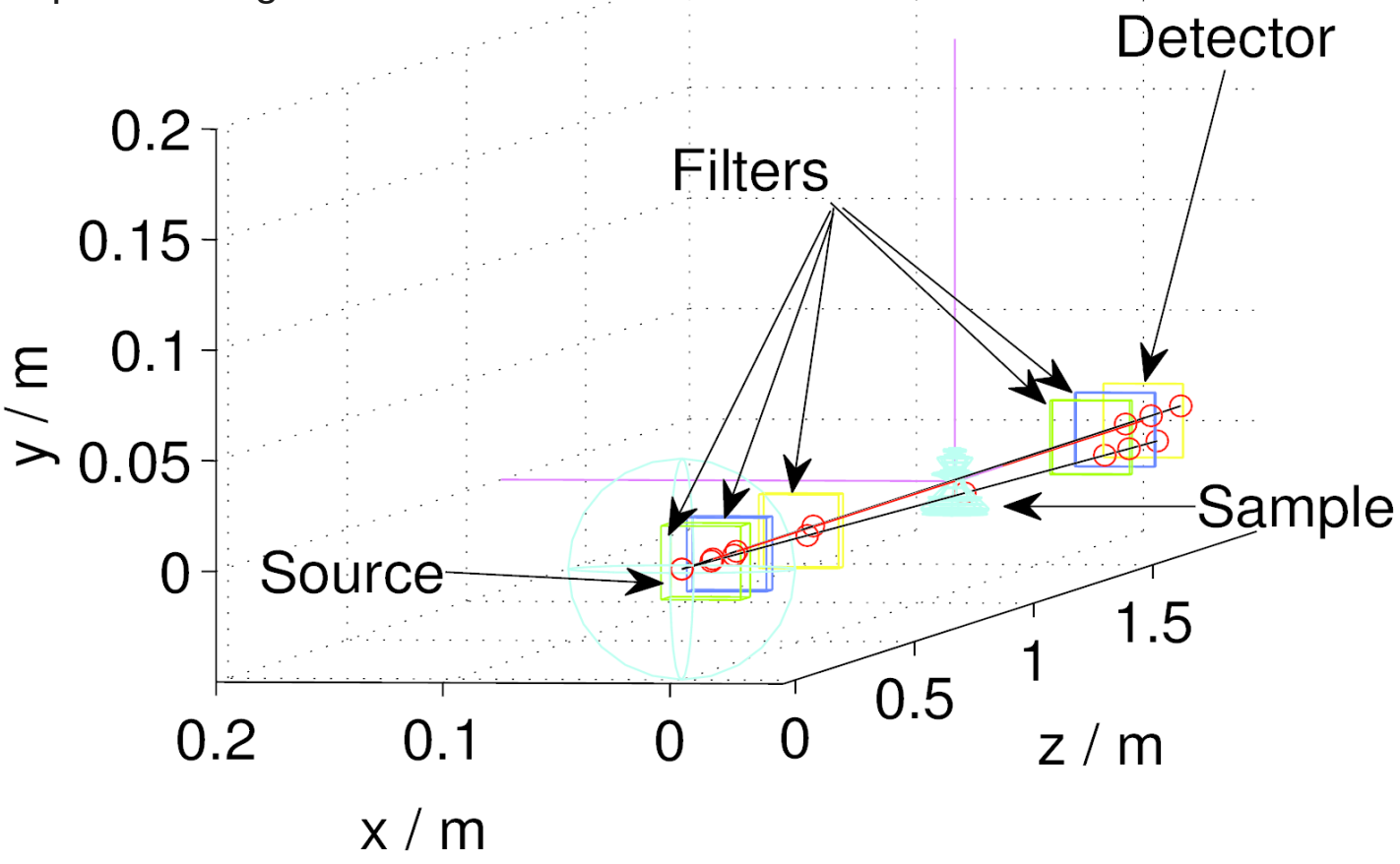


Time resolved, difference signal

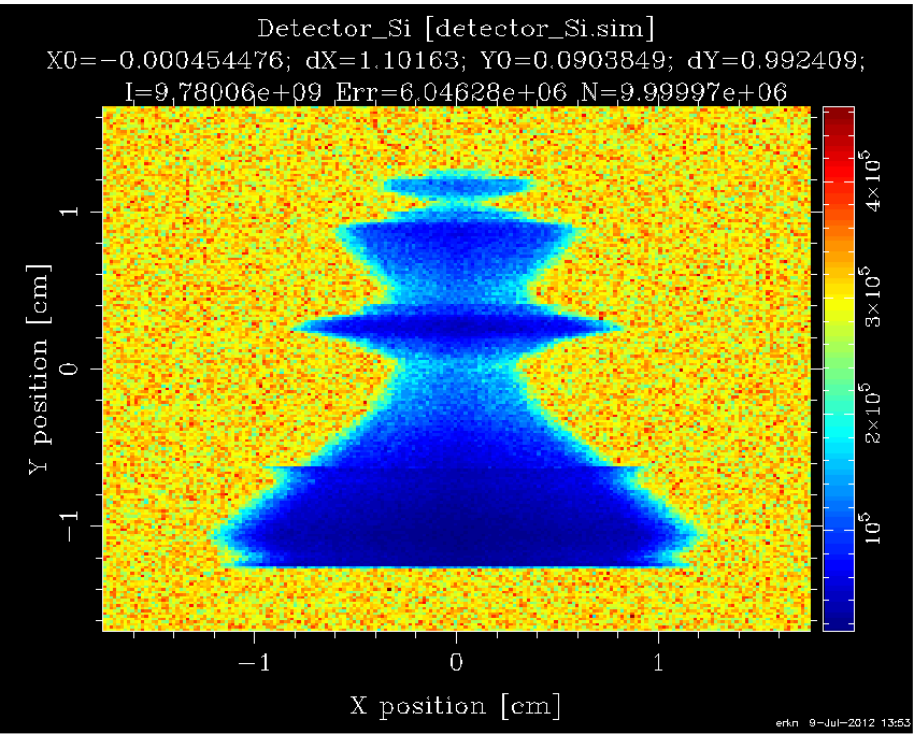


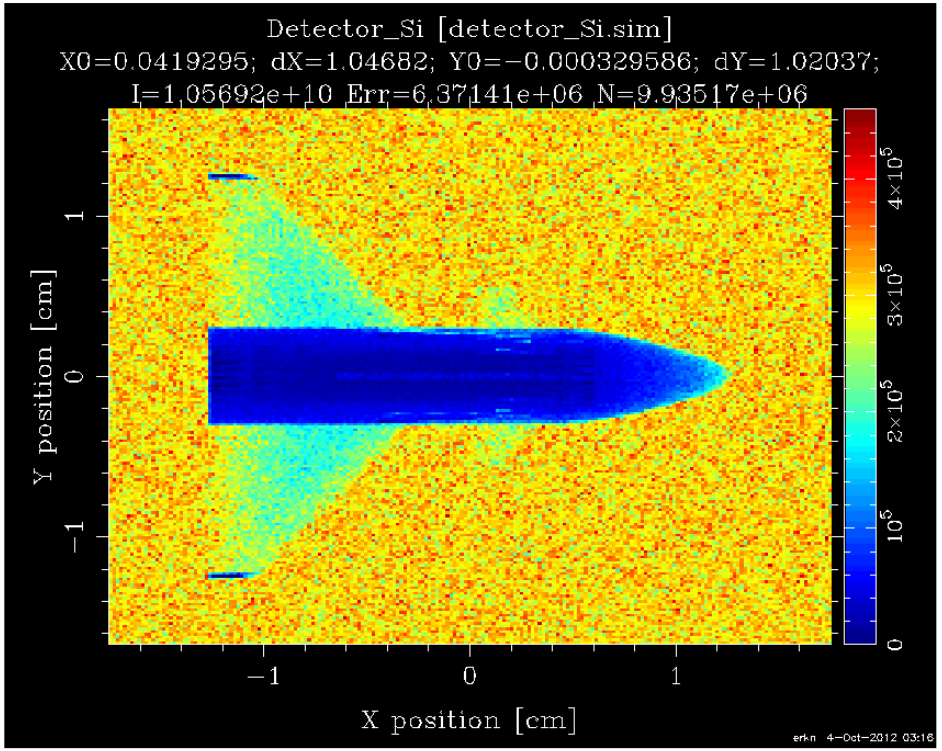
Tomography

Setup mimicking that of TU München

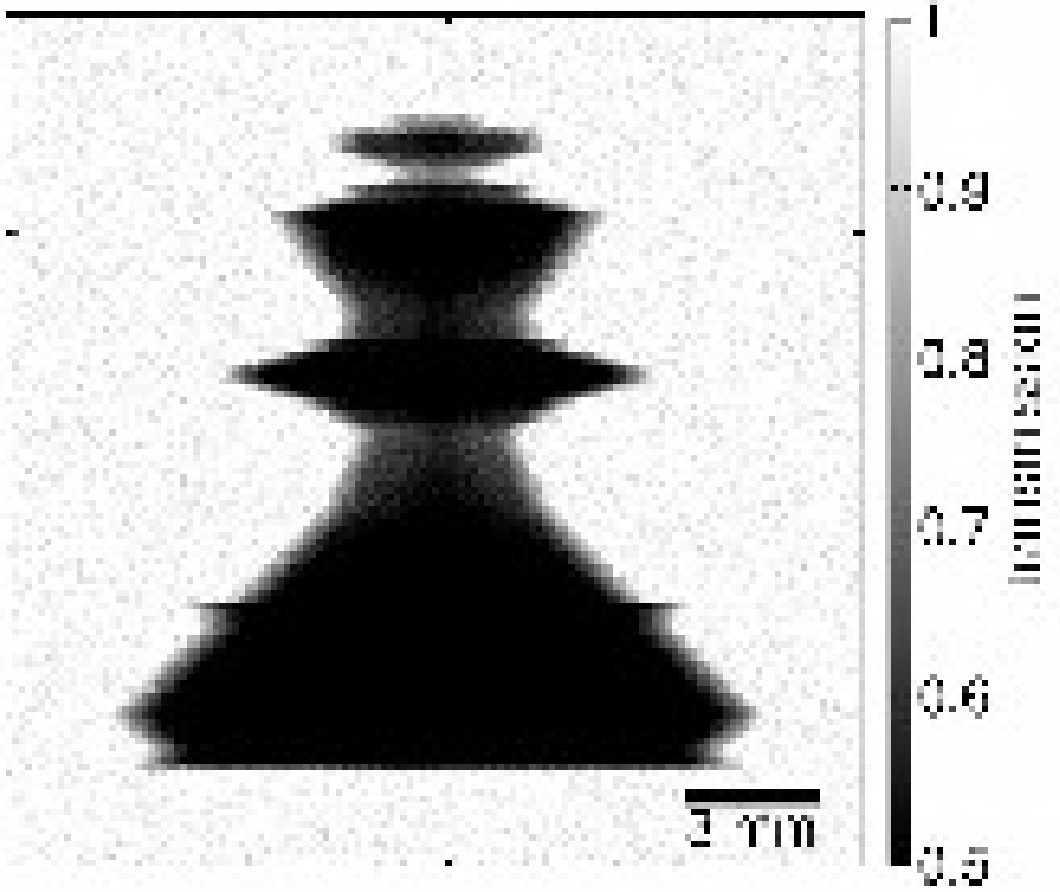


Anyshape tomography

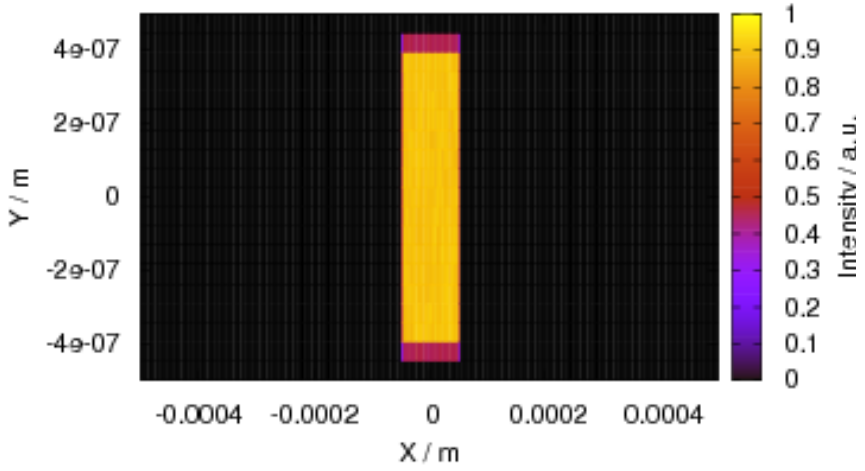


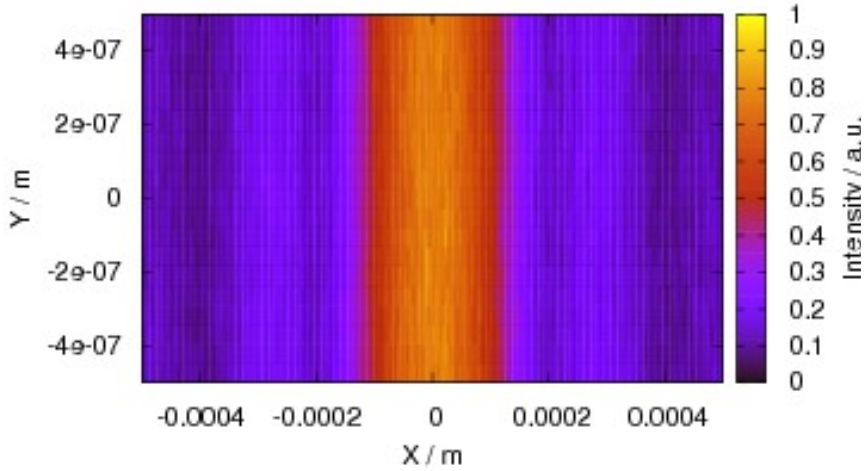


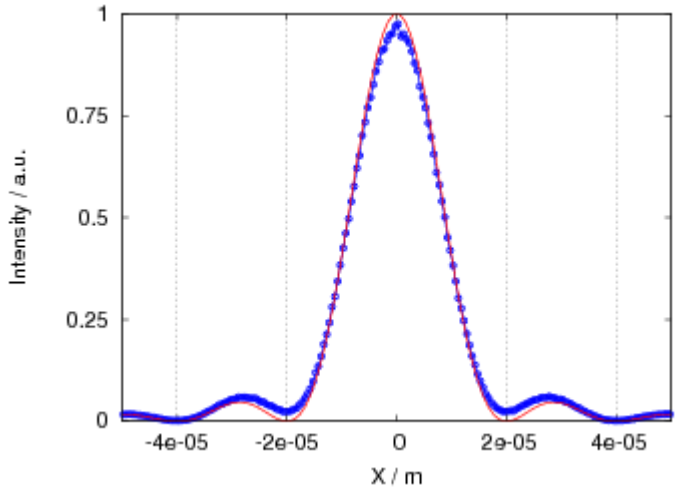
Anyshape Reconstruction



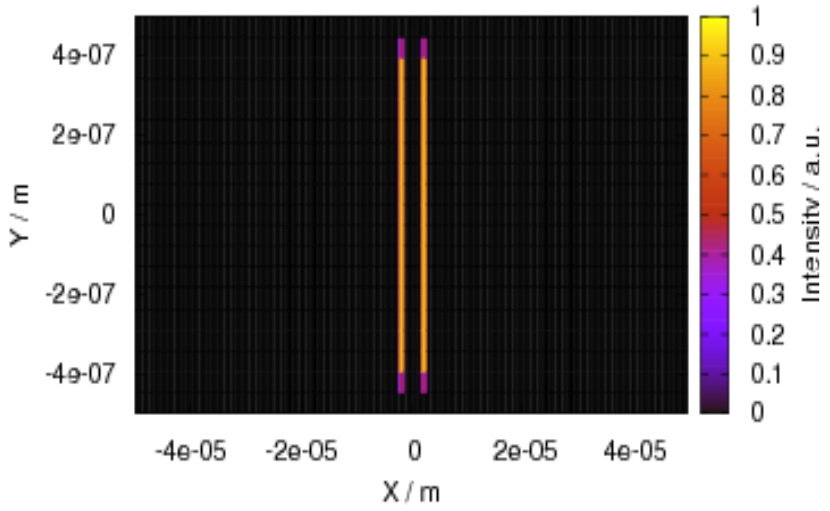
Single Slit

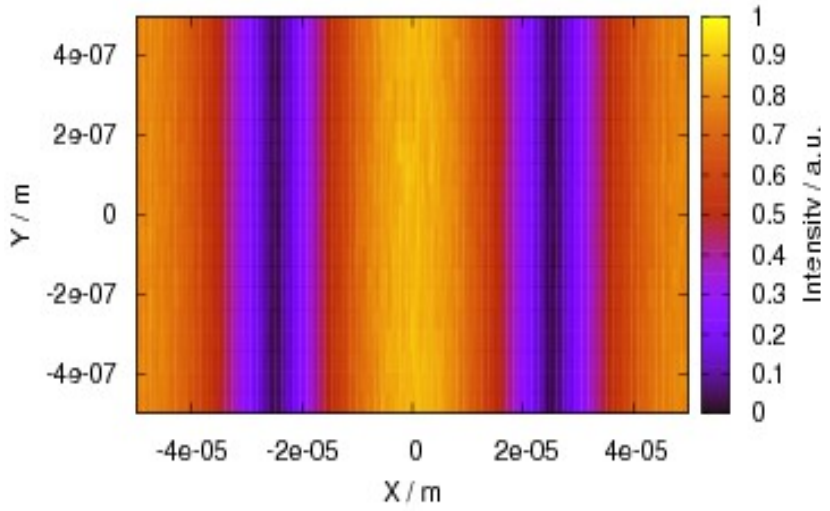

4e-07
2e-07
0
-2e-07
-4e-07
Y / m
-0.0004
