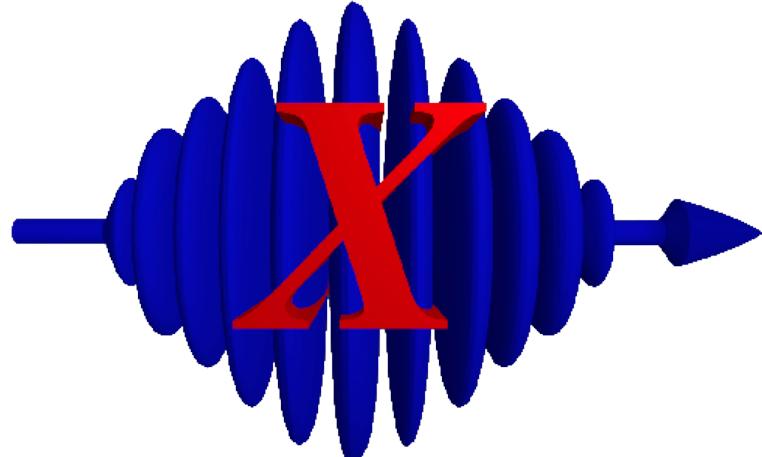




McXtrace



Powered by McStas technology

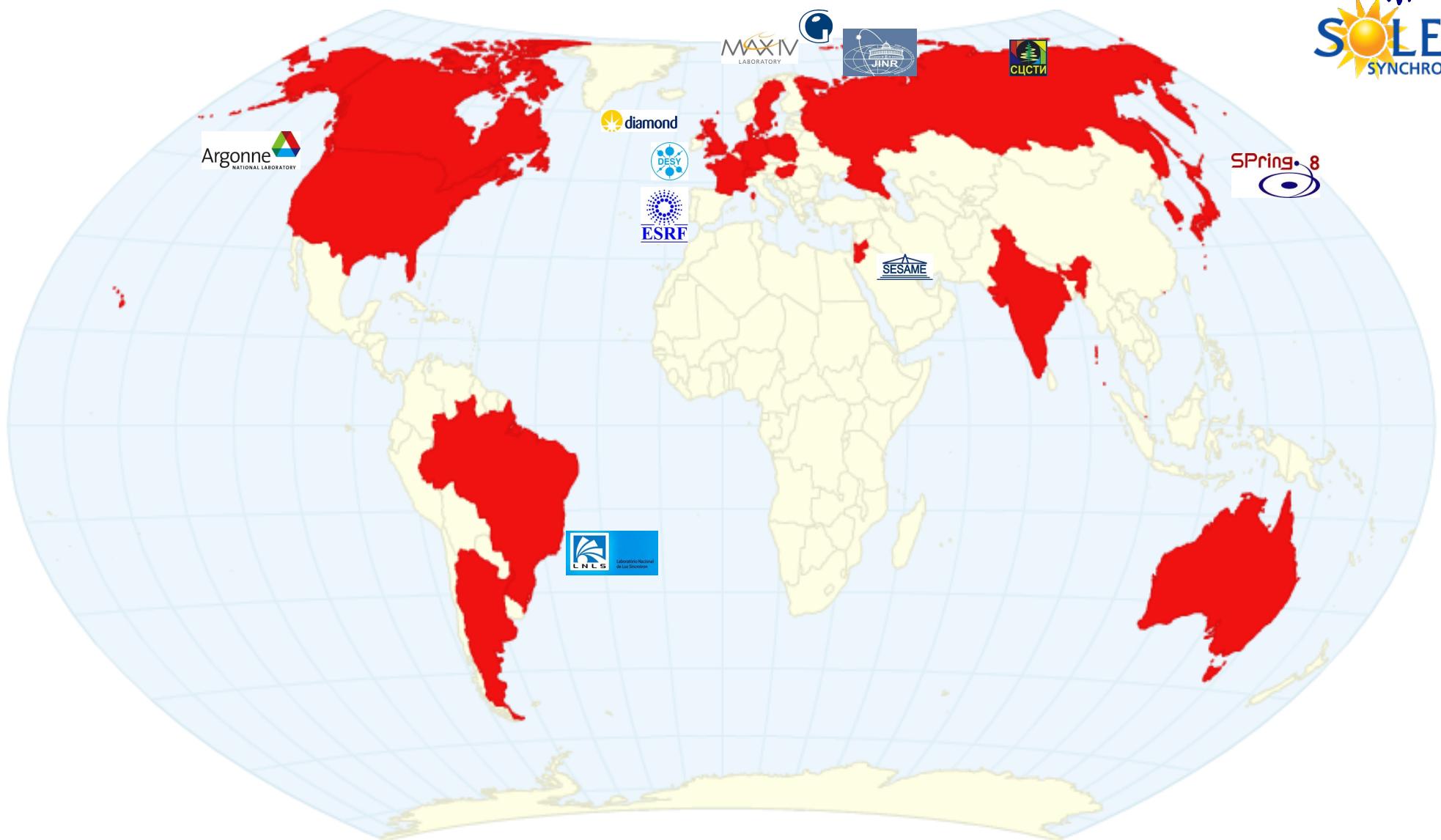
"McXtrace: a Monte Carlo software package for simulating X-ray optics, beamlines and experiments",

Journal of Applied Crystallography, vol. 46, part 3, June 2013

Erik Bergbäck Knudsen (erkn@fysik.dtu.dk)



Where?



What is it?

- Built on proven base of McStas for neutron ray tracing
- K. Lefmann and K. Nielsen, Neutron News 10, 20, (1999).
- Release 1.5
 - Portable code (Unix/Linux/Mac/Windows, 32 and 64 bit support)

Has run on all from iPhone to FERMI (world no. 7)



Project website at
<http://www.mcxttrace.org>

Project mailing list at
mcxttrace-users@mcxttrace.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 (python3/qt4 or perl/tk for gui).
- Permanent staff at DTU Physics maintaining the code



Github



McStasMcXtrace/McCode - Mozilla Firefox

GitHub, Inc. (US) | https://github.com/McStasMcXtrace/McCode

Most Visited Getting Started Portscout Port Up... Getting Started Bright: New beamlin... Astro-Update Hea... Portscout Port Up... Tinkercad | Create 3...

This repository Search Pull requests Issues Marketplace Gist

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McStasMcXtrace / McCode

Code Issues 63 Pull requests 0 Projects 0 Wiki Settings Insights

http://www.mccode.org Edit

c neutron x-ray scientific-computing simulation raytracing Manage topics

6,977 commits 15 branches 6 releases 14 contributors

Branch: master New pull request Create new file Upload files Find file Clone or download

climbcat	added a version using the native iFit python-matlab interface, now de...	Latest commit 0194107 2 days ago
cmake	A couple of @MCCODE_PREFIX@ needed	2 months ago
common	descriptive files that are now in the comps-package	2 months ago
doc	Update manual for 2.4.1	2 months ago
docpkg/manuals	Update manual for 2.4.1	2 months ago
mcstas-comps	Remove 1.12c style parameter line	a month ago
mcstas	Increase symbol table length to accomodate MACS instrument from Mads ...	4 months ago
mxtrace-comps	this had apparently not been committed	2 months ago
mxtrace	Make the Component Blah AT (x,y,z) location status in trace mode incl...	5 months ago
meta-pkgs	We only build 32 bit...	2 months ago
obsolete-files	Removing Yosemite scripts as the build server is being migrated to DM...	7 months ago
support	Adding binary for NeXus libs (distributed as "extras" for Windows)	3 months ago
tools	added a version using the native iFit python-matlab interface, now de...	2 days ago
BUILD_DEPS.TXT	added rpm dependence to RPMs build	a year ago
CHANGES_McStas	Update release no in one spot..	a month ago
CHANGES_McXtrace	this is not finished	2 months ago
COPYING	From our release, McStas is GPL 2 only	10 years ago

Beta:

- a. First package build of McXtrace Linux and Windows XP
- b. 2 Example beamlines
- c. Few components
- d. Optimized packaging, Linux, Windows7, XP and Mac OSX

1.0:

- 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

1.2:

- r. improved polarisation handling
- s. homogenized source physics
- t. SAXS-samples suite
- u. web interface
- v. Windows 8,8.1

1.4:

- v. polycrystal sample
- w. New GUI
- x. More examples instrument files
- y. DEPENDENCY keyword
- z. MCPL-interface
- aa. Automatic FreeBSD build
- ab. SPECTRA source interface
- ac. Undulator source

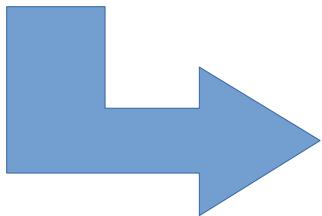
1.5:

- ad. Reflectivity library
- ae. MAX_Bloch
- af. Laue crystal model
- ag. MAXIV_DanMAX
- ah. MAXIV_FemtoMAX
- ai. NIST reflectometer
- aj. Reflective grating
- ak. Johann Spectrometer
- al. Powder Incoherent scattering
- am. More accurate Source_lab

Next-generation:

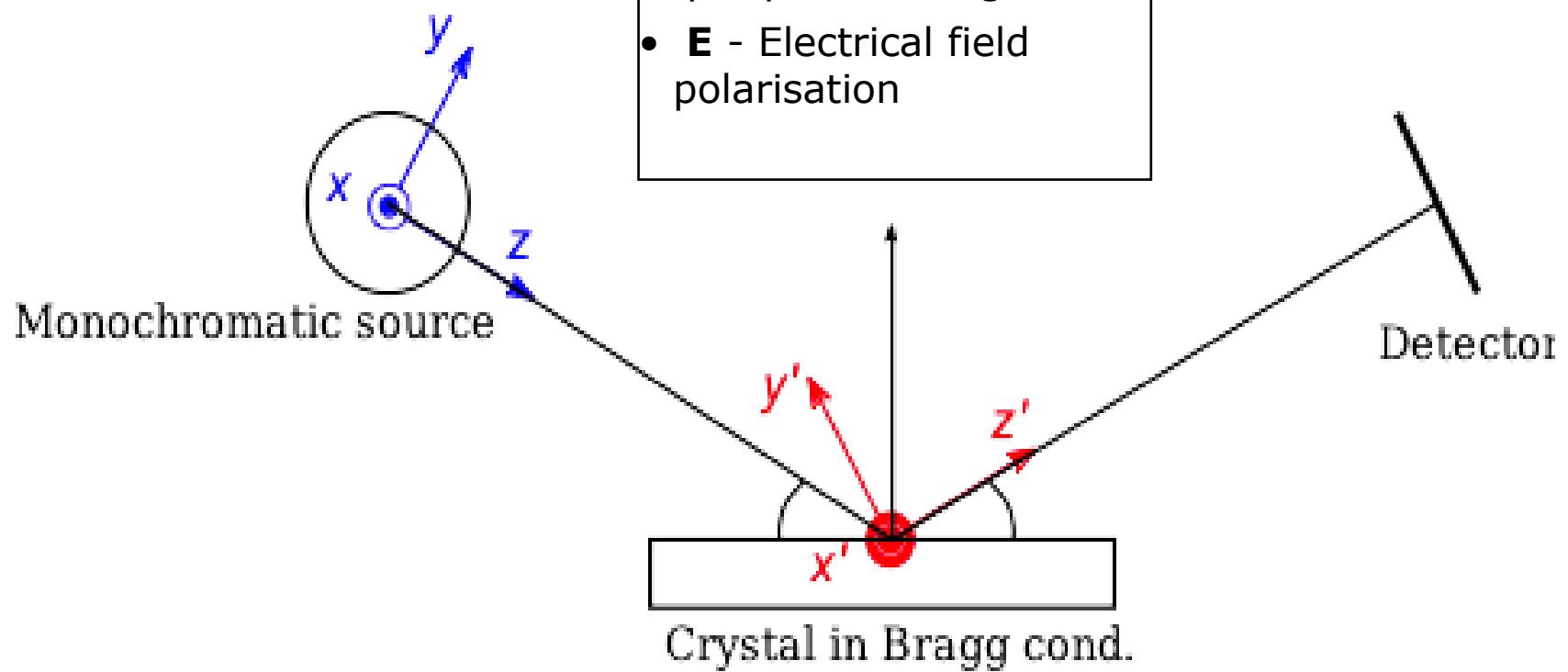
- an. GPU support (~ 40 x speedup)
- ao. Union
- ap. Reverse option

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

- Photon ray/package:
- $(\mathbf{r}, \mathbf{k}, \phi, t, p, \mathbf{E})$
- \mathbf{r} - spatial coordinates
- \mathbf{k} - wave vector
- ϕ - phase
- t - time
- p - photon weight
- \mathbf{E} - Electrical field polarisation

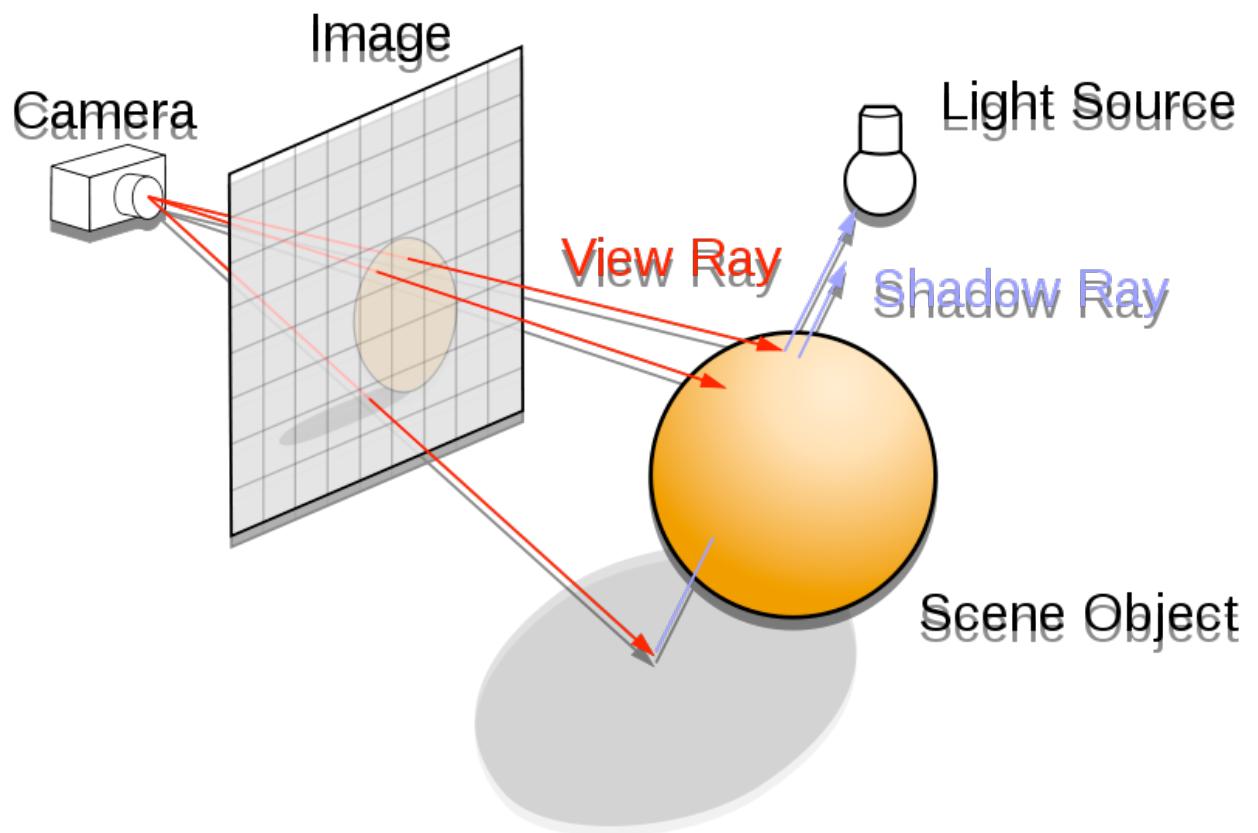




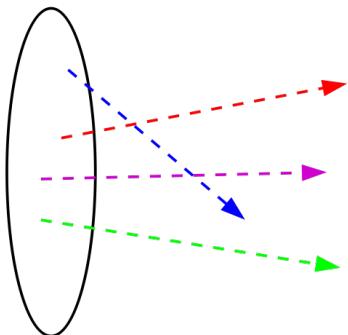
- During WW2, “numerical experiments” were applied at Los Alamos for solving mathematical complications of computing fission, criticality, neutronics, hydrodynamics, thermonuclear detonation etc.



- 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

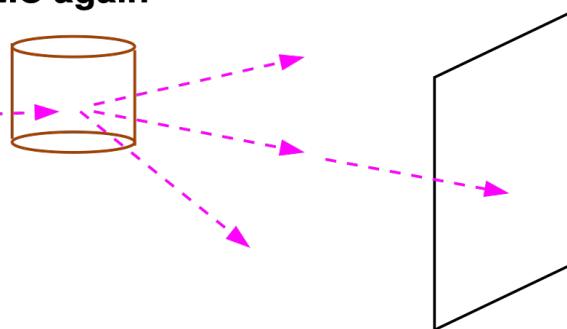


1. Particles emitted with random starting conditions via MC



2. Particles are "ray-traced" through space

3. Will eventually meet other objects e.g. a studied experimental sample and get scattered via MC again



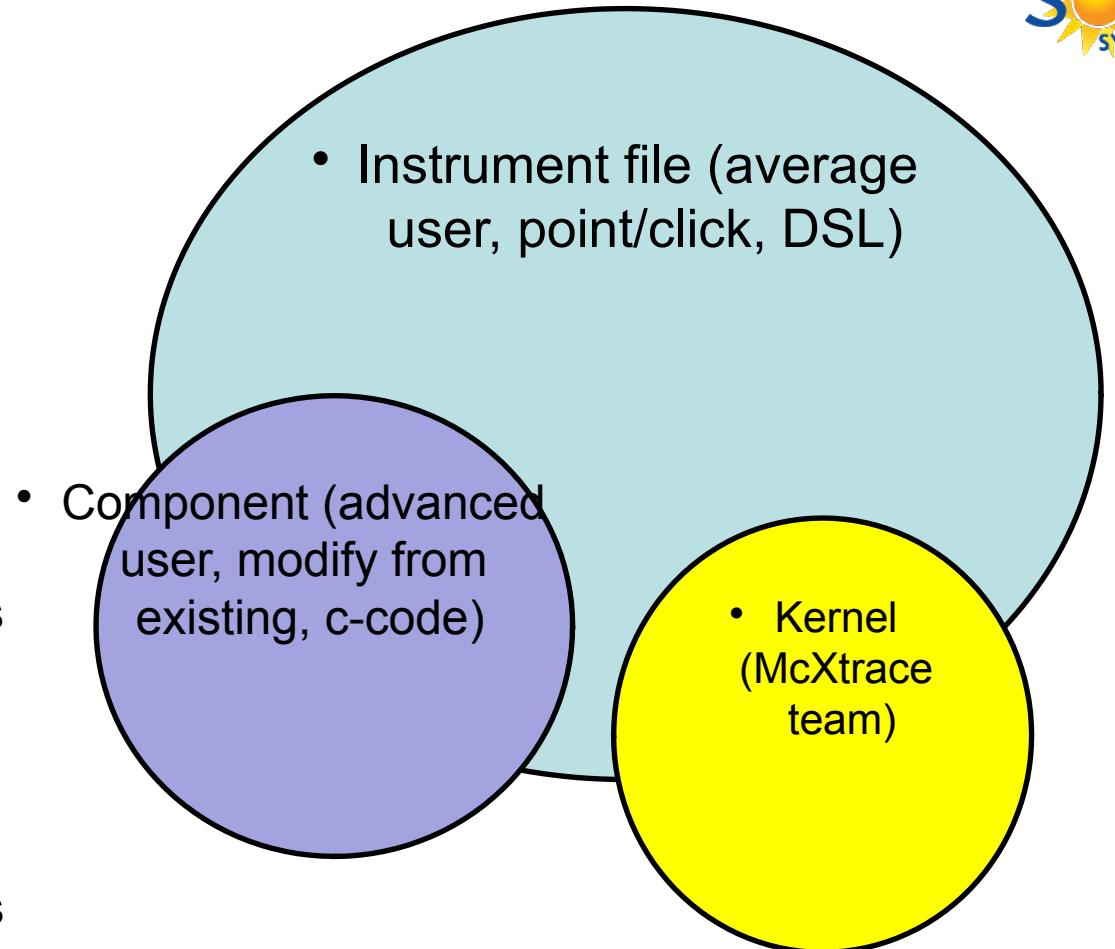
4. At various points in the instrument the particle states are measured in so-called monitors or detectors

- Important efficiency mechanisms:

✖ “Focusing” - e.g. lab source to first slit (4π vs. limited solid angle only)

✖ Rather vs. single particle description, absorption handled through statistics and downscaling the ray weight

- ◆ 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.)



