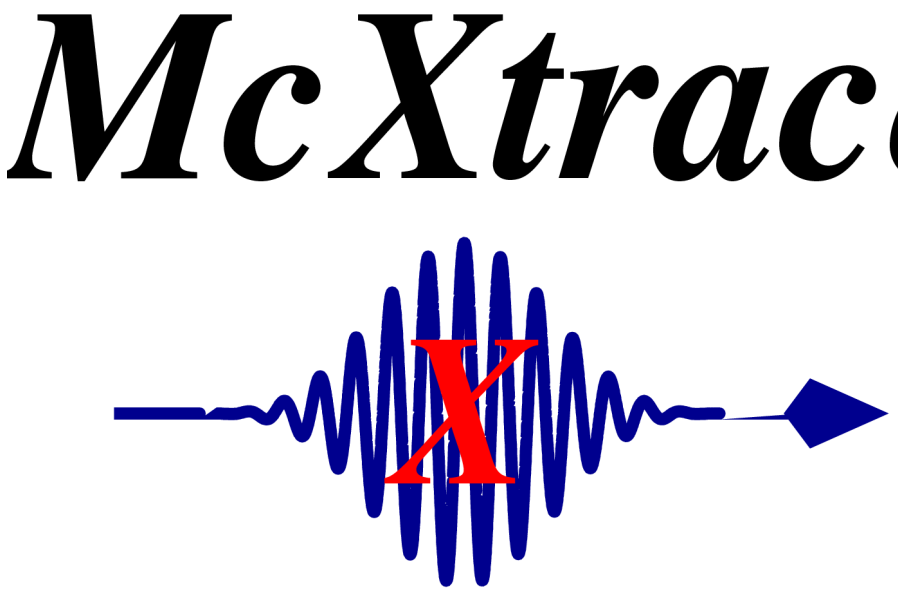
McXtrace

The McXtrace simulation package



E.B. Knudsen SRI 2012

Outline

- Introduce McXtrace
- McXtrace by examples
  - Tomography
  - Laue Camera for Crystallography
  - Powder diffraction beamline
  - XAFS/Diffraction beamline
  - Pump & Probe studies
  - Time Tracking for Pump & Probe
  - Coherent ray tracing
  - Strain measurements
  - ....
- Concluding remarks

McXtrace

- Built on proven base of McStas for neutron ray tracing
  - K. Lefmann and K. Nielsen, *Neutron News* 10, 20, (1999).
- Release 1.0 out now, 1.1 this summer!
- Portable code (Unix/Linux/Mac/Windows, 32 and 64 bit support)
- Has run on all from iPhone to 1000+ node clusters

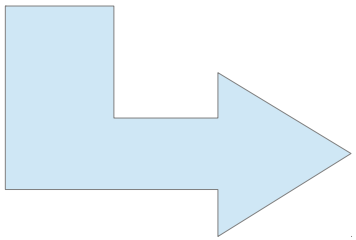



Project website at
http://www.mcxtrace.org

- 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).

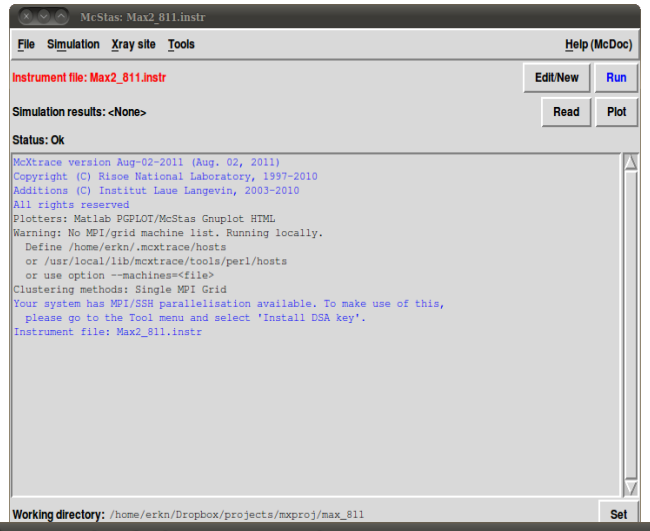
The McXtrace Way

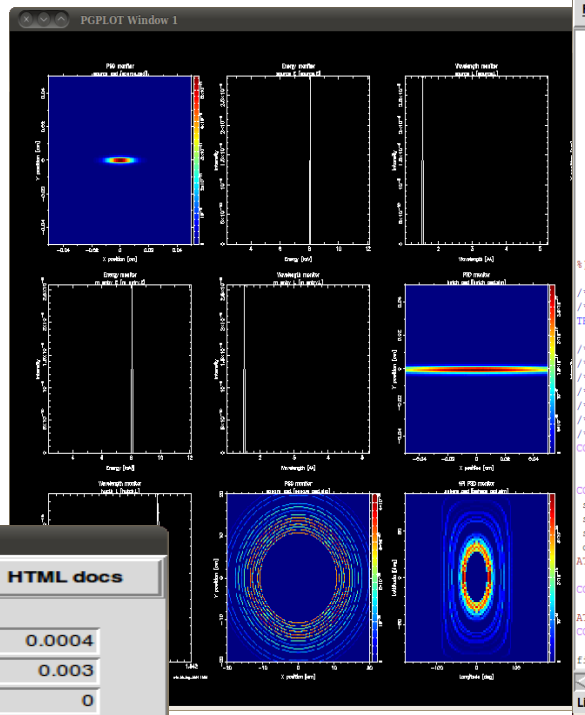
1. Describe your beamline in the McXtrace language (In a text file).
2. Automatically convert beamline into ANSI c
3. Compile
4. Run

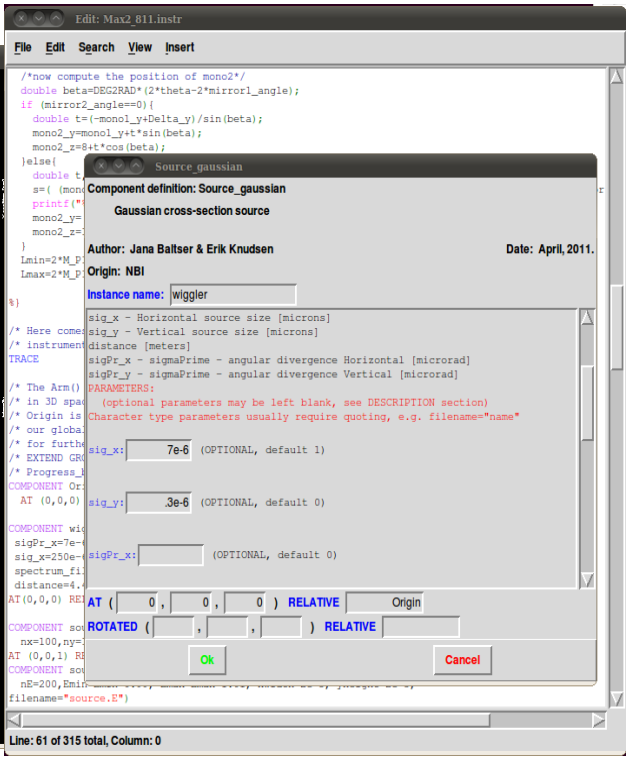


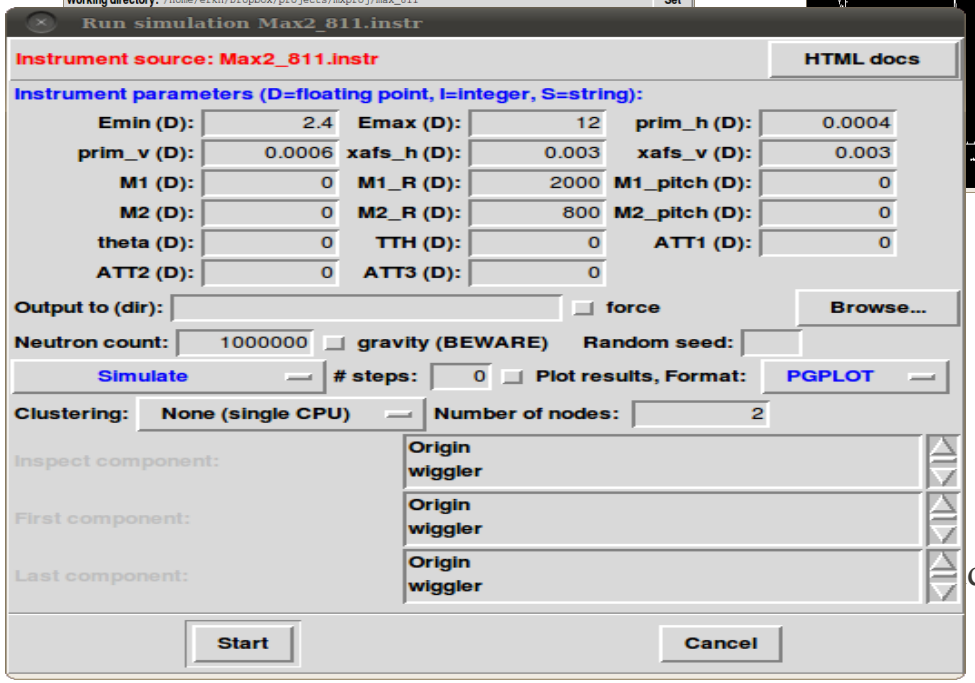
1. Optimized for your platform
2. Only includes what you use

GUI


McStas: Max2_811.instr
File Simulation Xray site Tools Help (McDoc)
Instrument file: Max2_811.instr
Edit/New
Run
Simulation results: <None>
Read
Plot
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
Set