-0.0002
0
0.0002
0.0004
X / m
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Intensity / a.u.


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.

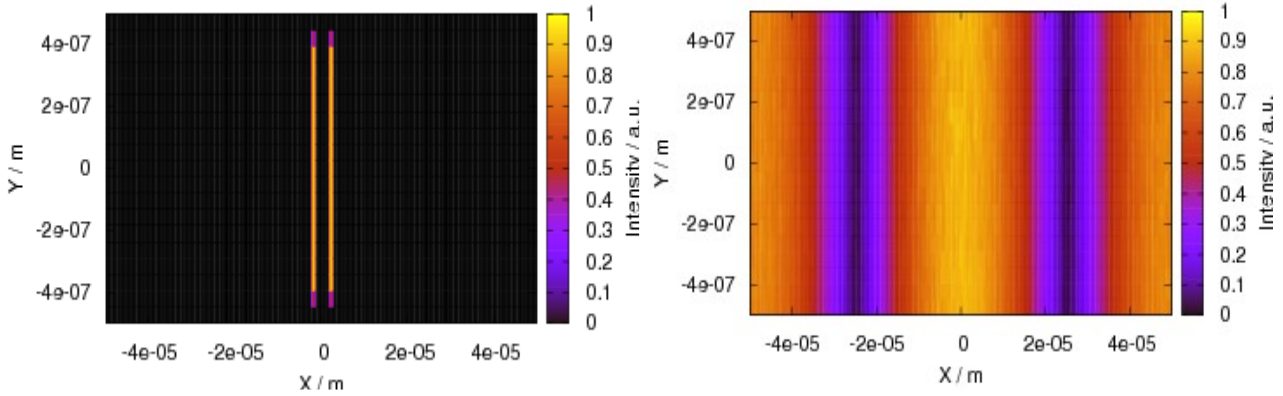

1
0.75
0.5
0.25
0
Intensity / a.u.
-4e-05
-2e-05
0
2e-05
4e-05
X / m

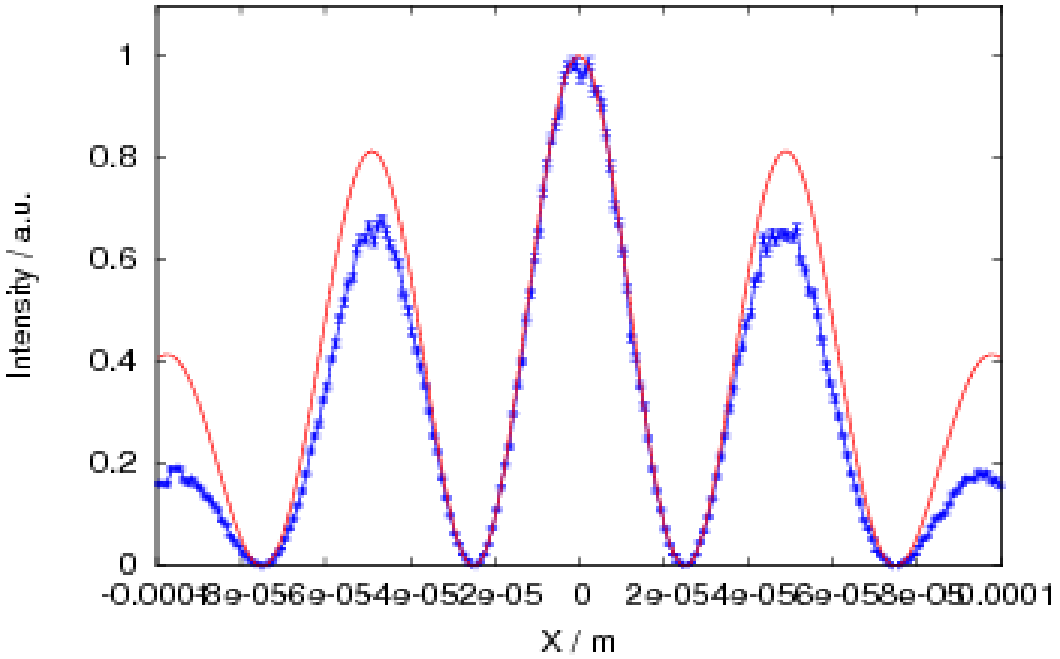
Double Slit


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.

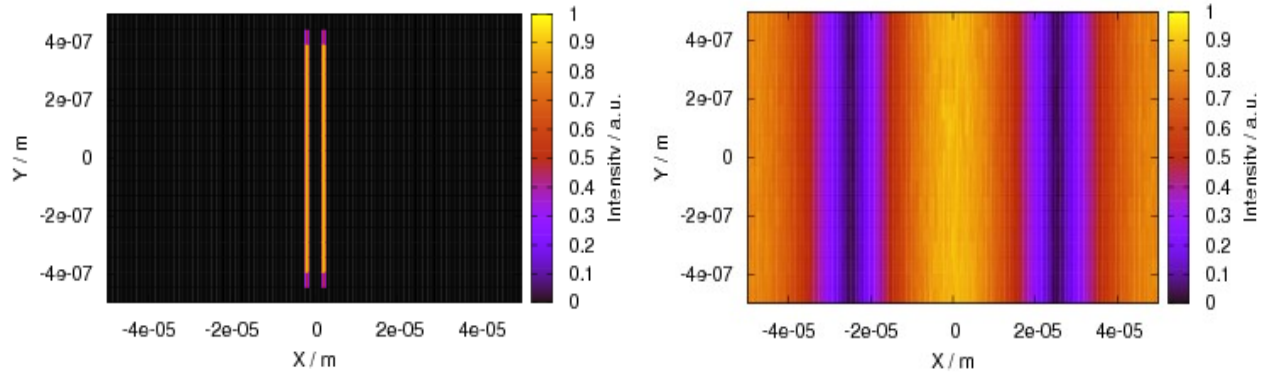

4e-07
2e-07
0
-2e-07
-4e-07
Y / m
-4e-05
-2e-05
0
2e-05
4e-05
X / m
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Intensity / a.u.