JJ_SAXS.instr + (~/Repositories/McCode/mcxtrace-comps/examples) - GVIM

File Edit Tools Syntax Buffers Window Help

```
*****
*      McXtrace instrument definition URL=http://www.mcxtrace.org
*
* Instrument: SAXS_saxlab (rename also the example and DEFINE lines below)
*
* %Identification
* Written by: Erik Knudsen (erkn@risoe.dtu.dk)
* Date: September 24th, 2009
* Origin: Ris&oslash; DTU, (Finnair flight AY67 to Hong Kong)
* Release: McXtrace
* Version: 0.1_alpha
* %INSTRUMENT_SITE: SAXSLAB
*
* Crude model of a laboratory SAXS-instrument mimicking the type sold by SAXSlab/JJ-Xray Systems.
*
* %Description
*
*
* %Parameters
* pin2_pos: [m] distance between 1st and 2nd pinhole in beam tube
* pin3_pos: [m] distance between 2nd and 3rd pinhole in beam tube
* optic_L: [m] length of the focusing optic
* sample_pos:[m] distance from 3rd pinhole to sample
* detector_pos: [m] distance from 3rd pinhole to detector
*
* %Example: pin2_pos=0.2 pin3_pos=0.4 optic_L=0.1 sample_pos=0.2 detector_pos=2 Detector: psd1_I=7.8629e-05
*
* %Link
* A reference/HTML link for more information
*
* %End
*****
```

```
DEFINE INSTRUMENT SAXS_saxlab(pin2_pos=0.2, pin3_pos=0.4, optic_L=0.1, sample_pos=0.2, detector_pos=2)
```

```
DECLARE
%{
%}

INITIALIZE
%{
%}

TRACE

COMPONENT Origin = Progress_bar()
    AT (0,0,0) ABSOLUTE

COMPONENT apparent_source=Source_flat(
    xwidth=8e-3,yheight=.04e-3,dist=0.1,focus_yh=0.001,focus_xw=0.01,lambda0=1.54,dlambda=0.1
)
AT (0,0,0) RELATIVE PREVIOUS

COMPONENT psd00=PSD_monitor(
    filename="psd00.dat",xwidth=0.2,yheight=0.2,restore_xray=1
)
AT(0,0,0.0999) RELATIVE PREVIOUS

    COMPONENT optic_arm=Arm()
    AT(0,0,0.1) RELATIVE apparent_source
    ROTATED(0,0,-90) RELATIVE apparent_source

    COMPONENT optic=Mirror_curved(
        radius=20,length=0.2)
    AT(0,0,0) RELATIVE optic_arm
    ROTATED(0,2.75,0) RELATIVE optic_arm
EXTEND
%{
    if (!SCATTERED) ABSORB;
%}
```

```
*****
COMPONENT beam_tube_axis=Arm()
AT(0,0,0.1) RELATIVE apparent_source
ROTATED (5.5,0,0) RELATIVE Origin

COMPONENT pinhole1=Slit(xwidth=0.1,yheight=0.1)
AT(0,0,0.15) RELATIVE beam_tube_axis

COMPONENT psd01=PSD_monitor(
    filename="psd01.dat",xwidth=0.2,yheight=0.2,restore_xray=1
)
AT(0,0,1e-3) RELATIVE PREVIOUS

COMPONENT pinhole2=Slit(xwidth=0.1,yheight=0.1)
AT(0,0,pin2_pos) RELATIVE beam_tube_axis

/*COMPONENT psd02=PSD_monitor(
    filename="psd02.dat",xwidth=0.2,yheight=0.2
)
AT (0,0,1e-3) RELATIVE PREVIOUS
*/
COMPONENT pinhole3=Slit(xwidth=0.1,yheight=0.1)
AT(0,0,pin3_pos) RELATIVE beam_tube_axis
COMPONENT psd03=PSD_monitor(
    filename="psd02.dat",xwidth=0.2,yheight=0.2
)
AT (0,0,1e-3) RELATIVE PREVIOUS

COMPONENT psd1=PSD_monitor(
    filename="psd1.dat",xwidth=0.4,yheight=0.4
)
AT (0,0,2) RELATIVE psd03

/* This section is executed when the simulation ends (C code). Other */
/* optional sections are : SAVE */
FINALLY
%{
%}
/* The END token marks the instrument definition end */
END
```

Repositories/McCode/mcxtrace-comps/examples/JJ_SAXS.instr [+] 55,1 Top Repositories/McCode/mcxtrace-comps/examples/JJ_SAXS.instr [+] 141,1 Bot

PSD_monitor.comp (~/Repositories/McCode/mcxtrace-comps/monitors) - GVIM10

```
File Edit Tools Syntax Buffers Window Help
DEFINITION COMPONENT PSD_monitor
DEFINITION PARAMETERS (nx=90, ny=90, nr=0, string filename=0, restore_xray=0)
  SETTING PARAMETERS (xmin=-0.05, xmax=0.05, ymin=-0.05, ymax=0.05, xwidth=0, yheight=0, radius=0)
OUTPUT PARAMETERS (PSD_N, PSD_p, PSD_p2)
/* X-ray parameters: (x,y,z,kx,ky,kz,phi,t,Ex,Ey,Ez,p) */

DECLARE
{
  double **PSD_N;
  double **PSD_p;
  double **PSD_p2;
}

INITIALIZE
{
  int i,j;
  double *p1,*p2,*p3;

  if (xwidth > 0) { xmax = xwidth/2; xmin = -xmax; }
  if (yheight > 0) { ymax = yheight/2; ymin = -ymax; }

  if ( ((xmin >= xmax) || (ymin >= ymax)) && !radius ) {
    printf("PSD_monitor: %s: Null detection area !\n"
          "        (xwidth,yheight,xmin,xmax,ymin,ymax,radius). Exiting",
          NAME_CURRENT_COMP);
    exit(0);
  }
  if(!radius){
    p1=calloc(nx*ny,sizeof(double));
    p2=calloc(nx*ny,sizeof(double));
    p3=calloc(nx*ny,sizeof(double));

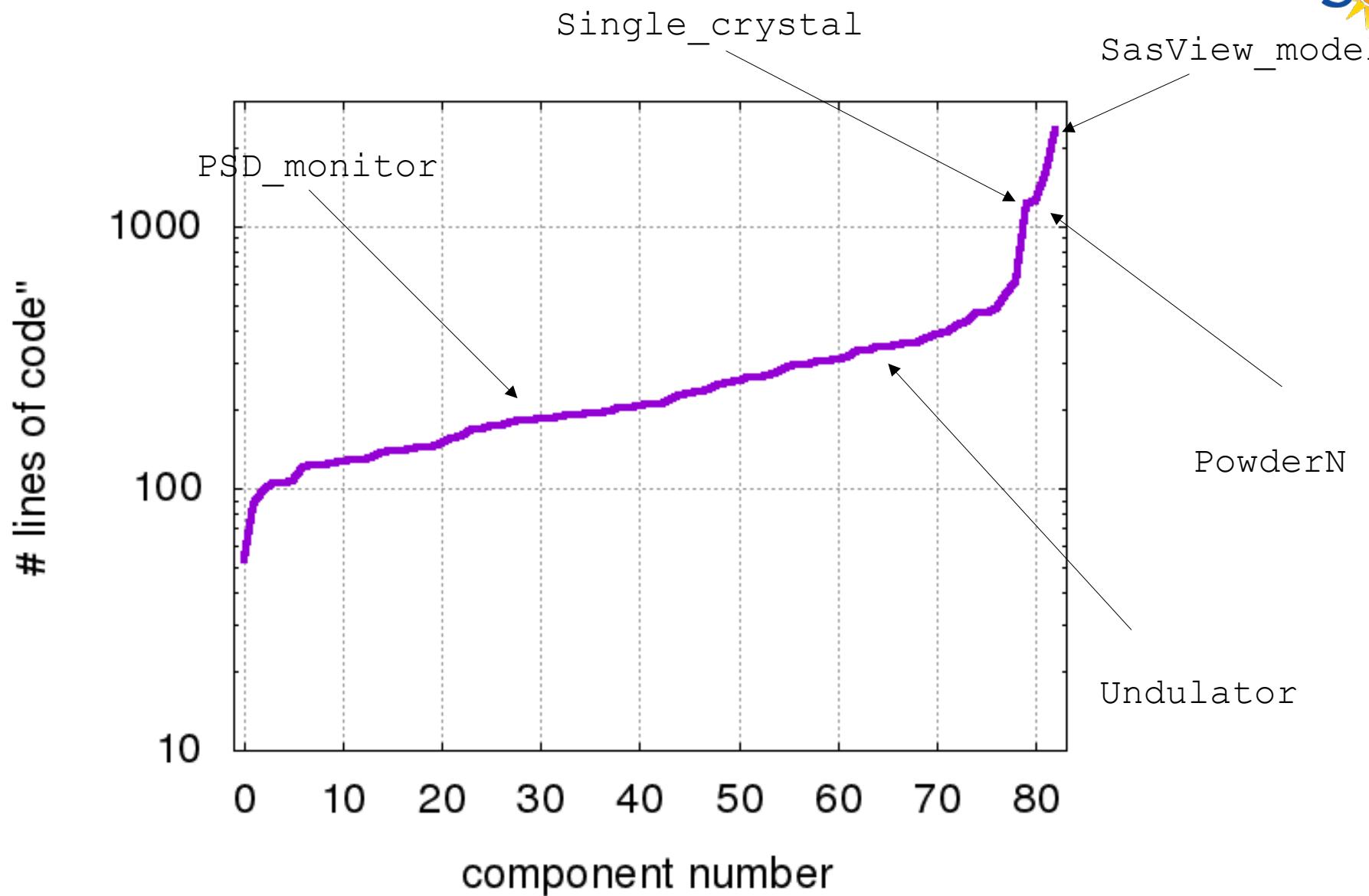
    PSD_N=calloc(nx,sizeof(double *));
    PSD_p=calloc(nx,sizeof(double *));
    PSD_p2=calloc(nx,sizeof(double *));

    for (i=0; i<nx; i++){
      PSD_N[i]=(p1+i*ny); //calloc(ny,sizeof(double));
      PSD_p[i]=(p2+i*ny); //calloc(ny,sizeof(double));
      PSD_p2[i]=(p3+i*ny); //calloc(ny,sizeof(double));
    }
  }else{
    PSD_N=calloc(1,sizeof(double *));
    PSD_p=calloc(1,sizeof(double *));
    PSD_p2=calloc(1,sizeof(double *));
    *PSD_N=calloc(nr,sizeof(double));
    *PSD_p=calloc(nr,sizeof(double));
    *PSD_p2=calloc(nr,sizeof(double));
  }
}

TRACE
{
  int i,j;
  PROP_Z0;
  if (!radius){
    if (x<xmin && x>xmax && y>ymin && y<ymax)
    {
      i = floor((x - xmin)*nx/(xmax - xmin));
      j = floor((y - ymin)*ny/(ymax - ymin));
      PSD_N[i][j]++;
      PSD_p[i][j] += p;
      PSD_p2[i][j] += p*p;
      SCATTER;
    }
  }else{
    double r=sqrt(x*x+y*y);
    if (<radius){
      i = floor(r*nr/radius);
      PSD_N[0][i]++;
      PSD_p[0][i] += p;
    }
  }
}

END
-
```

Component size



Why bother?

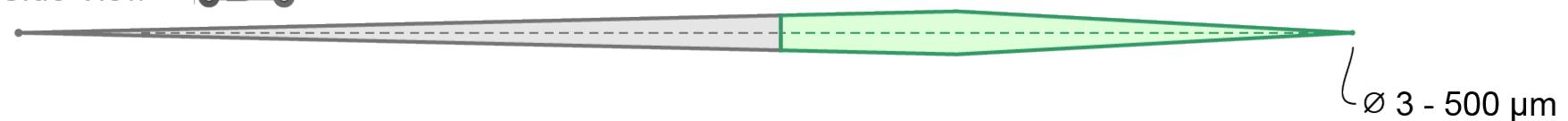
- 1) Why simulate when you can just do the experiment?
- 2) Why McXtrace and not sim. package X?

- Users don't have the luxury you have!
 - Prospective users may try out experiments.
 - Teach users how to do experiments.

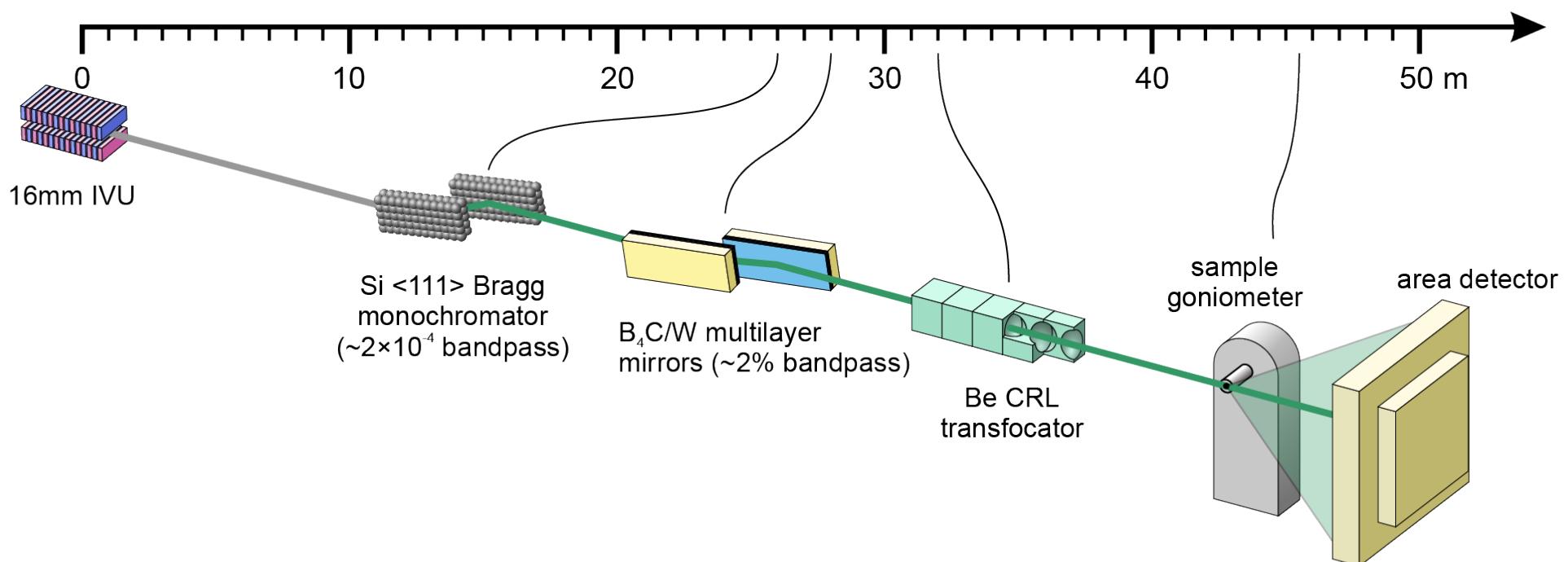
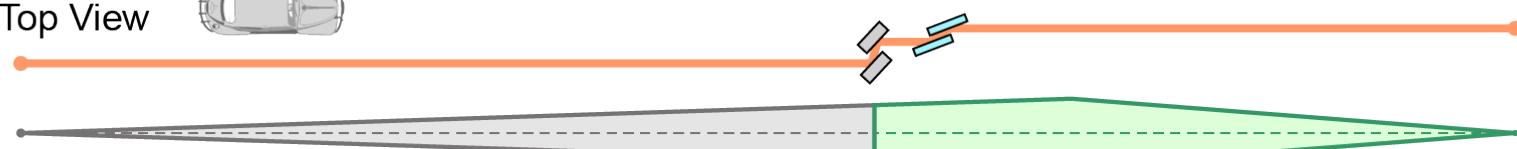
Why McXtrace

- Community driven code
- Fairly easy to extend - write a new component and it automatically fits into the framework.
- Portable (need a c-compiler).
- Several included standard sample models.
- Once written, a simulation/beamline is a real program in itself.
- ...but...
- Use whatever you prefer! XRT, SHADOW, SRW, Ray,...<insert package here>...

Side View 



Top View 



Instrument - Chromium

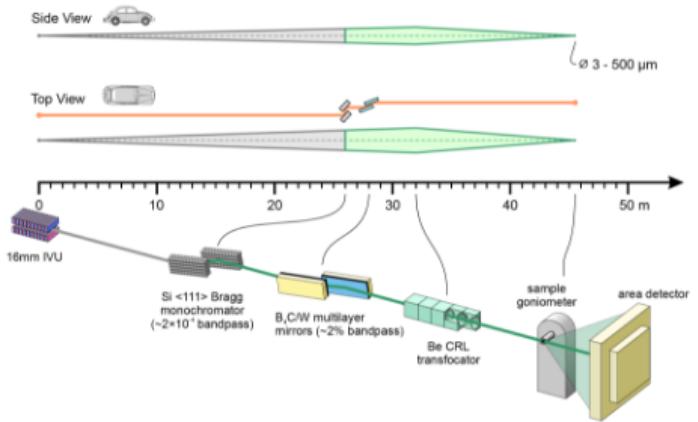
Instrument Simulation Data

<https://sim.e-neutrons.org/instrument/xrd/DanMAX>

Apps Debian.org Latest News Help

Logged in as ebknudsen ([see recent simruns](#)) Logout

DanMAX (click for documentation)



Side View: $\varnothing 3 - 500 \mu\text{m}$

Top View: $\varnothing 3 - 500 \mu\text{m}$

Detailed Schematic:

- 16mm IVU
- Si <111> Bragg monochromator ($\sim 2 \times 10^4$ bandpass)
- B₄C/W multilayer mirrors ($\sim 2\%$ bandpass)
- Be CRL transfocator
- sample goniometer
- area detector

Parameters for DanMAX

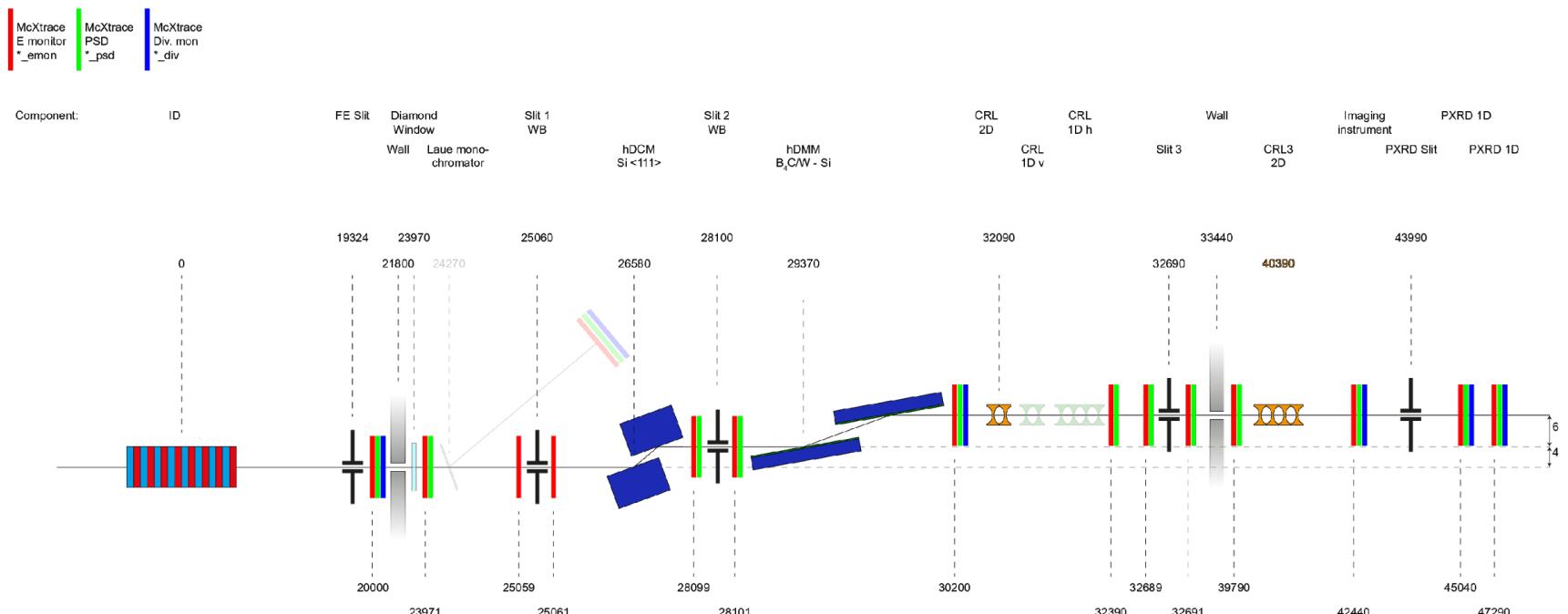
spectra_sfiles []:	/usr/local/mcxtrace/1.2/data/	Filename stem (comp will add .x.dta) for source files containing output from spectra calc. (/usr/local/mcxtrace/1.2/data/dm_2d_15keVpm0p5)
SRC []:	2	Choose which source model to use (2)
E0 [keV]:	15	The central energy to sample from source model. (15)
DE [keV]:	0.5	Spectral width (std. dev. if gaussian source) to sample from source model. (0.5)
DCM_e0 [keV]:	15	The energy to tune the Si monochromator to. May be different from E0. If 0 the monochromator is controlled by DCM_angle. (15)
DMM_e0 [keV]:	15	The energy to tune the Multilayer monochromator to. May be different from E0. If 0 the monochromator is controlled by DMM_angle. (15)
oh_premonoh [m]:	0.005	Vertical (height) opening of aperture in front of the monochromator. (0.005)
oh_premonow [m]:	0.005	Horizontal (width) opening of aperture in front of the monochromator. (0.005)
oh_midmonoh [m]:	0.005	Vertical (height) opening of aperture in the middle of the monochromator (between DCM and DMM). (0.005)
oh_midmonow [m]:	0.005	Horizontal (width) opening of aperture in the middle of the monochromator (between DCM and DMM). (0.005)
oh_endh [m]:	0.005	Vertical (height) opening of aperture at the end of the optical hutch. (0.005)
oh_endw [m]:	0.005	Horizontal (width) opening of aperture at the end of the optical hutch. (0.005)
PXRDsampleap_h [m]:	0.002	Vertical (height) opening of the guard aperture in front of the PXRD sample. (0.002)

