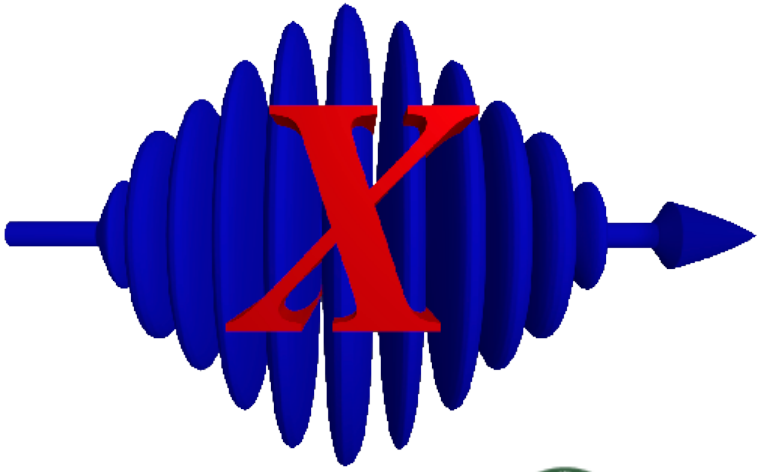
McXtrace



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

Peter Willendrup <pkwi@fysik.dtu.dk>
(slides from Erik Bergbäck Knudsen)

What is it?

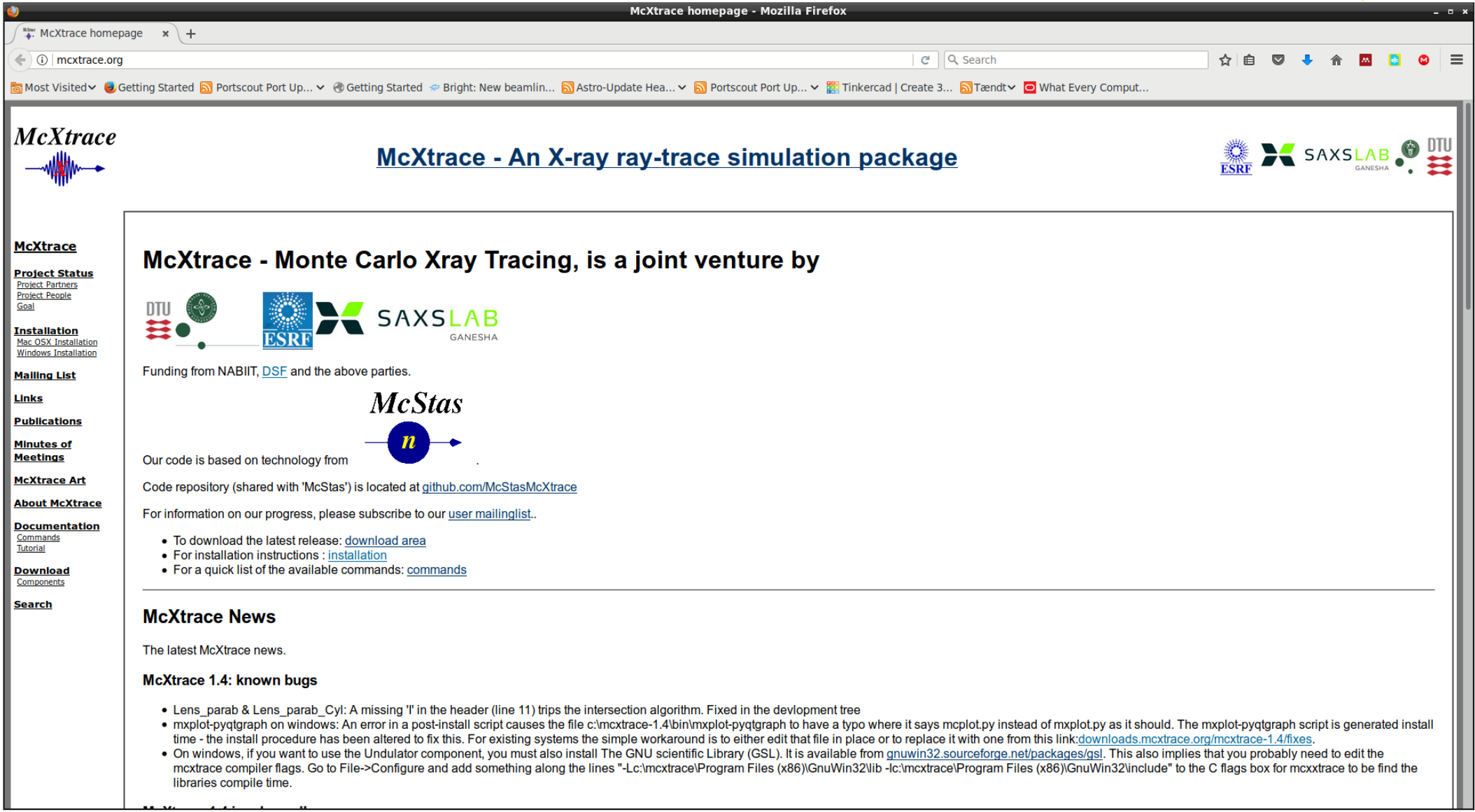
- Built on proven base of McStas for neutron ray tracing
  K. Lefmann and K. Nielsen, Neutron News 10, 20, (1999).
- Releases 1.7.1 and 3.1 (GPU support). New releases after SOLEIL school.
- Portable code (Unix/Linux/Mac/Windows, 32 and 64 bit support)
  Has run on all from iPhone to FERMI (world no. 7)

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

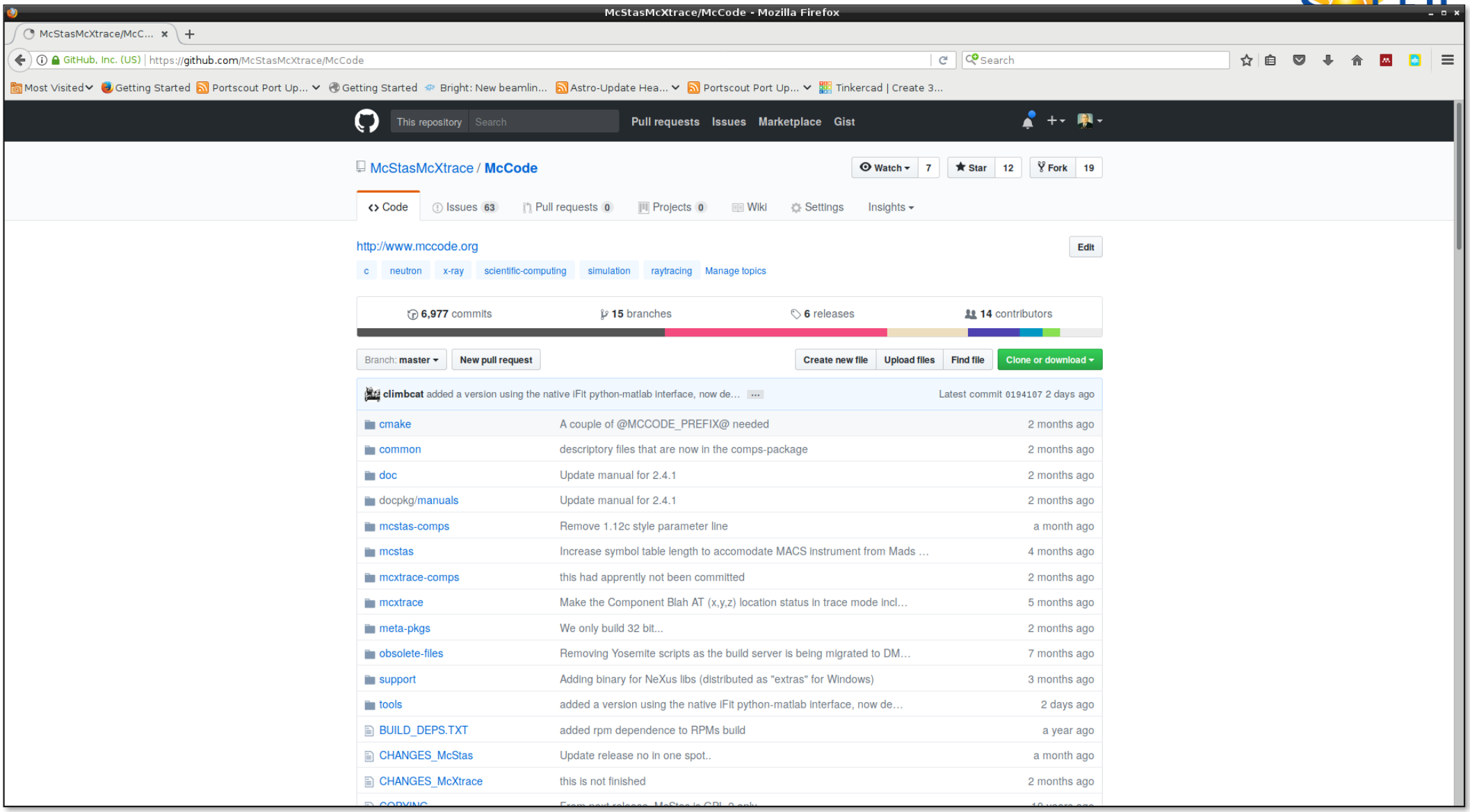
Project mailing list at
mcxtrace-users@mcxtrace.org