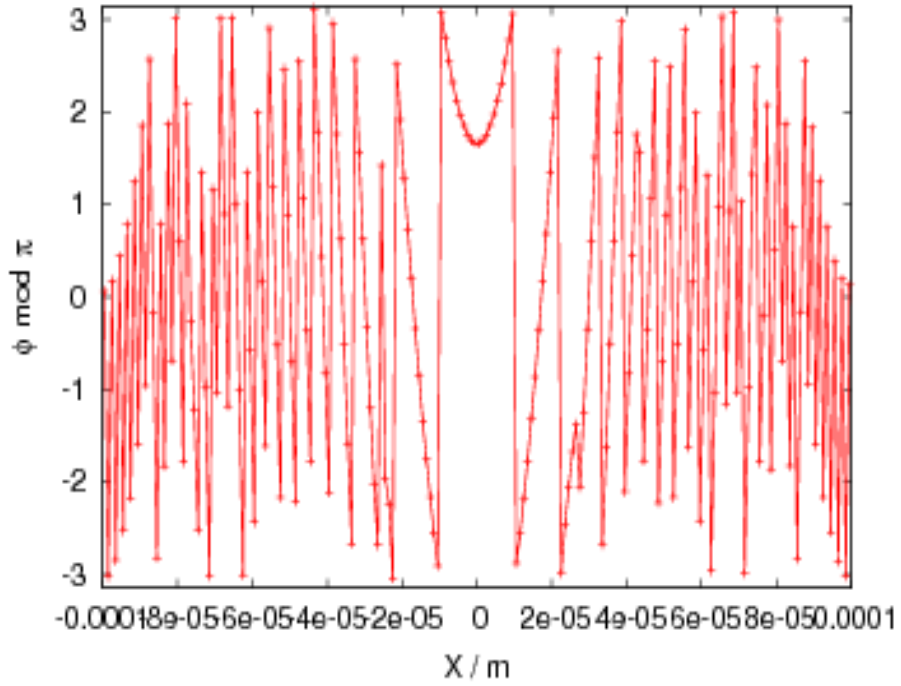
Double Slit


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

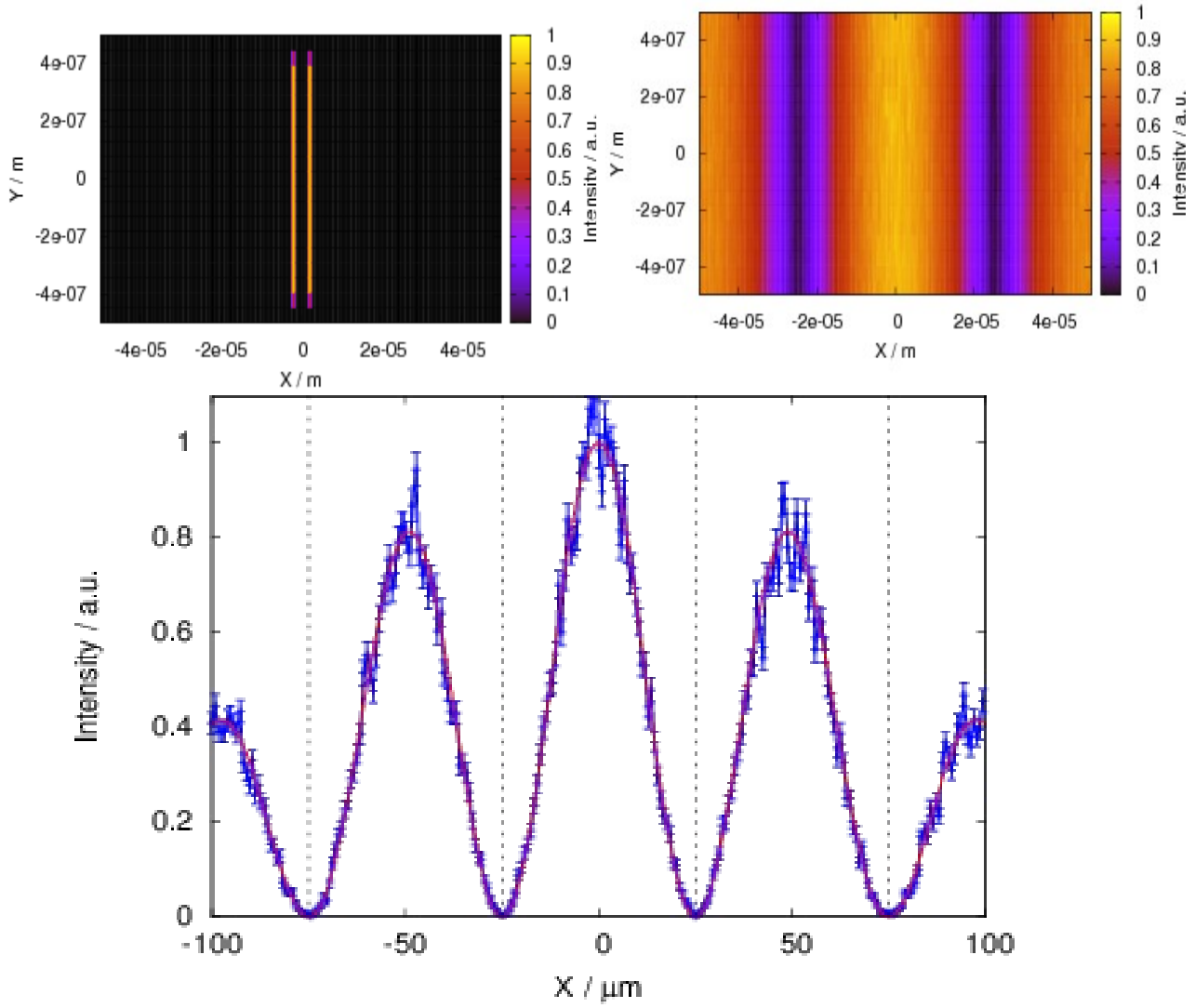

Intensity / a.u.
1
0.8
0.6
0.4
0.2
0
-0.0001
-8e-05
-6e-05
-4e-05
-2e-05
0
2e-05
4e-05
6e-05
8e-05
0.0001
X / m

Double Slit

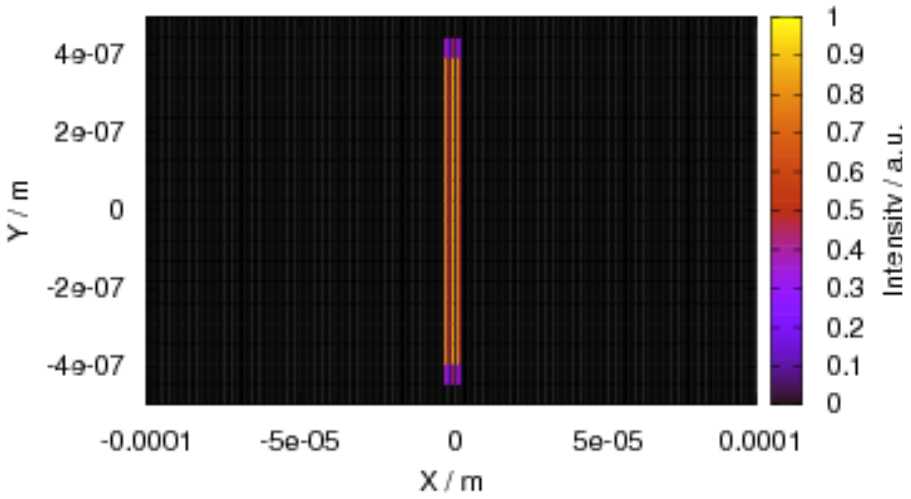

4e-07
2e-07
0
-2e-07
-4e-07
Y / m
-4e-05
-2e-05
0
2e-05
4e-05
X / m
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Intensity / a.u.

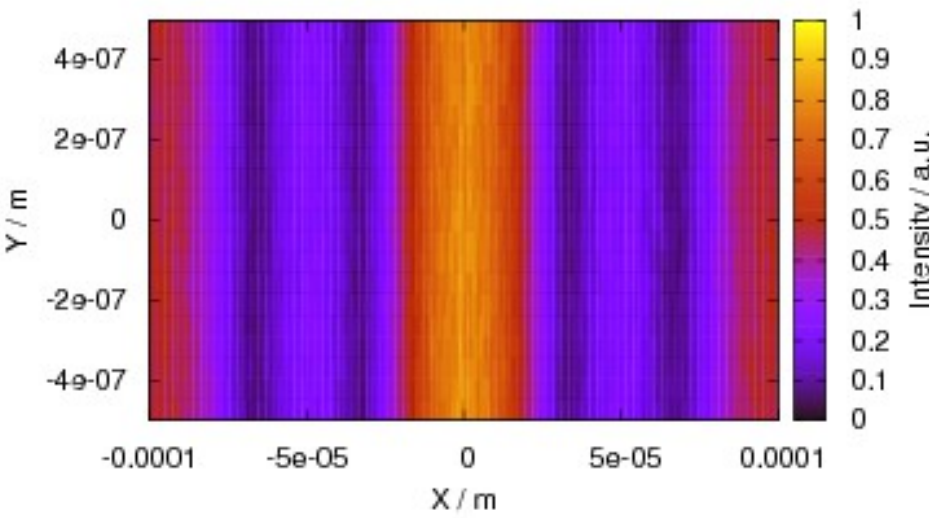

3
2
1
0
-1
-2
-3
φ mod π
-0.0001
8e-05
6e-05
4e-05
2e-05
0
2e-05
4e-05
6e-05
8e-05
0.0001
X / m

Double Slit


4e-07
2e-07
0
-2e-07
-4e-07
Y / m
-4e-05
-2e-05
0
2e-05
4e-05
X / m
Intensity / a.u.
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Intensity / a.u.
-100
-50
0
50
100
X / µm

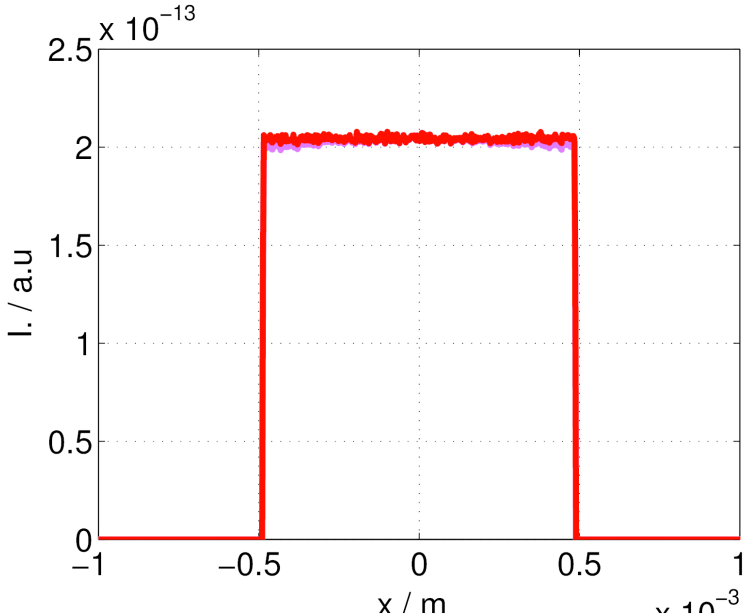
Triple Slit


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.

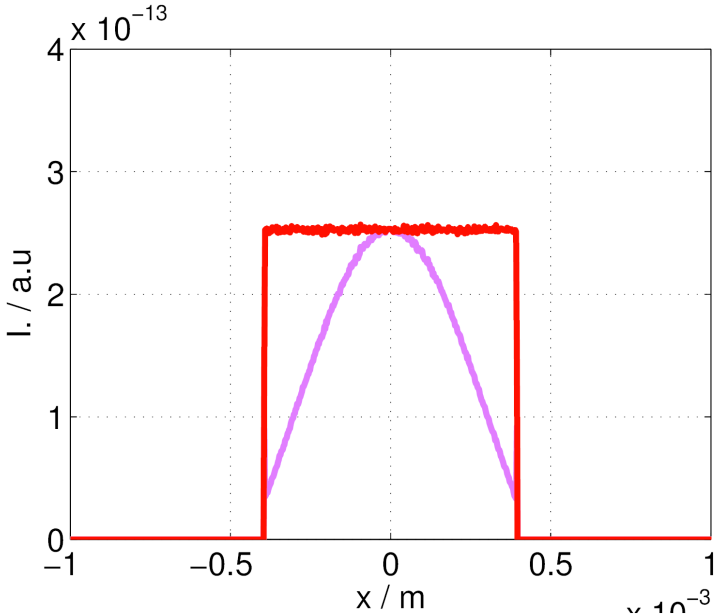

4e-07
2e-07
0
-2e-07
-4e-07
Y / m
-0.0001
-5e-05
0
5e-05
0.0001
X / m
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Intensity / a.u.