DanMAX simulation effort

McXtrace main simulation vehicle with connections to:

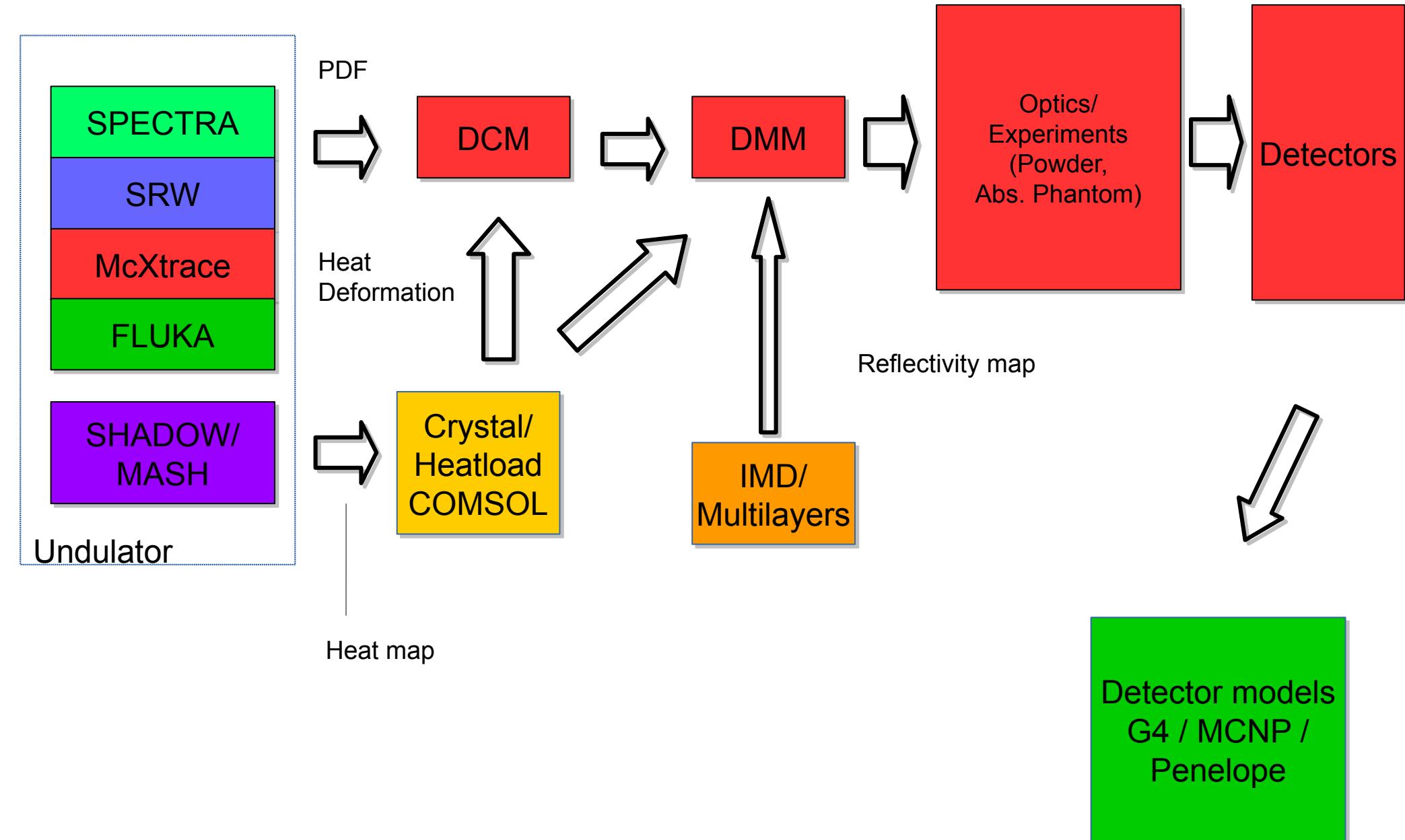
- SPECTRA / SRW for source (undulator) calculation benchmarking
- COMSOL + SHADOW + MASH - heatload calculations
- IMD - multilayer reflectivity calculations

DanMAX - McXtrace model - cheat sheet

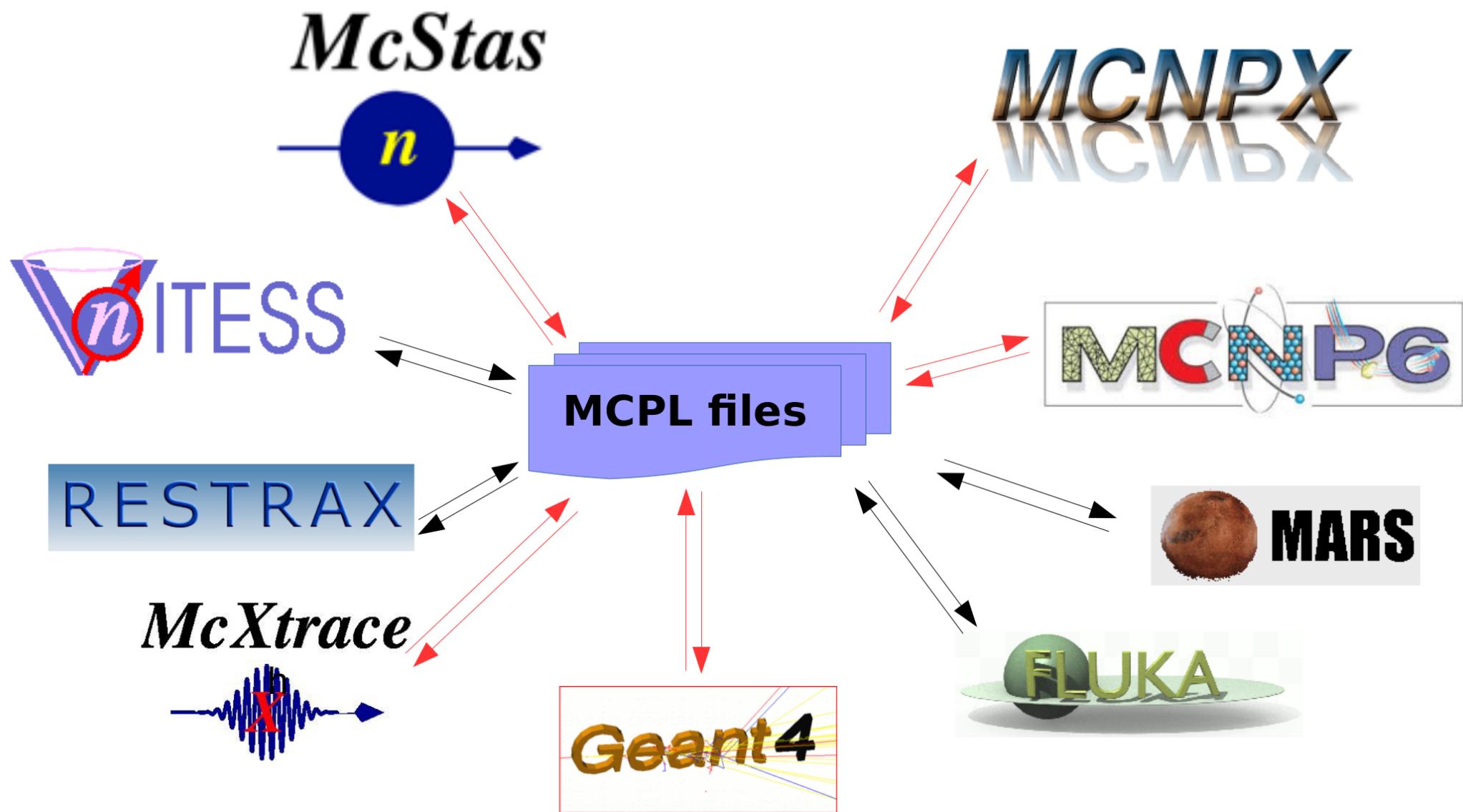


McXtrace name:	Origin	oh_diamond_filter1	DCMO	DMM0	oh_1dcrl	oh_end_ap	PXRDsample_ap
	FEMM	oh_premono_ap	oh_midmono_ap	oh_2dcrl	oh_1dorlh	eh_2dcrl	
McXtrace monitor name:	source	oh_alter_dia	oh_premono1	oh_midmono1	oh_postfocus	oh_end1	tomosample
	postfe	oh_premono0	oh_midmono0	oh_postmono	oh_end0	eh_start	PXRDsample1
On/Off flag:		DCM	DMM	OH_CRL_1Dh_n OH_CRL_2D_n OH_CRL_1Dv_n		EH_CRL_2D_n	
Parameters:	E0 DE	SI_angle oh_premonoh oh_premonow	ML_angle ML_RBW oh_midmonoh oh_midmonow				PXRDsampleap_h PXRDsampleap_w

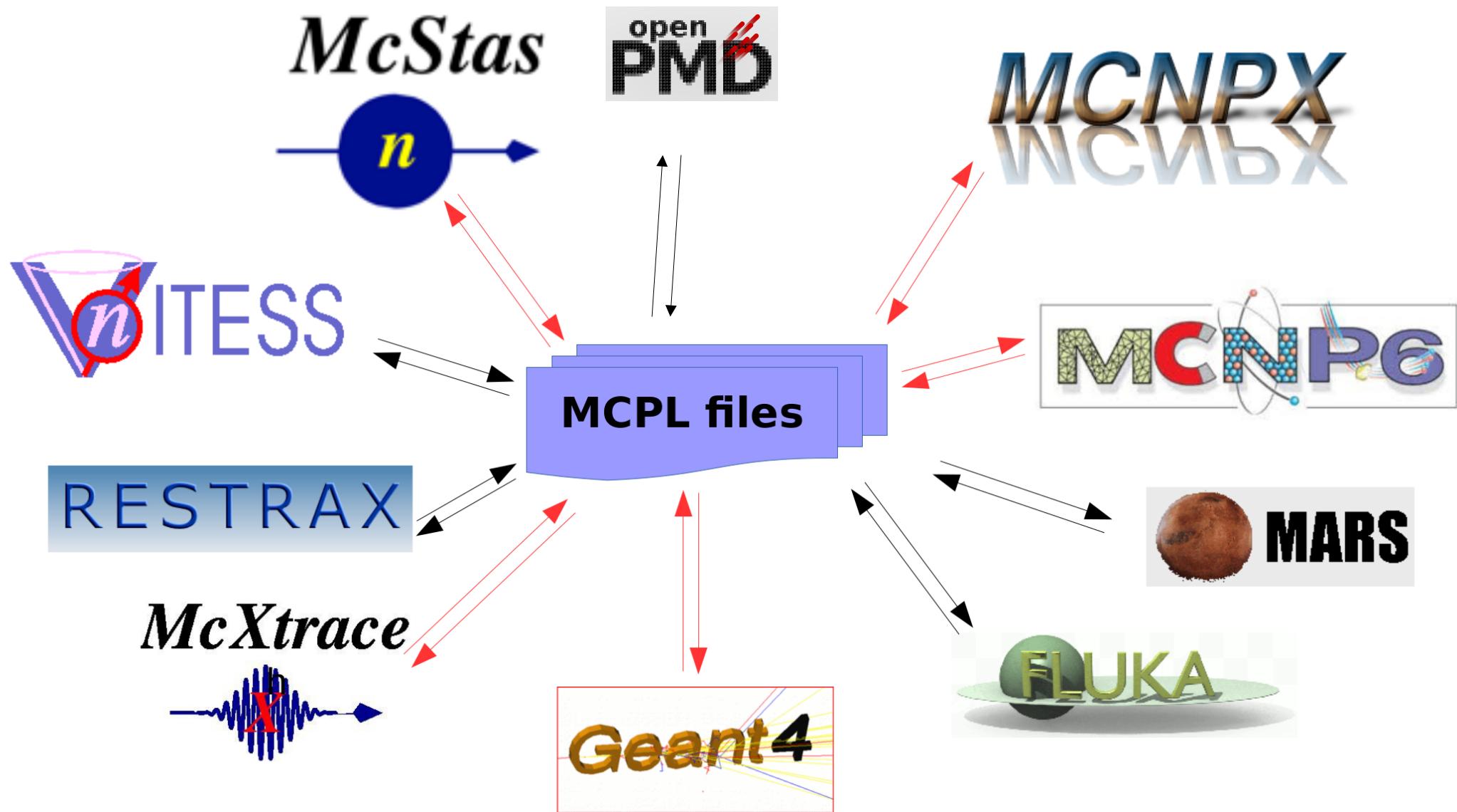
DanMAX simulation workflow



Monte Carlo Particle List-format



Monte Carlo Particle List-format

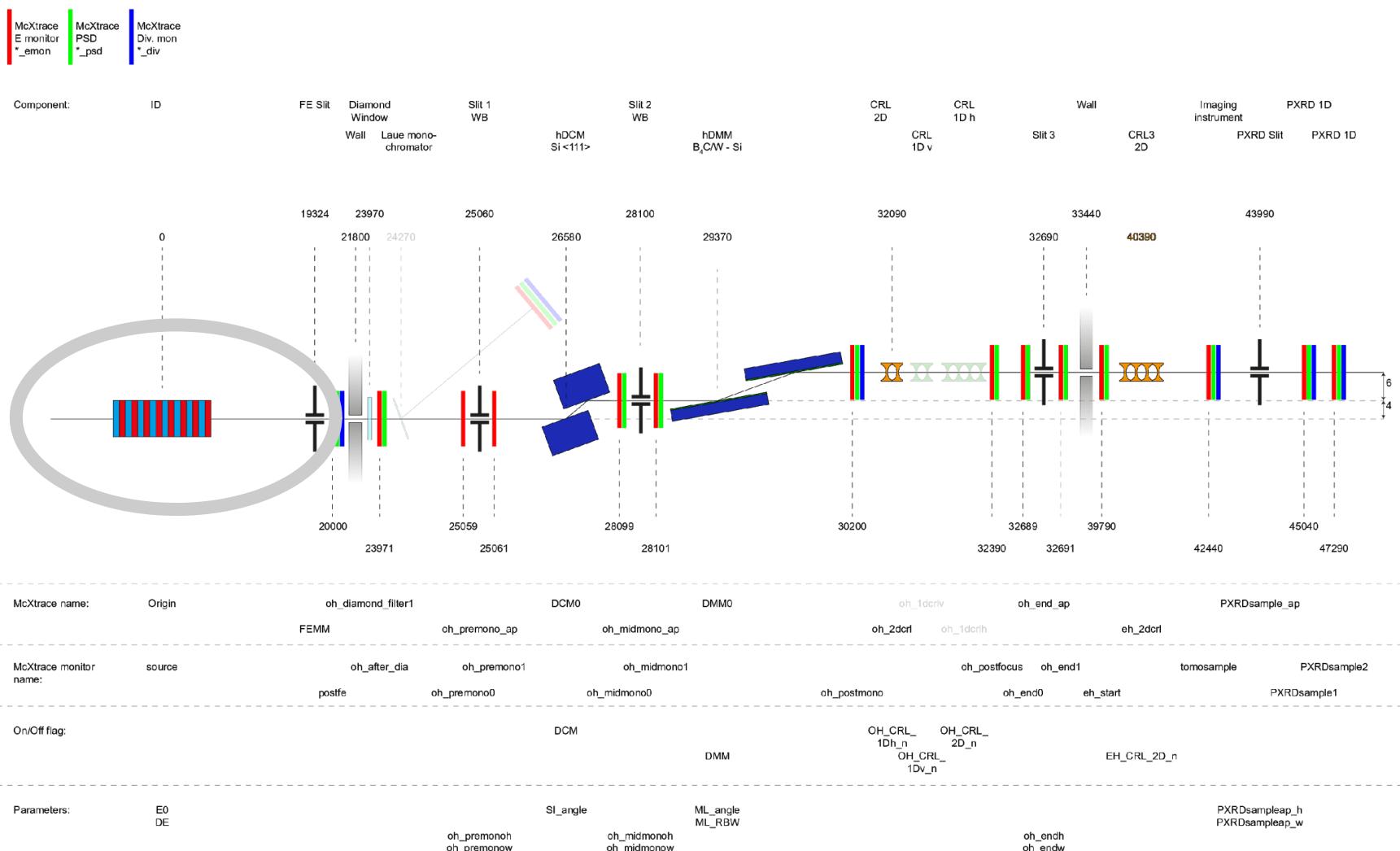


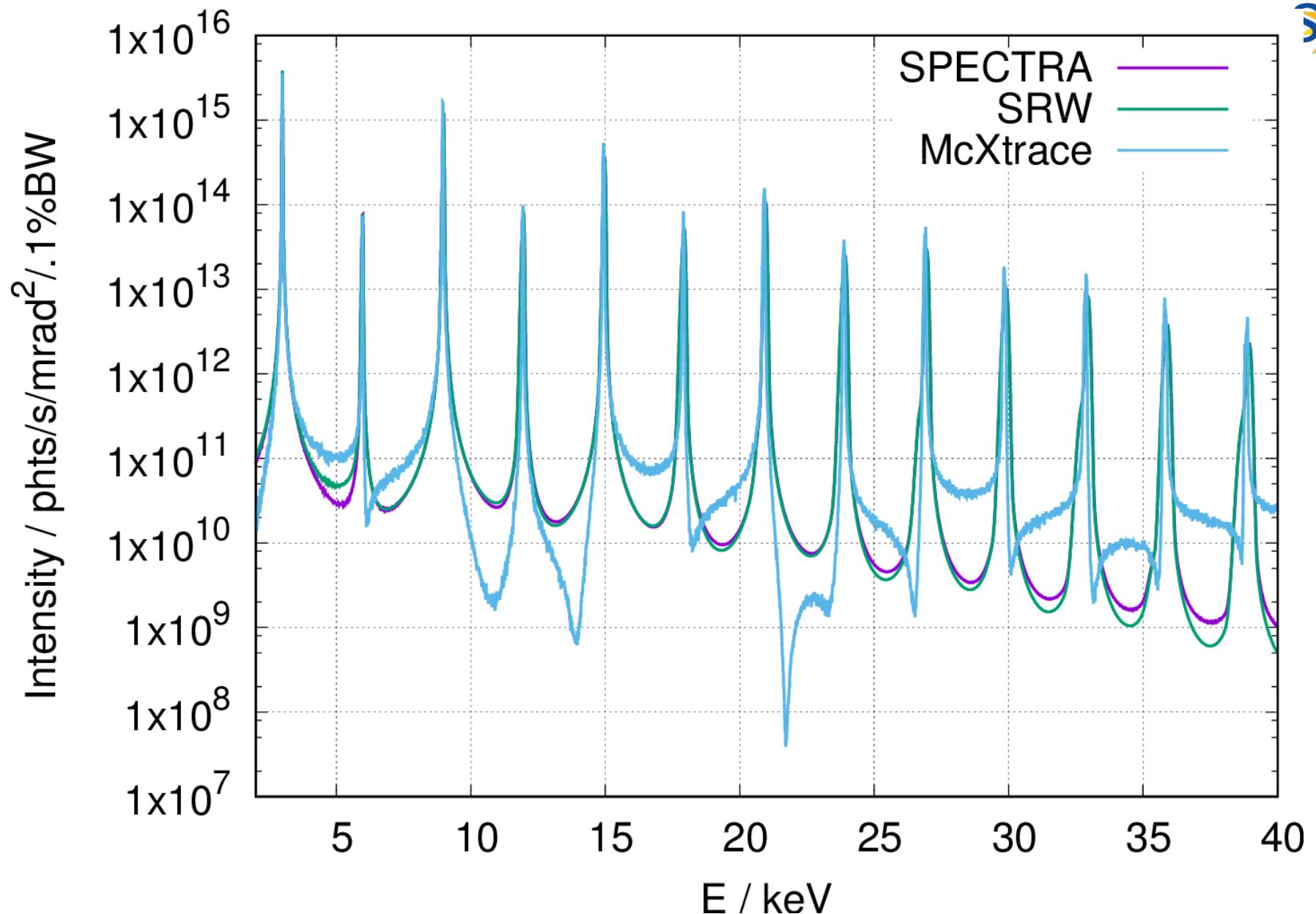
DanMAX simulation effort

McXtrace main simulation vehicle with connections to:

- SPECTRA / SRW for source (undulator) calculation benchmarking
- COMSOL + SHADOW + MASH - heatload calculations
- IMD - multilayer reflectivity calculations