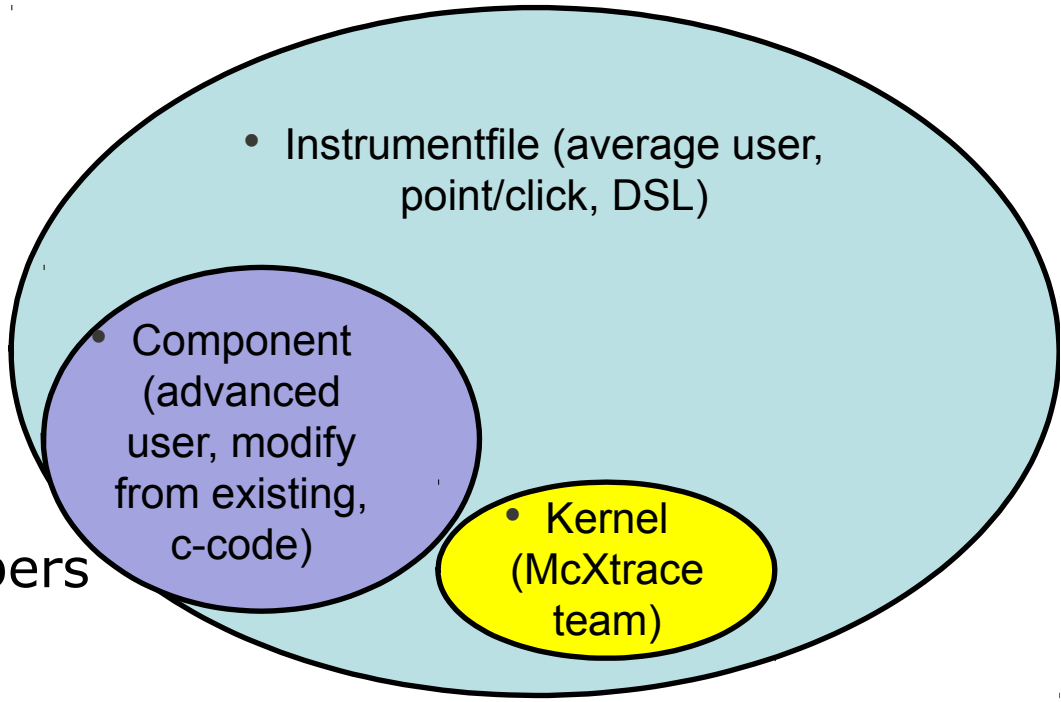

PGPLOT Window 1


Edit: Max2_811.instr
File Edit Search View Insert
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
Line: 61 of 315 total, Column: 0

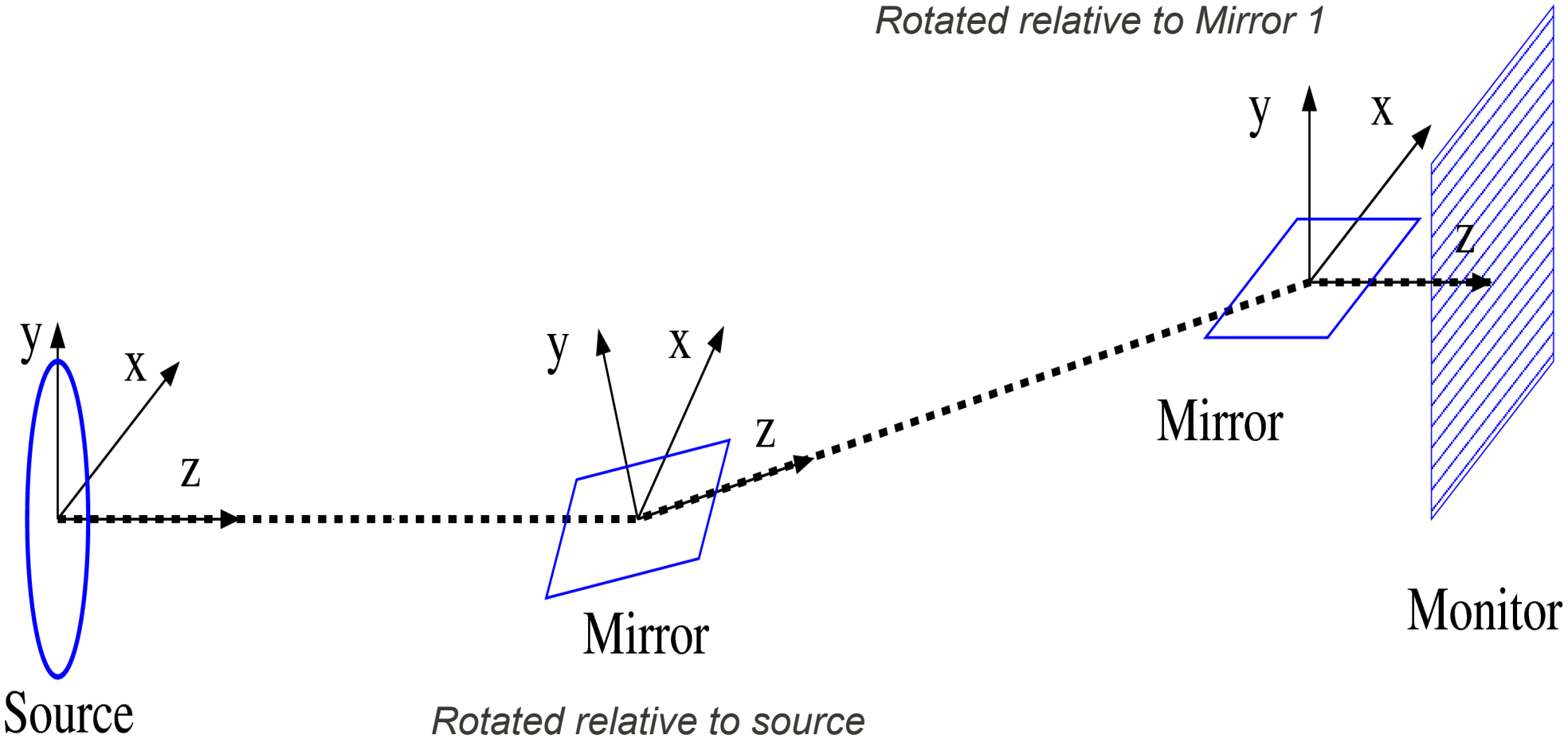

Run simulation Max2_811.instr
Instrument source: Max2_811.instr
HTML docs
Instrument parameters (D=floating point, I=integer, S=string):
Emin (D): 2.4
Emax (D): 12
prim_h (D): 0.0004
prim_v (D): 0.0006
xafs_h (D): 0.003
xafs_v (D): 0.003
M1 (D): 0
M1_R (D): 2000
M1_pitch (D): 0
M2 (D): 0
M2_R (D): 800
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

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.)