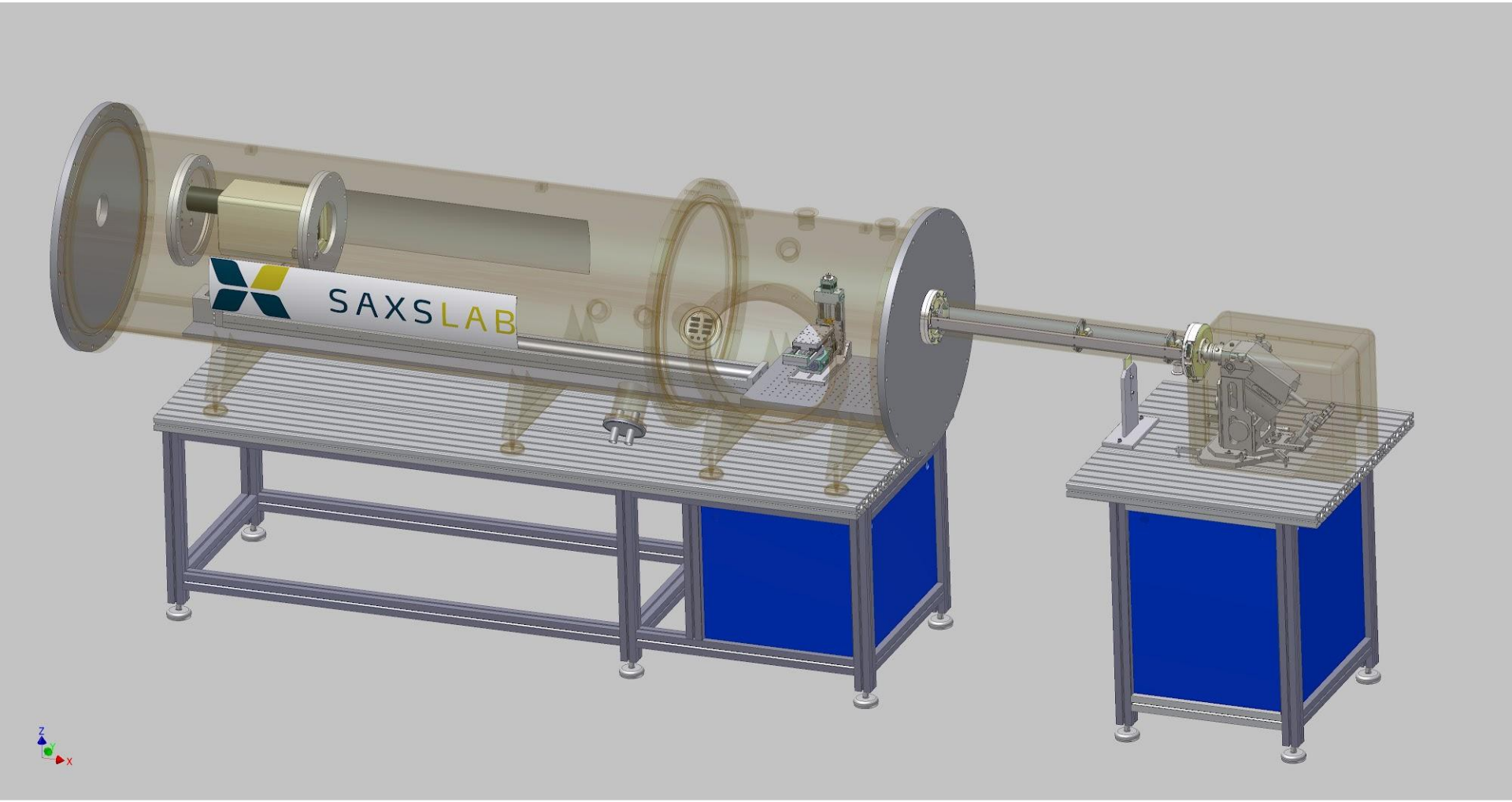
Coherent examples

1 Be refractive lens:
Red: Incoherent
Magenta: Fully coherent, in phase

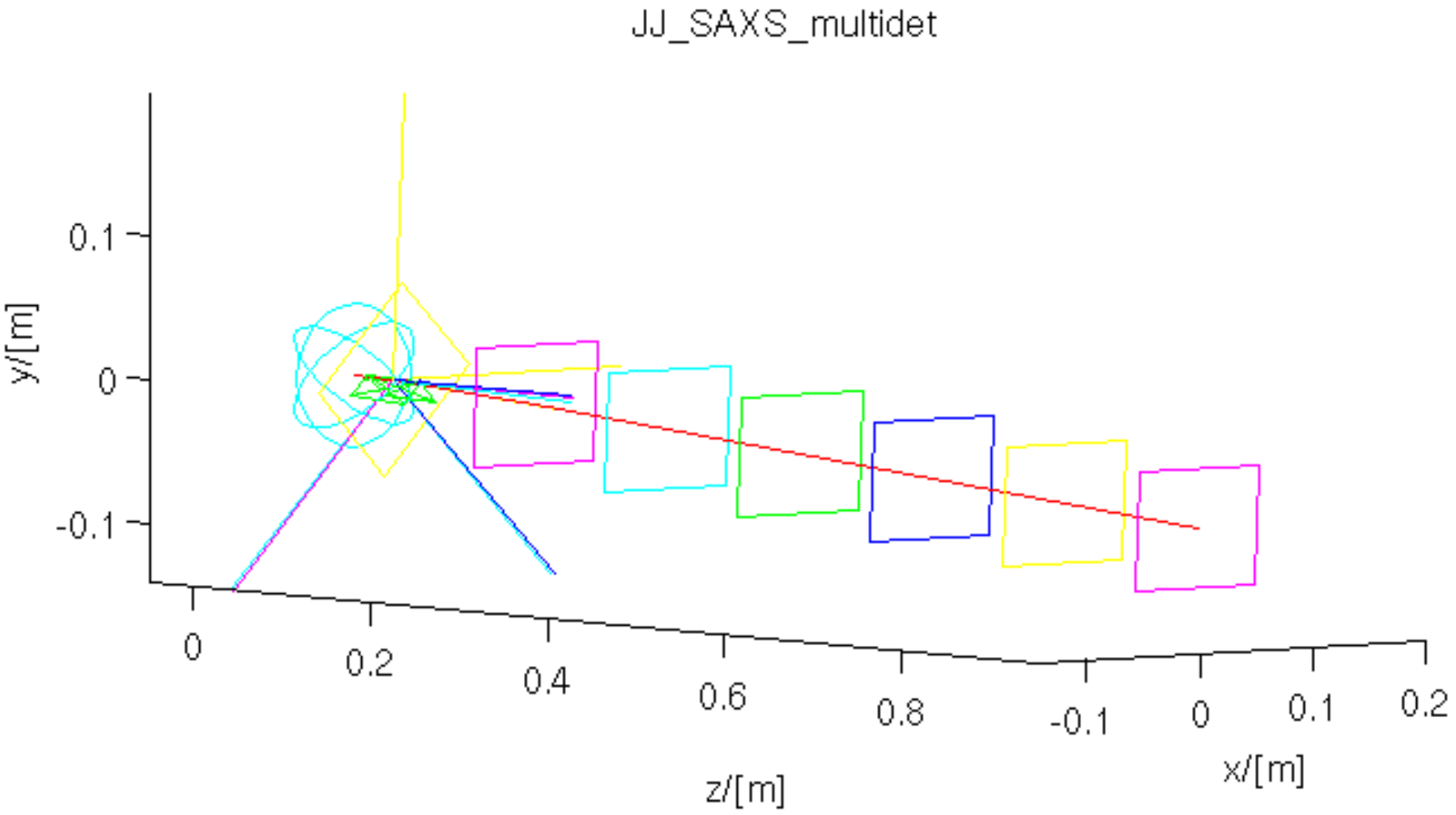


8 Be refractive lenses:
Red: Incoherent
Magenta: Fully coherent, in phase

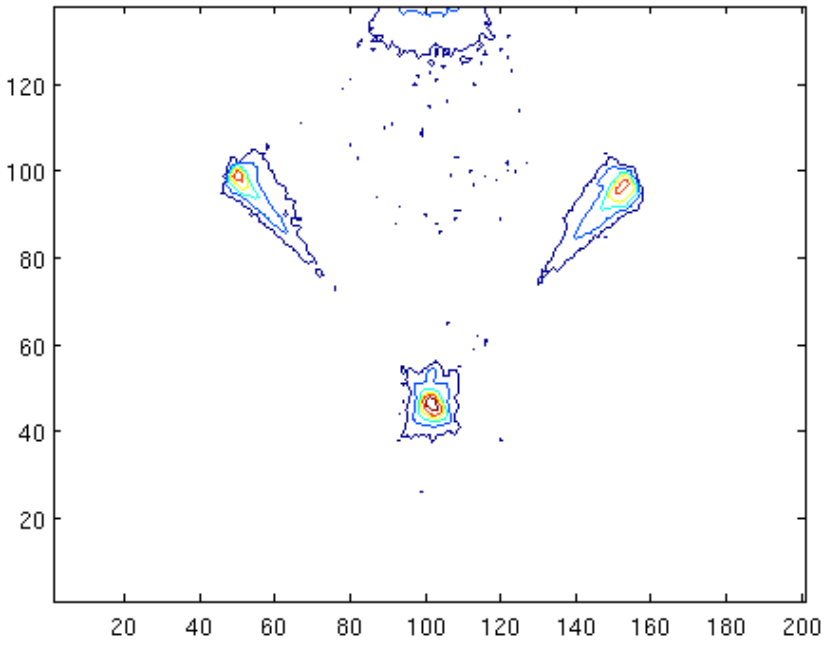


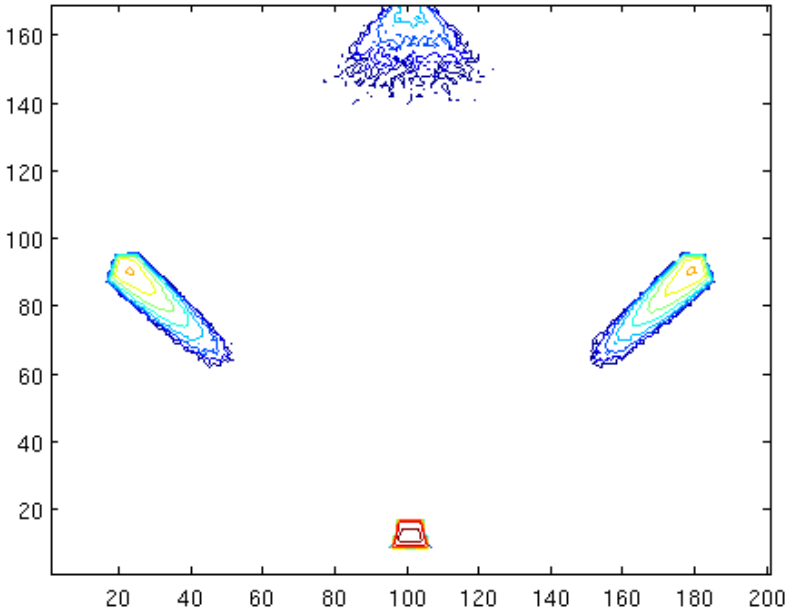

SAXSLAB

McXtrace Simulation



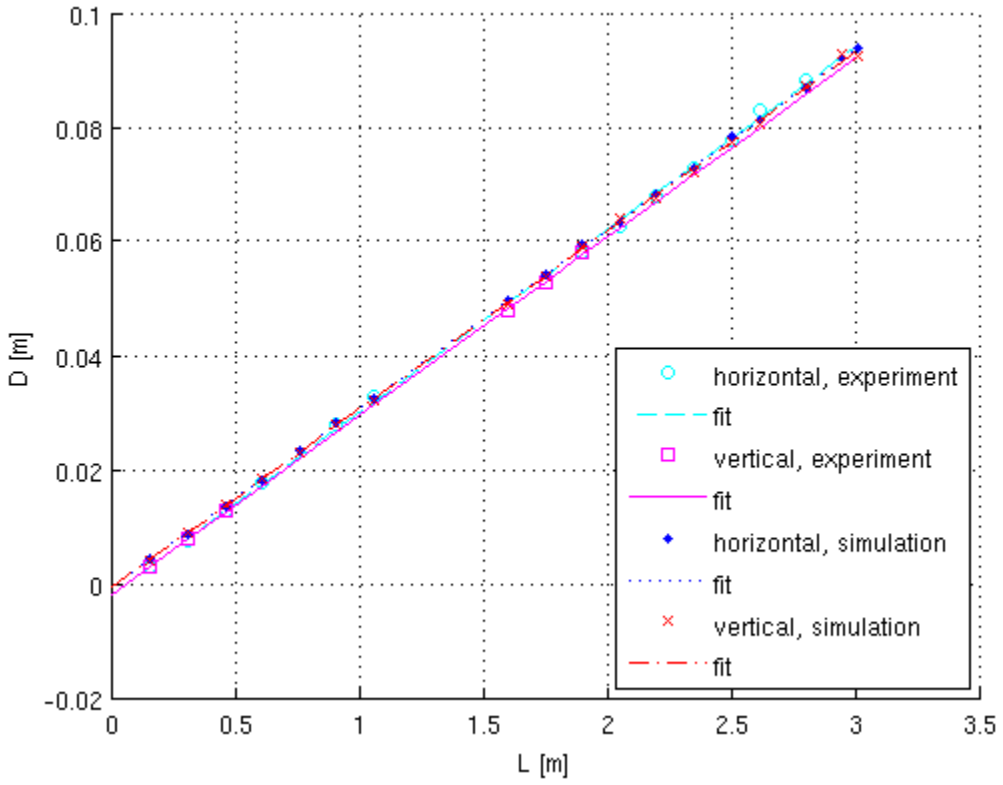
Test Data


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

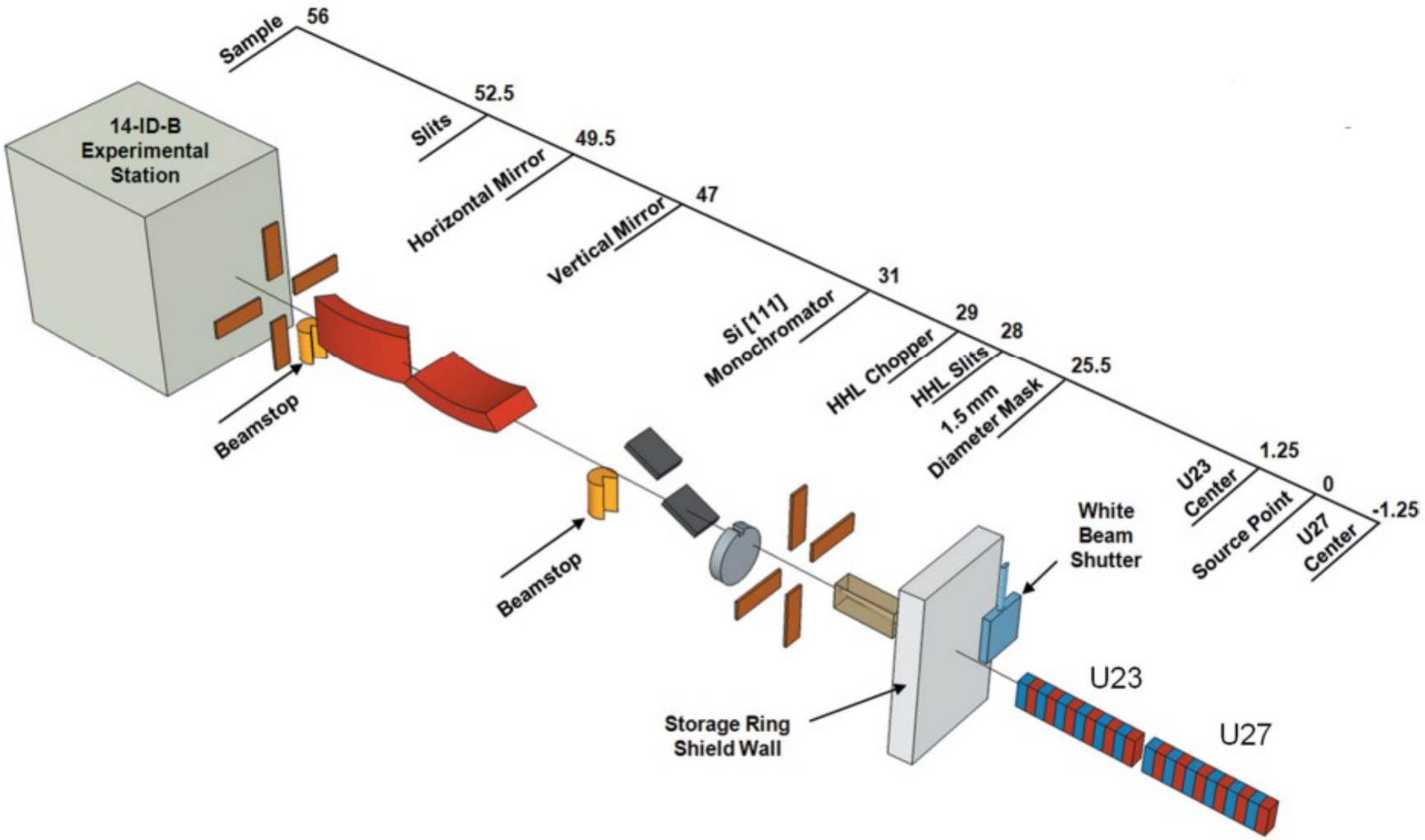

160
140
120
100
80
60
40
20
20 40 60 80 100 120 140 160 180 200

Difference?