DanMAX - McXtrace model - cheat sheet





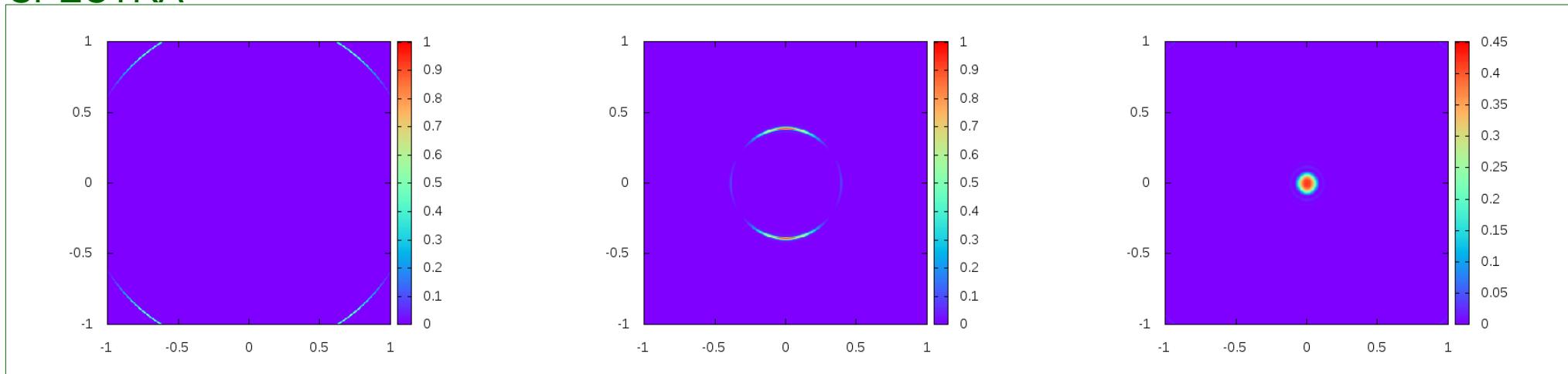
Tuned to have 11th Harmonic at 33 keV

25.3 keV

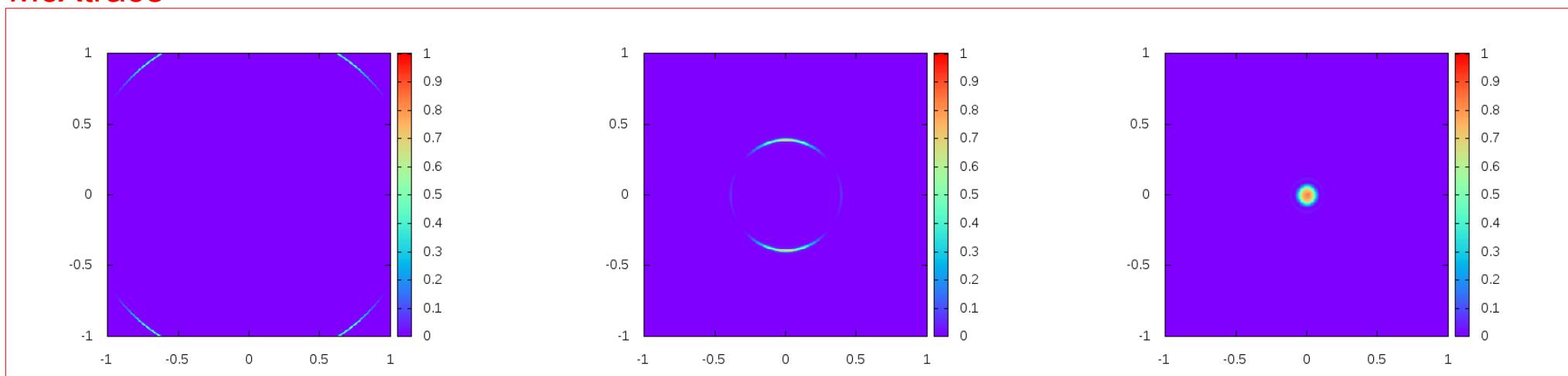
26.8 keV

33 keV

SPECTRA



McXtrace



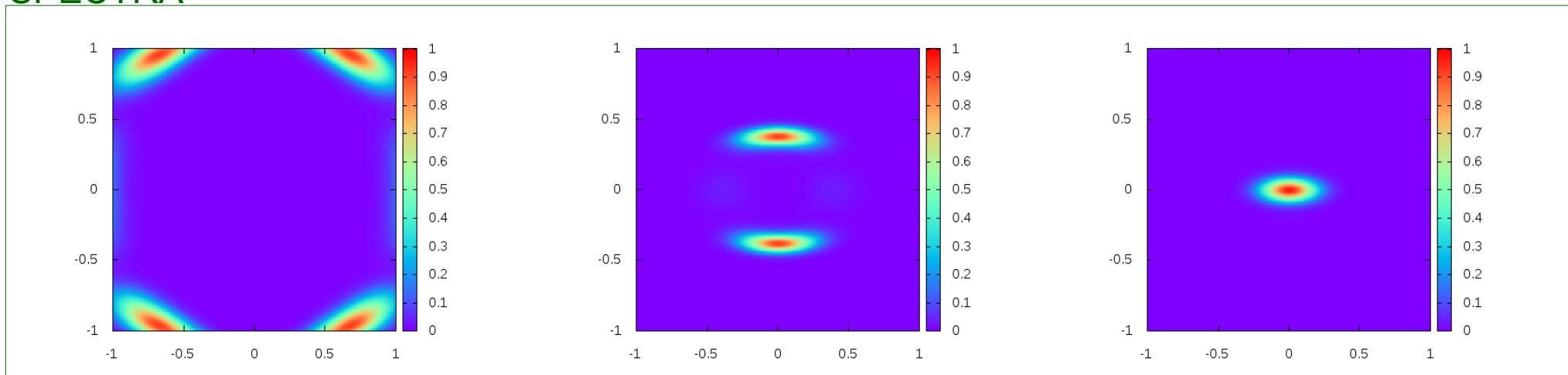
Tuned to have 11th Harmonic at 33 keV With emittance

25.3 keV

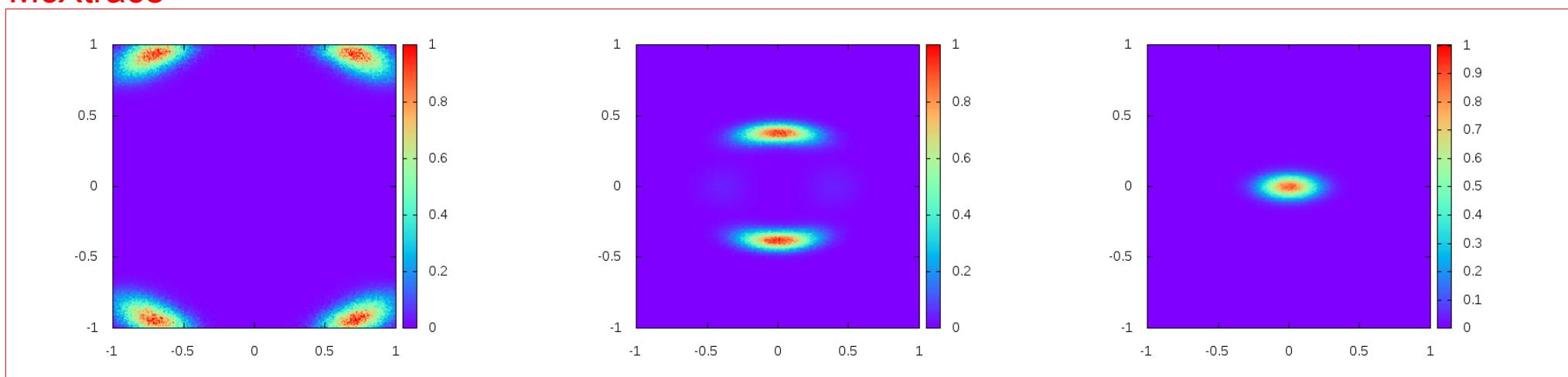
26.8 keV

33 keV

SPECTRA



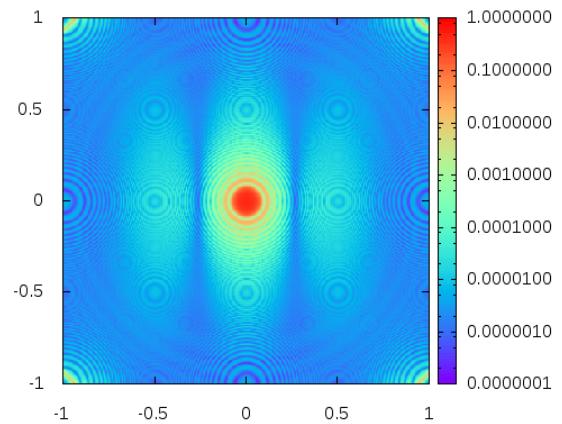
McXtrace



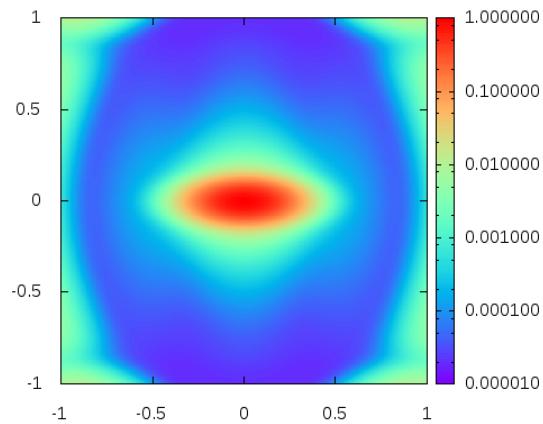
Log-plots. 33 keV

SPECTRA

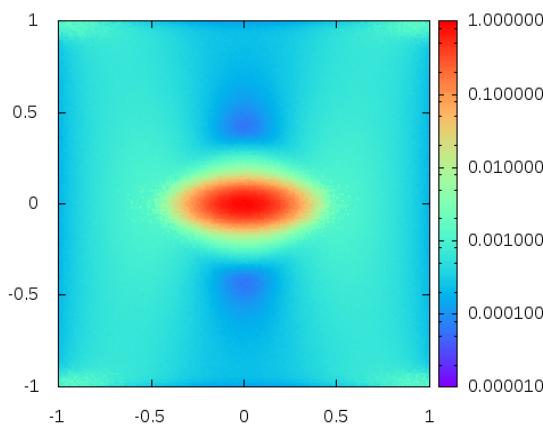
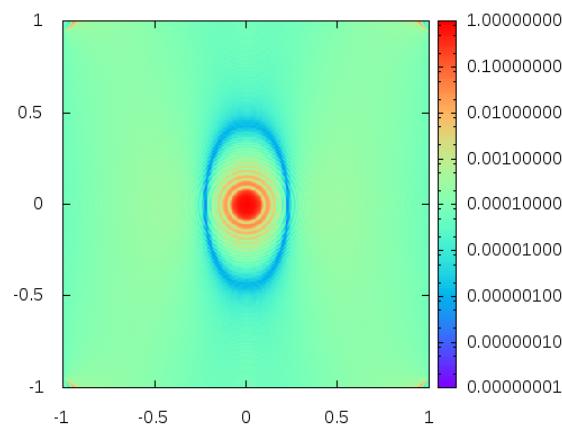
No emittance



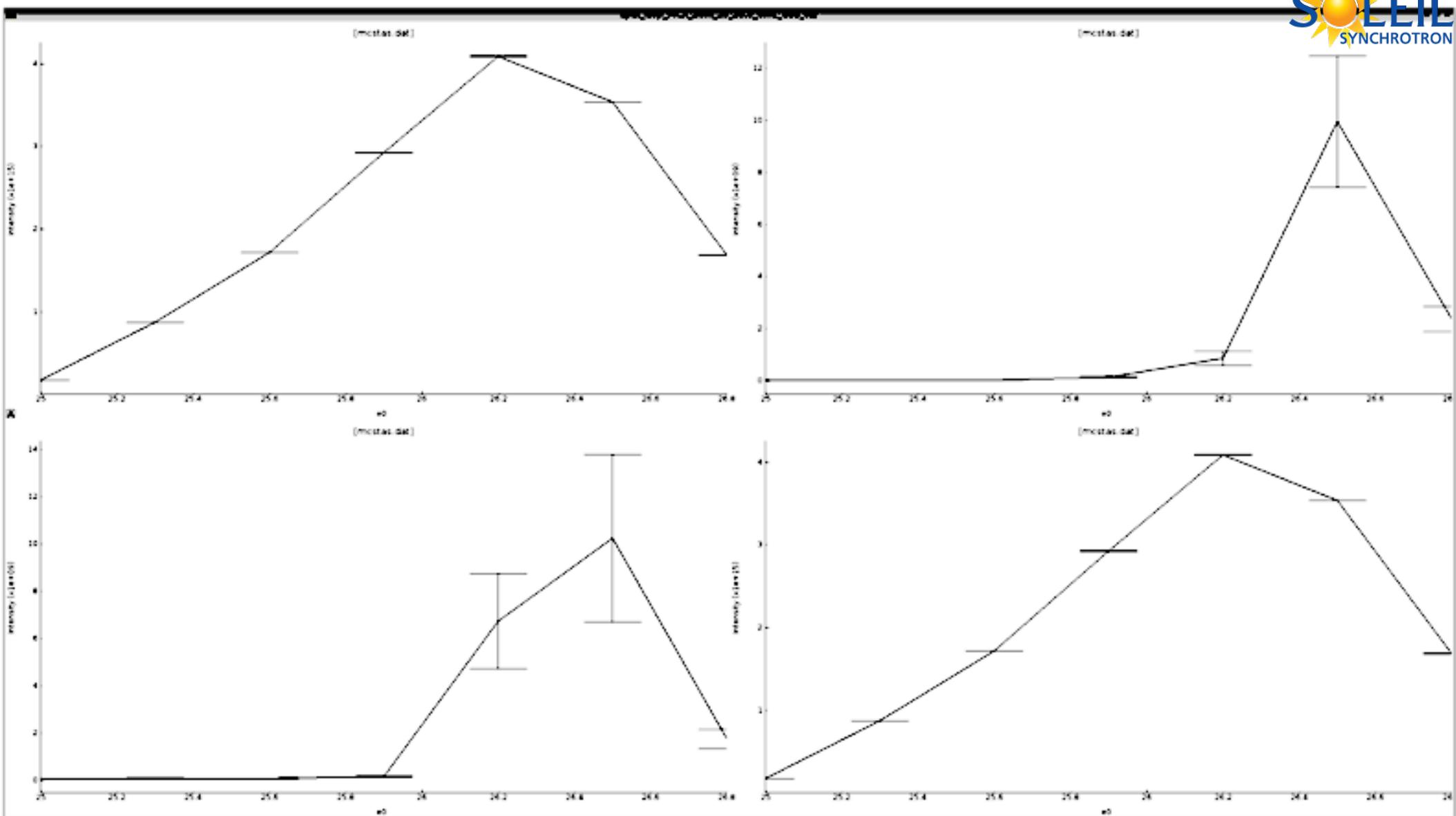
With emittance



McXtrace



Plot scan results



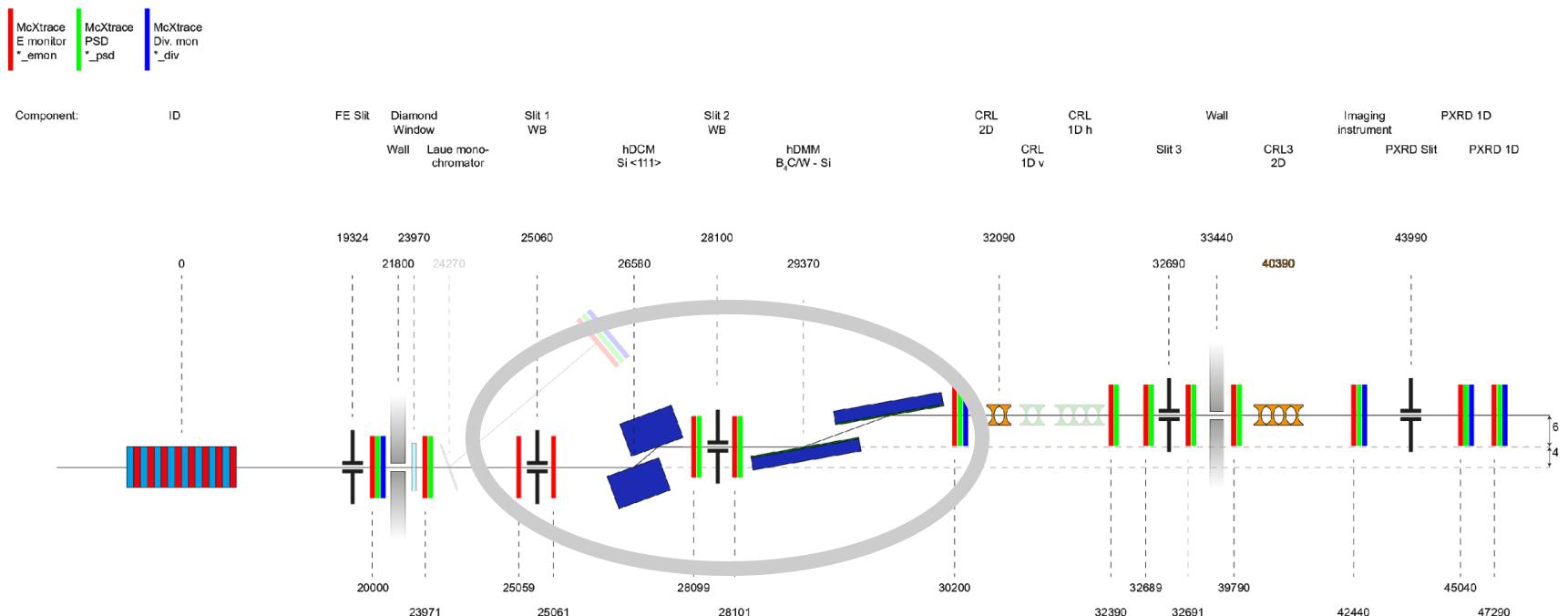
Plot scan results

DanMAX simulation effort

McXtrace main simulation vehicle with connections to:

- SPECTRA / SRW for source (undulator) calculation benchmarking
- COMSOL + SHADOW + MASH - heatload calculations
- IMD - multilayer reflectivity calculations

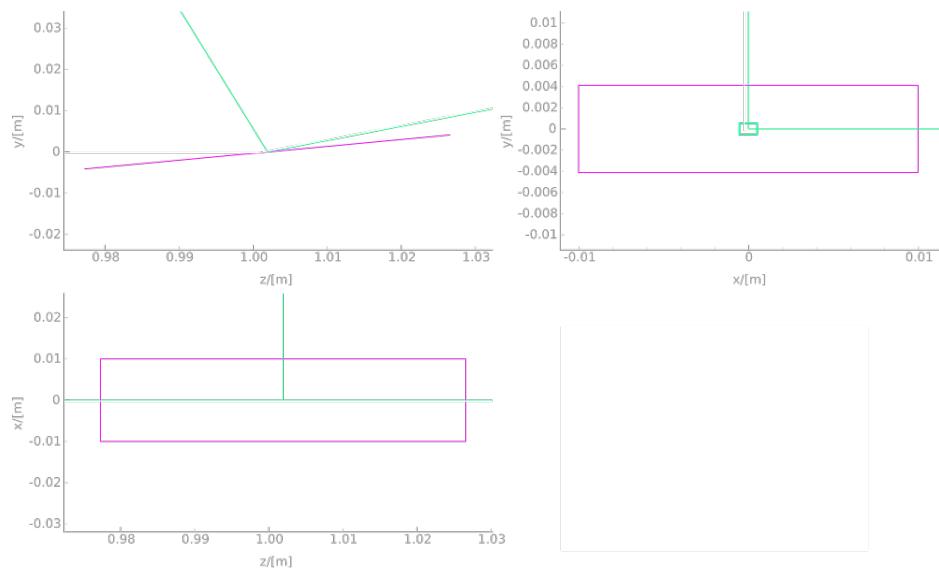
DanMAX - McXtrace model - cheat sheet



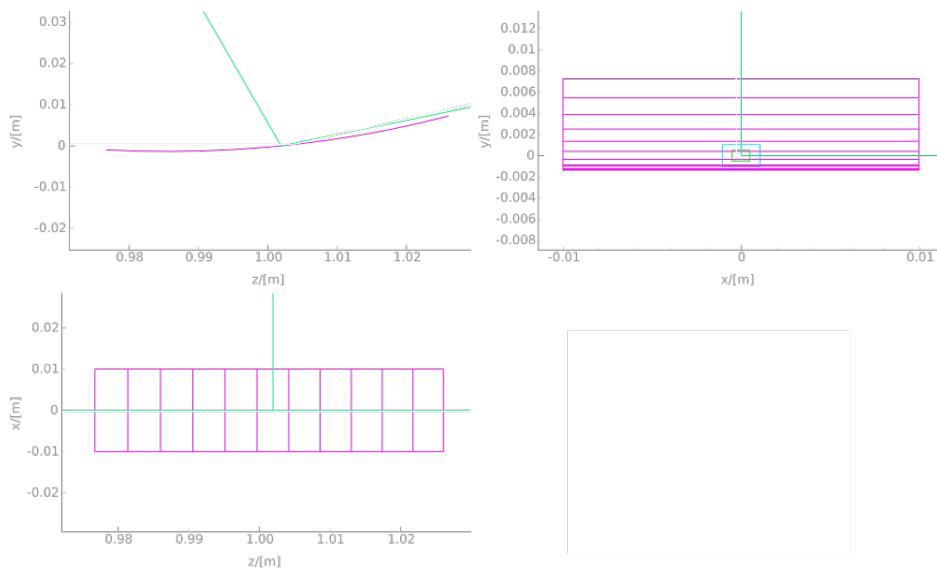
McXtrace name:	Origin	oh_diamond_filter1	DCMO	DMM0	oh_1dcrl	oh_end_ap	PXRDsample_ap	
	FEMM	oh_premono_ap	oh_midmono_ap		oh_2dcrl	oh_1dorlh	eh_2dcrl	
McXtrace monitor name:	source	oh_alter_dia	oh_premono1	oh_midmono1		oh_postfocus	oh_end1	tomosample
	postfe	oh_premono0	oh_midmono0		oh_postmono	oh_end0	eh_start	PXRDsample1
On/Off flag:			DCM	DMM	OH_CRL_1Dh_n OH_CRL_2D_n OH_CRL_1Dv_n		EH_CRL_2D_n	
Parameters:	E0 DE		SI_angle oh_premonoh oh_premonow	ML_angle ML_RBW oh_midmonoh oh_midmonow		oh_endh oh_endw	PXRDsampleap_h PXRDsampleap_w	