- 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 (python3/qt5 or perl/tk for gui).
- Permanent staff at DTU Physics maintaining the code

Website at
https://www.mcxtrace.org



Github


McStasMcXtrace/McCode - Mozilla Firefox
McStasMcXtrace/McC...
GitHub, Inc. (US) | https://github.com/McStasMcXtrace/McCode
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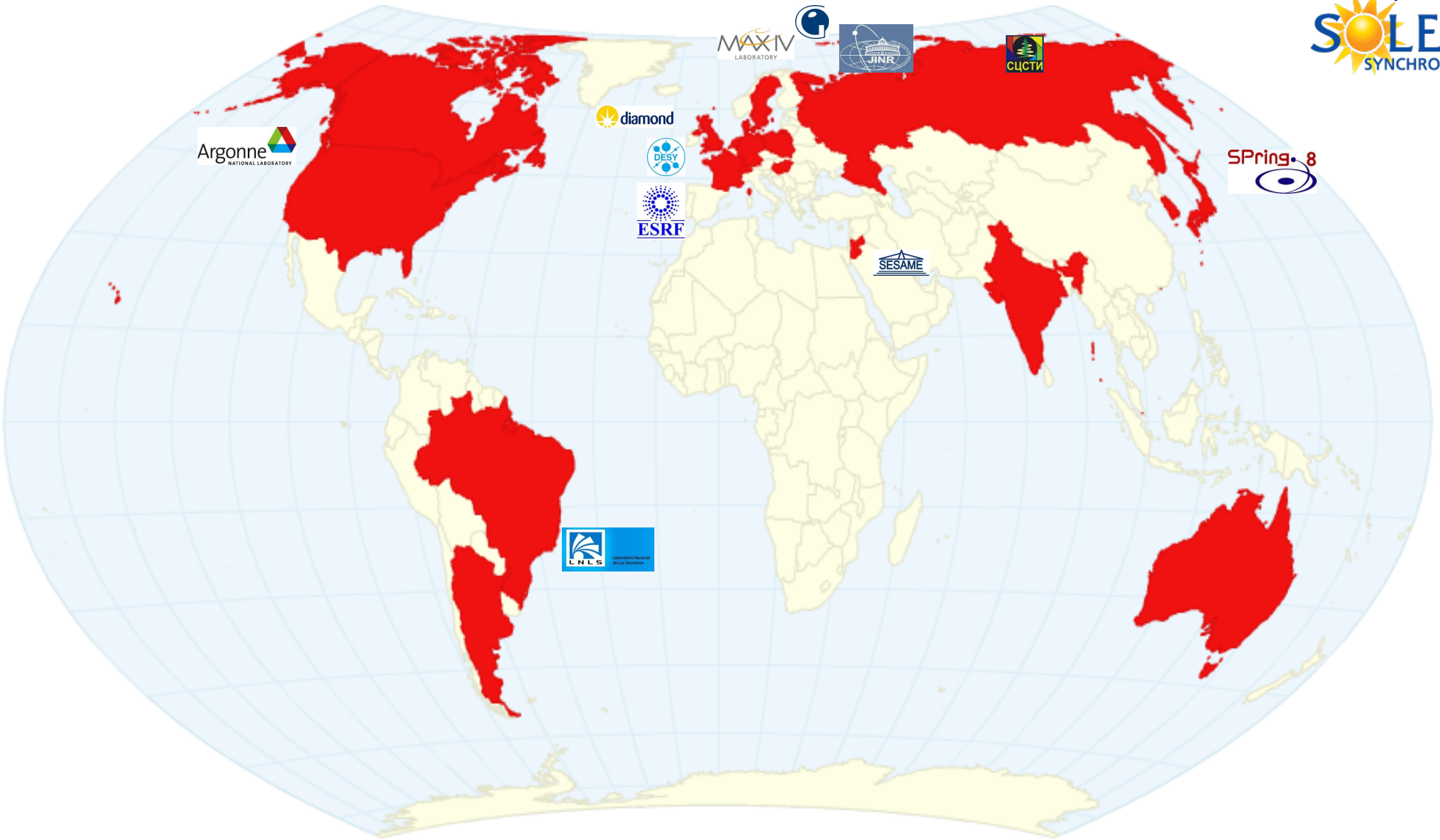
Manage topics
6,977 commits
15 branches
6 releases
14 contributors
Branch: master
New pull request
Create new file
Upload files
Find file
Clone or download
climbcat added a version using the native iFit python-matlab interface, now de...
Latest commit 0194107 2 days ago
cmake A couple of @MCCODE_PREFIX@ needed 2 months ago
common descriptory 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
mcxtrace-comps this had apprently not been committed 2 months ago
mcxtrace 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

Where?


MAX IV
LABORATORY
JINR
CLICTN
diamond
Argonne
NATIONAL LABORATORY
DESY
SPring-8
ESRF
SESAME
LNLS

Feature History - and plans for NG (not fully up-to-date)

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:

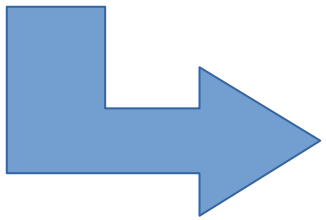
ad. Reflectivity library
ae. MAX_Bloch
af. Laue crystal model
ag. MAXIV_DanMAX
ah. MAXIV_FemtoMAX
ai. NIST reflectometer
aj. Reflective grating
ak. Johann Spectrometer
al. Powder Incoherent scattering
am. More accurate Source_lab

Next-generation:

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

The McXtrace way

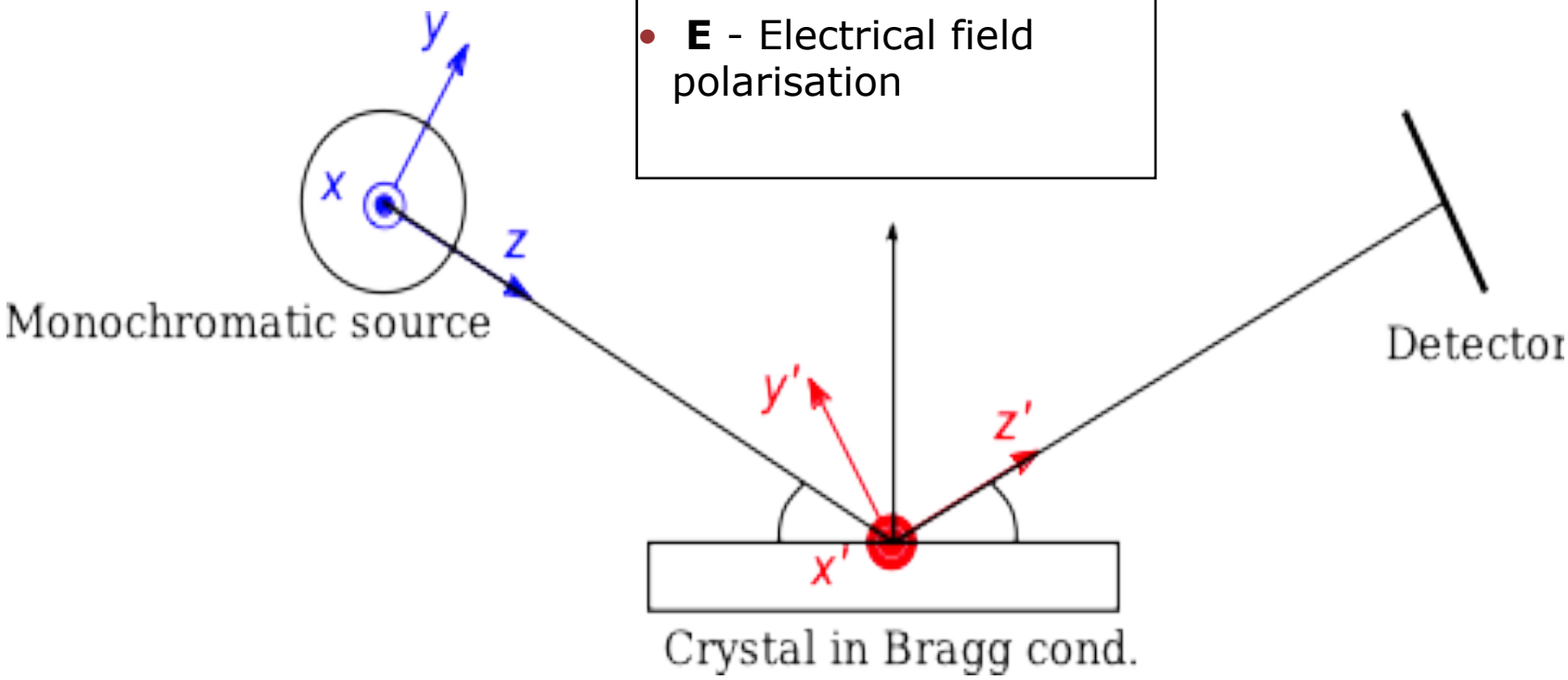
1. Describe your beamline in the McXtrace language (In a text file).
2. Automatically convert beamline into ANSI c
3. Compile
4. Run



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

How?