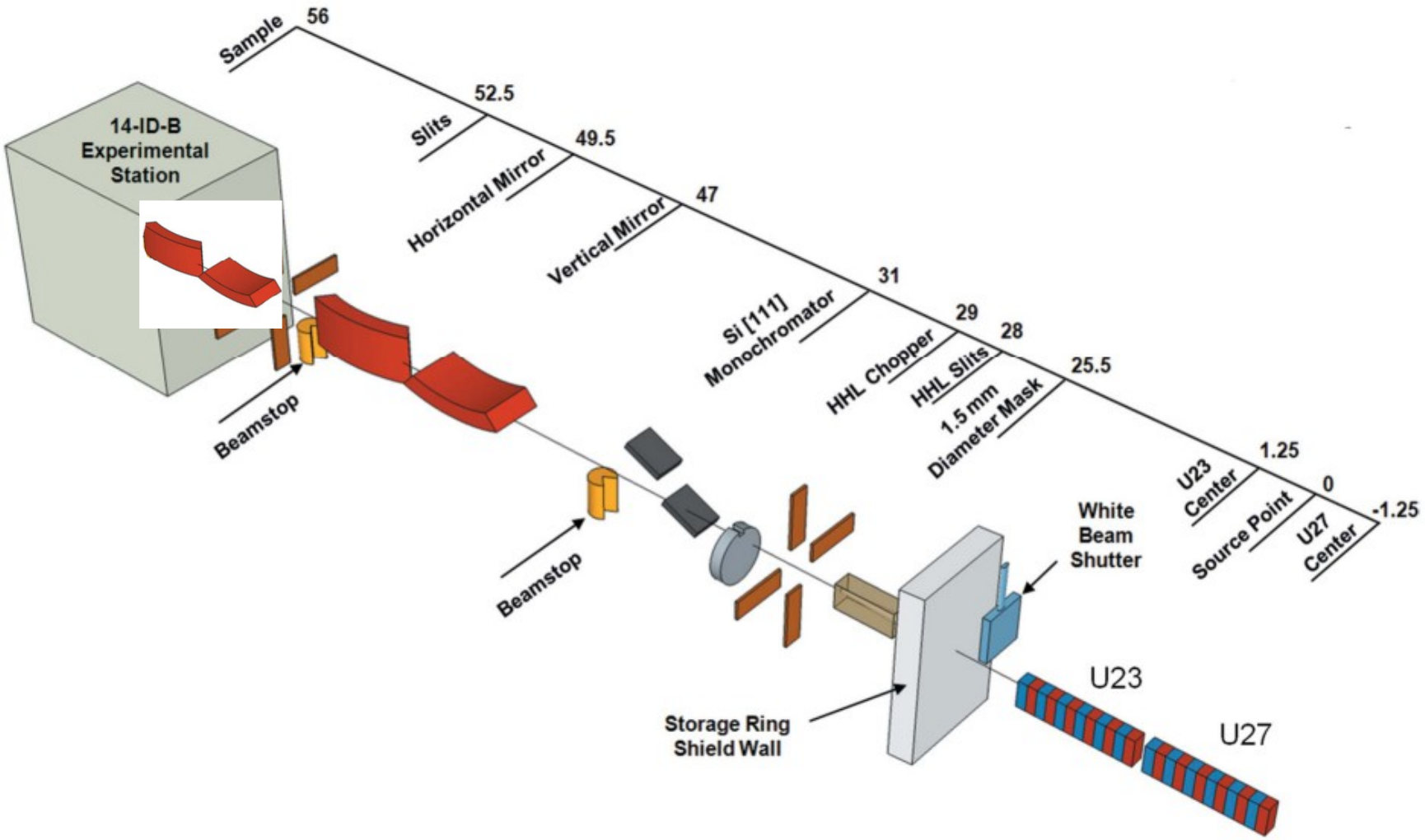
Add an *offset* slit after Side-by-Side KB-mirror