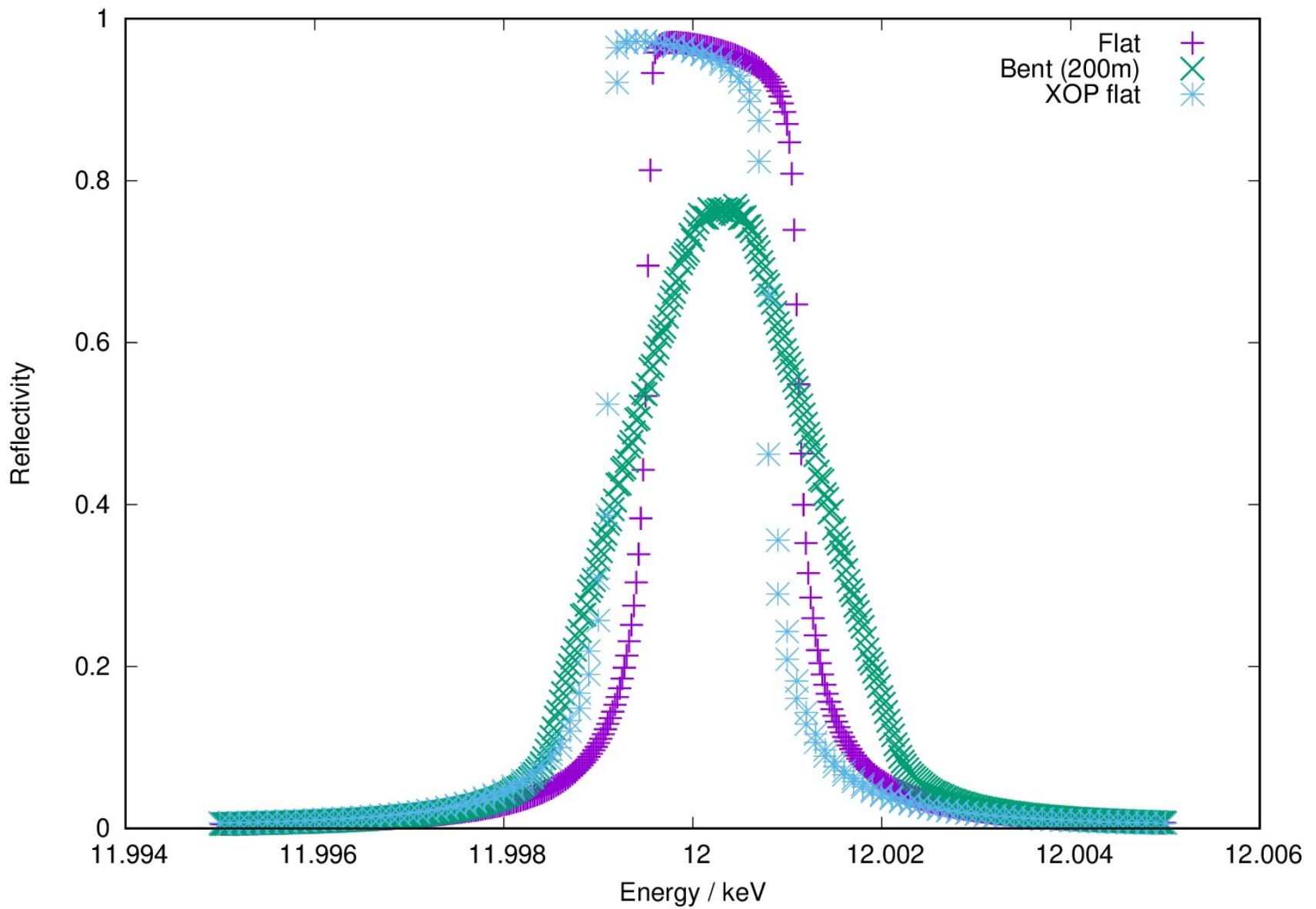
Monochromator Crystals

Flat



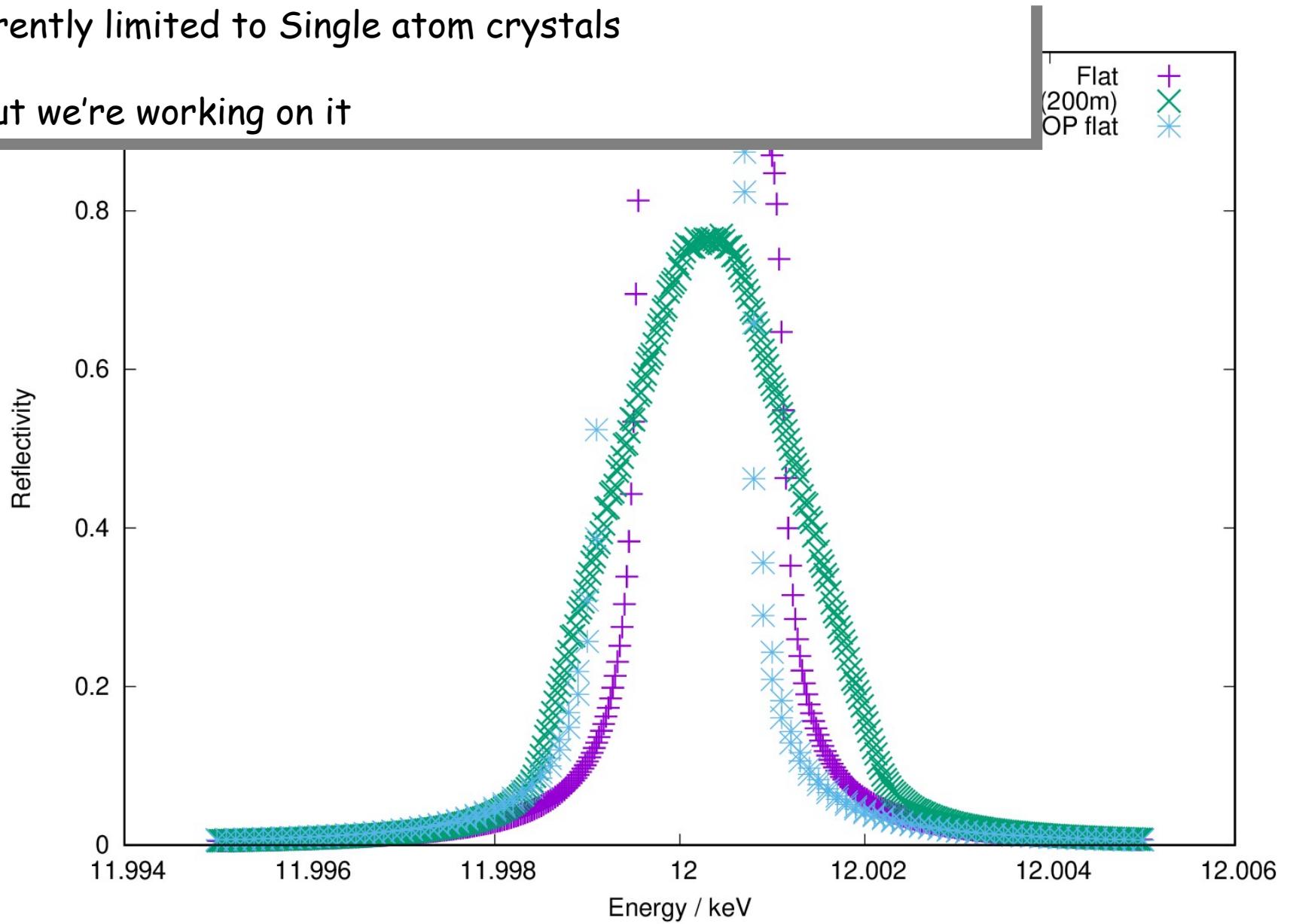
Bent ($r=200\text{m}$)

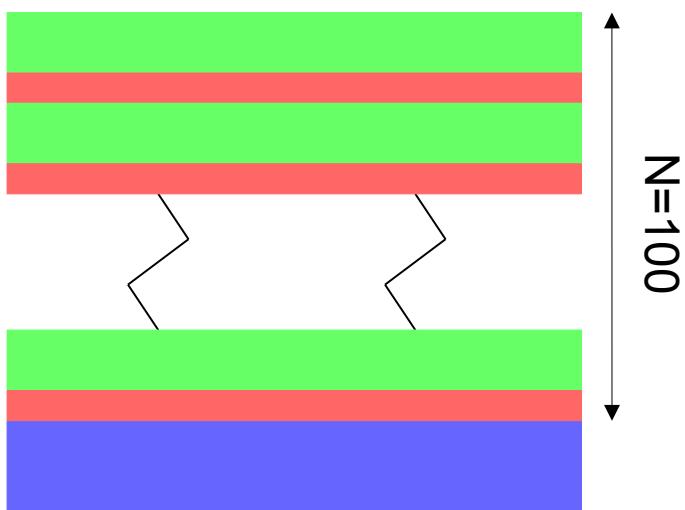




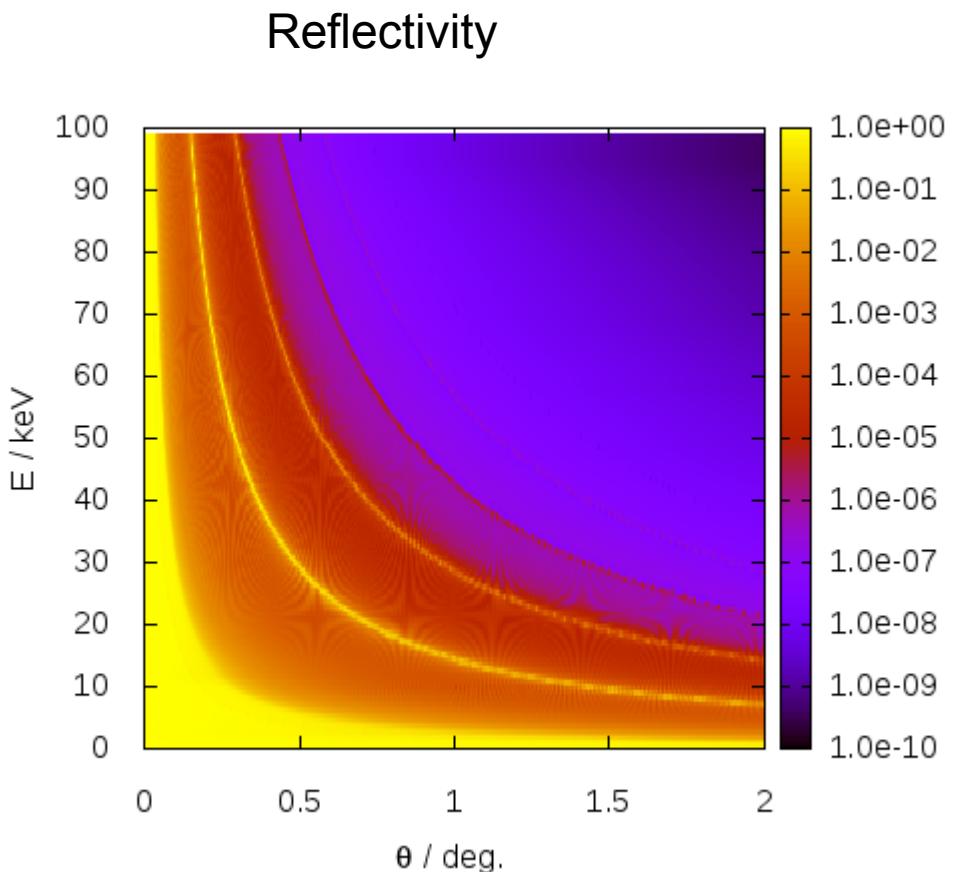
Currently limited to Single atom crystals

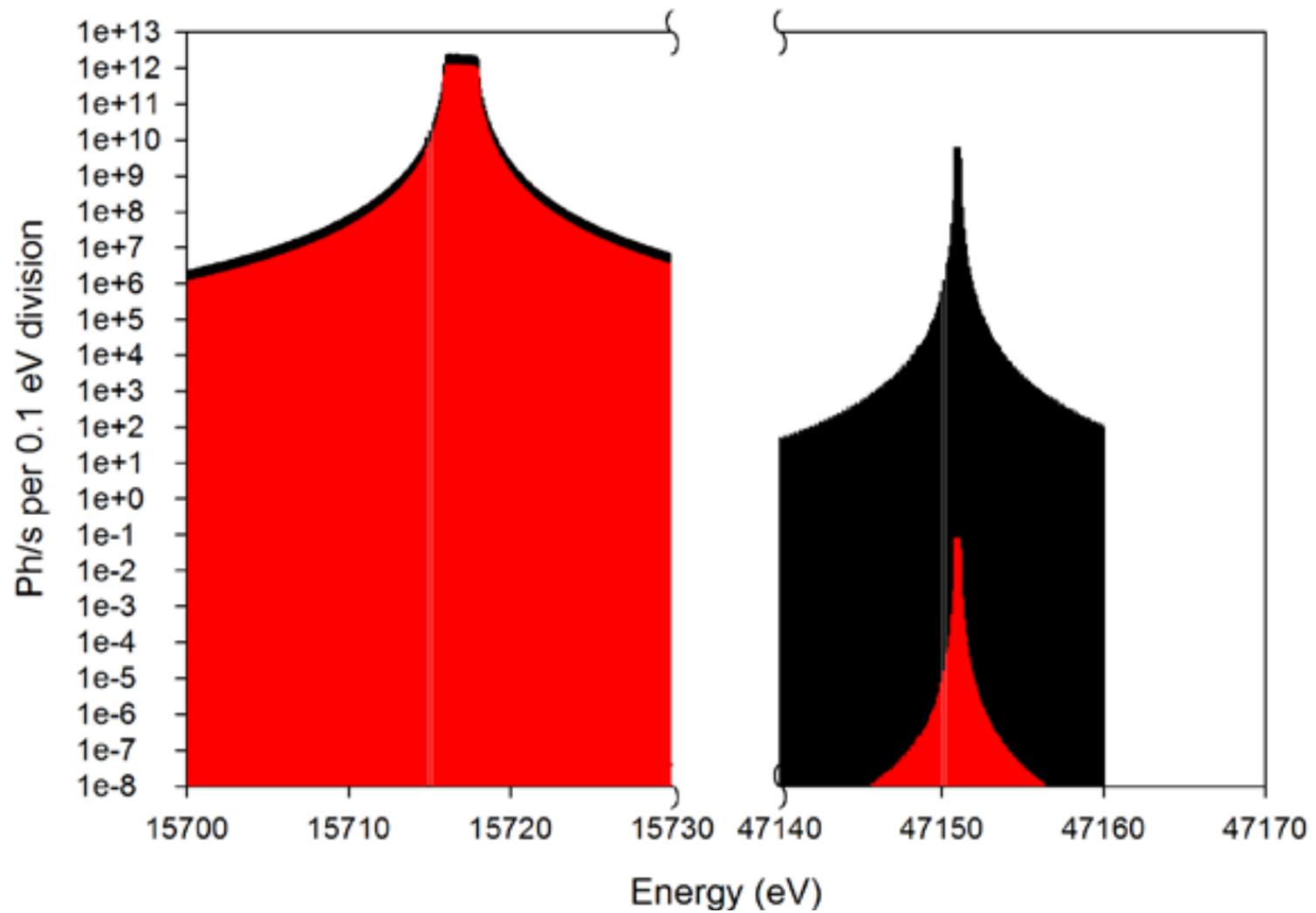
... but we're working on it





$\text{W},\text{B}_4\text{C}$: 17.5 Å, 7.5 Å
Si substrate





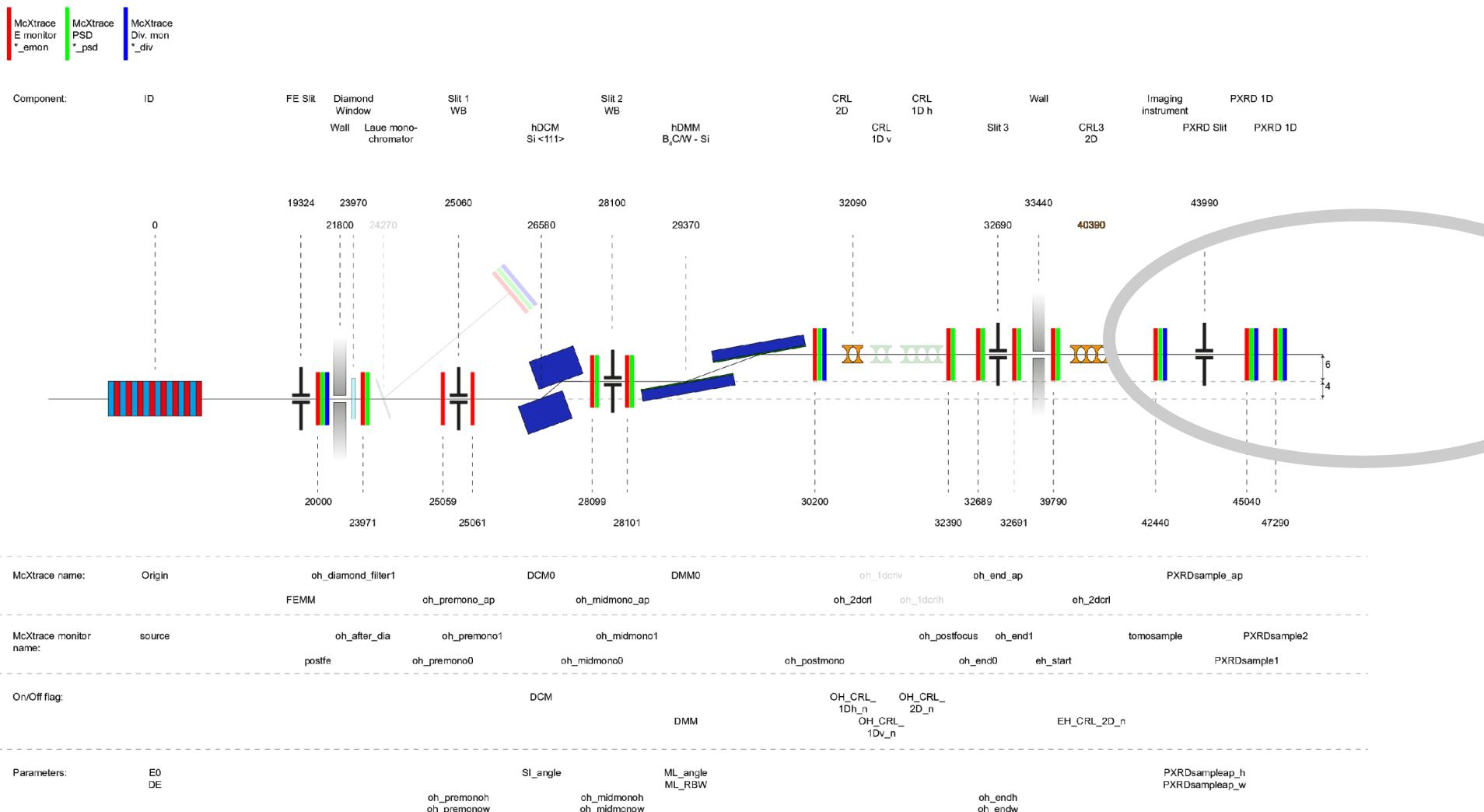
[I. Kantor]

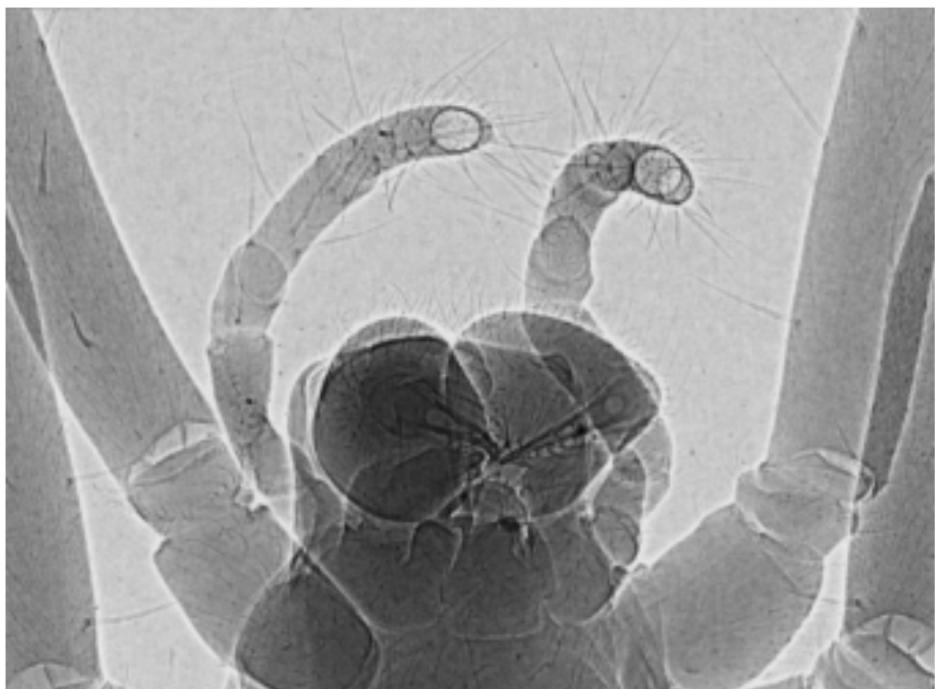
DanMAX simulation effort

McXtrace main simulation vehicle with connections to:

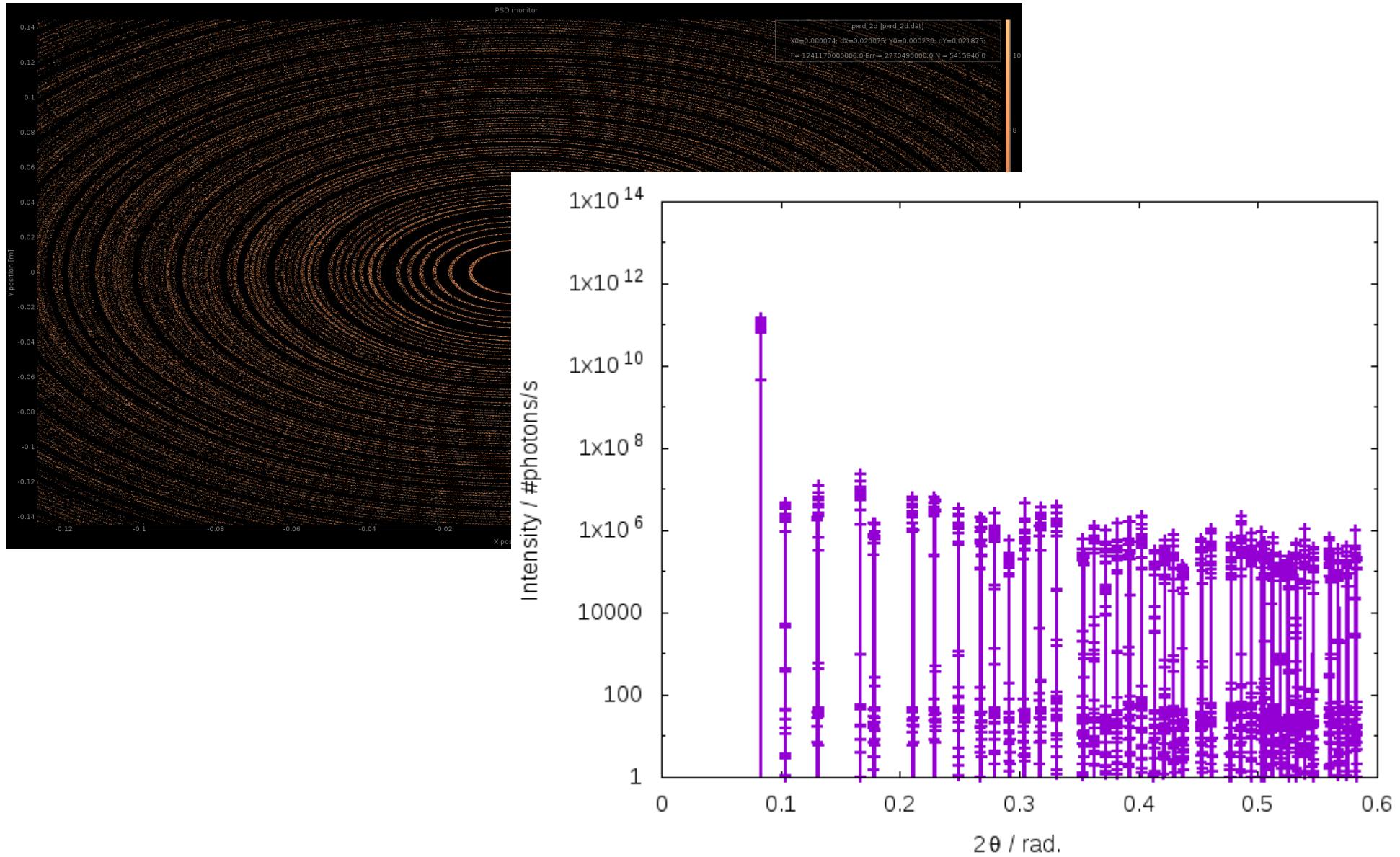
- SPECTRA / SRW for source (undulator) calculation benchmarking
- COMSOL + SHADOW + MASH - heatload calculations
- IMD - multilayer reflectivity calculations

DanMAX - McXtrace model - cheat sheet





[I. Kantor]



Other new features:

- A new set of modern, python based GUI and plotting tools
- Polycrystal sample model
- A homogenization of components of similar type, to make it easier for users to switch between models.
- More standardized installation on debian and FreeBSD class systems.
- New example simulations.
- Support for the Nexus-file format

Python based

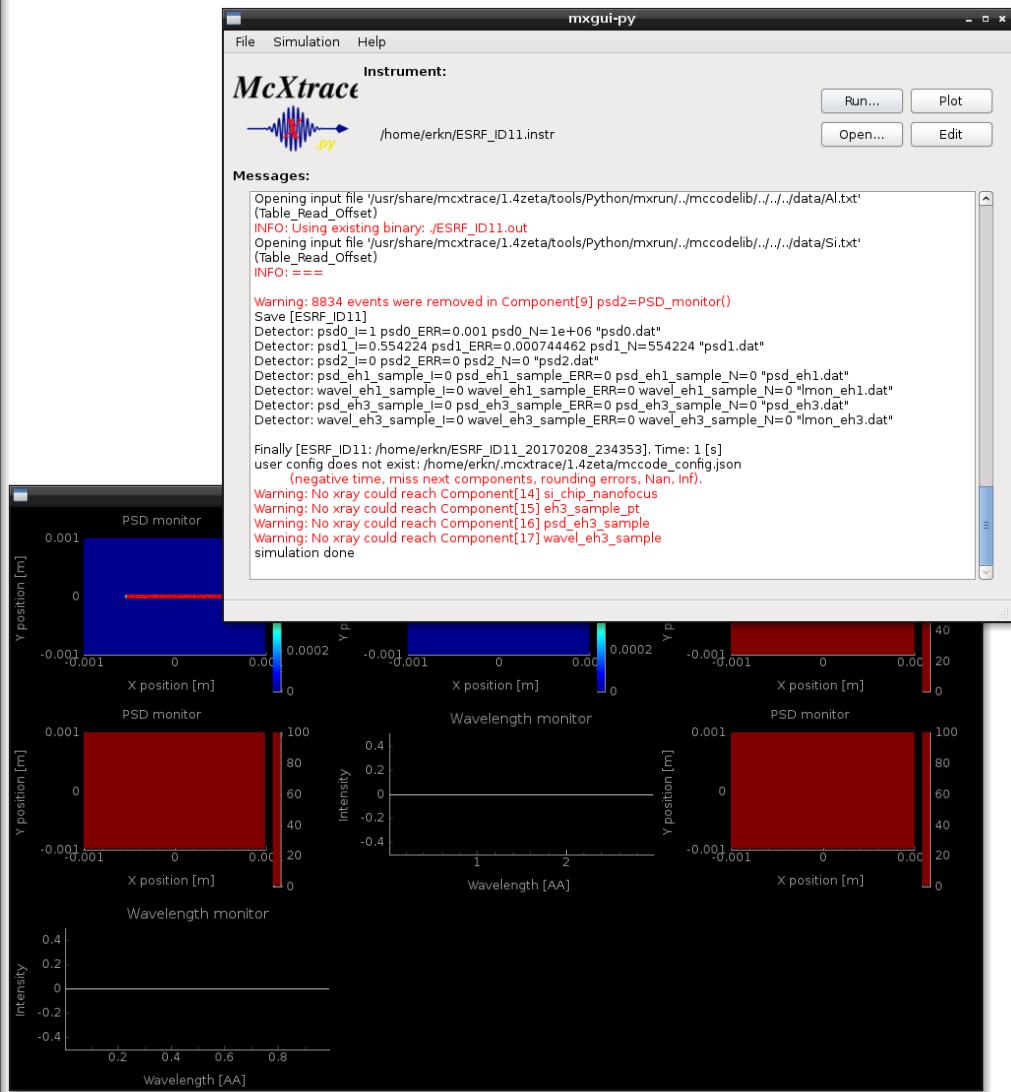
mxtrace: /home/erkn/ESRF_ID11.instr

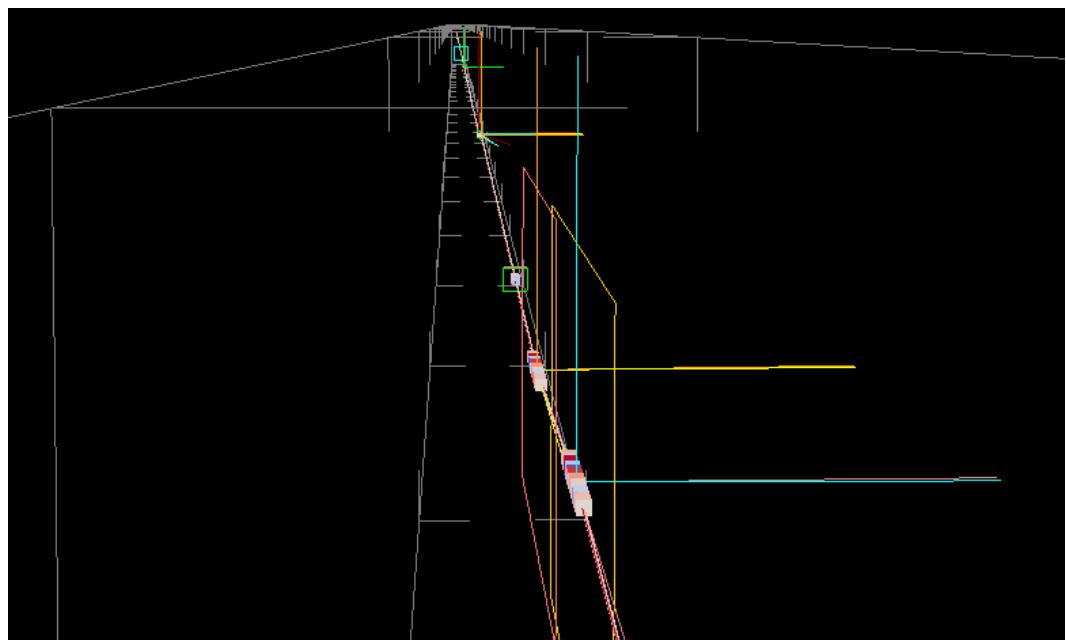
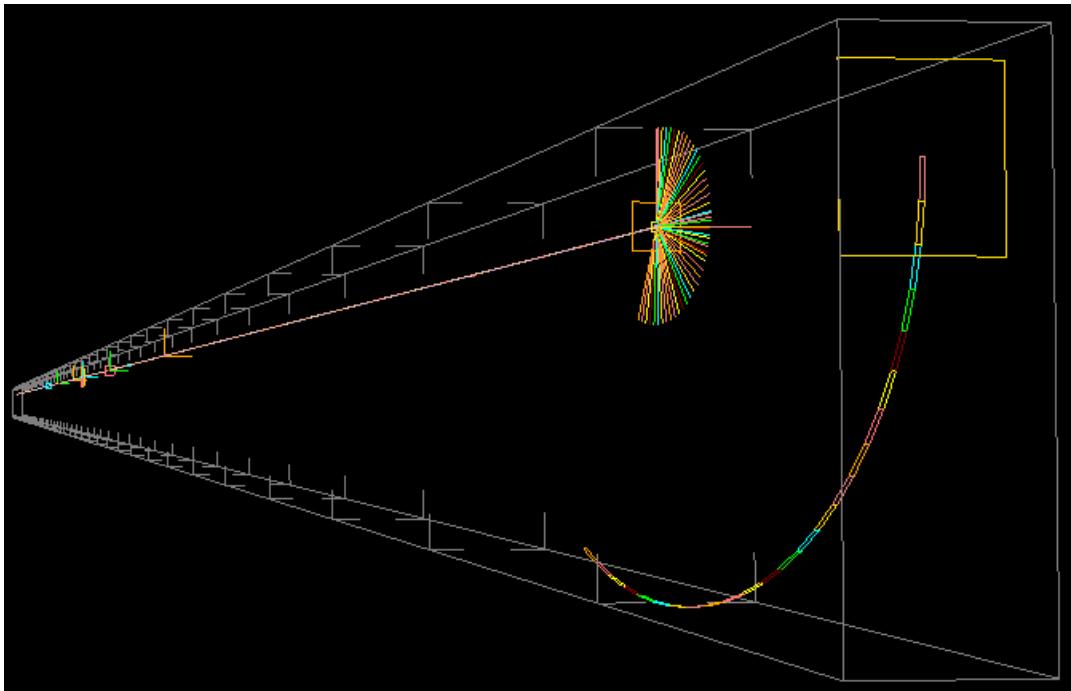
```

File Edit View Search Insert
1 ****
2 *      McXtrace instrument definition URL=http://www.mcxttrace.org
3 *
4 * Instrument: ESRF-ID11-nanofocus beamline
5 *
6 * %Identification
7 * Written by: E. Knudsen (erkn@risoe.dtu.dk)
8 * Date: Nov. 26th, 2009
9 * Origin: Risøslash; DTU
10 * Release: McXtrace 0.1_alpha
11 * Version: $Revision$
12 * %INSTRUMENT_SITE: ESRF
13 *
14 * %Description
15 * Model of the ESRF ID11 Transfocator based beamline.
16 *
17 * %Parameters
18 * ANGLE [deg] Rotation (misalignment) of first transfocator
19 * SOURCE [ ] 1) Choose rectangular source with defined divergence. 2) Choose Gaussian cross-s
20 * T1_N [ ] Number of Be lenses in 1st IVT transfocator @31.5m
21 * T2_N [ ] Number of Al lenses in 1st IVT transfocator @31.5m _currently deactivated by defau
22 * T3_N [ ] Number of Al lenses in 2nd IVT transfocator @92.25 m
23 * SI_N [ ] Number of Si lenses in Si microfocus chip transfocator @94 m
24 * IVT1BE [ ] If nonzero the set of Be-lenses is chosen for the IVT @31.5m. If 0 the Al set is
25 *
26 * %Example: ESRF_ID11.instr ANGLE=0 Detector: psd_eh3_sample_I=0.285899
27 * %Link
28 * http://www.esrf.eu/UsersAndScience/Experiments/StructMaterials/ID11/ID11Source
29 * %End
30 ****
31
32 DEFINE INSTRUMENT ESRF_ID11(ANGLE=0,SOURCE=0,T1_N=16,T2_N=16,T3_N=16,SI_N=2, IVT1BE=1)
33
34
35 DECLARE
36 %{
37   const double source_h=57e-6*FWHM2RMS;
38   const double source_v=10e-6*FWHM2RMS;
39   const double source_div_h=88e-6*FWHM2RMS;
40   const double source_div_v=5e-6*FWHM2RMS;
41
42   double eh1_sample_offset,EH3TFOC_offset,chip2sample,eh3_sample_offset;
43 %}
44
45
46 INITIALIZE
47 %{
48   /*set some geometry parameters*/
49   eh1_sample_offset=0;
50   EH3TFOC_offset=0;
51   chip2sample=0.1;
52   eh3_sample_offset=0;
53 %}
54
55 TRACE

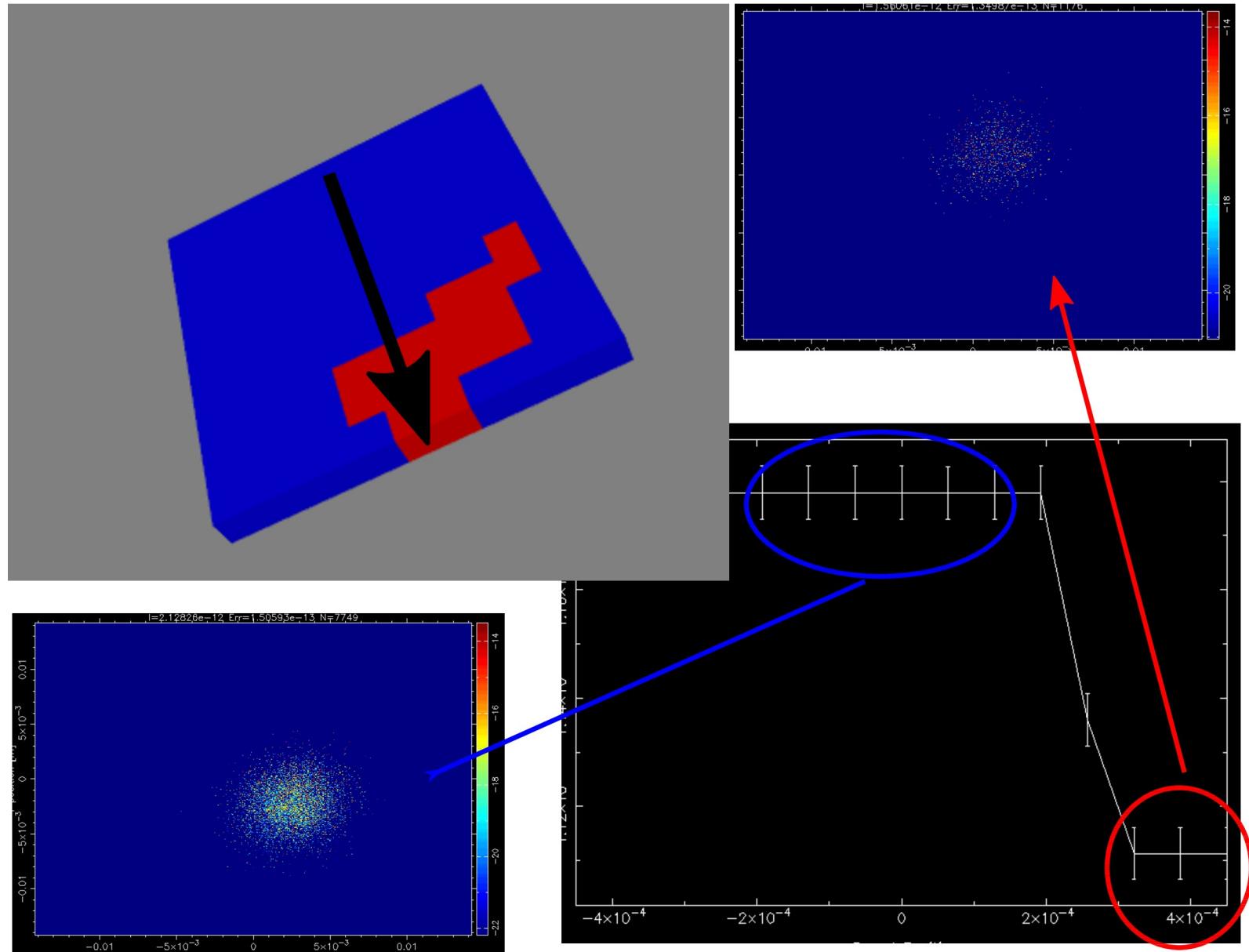
```

search... erkn@elwing: ~ mxcode_config.p... mxgui-p... mxtrace: /home/erkn/ESRF_ID11.instr