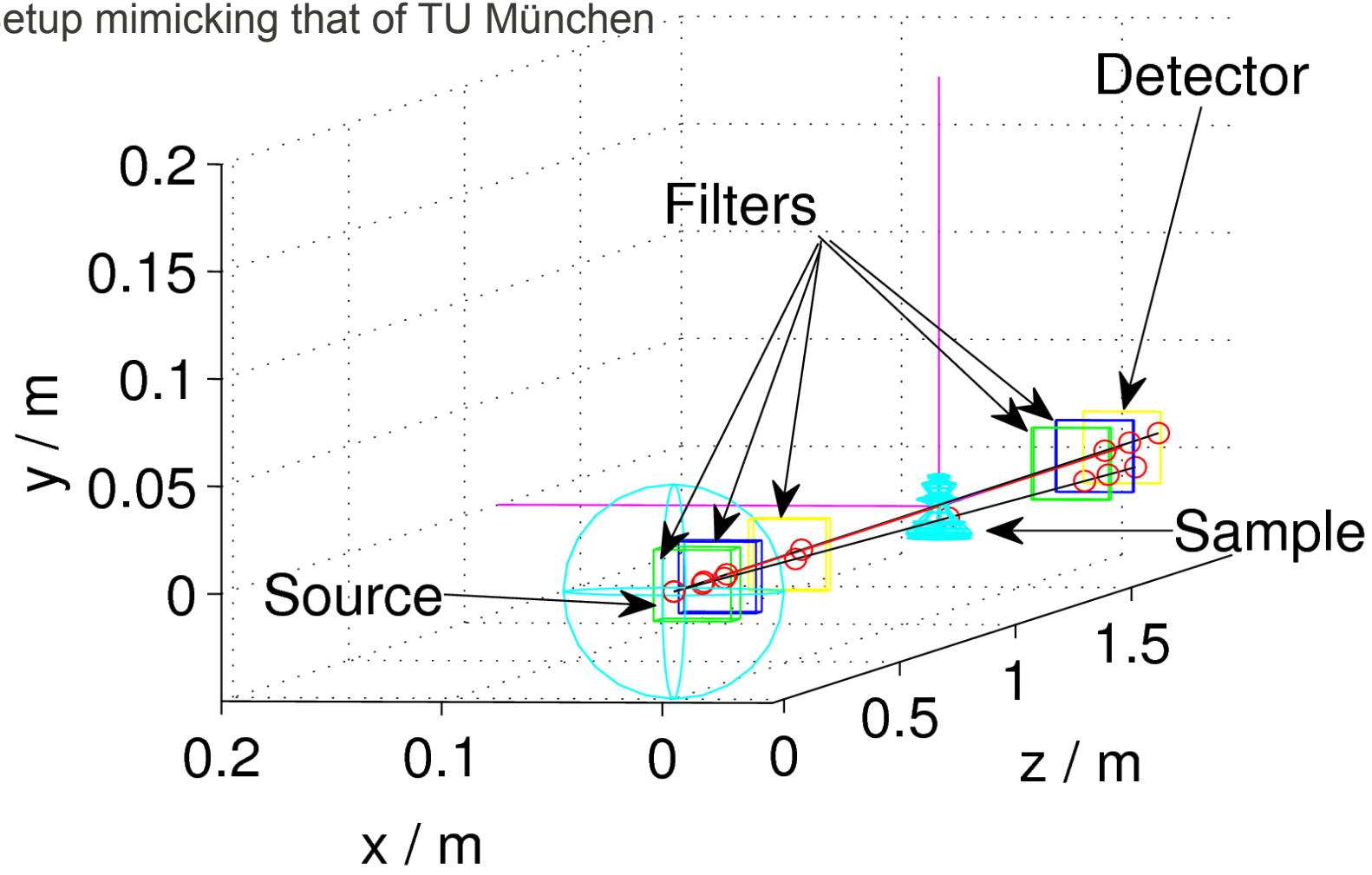


McXtrace positioning scheme

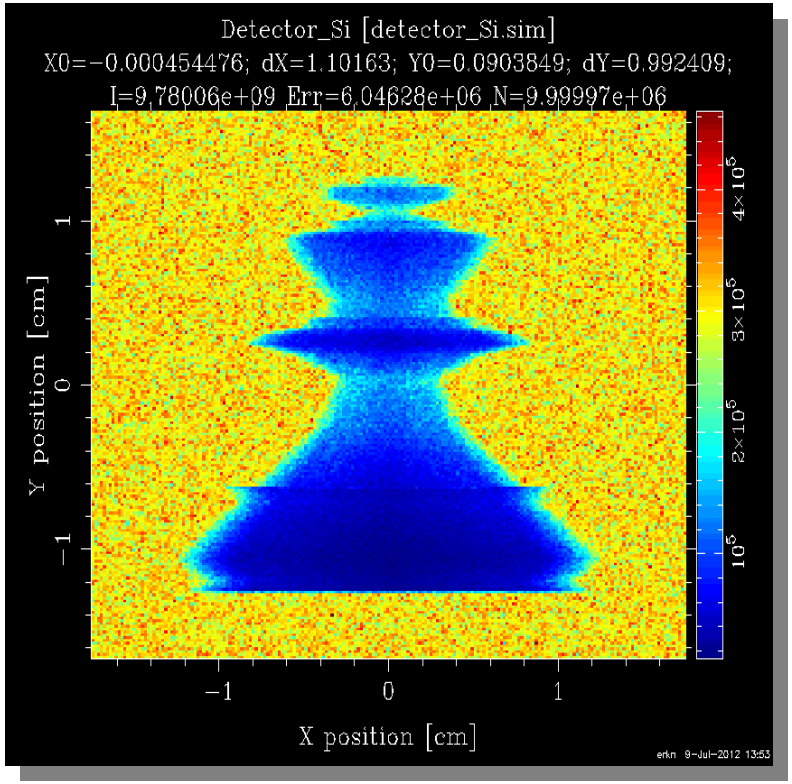


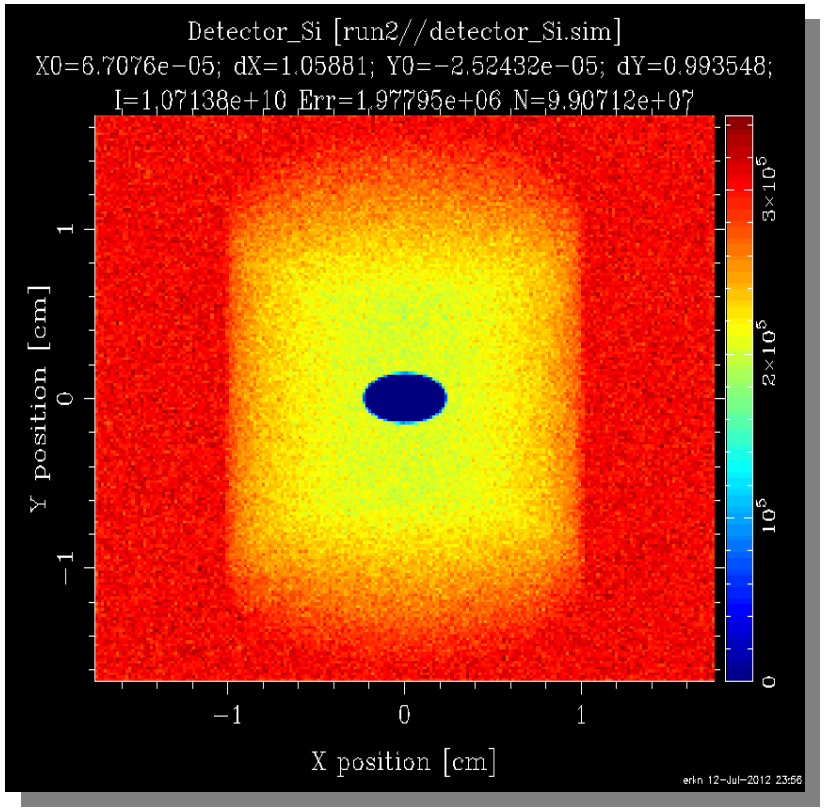
Tomography

Setup mimicking that of TU München

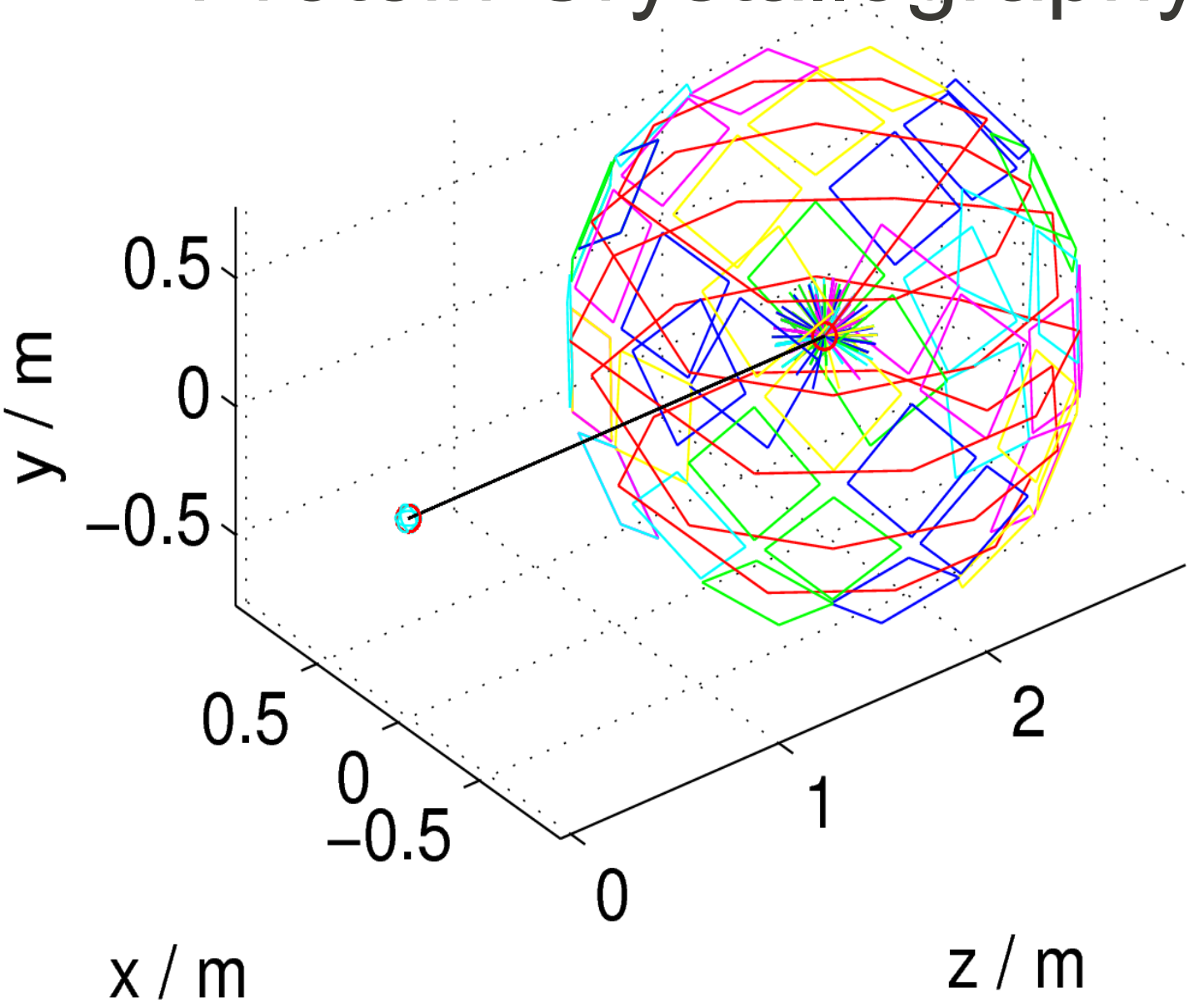


Tomography

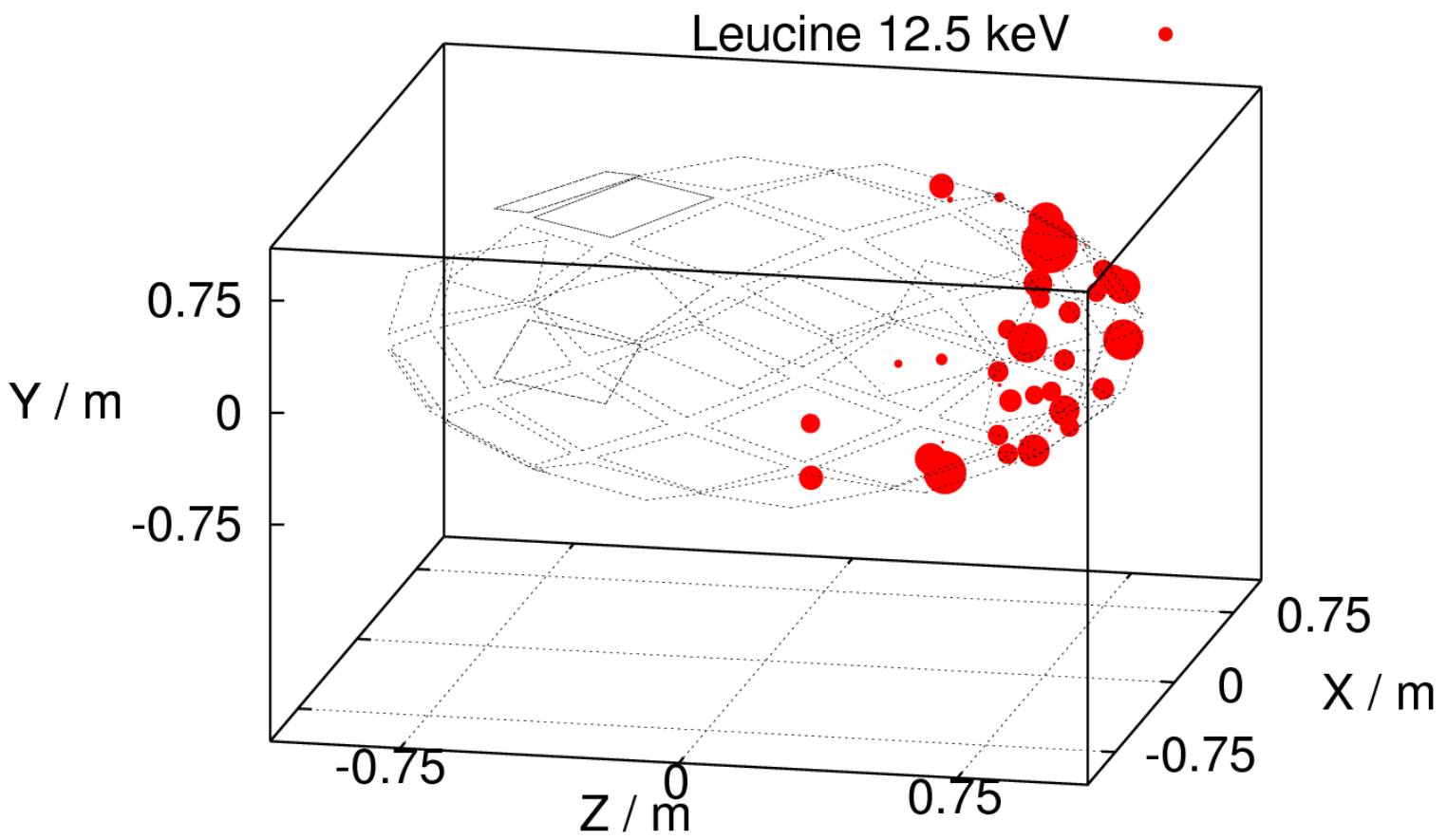

Detector_Si [detector_Si.sim]
X0=-0.000454476; dX=1.10163; Y0=0.0903849; dY=0.992409;
I=9.78006e+09 Err=6.04628e+06 N=9.99997e+06
Y position [cm]
X position [cm]
erkn 9-Jul-2012 13:53


Detector_Si [run2//detector_Si.sim]
X0=6.7076e-05; dX=1.05881; Y0=-2.52432e-05; dY=0.993548;
I=1.07138e+10 Err=1.97795e+06 N=9.90712e+07
Y position [cm]
X position [cm]
erkn 12-Jul-2012 23:56