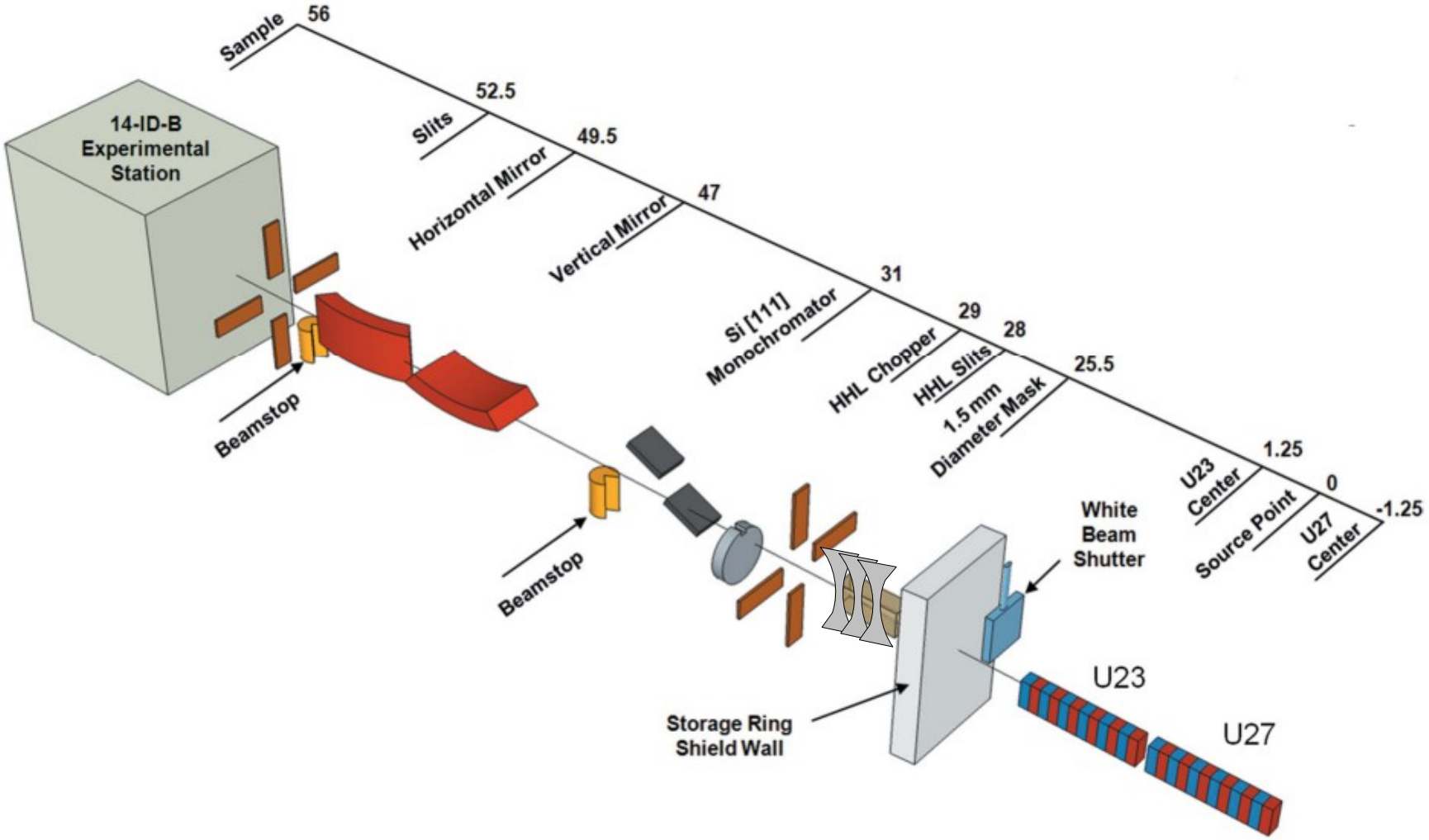
APS ID14 Bio CARS



APS ID14 High Focus option 1

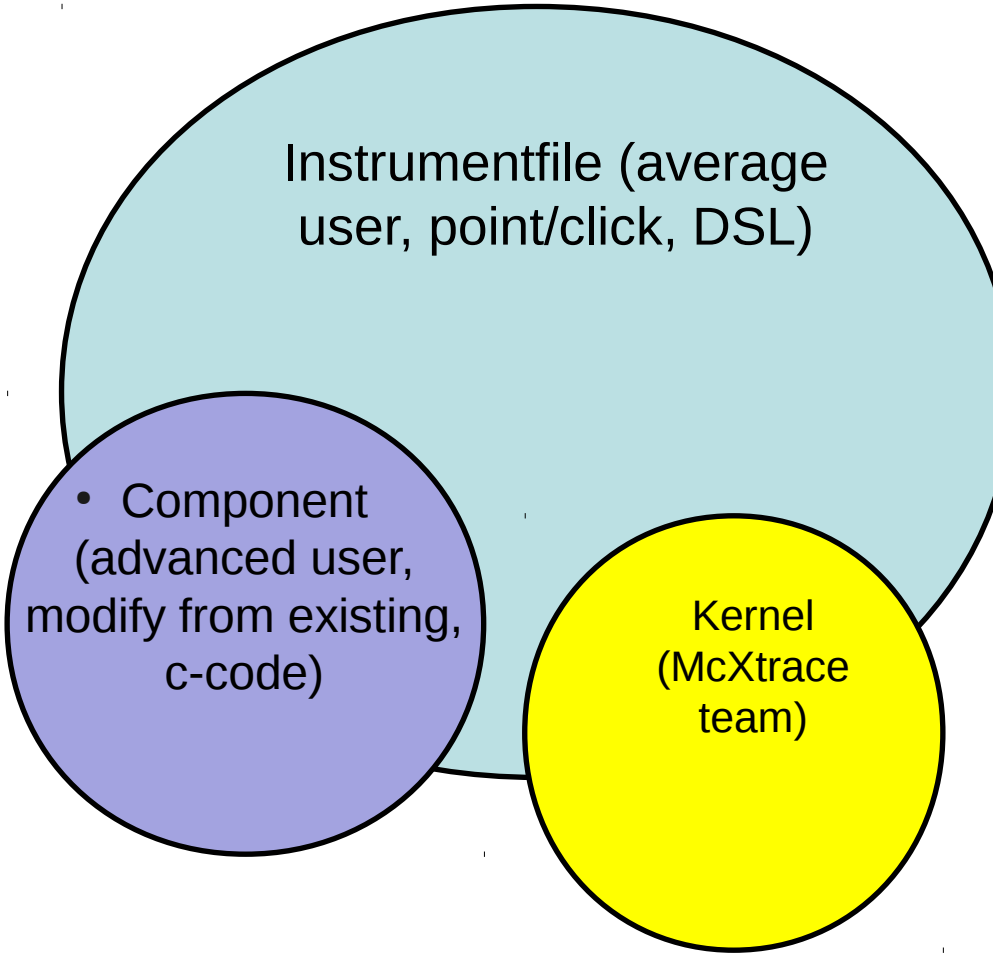


APS ID14 High Focus option 2

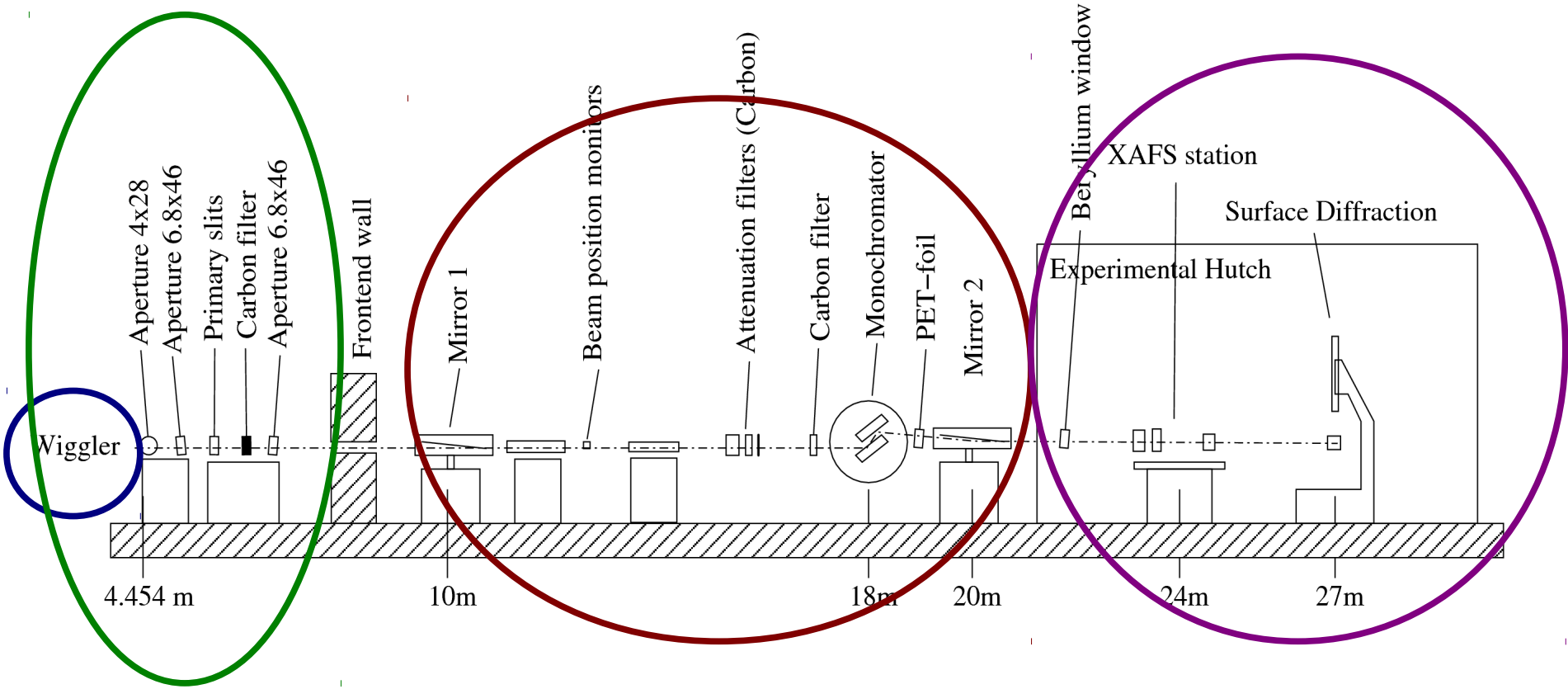


Levels of Code revisited

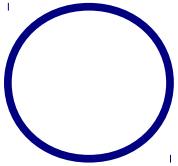
- **Instrument file – all users**
  - **existing examples**
  - **user written – GUI assisted**
- Component files – some users
  - Short pieces of code
  - Easy to modify from existing
- Kernel code – McXtrace developers
  - Propagation routines
  - Intersections
- Generated ISO-C code – “no” users
  - Assembled by code generation
  - Very low overhead of unneeded code
  - Includes runtime libs that comps rely on (propagation etc.)



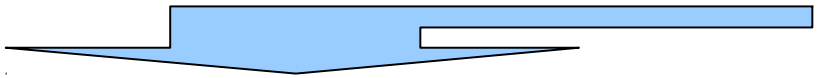
Modelling the Max II beamline 811



Wiggler

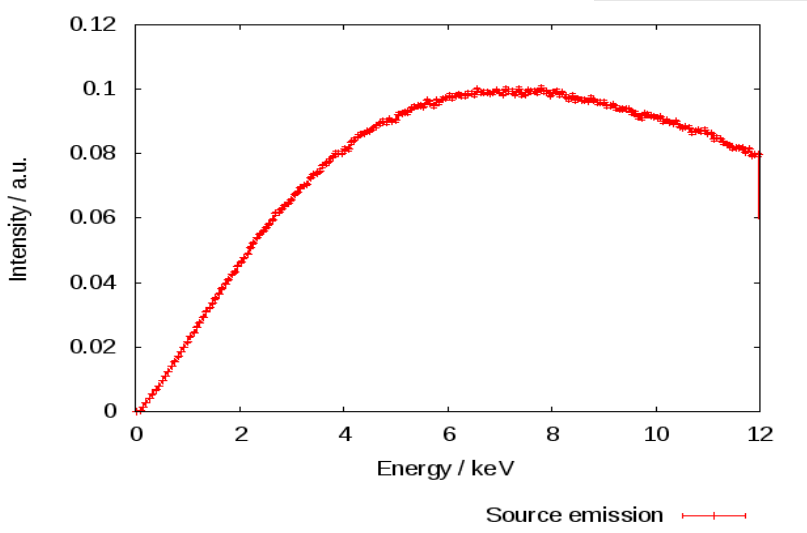


Carlsson et.al., *J. Synch. Rad*, vol 13, pt. 5, pp 359, **2006**



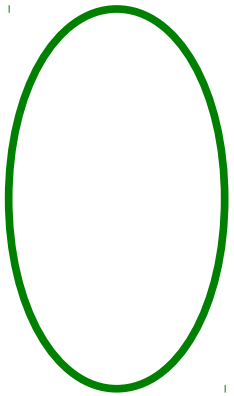
```
137 COMPONENT wiggler = Source_gaussian(
138  sigPr_x=7e-6*FWHM2RMS, sigPr_y=0.3e-6*F
139  sig_x=250e-6*FWHM2RMS, sig_y=50e-6*FWHM
140  spectrum_file="characteristics.dc0",E0=
141  distance=4.454,dlambda=0)
142 AT(0,0,0) RELATIVE Origin
```

From SPECTRA

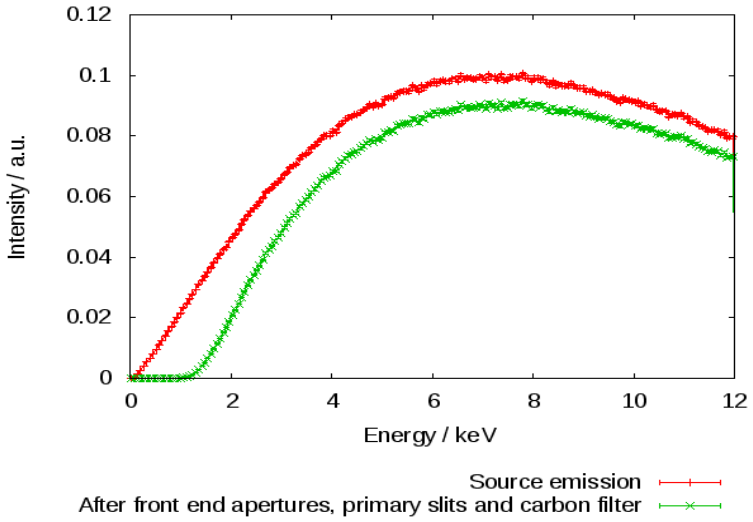


Ring Current	250 mA
Source	Superconducting Wiggler
Magnetic Field	3.5 T
Magnet Period	65 mm
Number	49
	.1%
	^-1
	0 µm (v
	6.0
	)
	ce
Front-end Slits	6.4 m from source

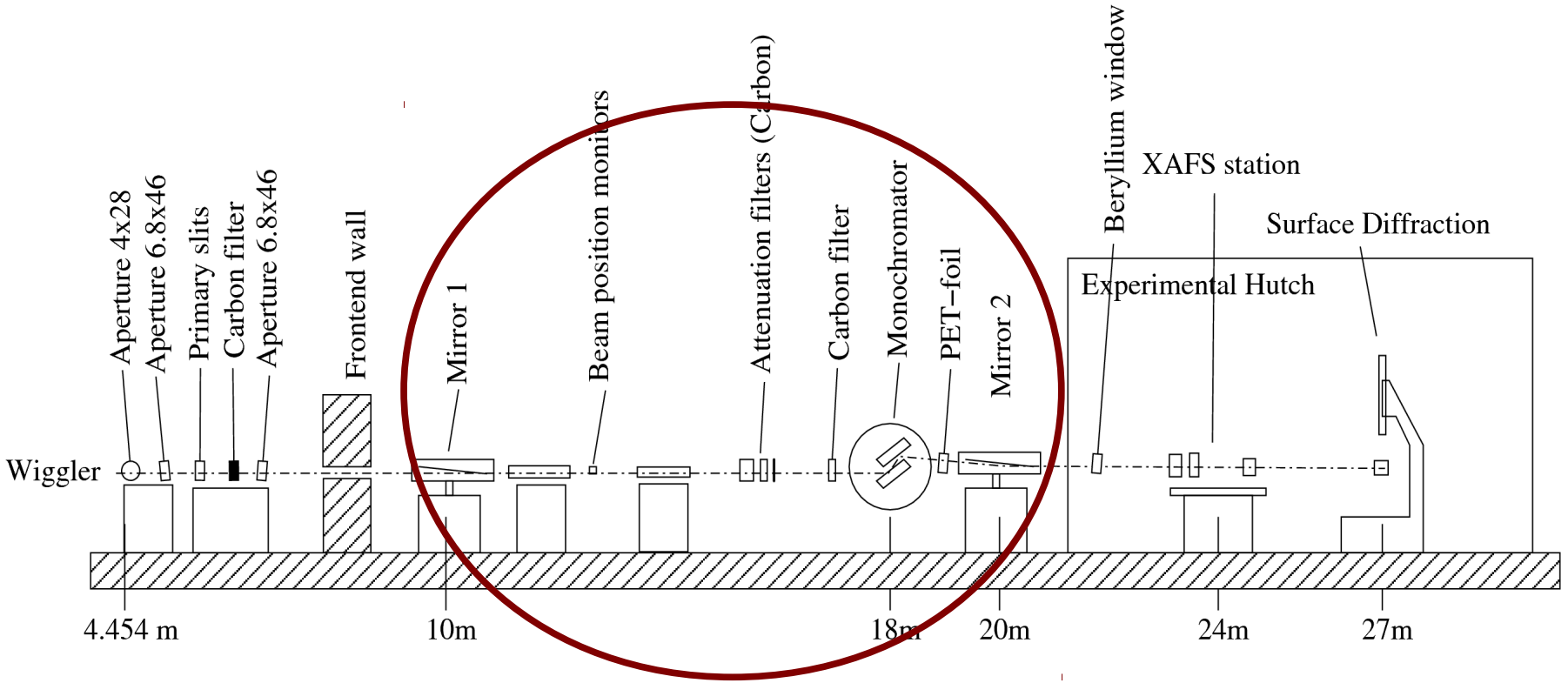
Front-end fixed apertures and Slits



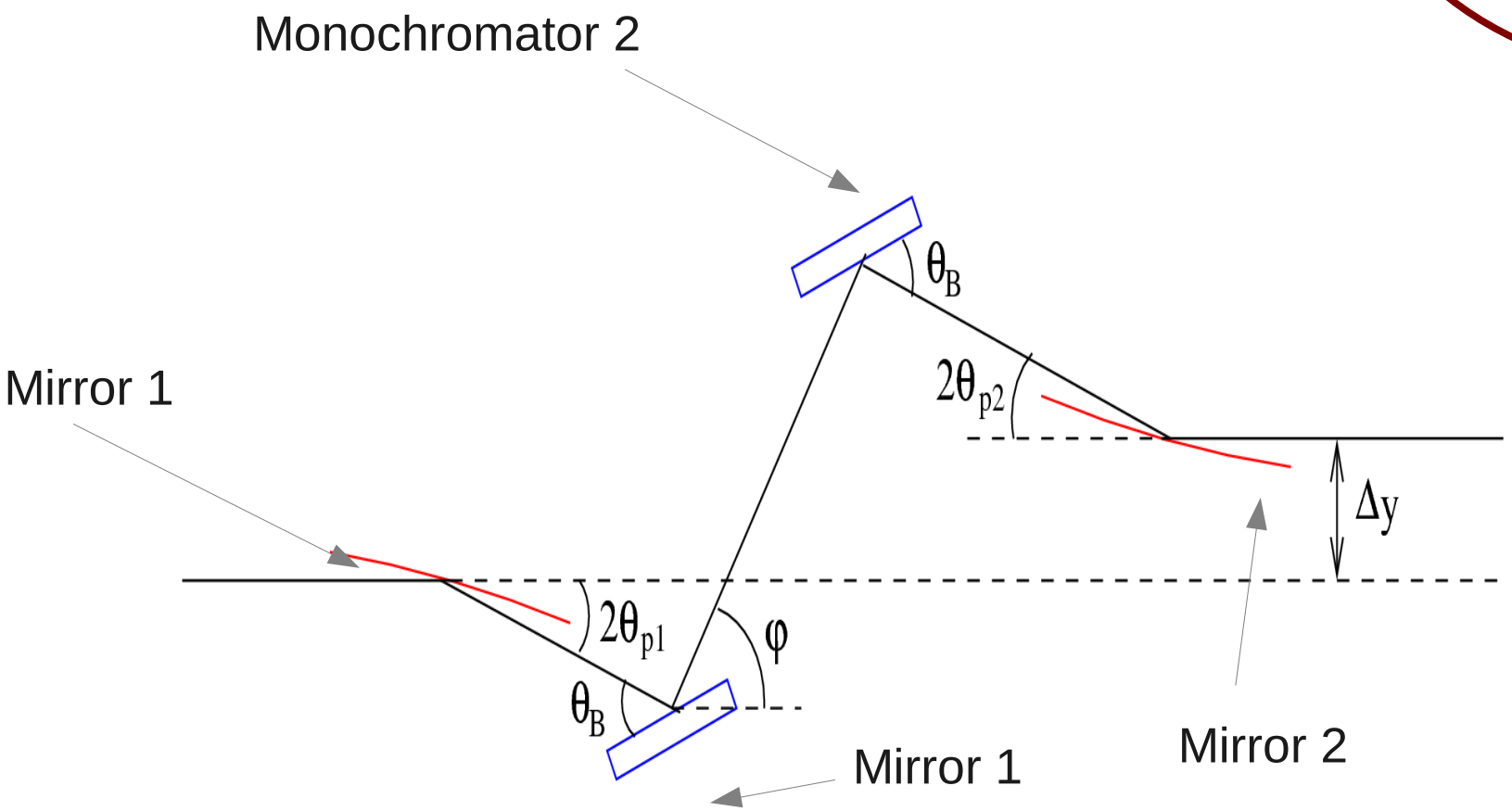
```
156 COMPONENT ap1 = Slit(
157   yheight=4e-3, xwidth=28e-3)
158 AT(0,0,4.454) RELATIVE wiggler
159
160 COMPONENT ap2 = Slit(
161   yheight=6.8e-3,xwidth=46e-3)
162 AT(0,0,6) RELATIVE wiggler
163
164 /*Frontend carbon Filter*/
165 COMPONENT  fe_c_filter= Filter(
166   material_datafile="C.txt", xwidth
167 AT(0,0,6.3) RELATIVE wiggler
168
169 /*Primary Slits*/
170 COMPONENT prim_slitv = Slit(
171   xwidth=.1,yheight=prim_v)
172 AT(0,0,6.4) RELATIVE wiggler
173 COMPONENT prim_slith = Slit(
174   xwidth=prim_h,yheight=.1)
175 AT(0,0,15e-3) RELATIVE PREVIOUS
176
177 COMPONENT ap3 = COPY(ap2)
178 AT(0,0,7) RELATIVE wiggler
```