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



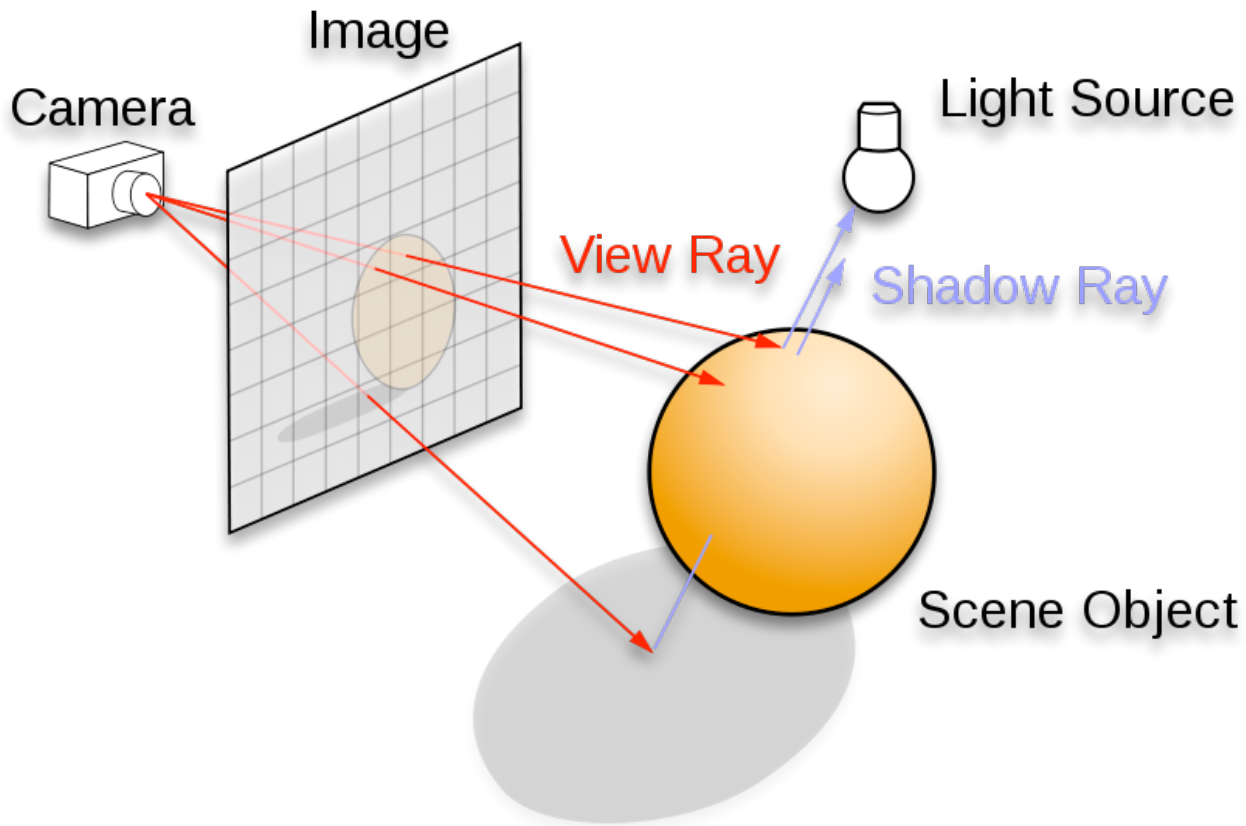
Monte Carlo techniques

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



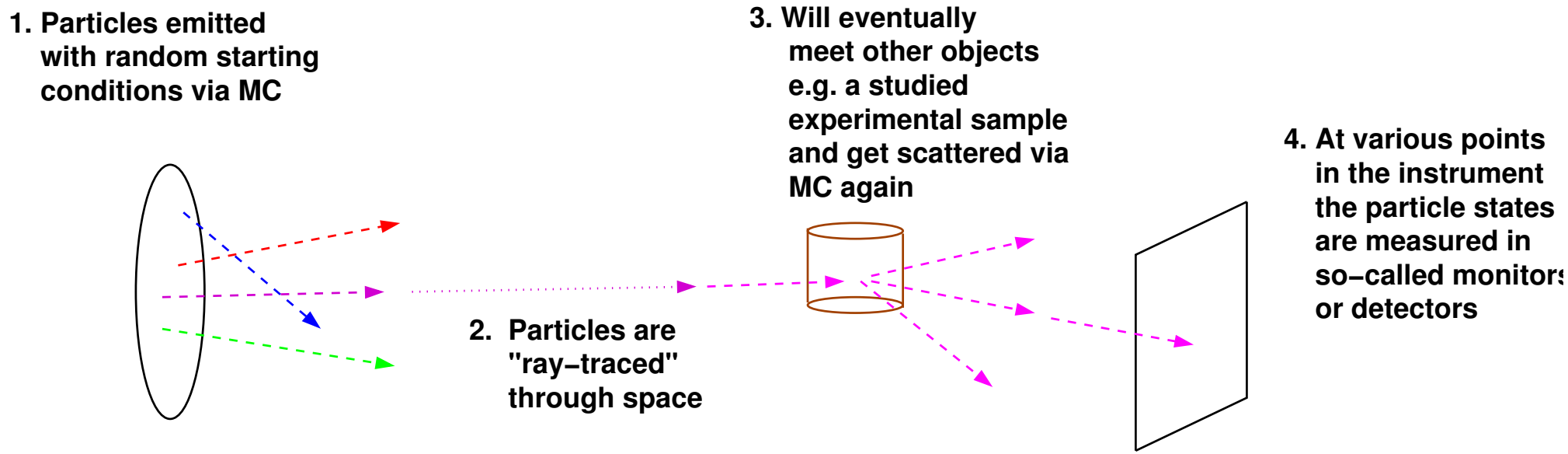
- Notable fathers: John v. Neumann Stanislav Ulam Nicholas Metropolis
- Named “Monte Carlo” after Ulam’s fathers frequent visits to the Monte Carlo casino in Las Vegas
- Initially “implemented” by letting large numbers of women use tabularized random numbers and hand calculators for individual particle calculations
- Later, analogue and digital computing devices were used

Ray-tracing methods



- When particles move in “free space”, we use ray-tracing
  - but in most cases in direction source -> detector

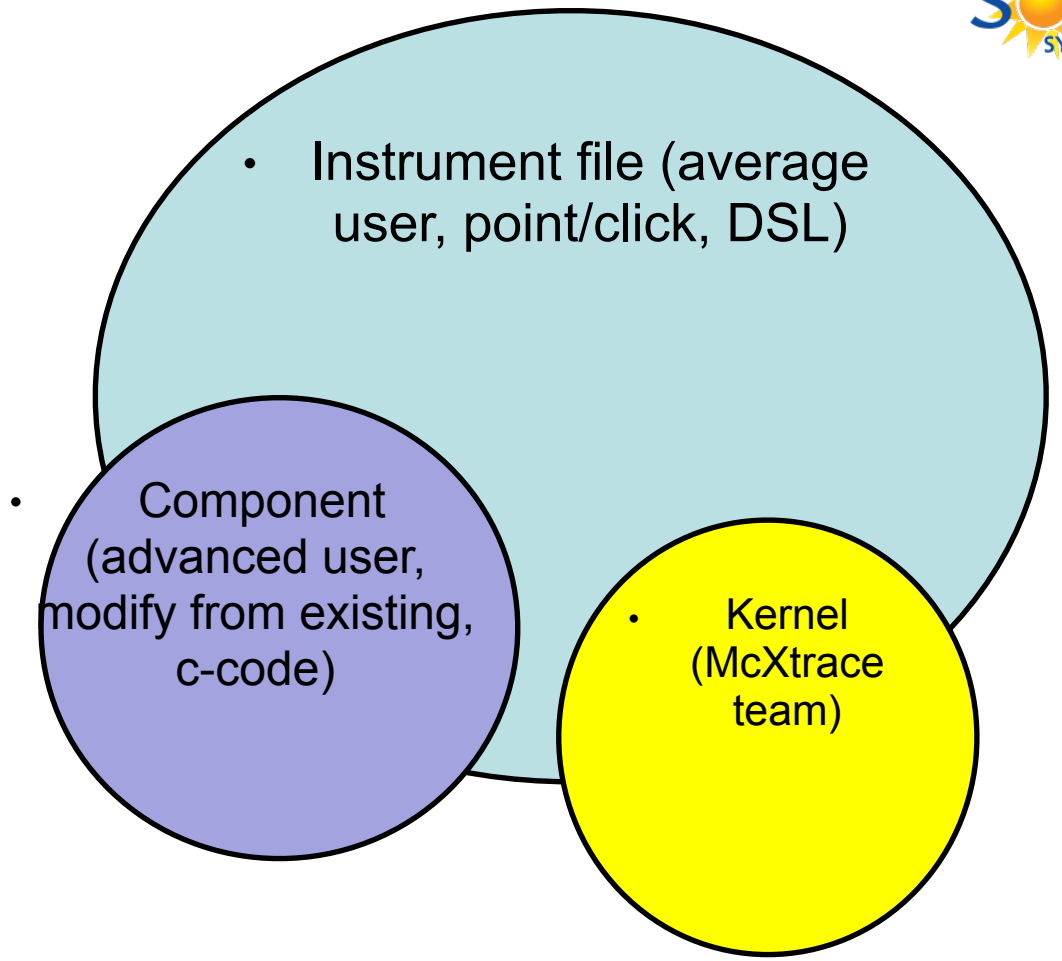
Overall picture: Monte Carlo Ray-Tracing