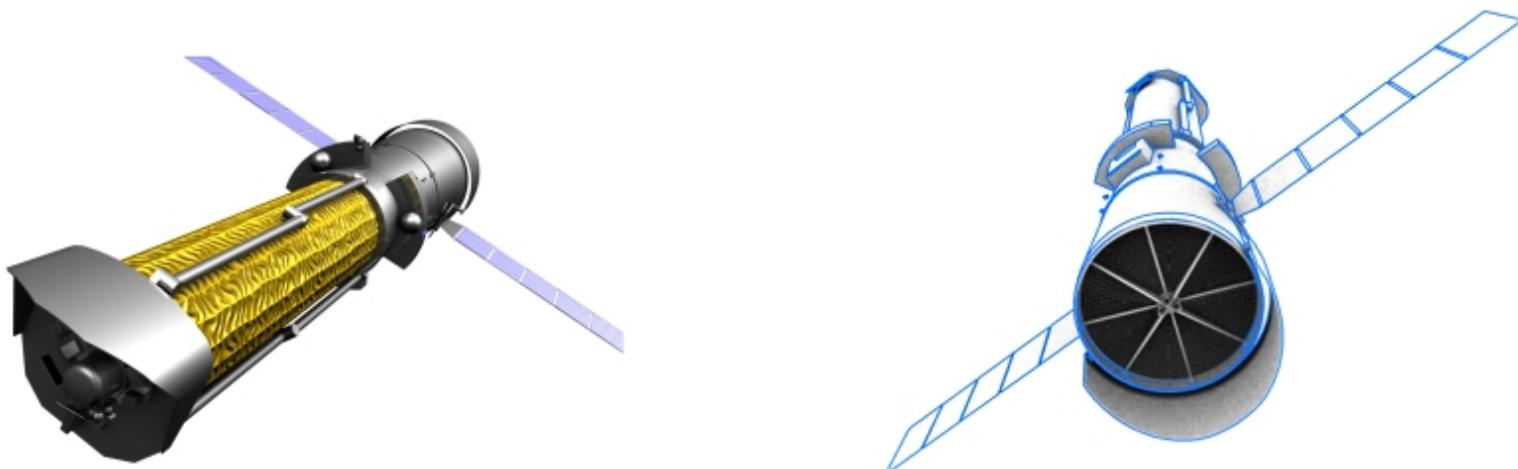




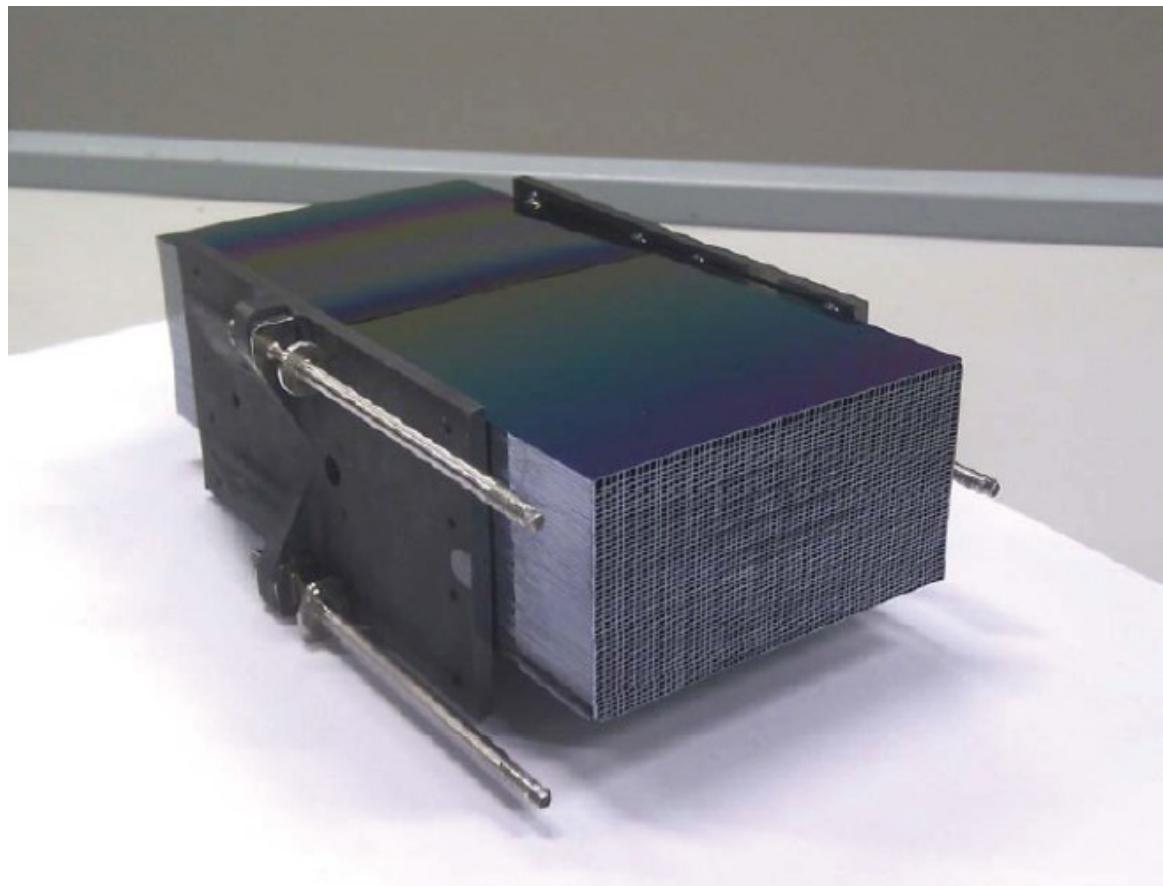
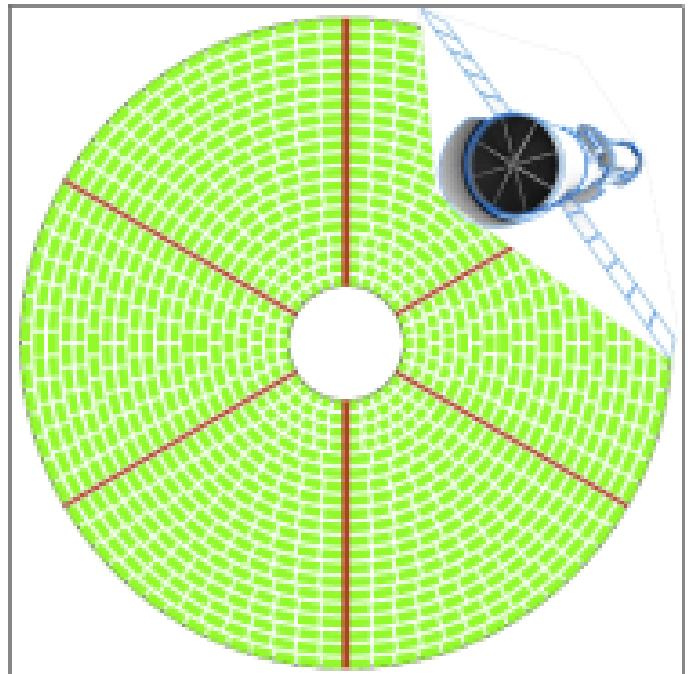
Ge-bicrystal wafer scanned by a monochromatic microbeam along the arrow. The red crystal has a .7% greater lattice spacing.

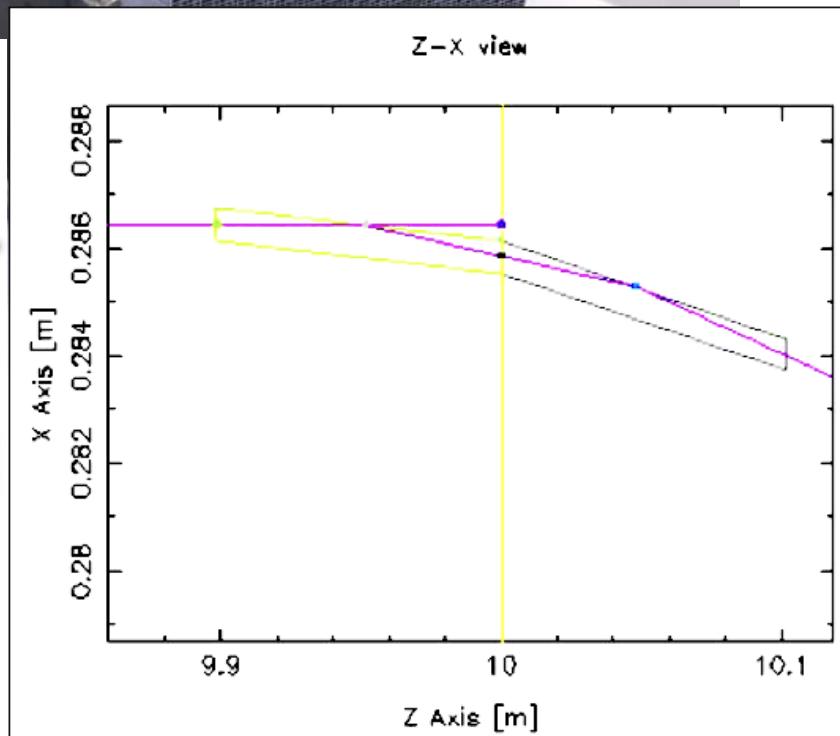
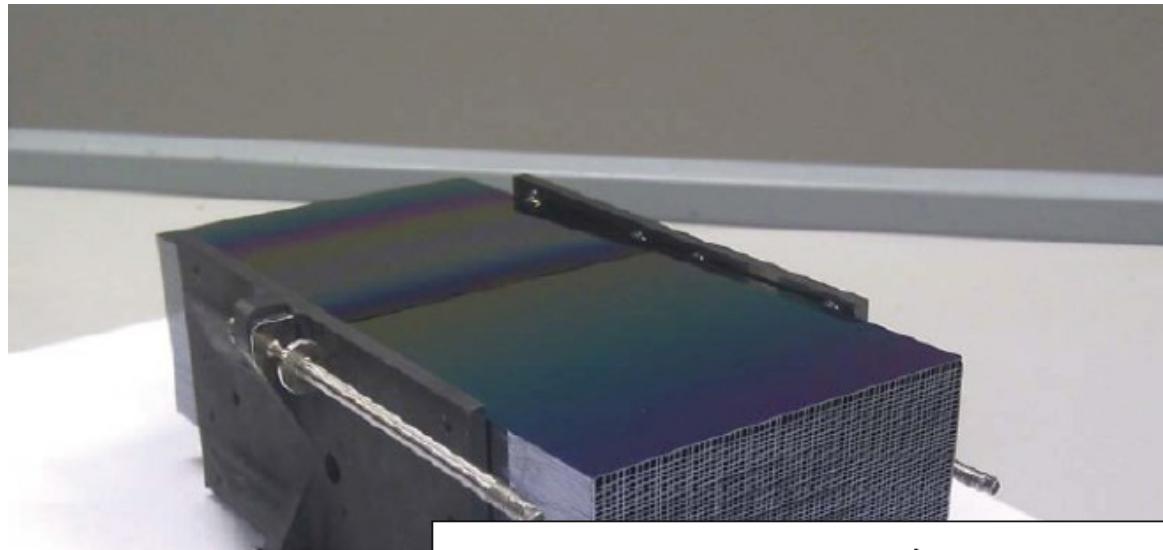
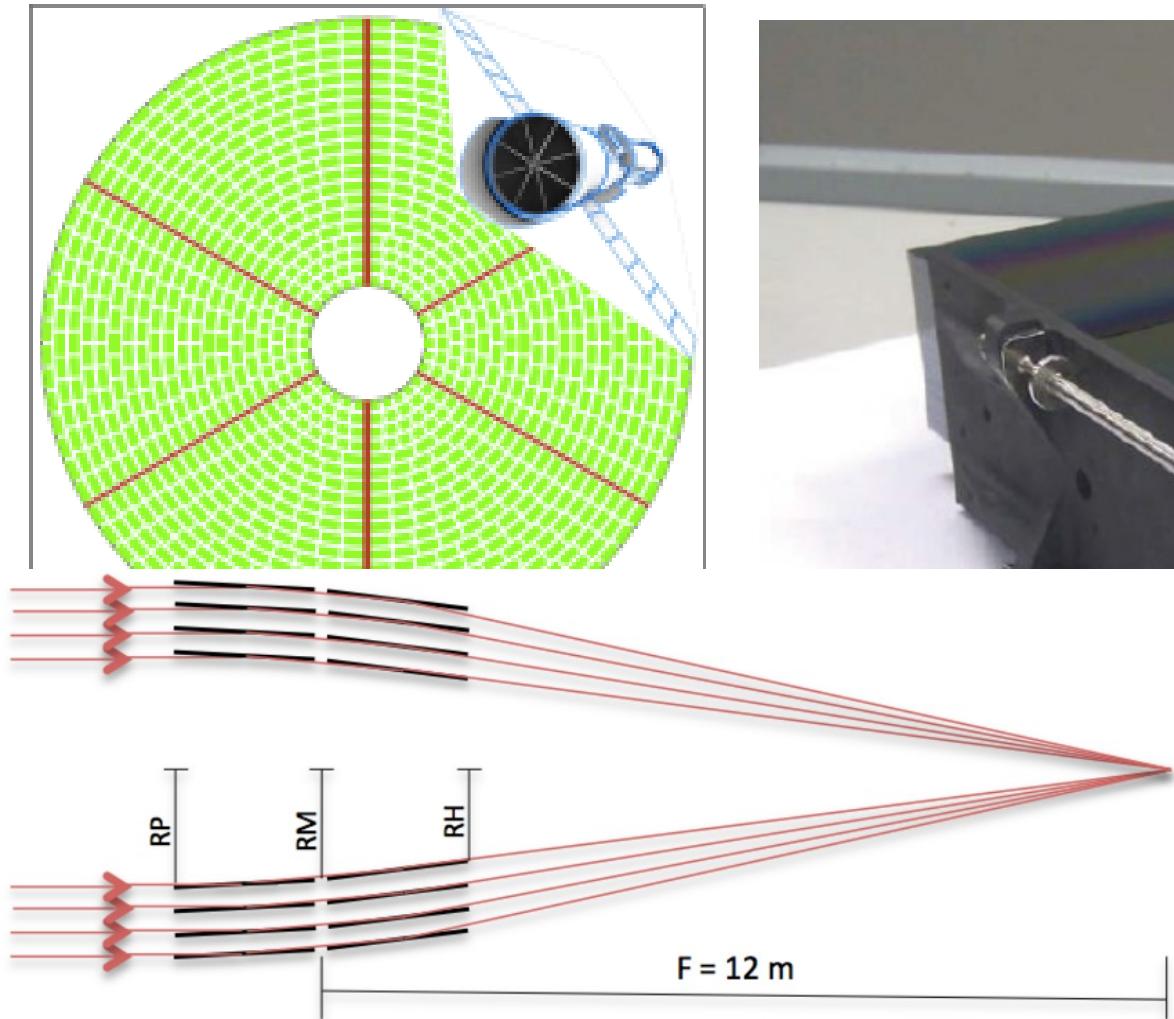


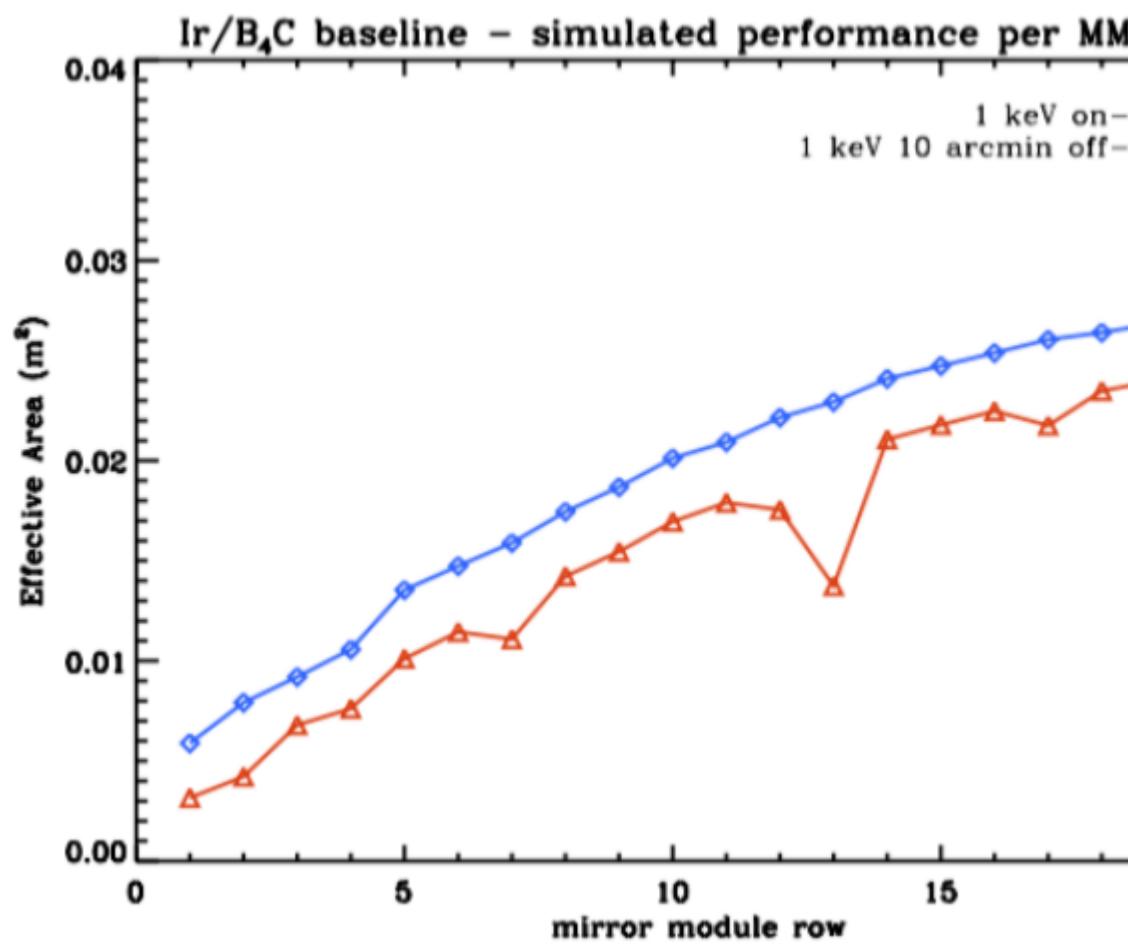
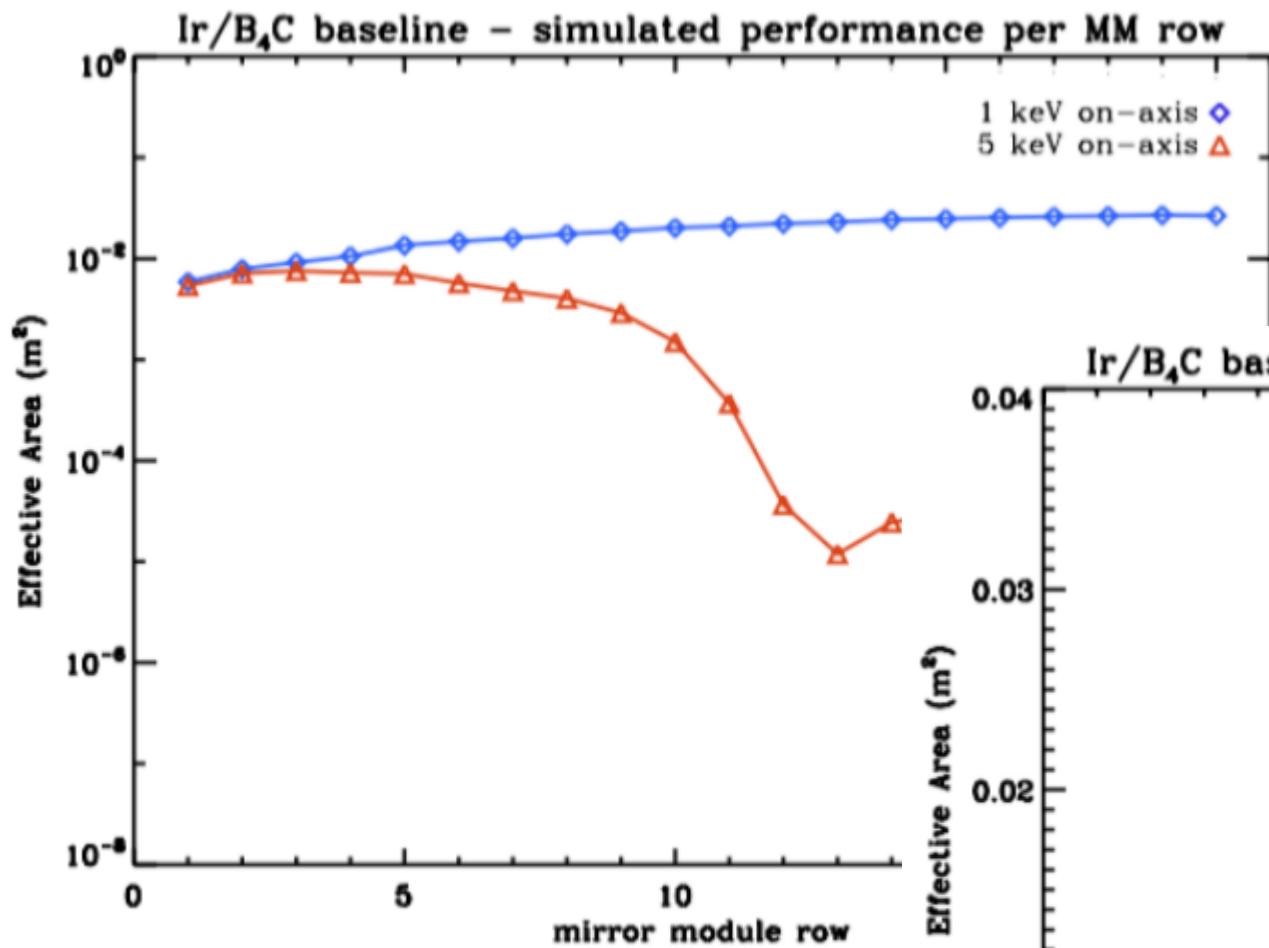
X-Ray satellite telescope



ATHENA X-ray space telescope: <http://sci.esa.int/ixo/>







McXtrace homepage - Mozilla Firefox

mcxtrace.org

Most Visited Getting Started Portscout Port Up... Getting Started Bright: New beamlin... Astro-Update Hea... Portscout Port Up... Tinkercad | Create 3... Tændt What Every Comput...

McXtrace

McXtrace - An X-ray ray-trace simulation package

McXtrace - Monte Carlo Xray Tracing, is a joint venture by

Funding from NABIIT, [DSF](#) and the above parties.

McStas

Our code is based on technology from .

Code repository (shared with 'McStas') is located at github.com/McStasMcXtrace

For information on our progress, please subscribe to our [user mailinglist](#).

- To download the latest release: [download area](#)
- For installation instructions : [installation](#)
- For a quick list of the available commands: [commands](#)

McXtrace News

The latest McXtrace news.