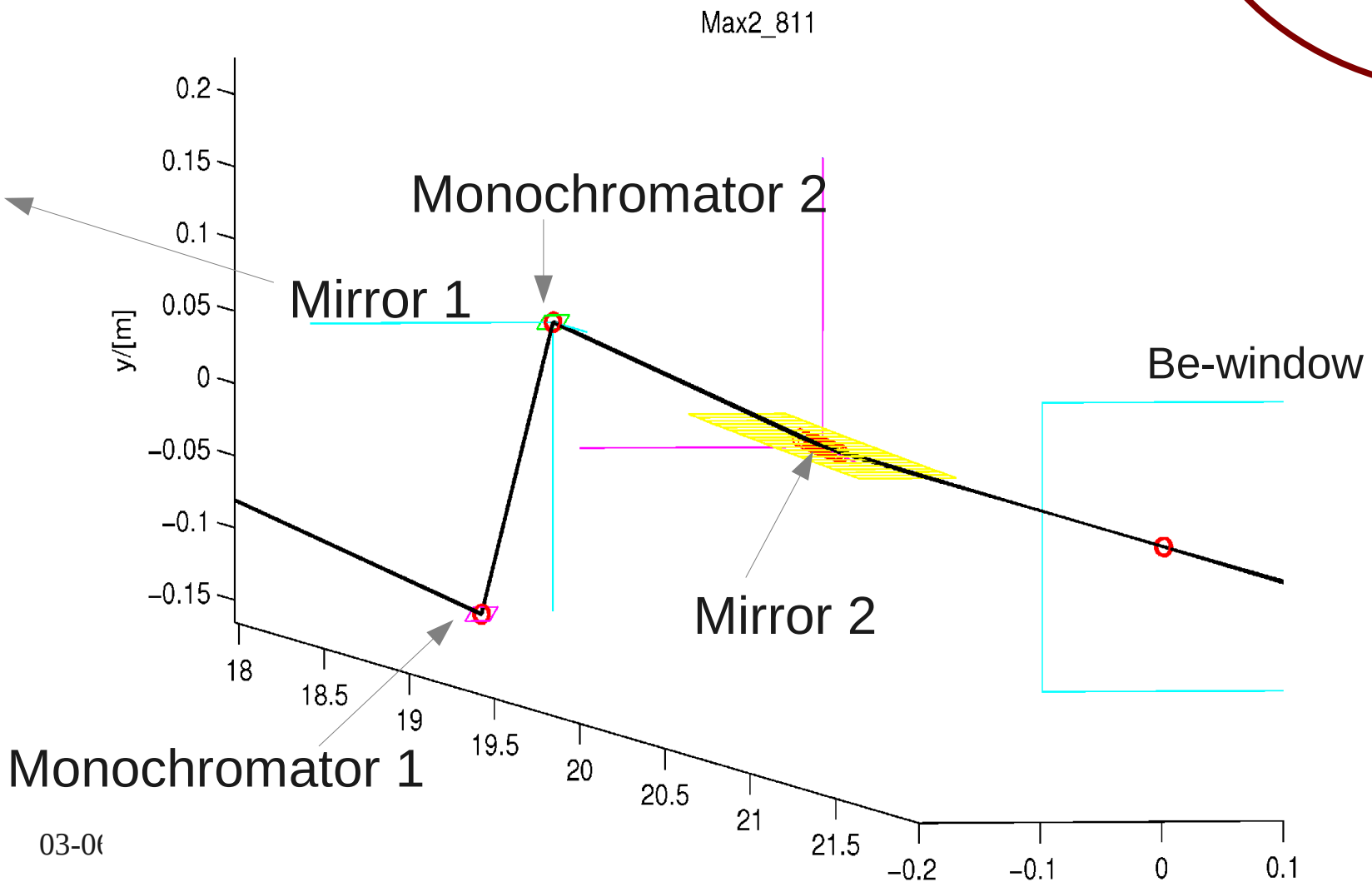
Mirror/Monochromator Layout



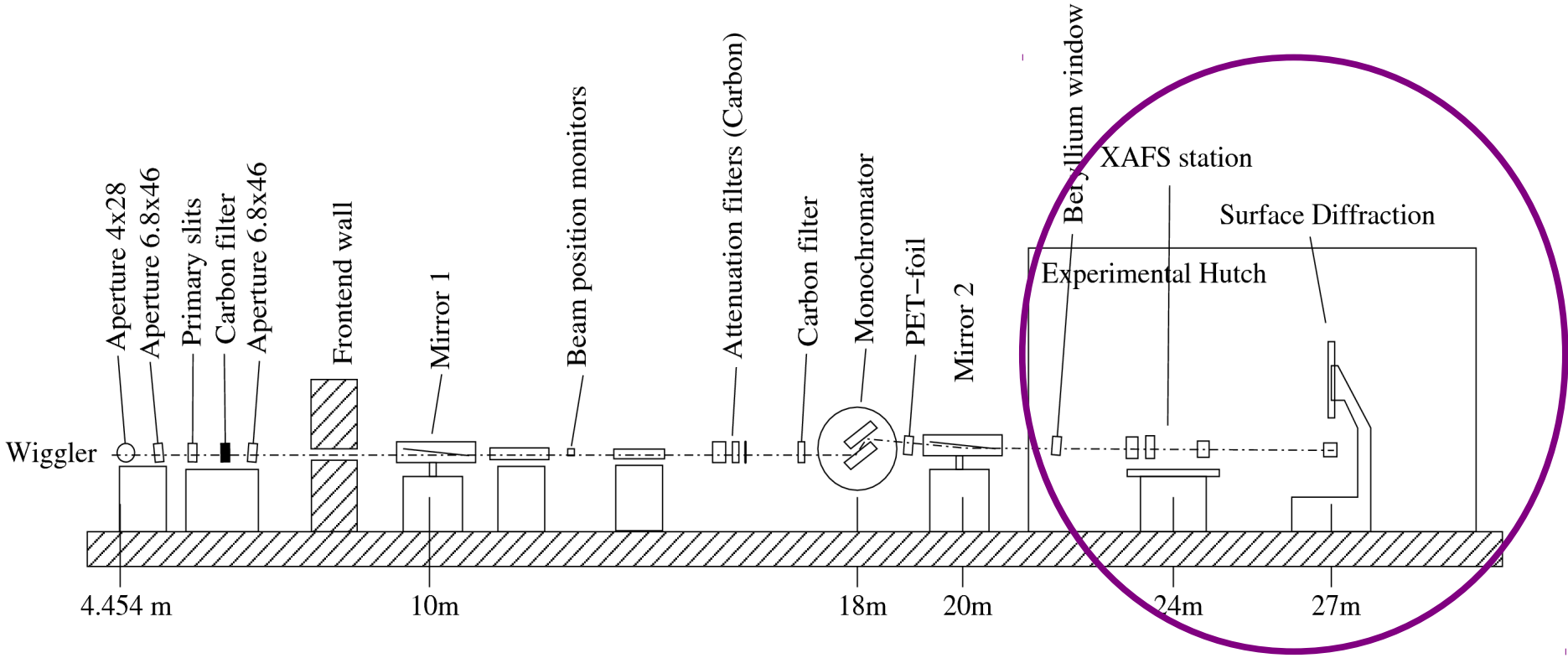
Mirror/Monochromator Layout



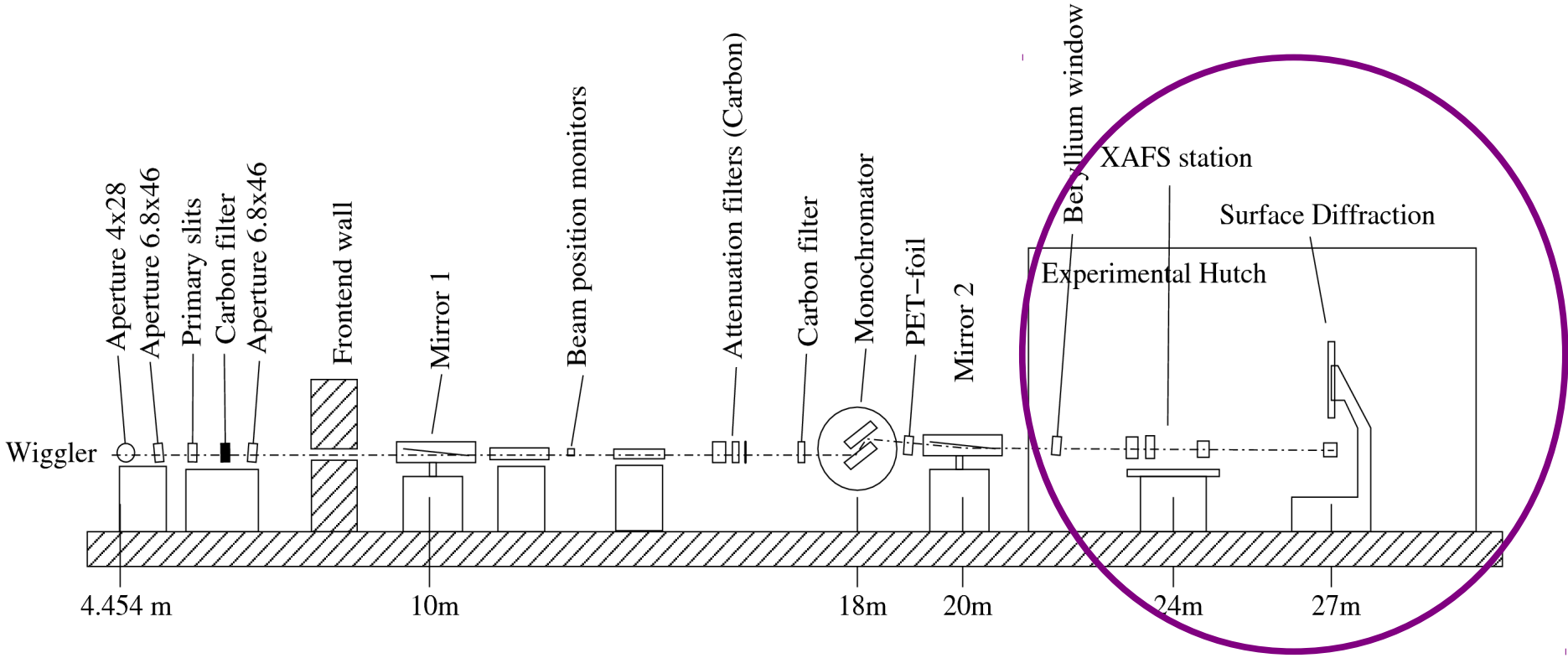
Mirror/Monochromator Layout trace



Experimental Hutch

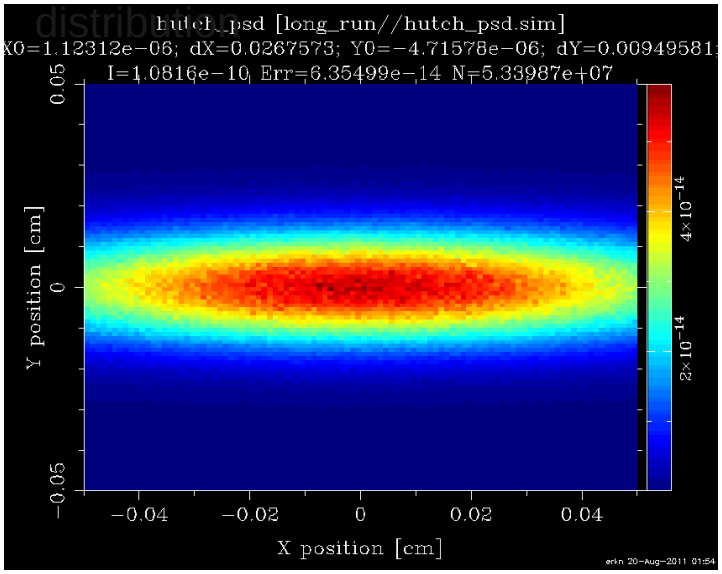


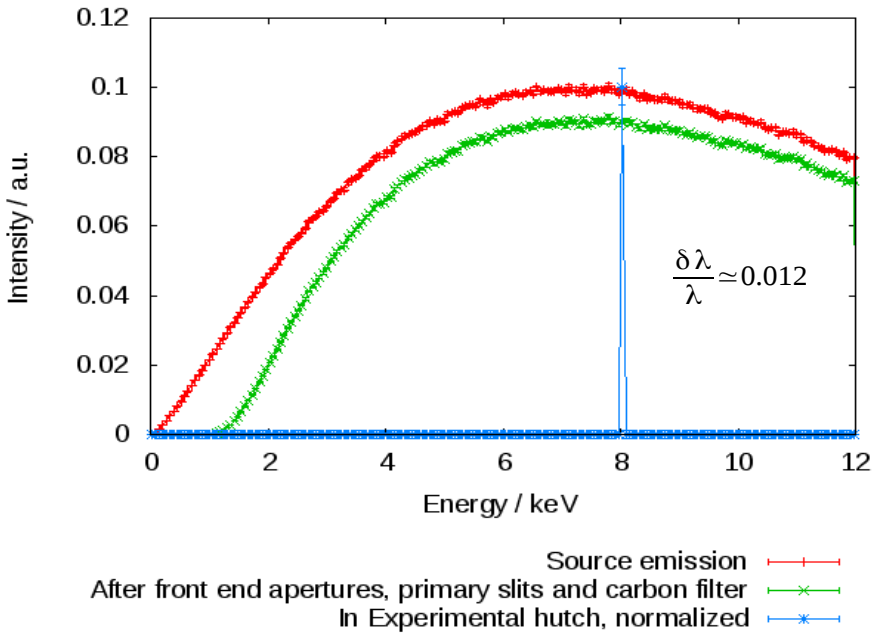
Experimental Hutch



Experimental Hutch

Unslit Spatial beam



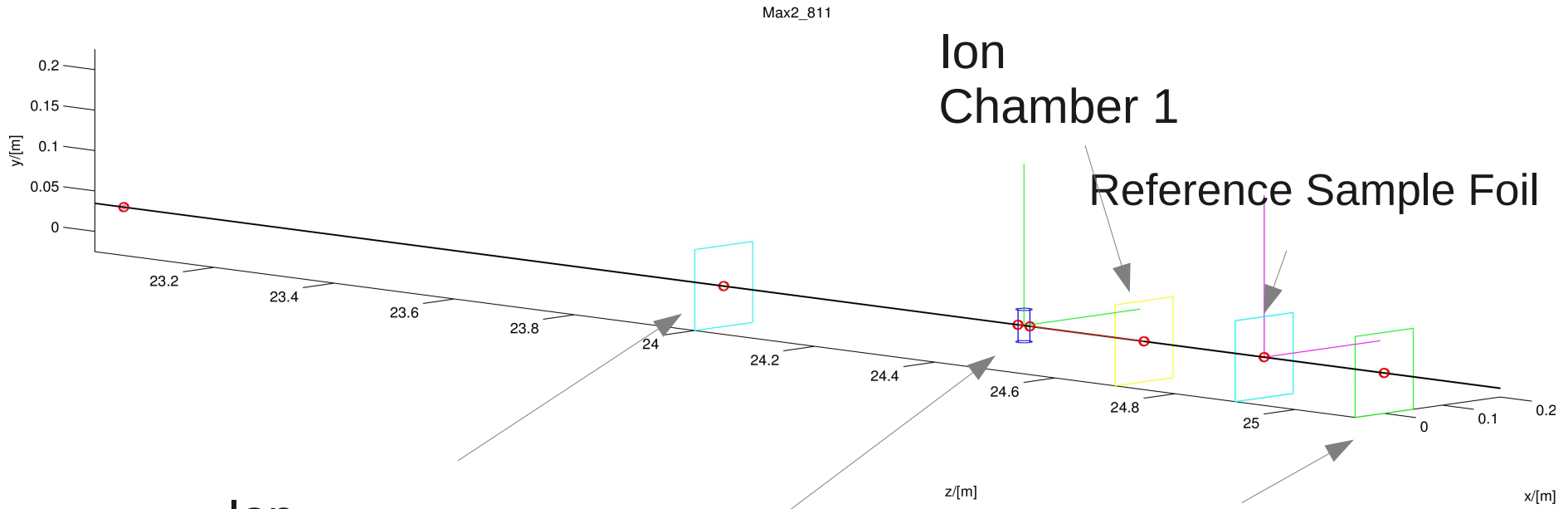


Ratio between photons emitted and on sample match up OK:

real: [2000..20000] reported, virtual: 20800

Experimental Hutch, XAFS Station

Ion chambers have so far been approximated by Integrating Intensity monitors



Ion Chamber 1

Reference Sample Foil

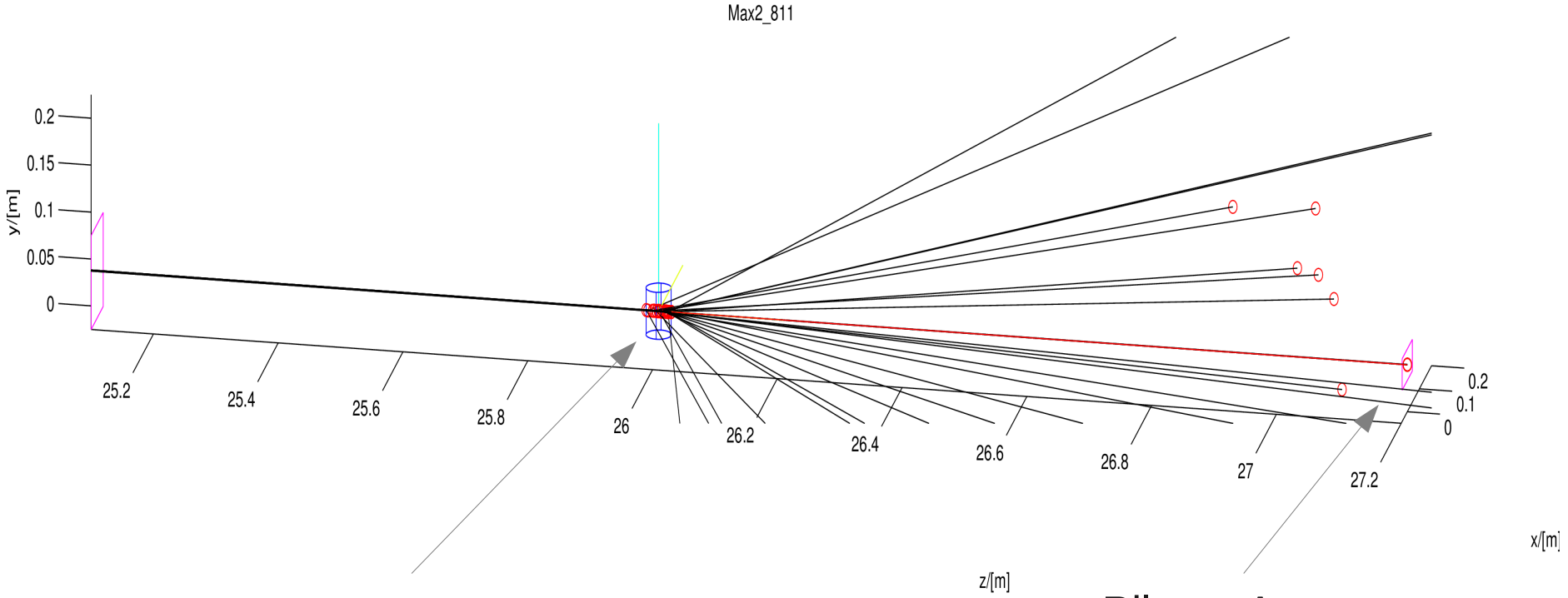
Ion Chamber 0

Sample