- Important efficiency mechanisms:
  - "Focusing" - e.g. lab source to first slit (4π vs. limited solid angle only)
  - Rather vs. single particle description, absorption handled though statistics and downscaling the ray weight

Code Levels

- **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.)



Instrument file

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_saxslab (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

-- INSERT --

Component file

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

File Edit Tools Syntax Buffers Window Help

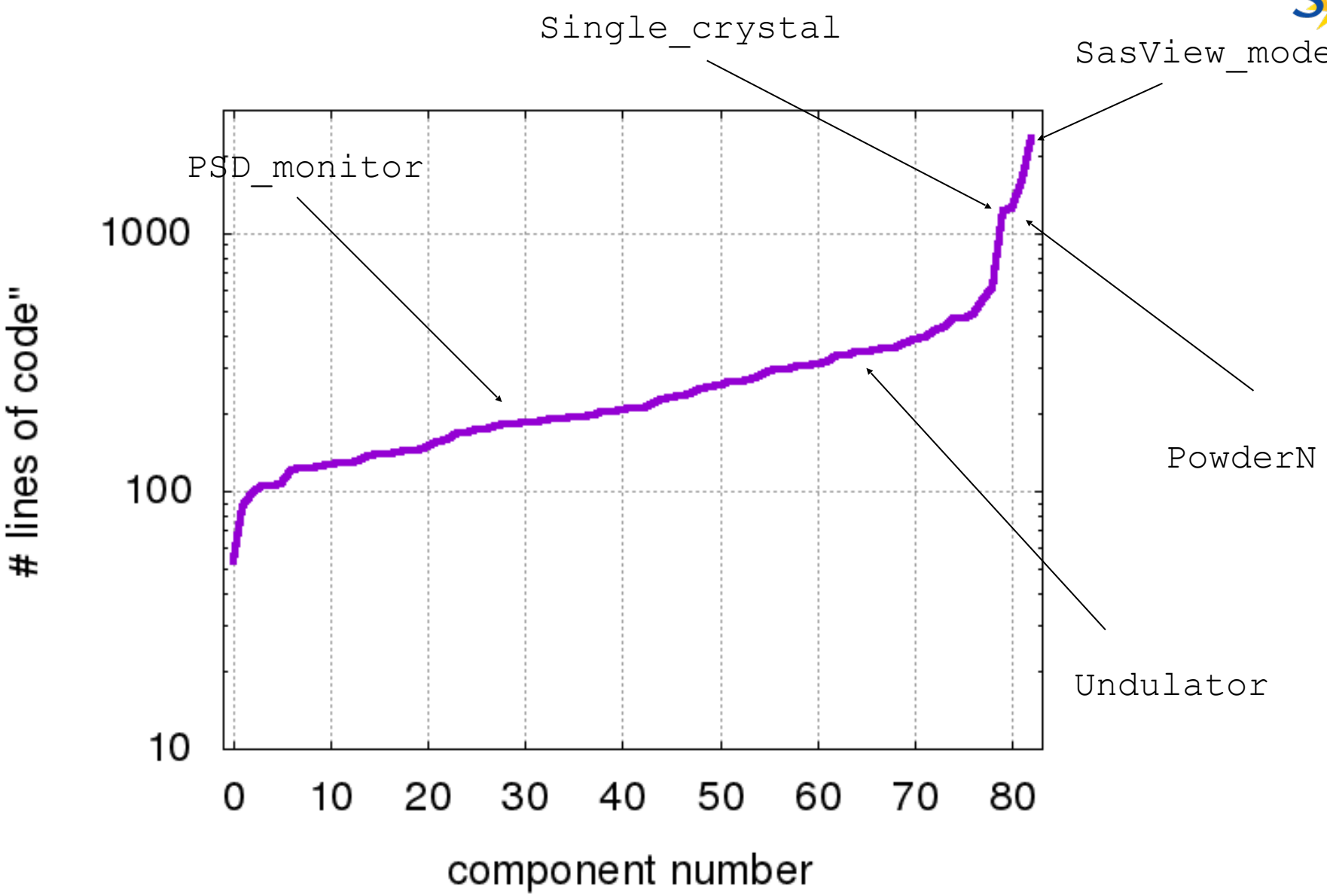
```
DEFINE COMPONENT PSD_monitor
DEFINITION PARAMETERS (nx=90, ny=90,nr=0, string filename=0, restore_xray=0)
  SETTING PARAMETERS (xmin=-0.05, xmax=0.05, ymin=-0.05, ymax=0.05, xwidth=0, yheight=0, radius=0)
OUTPUT PARAMETERS (PSD_N, PSD_p, PSD_p2)
/* X-ray parameters: (x,y,z,kx,ky,kz,phi,t,Ex,Ey,Ez,p)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

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"
                  "ERROR         (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 (r<radius){
        i = floor(r*nr/radius);
        PSD_N[0][i]++;
        PSD_p[0][i] += p;
```

../McCode/mcxtrace-comps/monitors/PSD_monitor.comp 75,61 52%

```
        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 (r<radius){
        i = floor(r*nr/radius);
        PSD_N[0][i]++;
        PSD_p[0][i] += p;
        PSD_p2[0][i] += p*p;
        SCATTER;
      }
    }
    if (restore_xray) {
      RESTORE_XRAY(INDEX_CURRENT_COMP, x, y, z, kx, ky, kz, phi, t, Ex, Ey, Ez, p);
    }
  %}
SAVE
  %{
    if(!radius){
      DETECTOR_OUT_2D(
          "PSD_monitor",
          "X position [m]",
          "Y position [m]",
          xmin, xmax, ymin, ymax,
          nx, ny,
          *PSD_N,*PSD_p,*PSD_p2,
          filename);
    }else{
      DETECTOR_OUT_1D(
          "PSD_monitor","Radial Position[m]", "Intensity", "R",
          0,radius,nr,&PSD_N[0][0],&PSD_p[0][0],&PSD_p2[0][0],filename);
    }

  %}

FINALLY
%{
    free(PSD_N[0]);
    free(PSD_N);
    free(PSD_p[0]);
    free(PSD_p);
    free(PSD_p2[0]);
    free(PSD_p2);
%}
MCDISPLAY
%{
  magnify("xy");
  multiline(5, (double)xmin, (double)ymin, 0.0,
               (double)xmax, (double)ymin, 0.0,
               (double)xmax, (double)ymax, 0.0,
               (double)xmin, (double)ymax, 0.0,
               (double)xmin, (double)ymin, 0.0);


END
```

../McCode/mcxtrace-comps/monitors/PSD_monitor.comp 131,5 Bot

Component size



Why bother?

1) Why simulate when you can just do the experiment?

2) Why McXtrace and not sim. package X?

Why simulate a full beamline?