Protein Crystallography

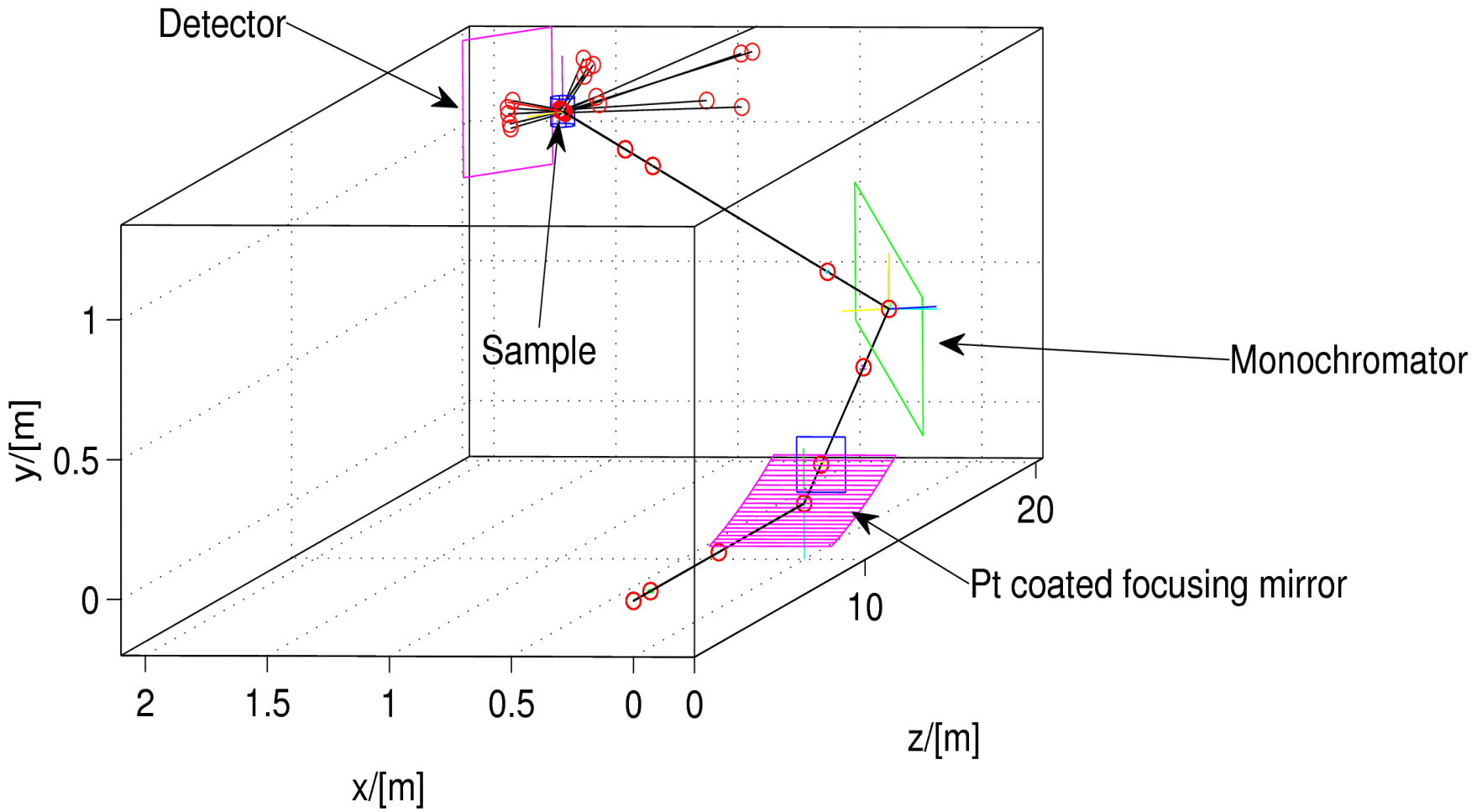


Protein Crystallography



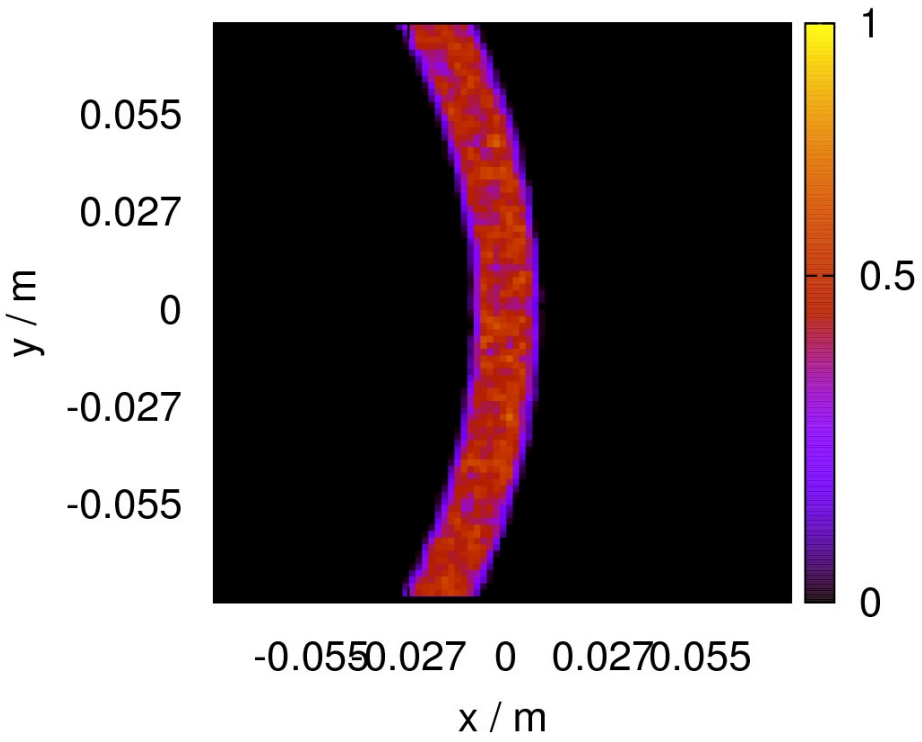
Powder Diffraction Beamline

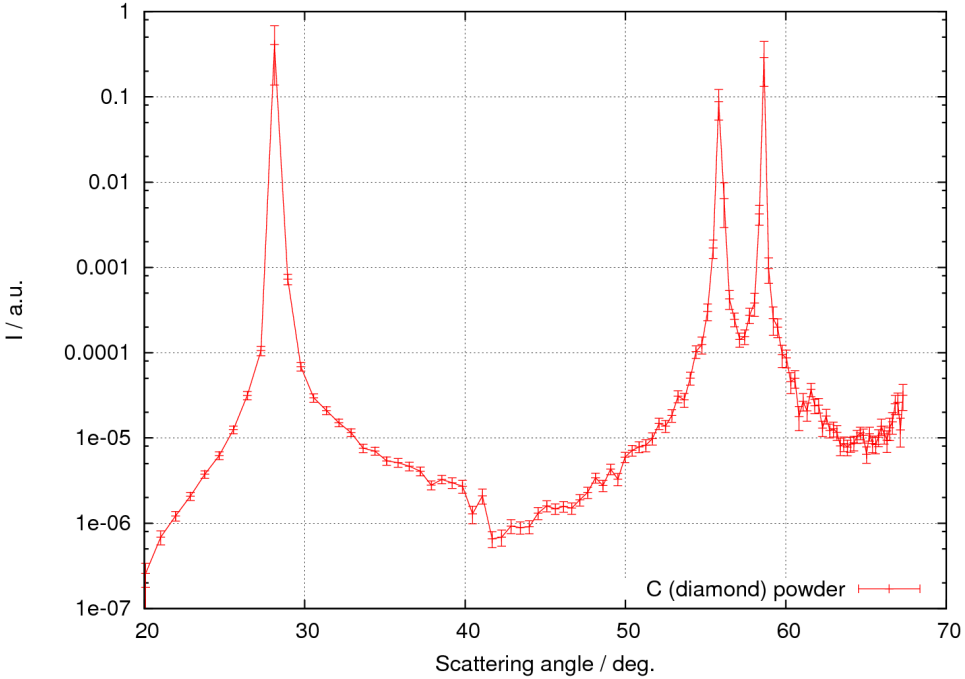
Powder Diffraction Beamline 711 @ MAX IV



Powder Diffraction Beamline

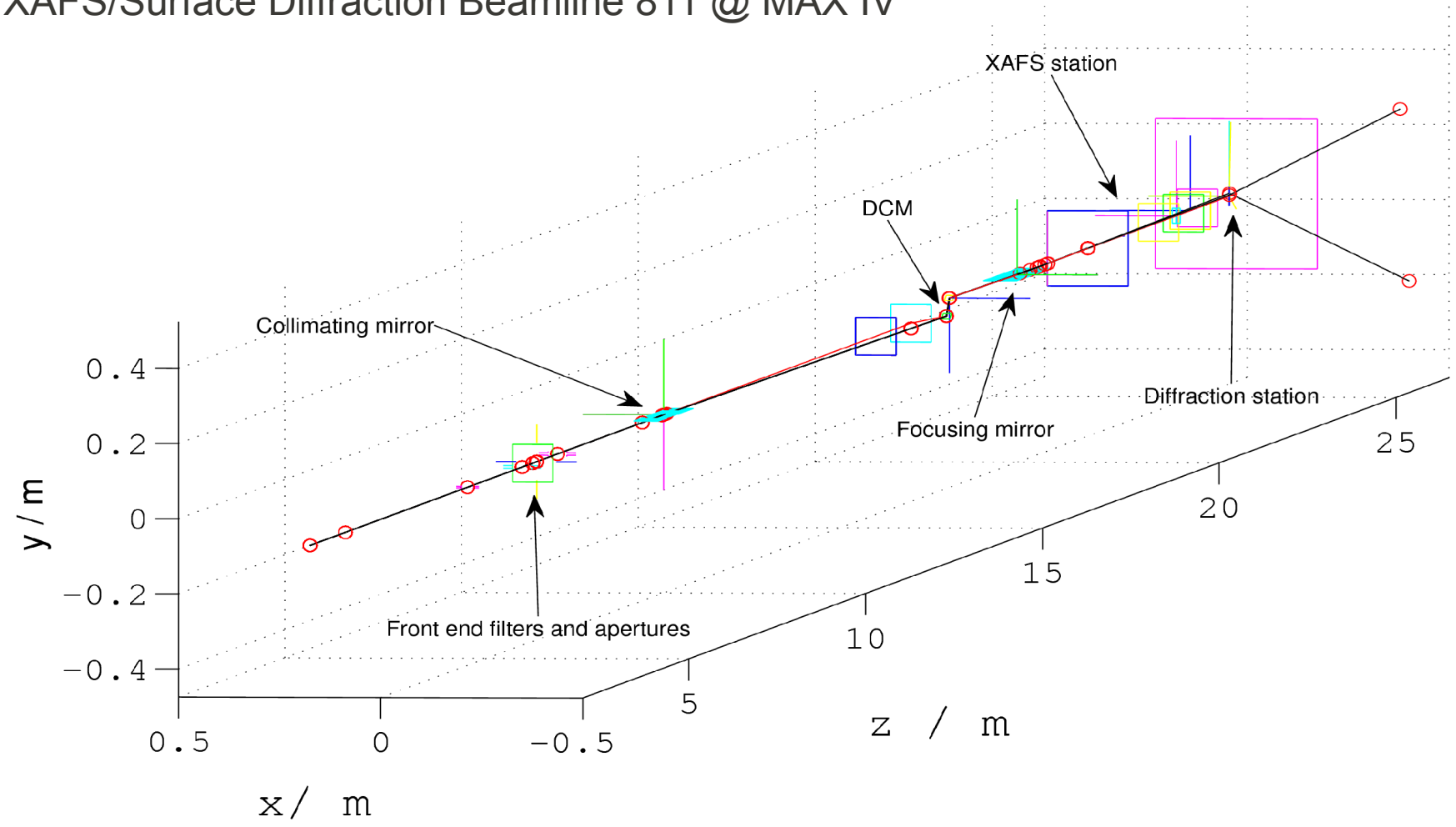
Powder Diffraction Beamline 711 @ MAX IV





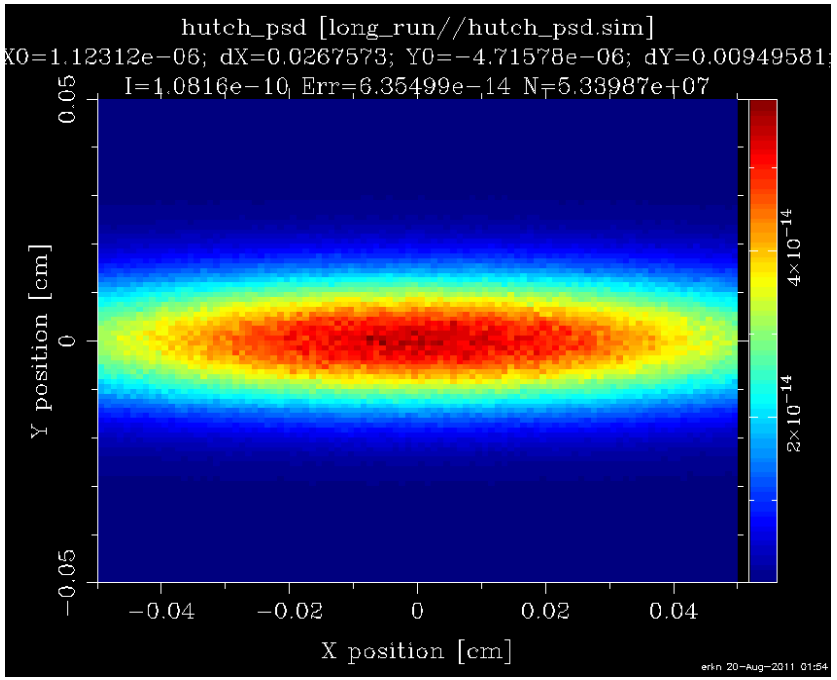
A Combination Beamline

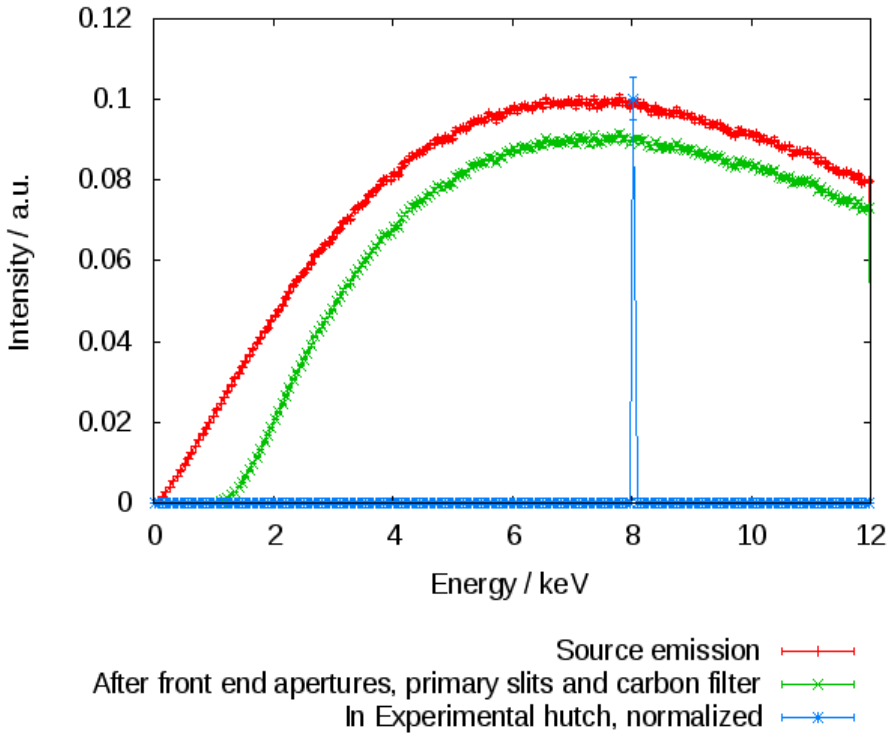
XAFS/Surface Diffraction Beamline 811 @ MAX IV