Ion Chamber 2

Experimental Hutch, Diffraction Station

Using a Silicon Powder sample

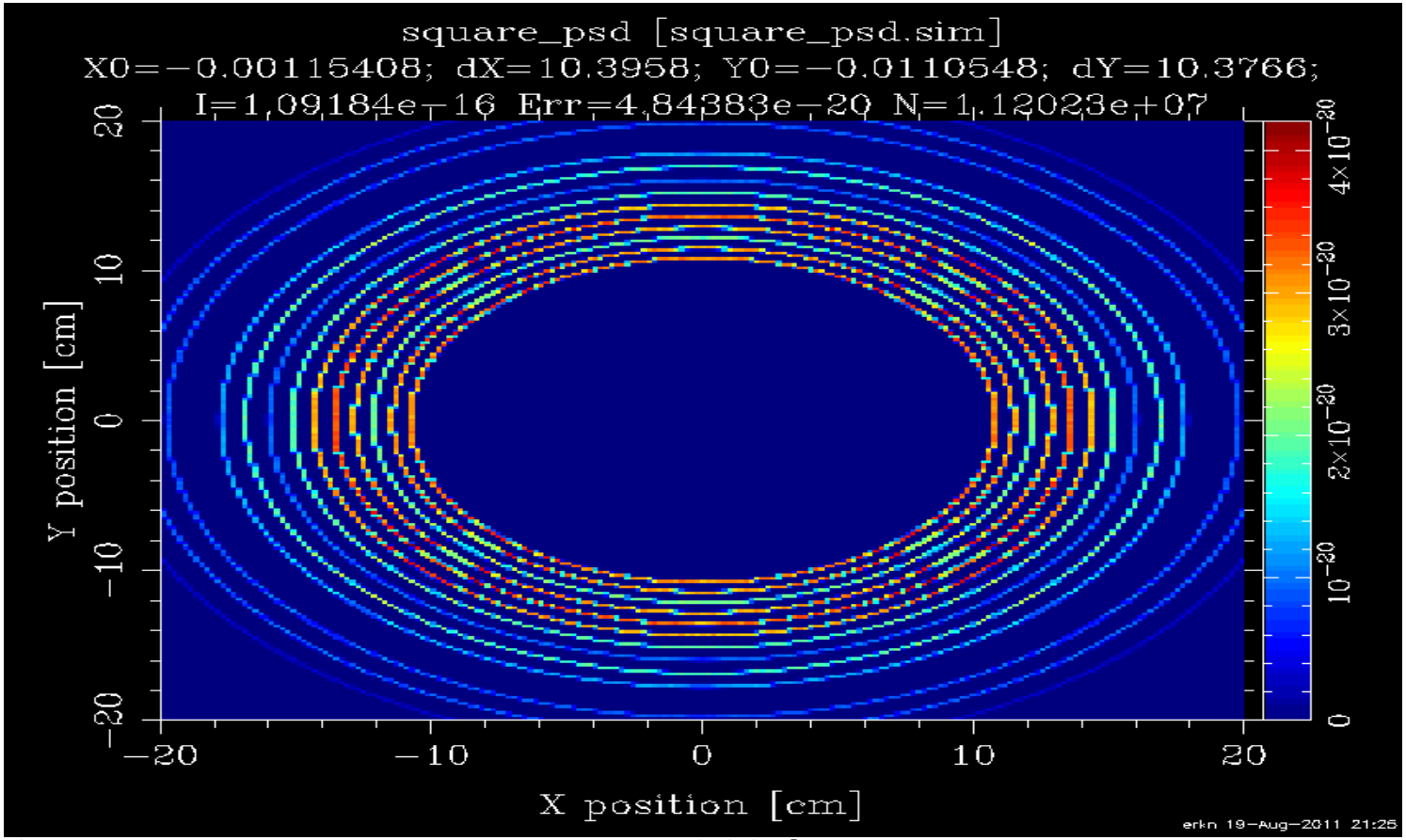


Sample

Pilatus Area Detector

Experimental hutch, Diffraction Station

Using a Silicon Powder sample



TODO

- Prove slit-scatter with crystal sample
- Revamp/Reorganize website again
- Publish manual POD (amazon?)
- Consolidate reflectivity models
- Partial Coherence Work integration
- Finish (a) SPECTRA and (b)SRW interfaces
- Allow python/ruby components?
- McXtrace under ROOT/cling?

Why McXtrace ?

- Open Source GPL.
- Extensible
- Fast/Scalable
- Portable
- Connectable/Embeddable to/in other tools
- Community friendly (crowdsourcing)
- 100+ page manual

McXtrace 1.1 release out!

THANK YOU FOR YOUR TIME AND ATTENTION!