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

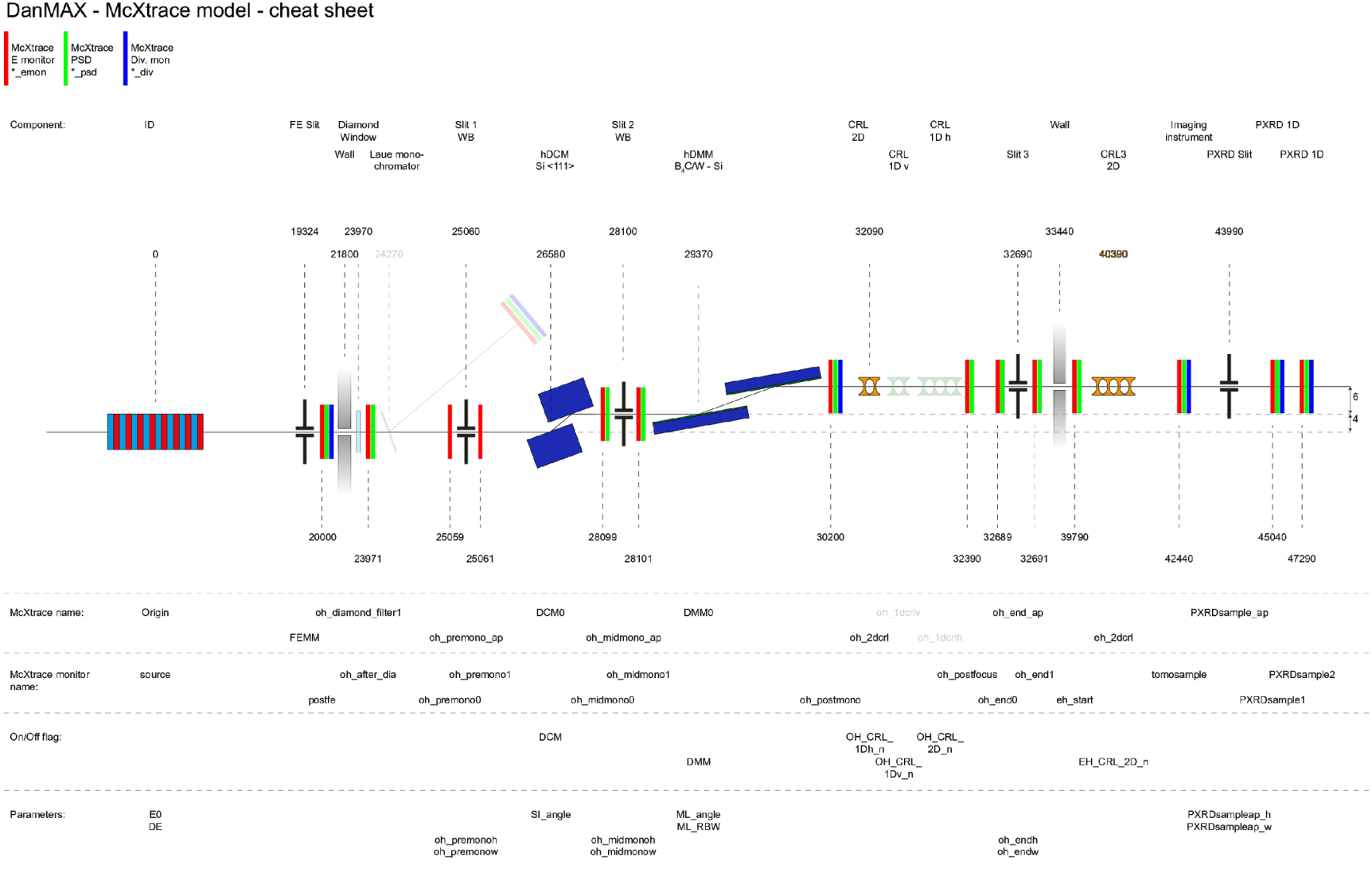
Why McXtrace

- 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>...

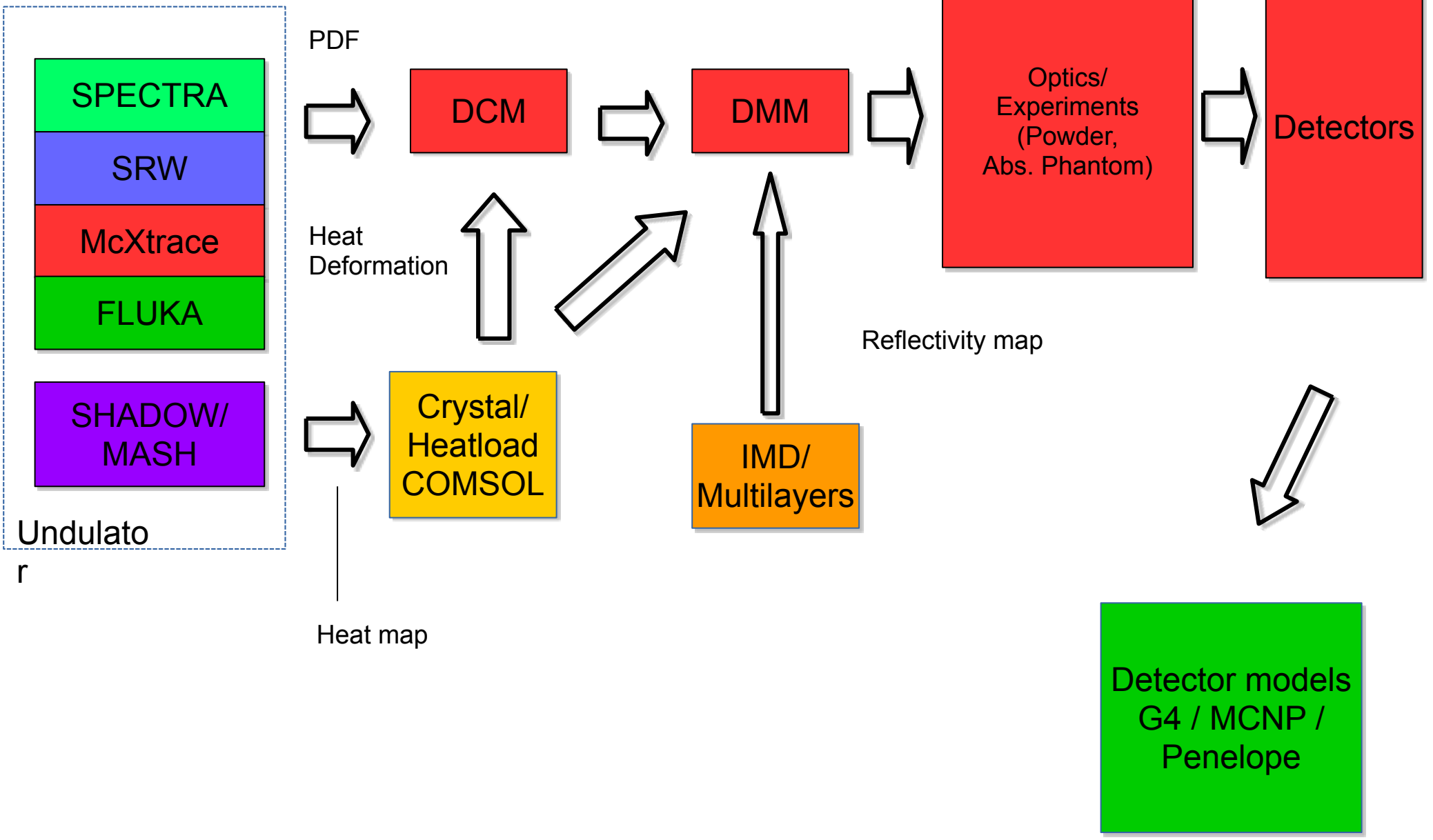
DanMAX simulation effort

McXtrace main simulation vehicle with connections to:

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

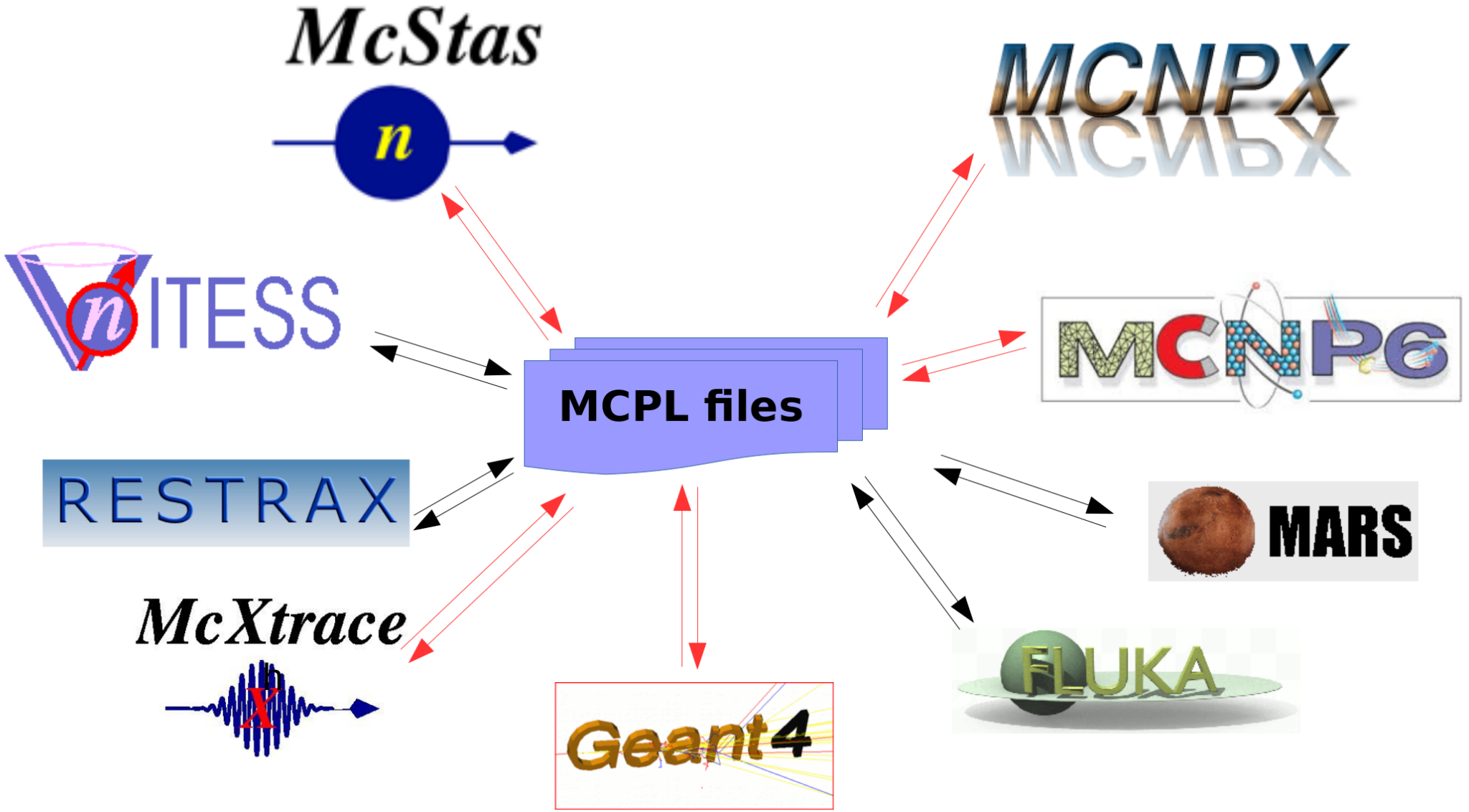


DanMAX simulation workflow



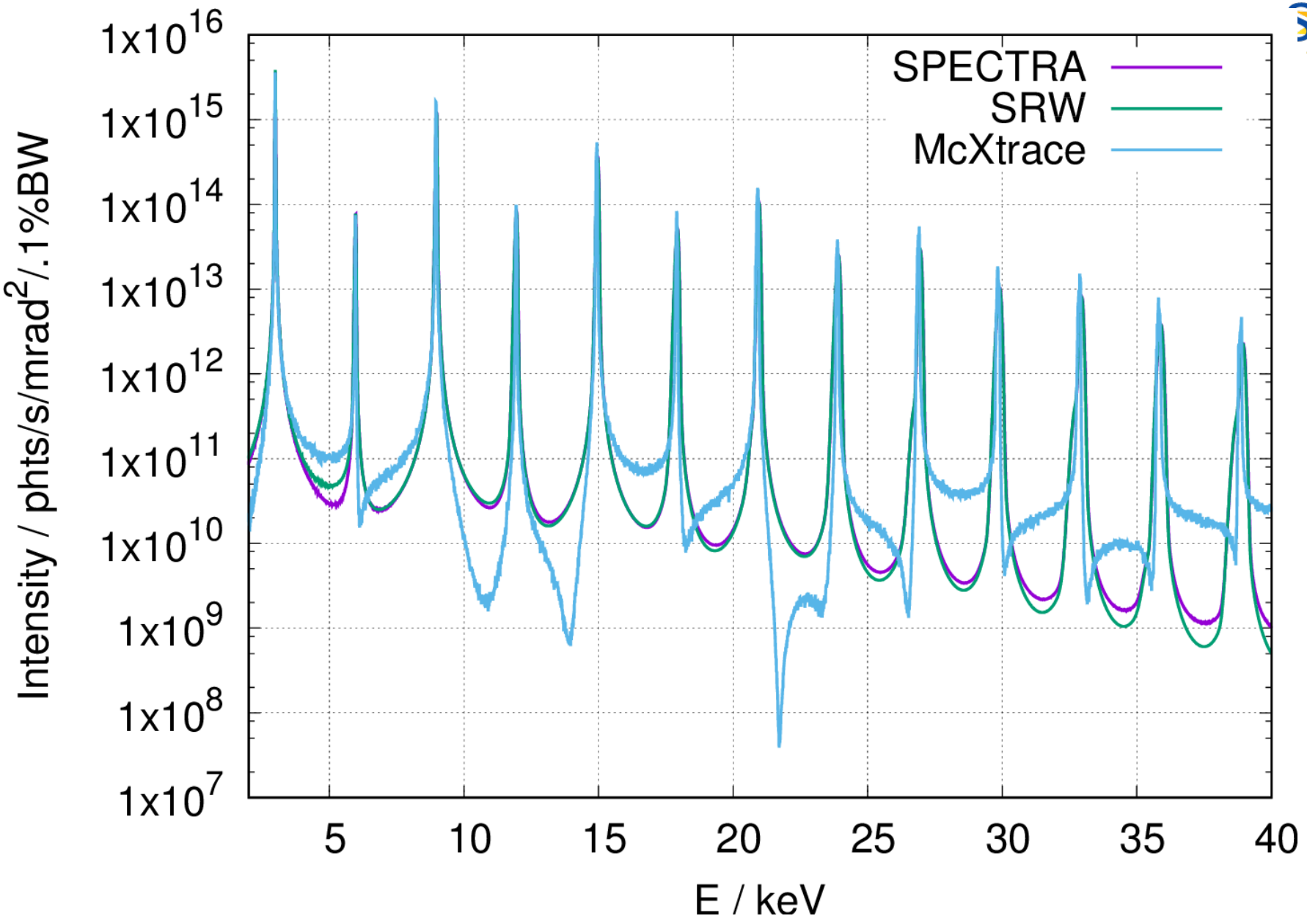
MCPL

Monte Carlo Particle List-format



Courtesy T. Kittelmann, ESS

Source: Undulator

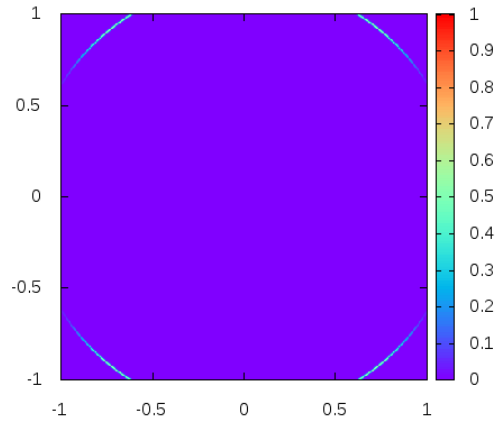


Undulator: Spatial distr.