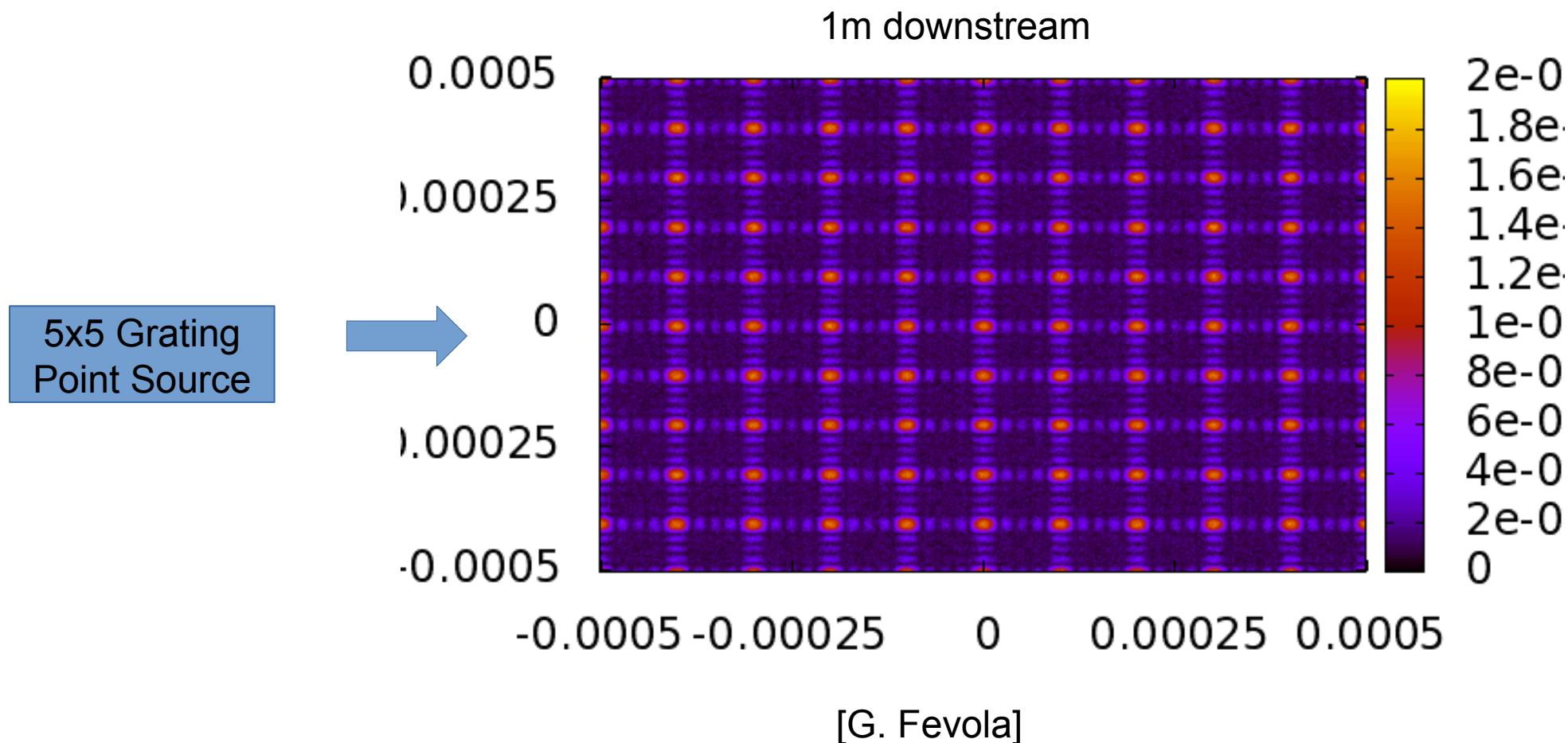
McXtrace 1.4: known bugs

- Lens_parab & Lens_parab_Cyl: A missing 'l' in the header (line 11) trips the intersection algorithm. Fixed in the development tree
- mxplot-pyqtgraph on windows: An error in a post-install script causes the file c:\mcxtrace-1.4\bin\mxplot-pyqtgraph to have a typo where it says mcplot.py instead of mxplot.py as it should. The mxplot-pyqtgraph script is generated install time - the install procedure has been altered to fix this. For existing systems the simple workaround is to either edit that file in place or to replace it with one from this link:downloads.mcxtrace.org/mcxtrace-1.4/fixes.
- On windows, if you want to use the Undulator component, you must also install The GNU scientific Library (GSL). It is available from gnuwin32.sourceforge.net/packages/gsl. This also implies that you probably need to edit the mcxtrace compiler flags. Go to File->Configure and add something along the lines "Lc:mcxtrace\Program Files (x86)\GnuWin32\lib -Ic:mcxtrace\Program Files (x86)\GnuWin32\include" to the C flags box for mcxtrace to be find the libraries compile time.

Current Projects

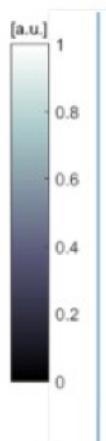
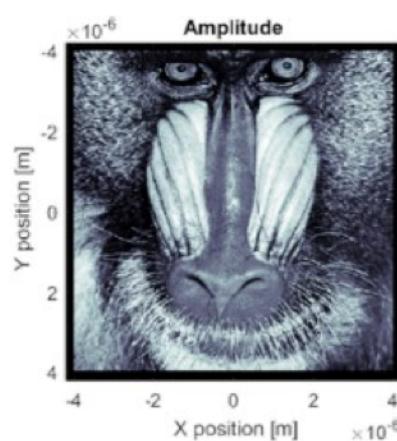
1. Interoperability
2. Ray Tracing Ptychography

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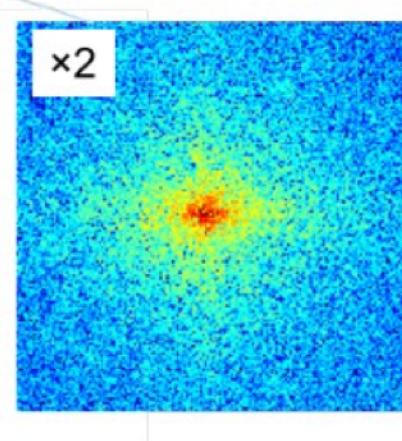
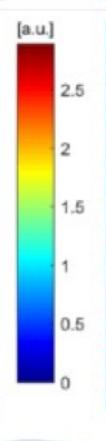
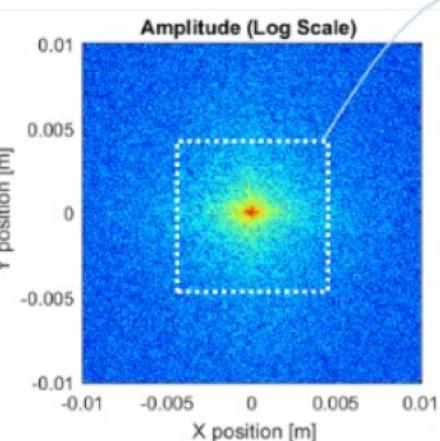


Raytracing diffraction

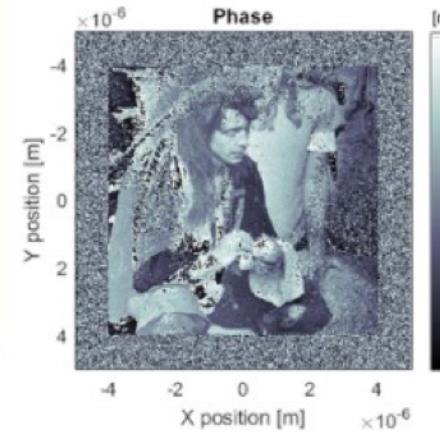
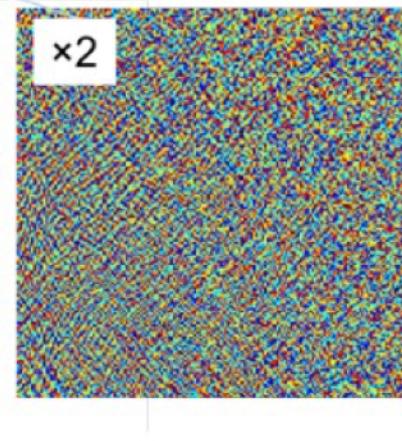
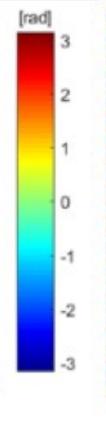
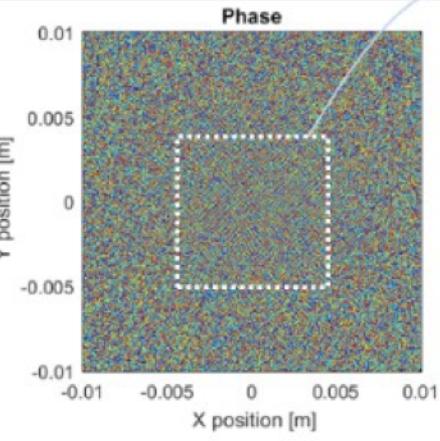
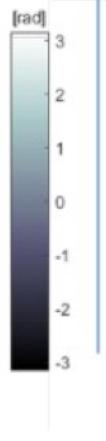
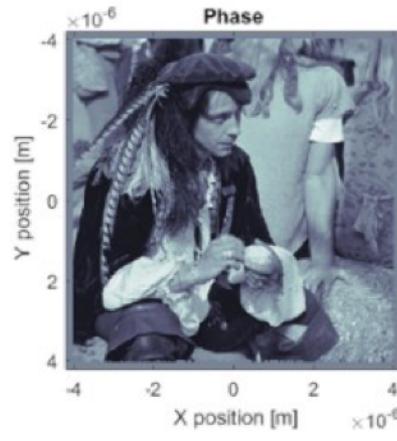
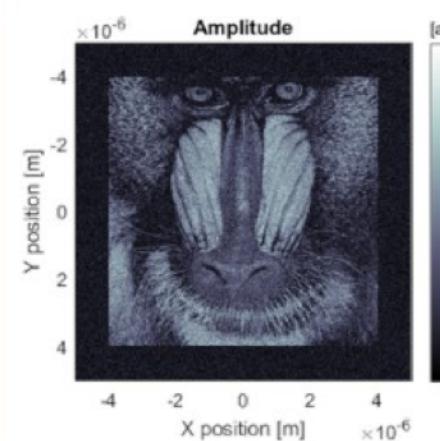
Exit Wavefield



Diffraction Pattern



Inverse Fourier Transform

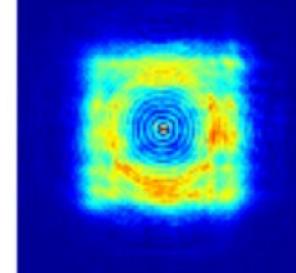


Amplitude**[a.u.]**

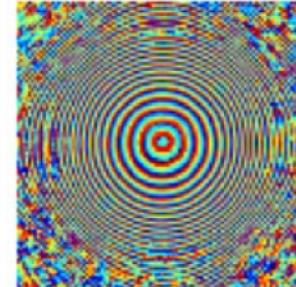
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1

Phase**[rad]**

3
2
1
0
-1
-2
-3

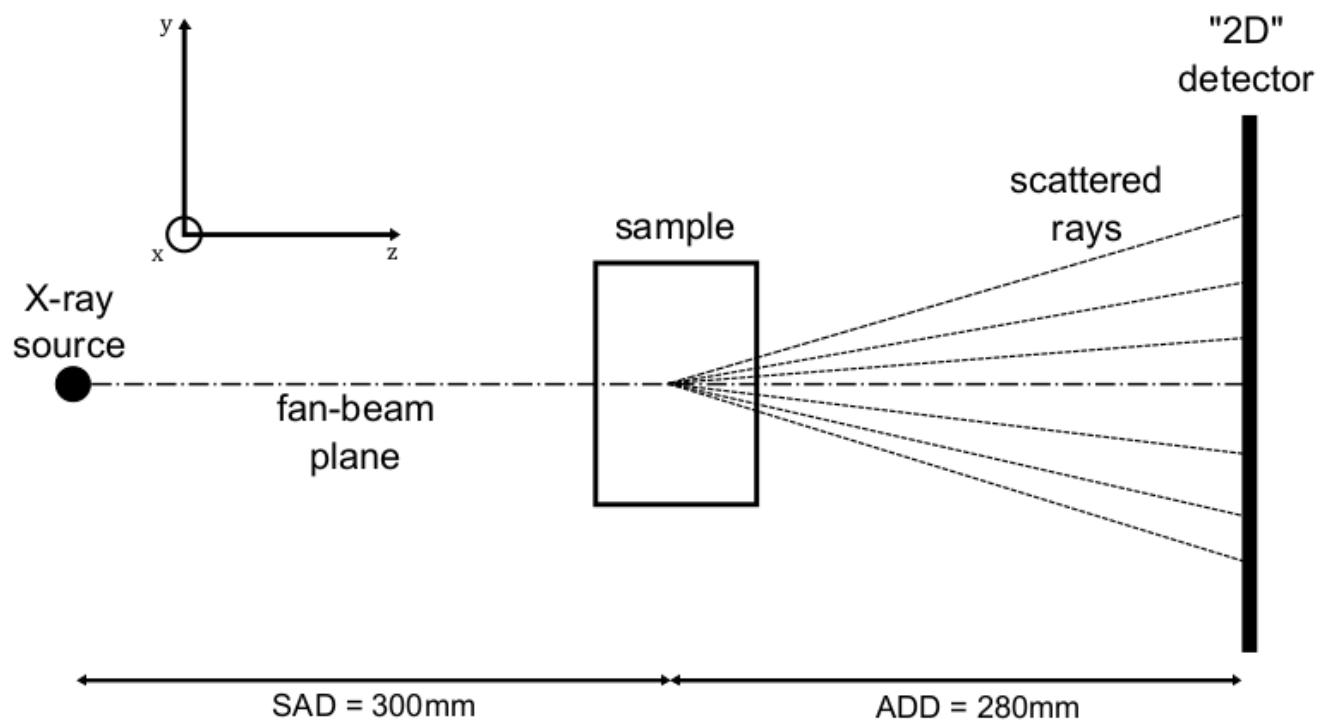
Amplitude**[a.u.]**

0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1

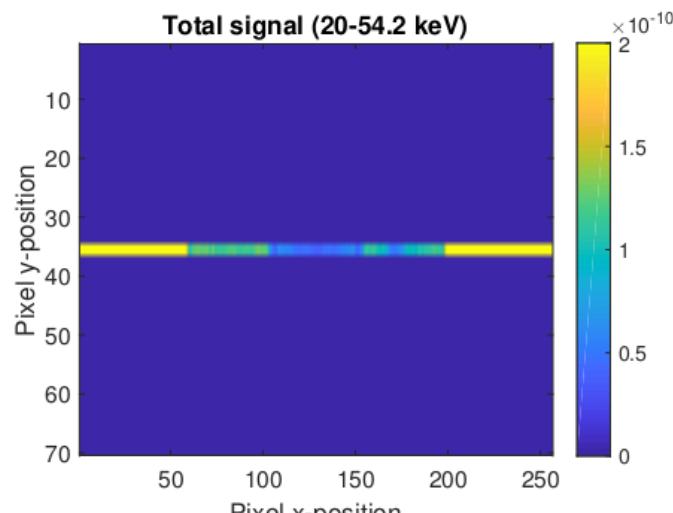
Phase

3
2
1
0
-1
-2
-3

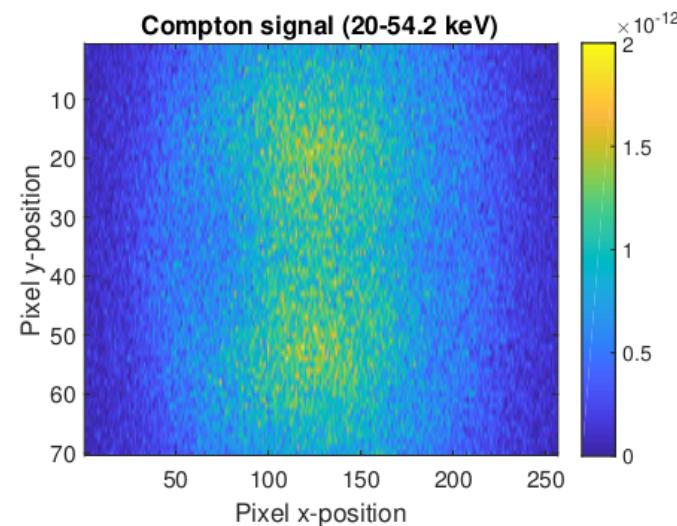
1. Interoperability
2. Ray Tracing Ptychography
3. NanoMAX simulation
4. Imaging simulations.



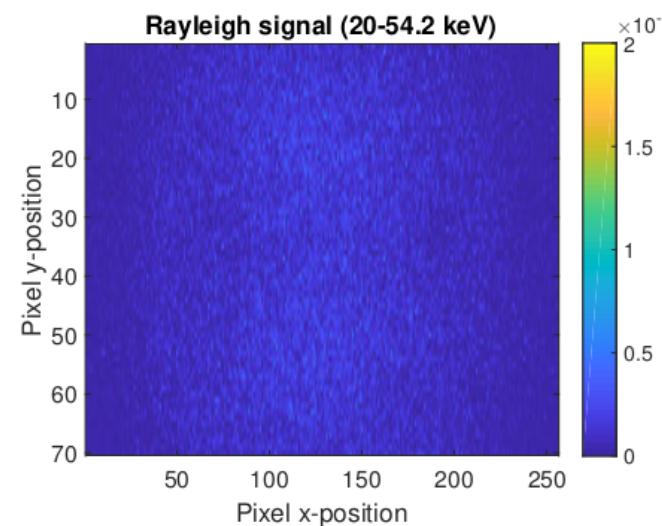
Current Projects



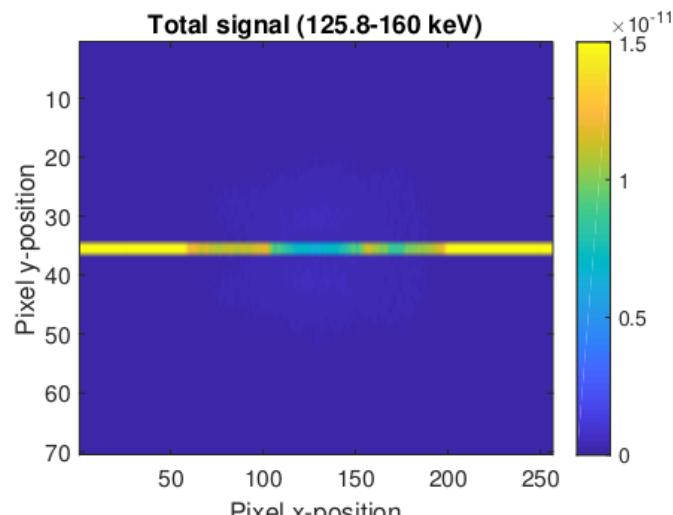
(a)



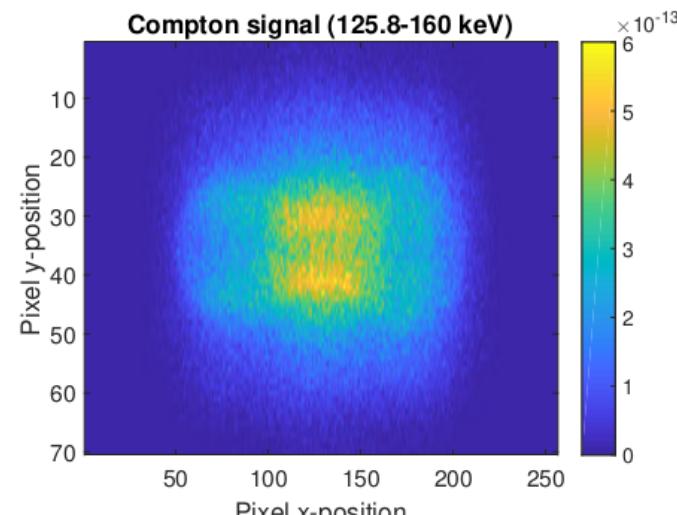
(b)



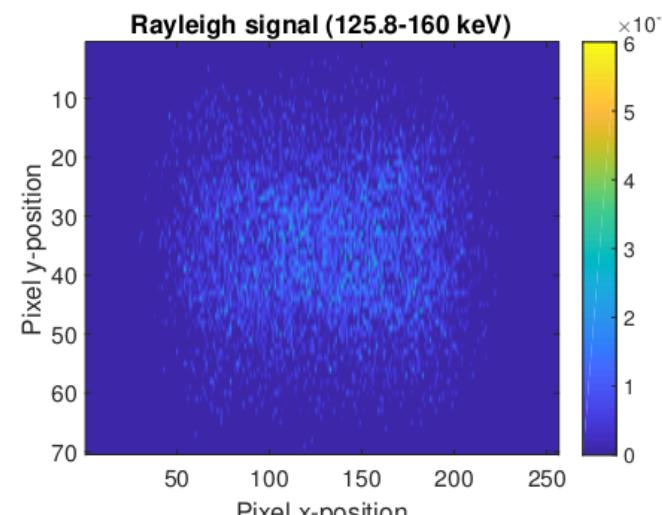
(c)



(d)



(e)



(f)



Thank you for your attention!

Peter Willendrup [1]

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 Cramer Petersen [3]

Robert Feidenhans'l [2]

Kim Lefmann [2]

Matteo Busi [1]

Innokenty Kantor [1,7]

Mads Ry Jørgensen[8,7]

Marcus Mendenhall [9]

Giovannin Fevola [10]



Region
Hovedstaden



Uddannelses- og
Forskningsministeriet

—
Styrelsen for Forskning og Innovation

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[9] NIST, Gaithersburg, MD, USA.

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