A Combination Beamline

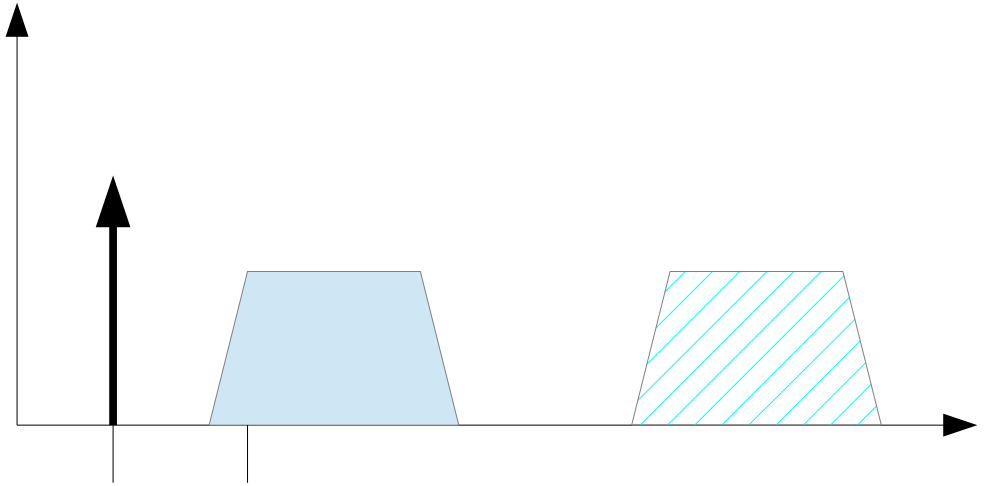
- Unslit Spatial beam distribution

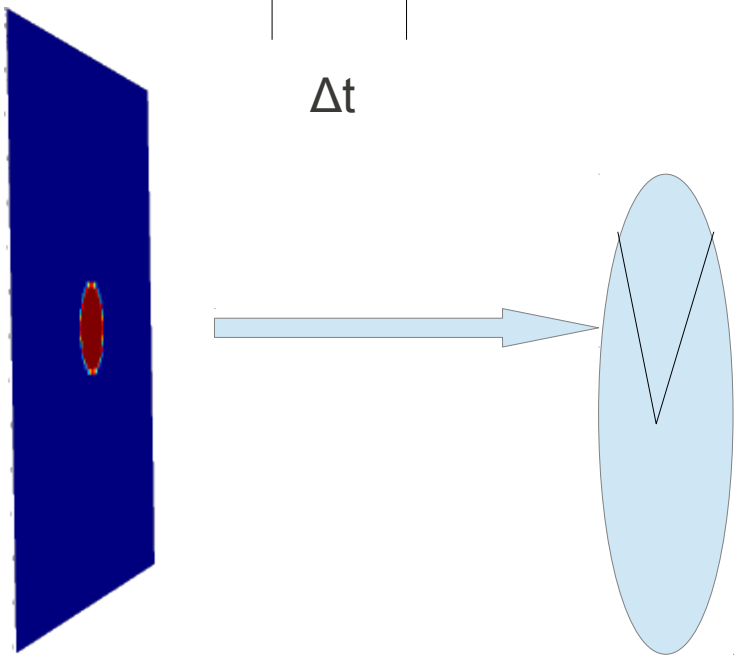


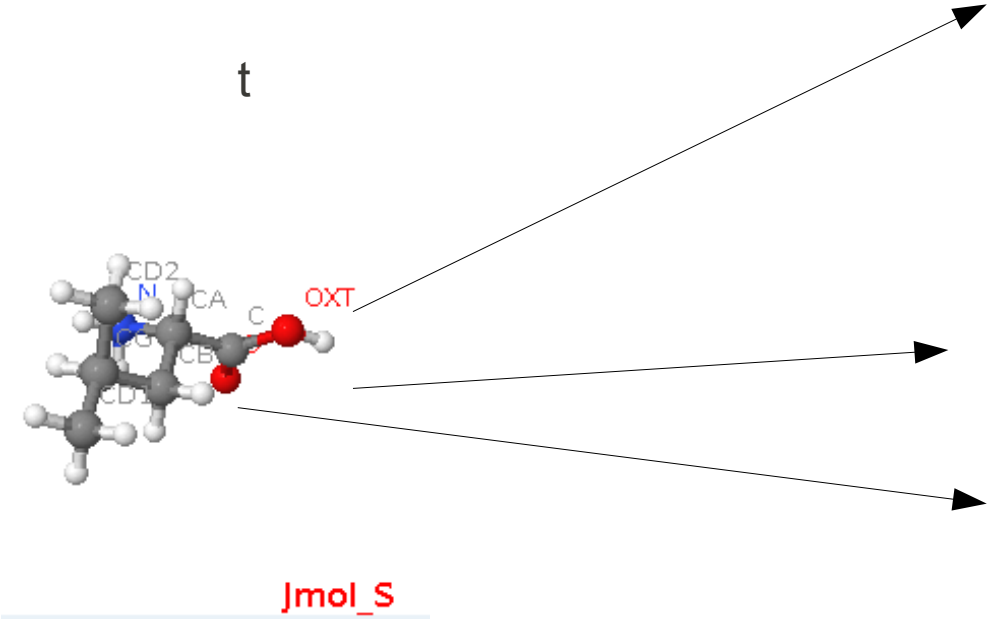


- Ratio between photons emitted and on sample match up OK:
- real: [2000..20000] reported, virtual: 20800