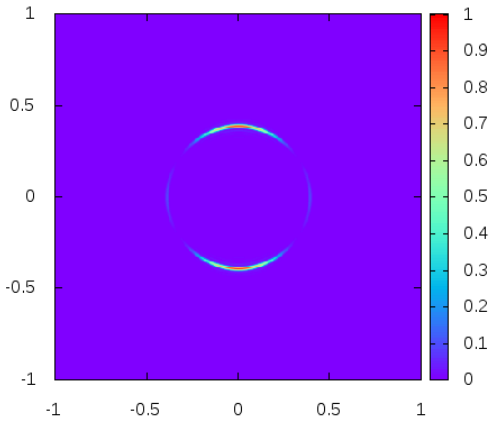
Tuned to have 11th Harmonic at 33 keV

SPECTRA

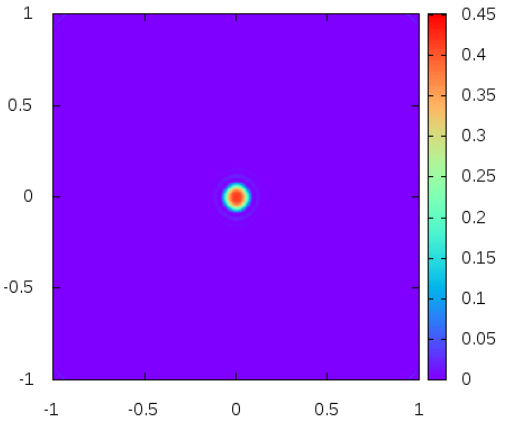
25.3 keV



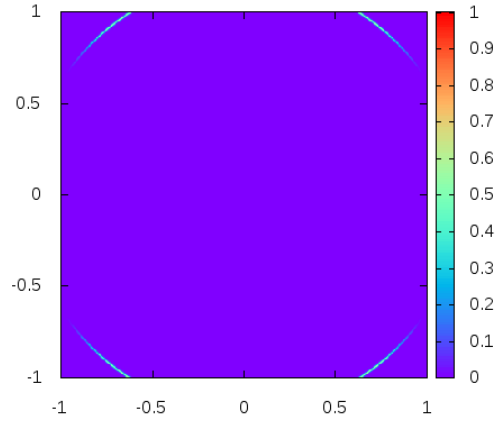
26.8 keV

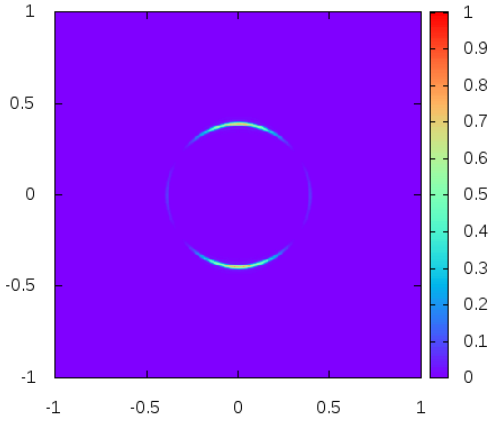


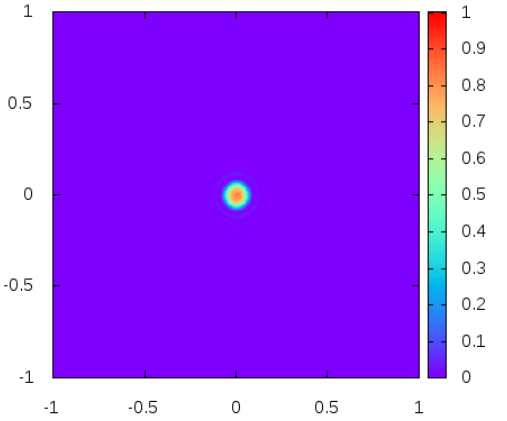
33 keV



McXtrace







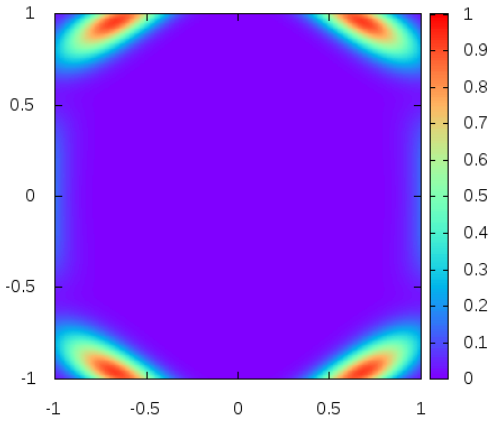
Undulator: Spatial distr.

Tuned to have 11th Harmonic at 33 keV

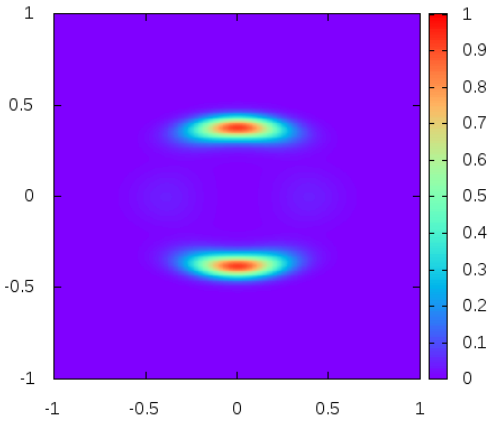
With emittance

SPECTRA

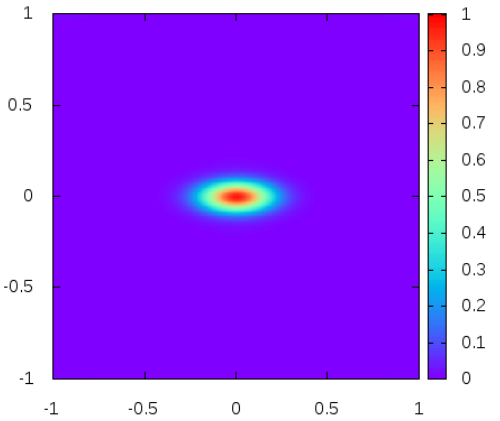
25.3 keV



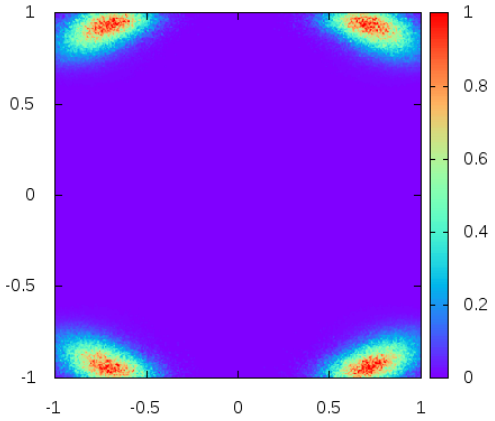
26.8 keV

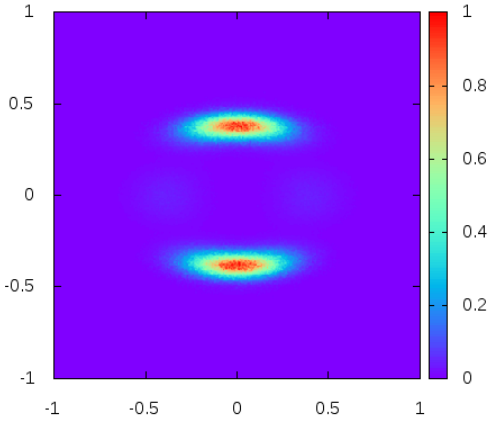


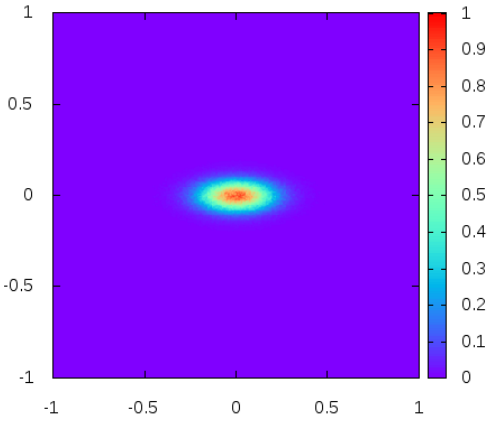
33 keV



McXtrace





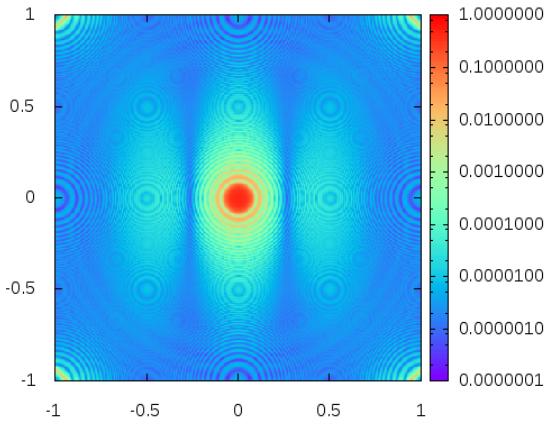


Undulator: Spatial distr.