Time Resolved Studies

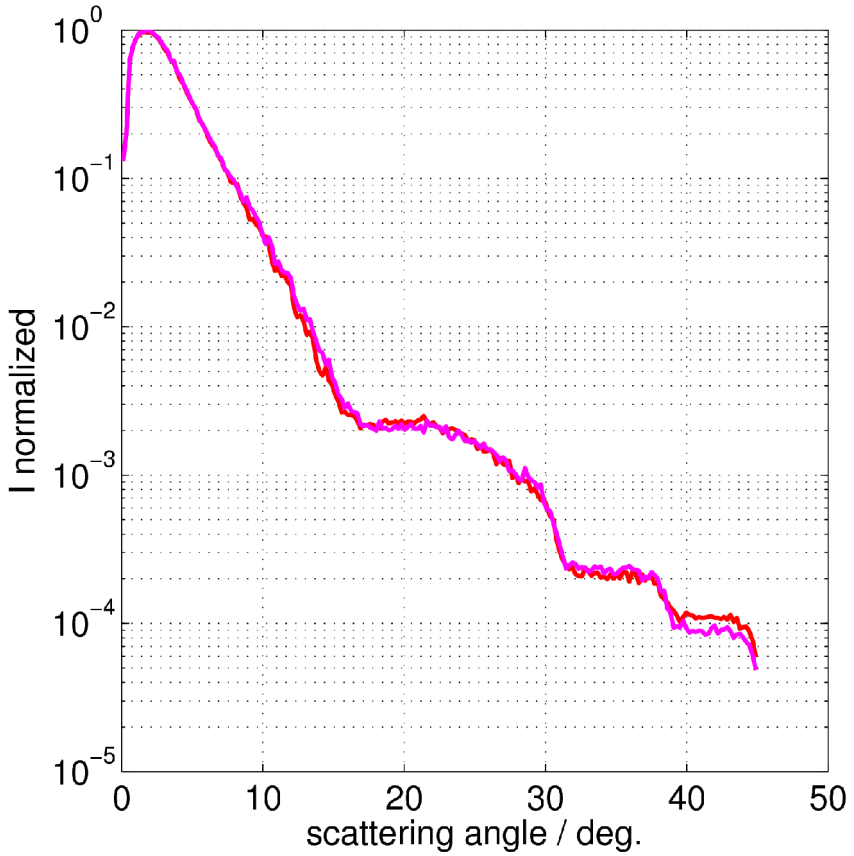


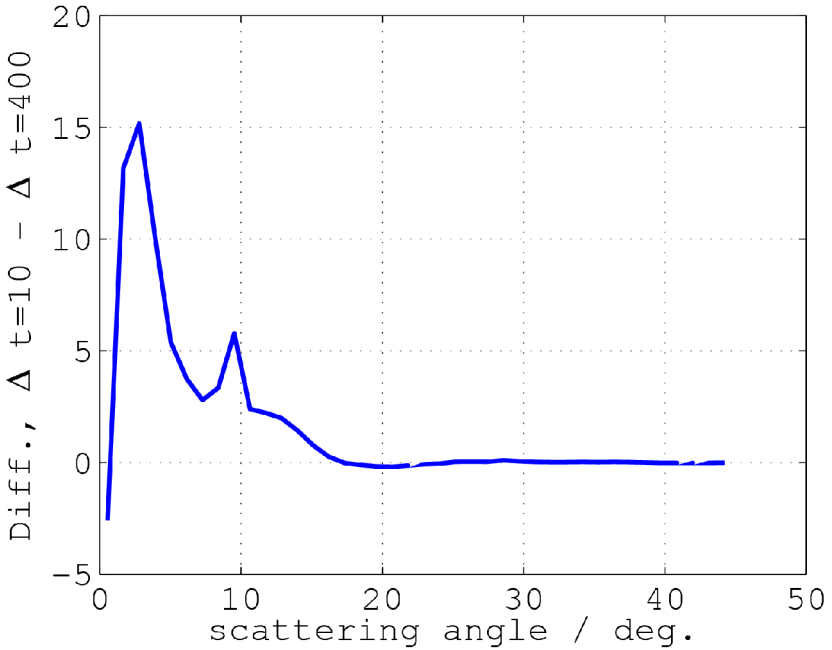




Time Resolved Studies

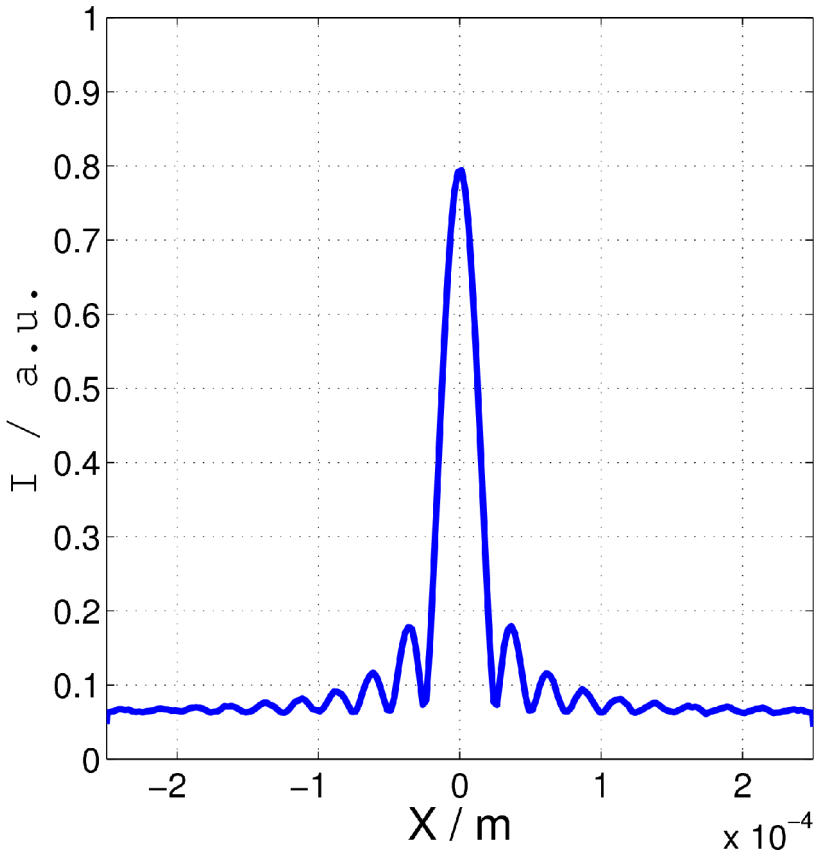
Fe (bpy)



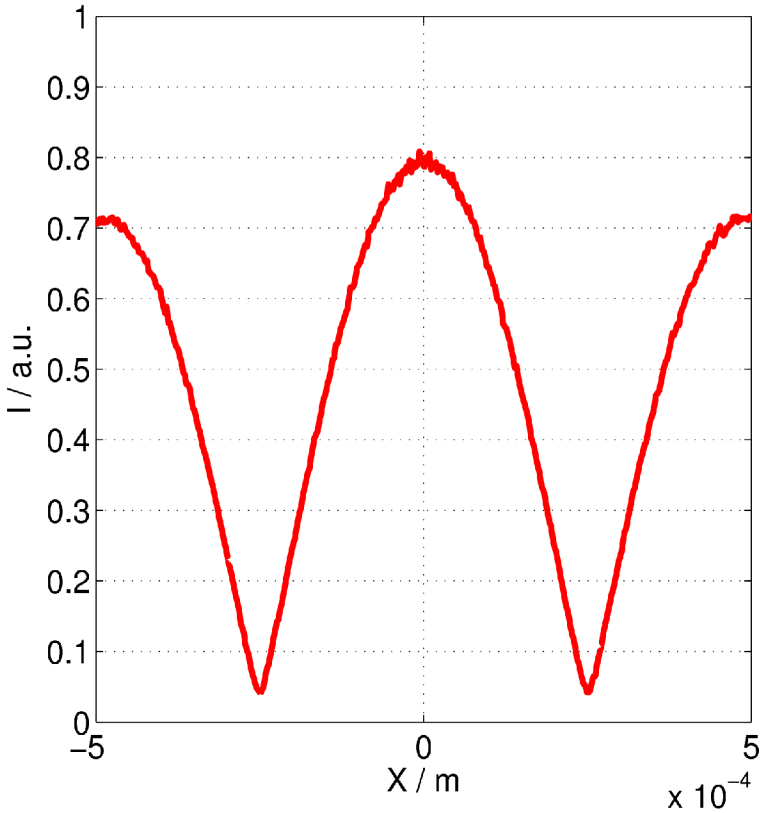


Coherent examples

Single slit diffraction
- λ = 1 Å
- Slit width 1 μm

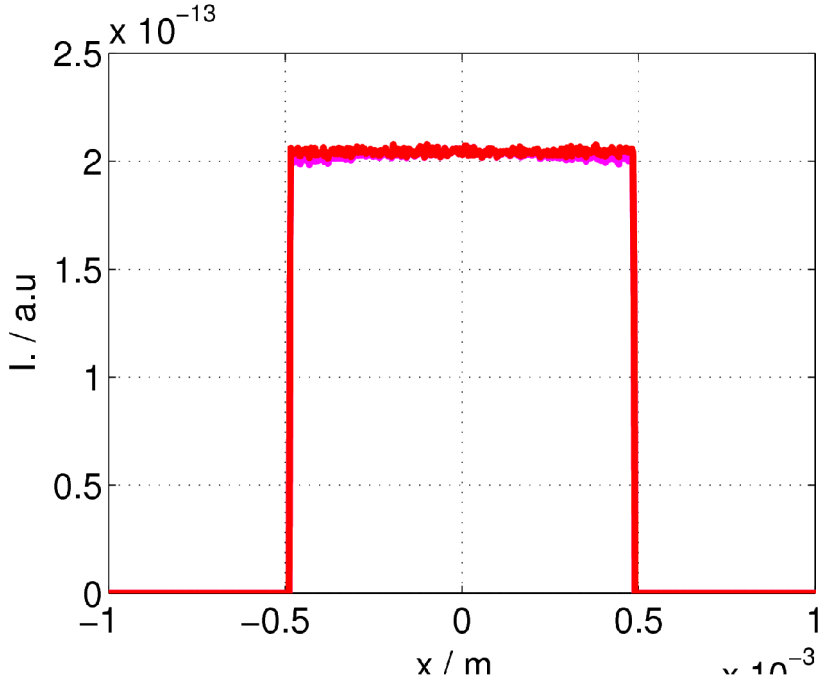


Double slit interference
- λ = 1 Å
- Slit width 1 μm
- Slit separation Δ=2 μm

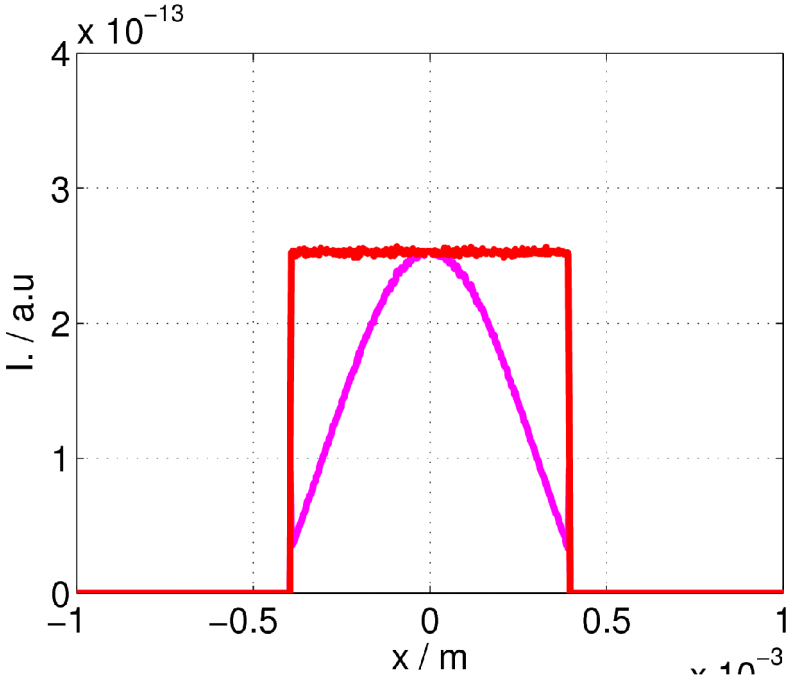


Coherent examples

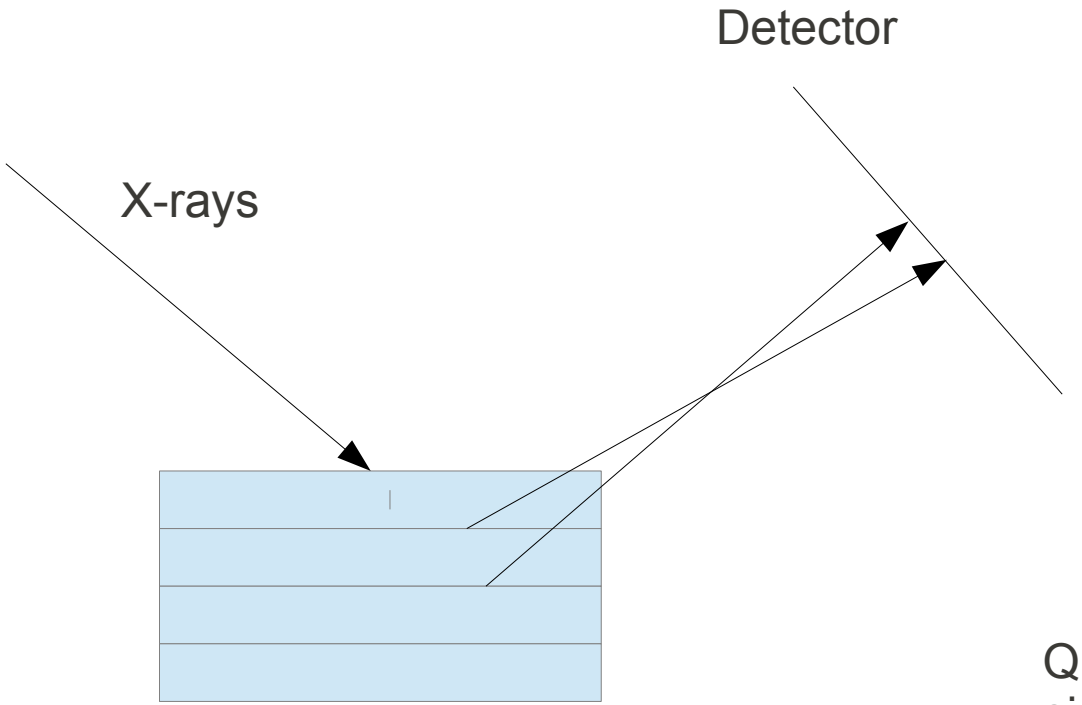
1 Be refractive lens:
Red: Incoherent
Magenta: Fully coherent, in phase



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

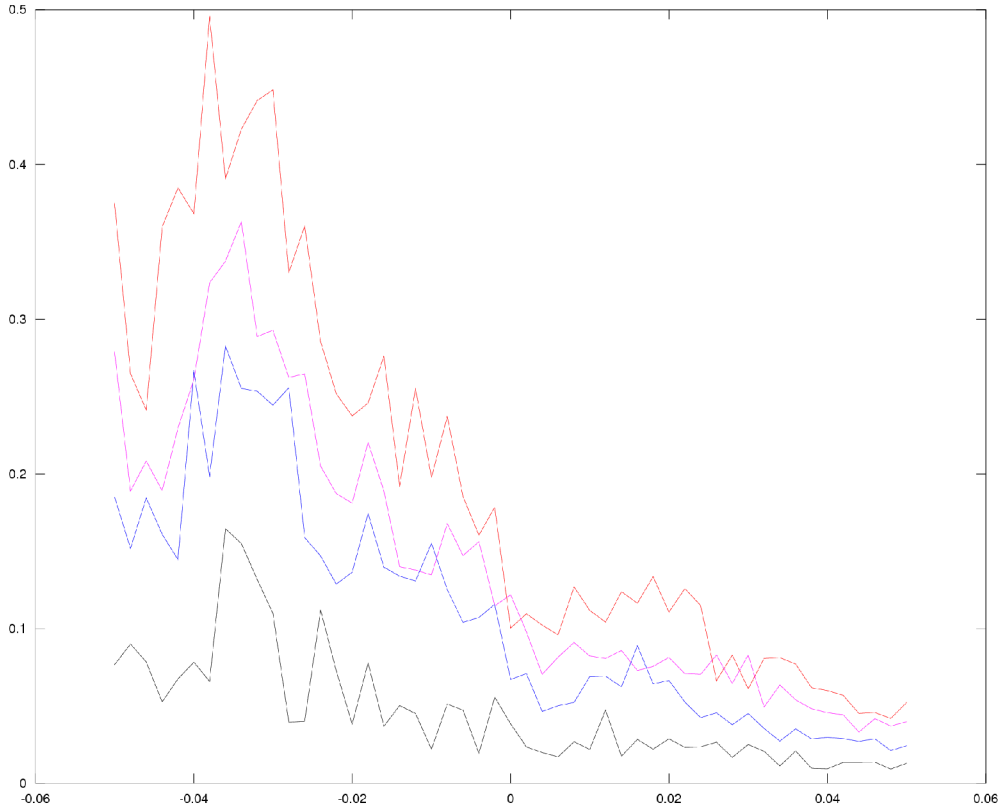


Portable bulk strain beamline

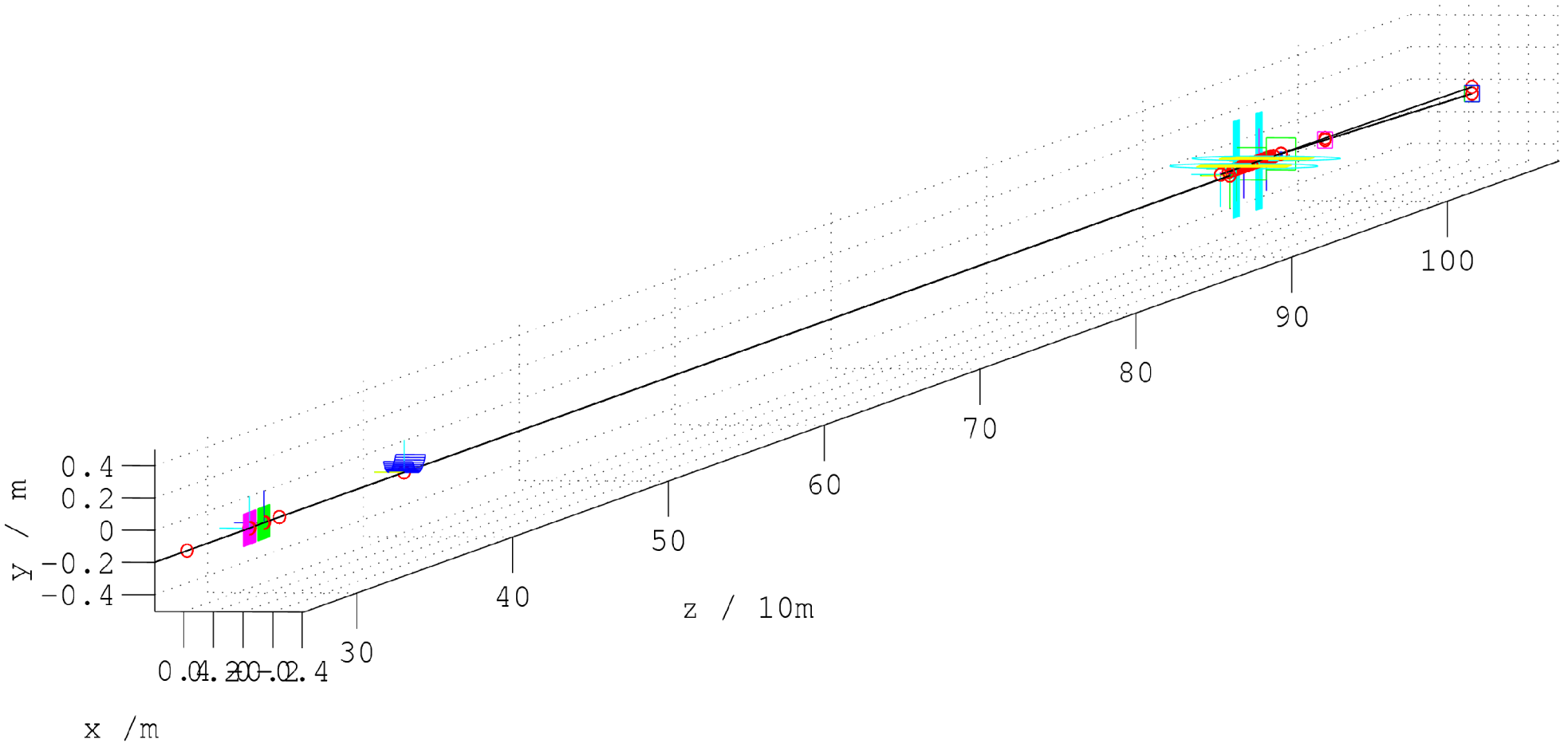


Question: Can we get an appreciable signal from the bulk of the sample?

Portable bulk strain beamline



Guerilla simulation / XFEL SPB



Why McXtrace ?

- Open Source GPL.
- Extensible
- Fast/Scalable
- Portable
- Connectable/Embeddable to other tools
- 100+ page manual.

McXtrace 1.1 release out soon!

McXtrace People

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Claudio Ferrero4
Karsten Joensen5
Kell Mortensen3
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Kim Lefmann2

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

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5SAXSLAB, Denmark (Formerly JJ X-RAY Systems)