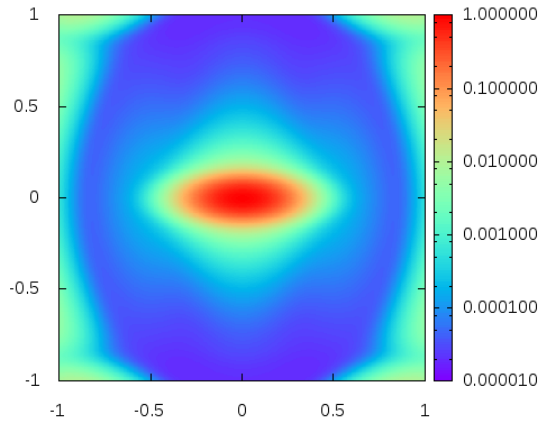
Log-plots. 33 keV

SPECTRA

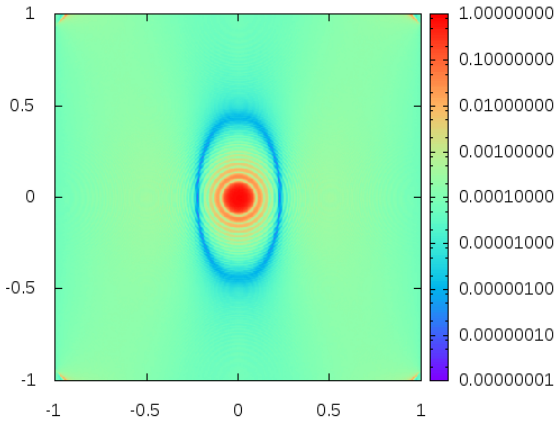
No emittance

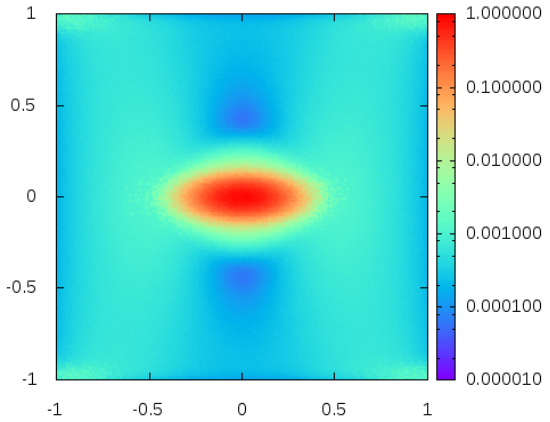


With emittance



McXtrace

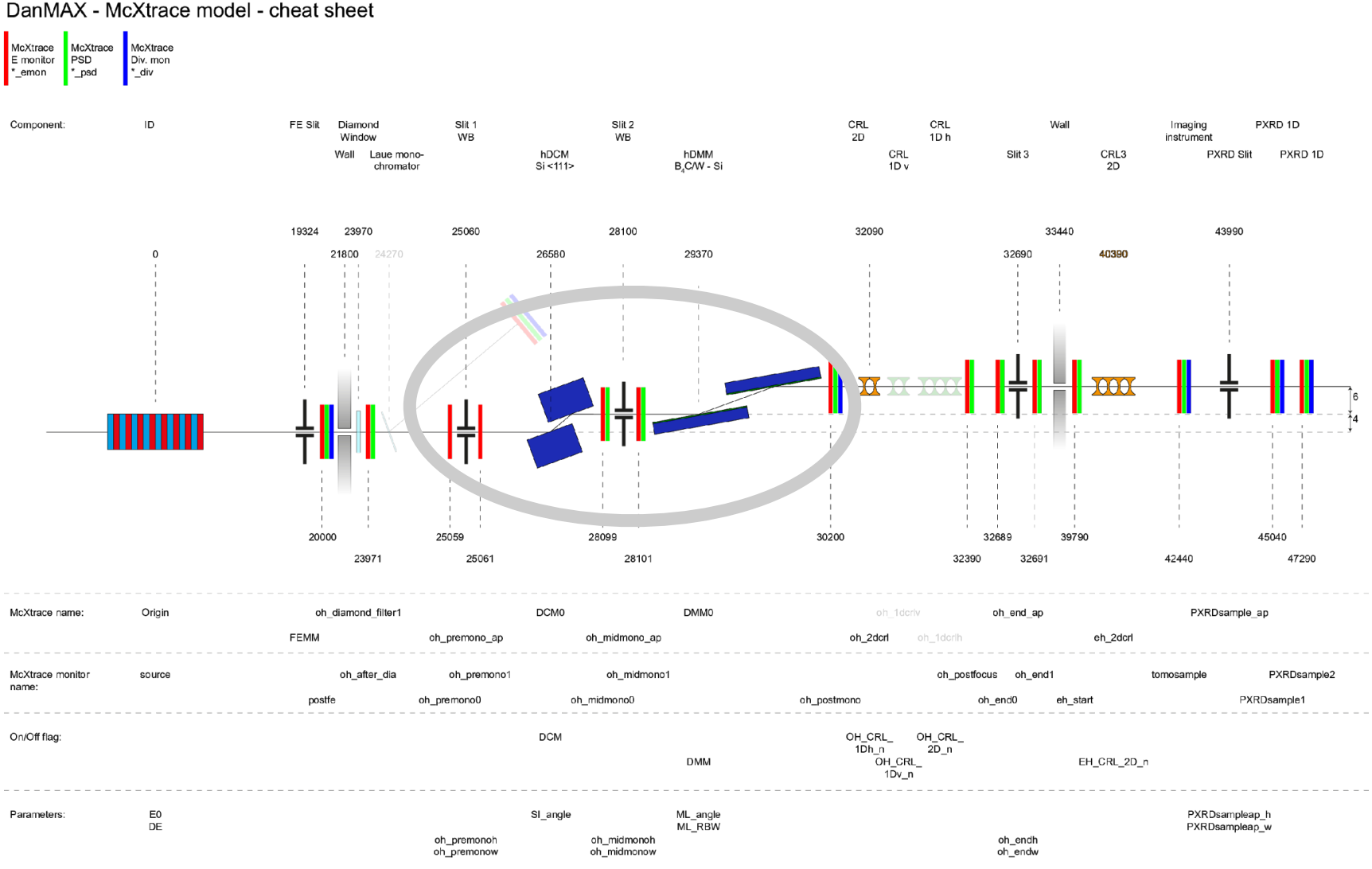




DanMAX simulation effort

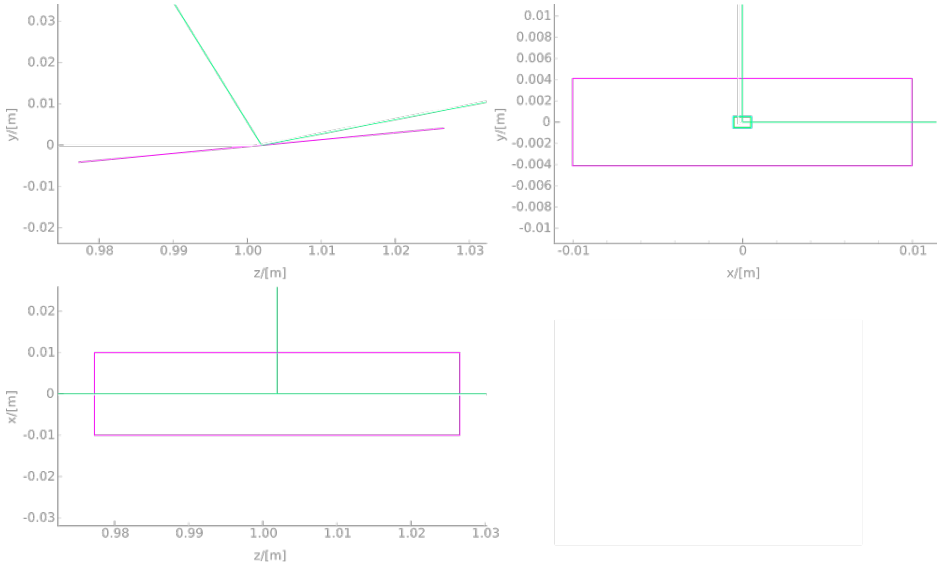
McXtrace main simulation vehicle with connections to:

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

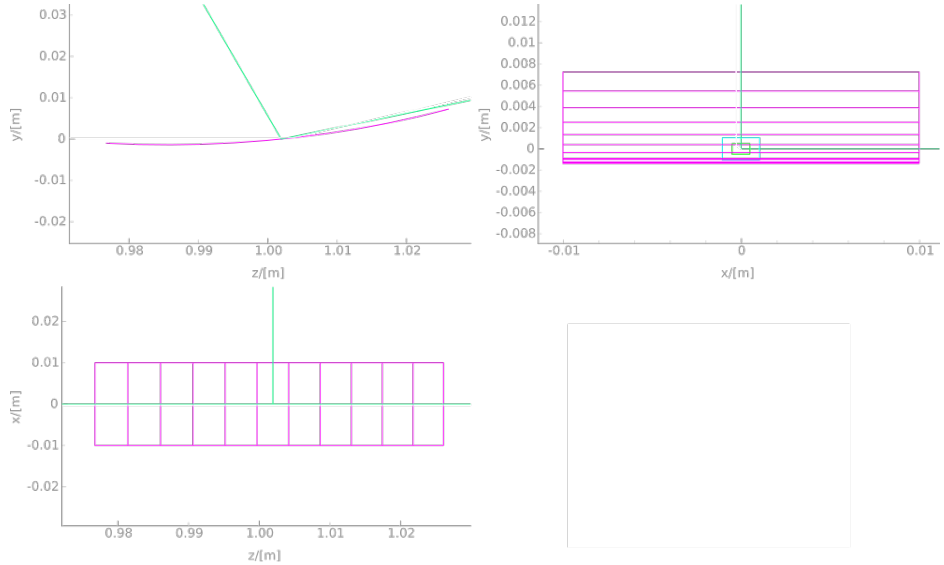


Monochromator Crystals

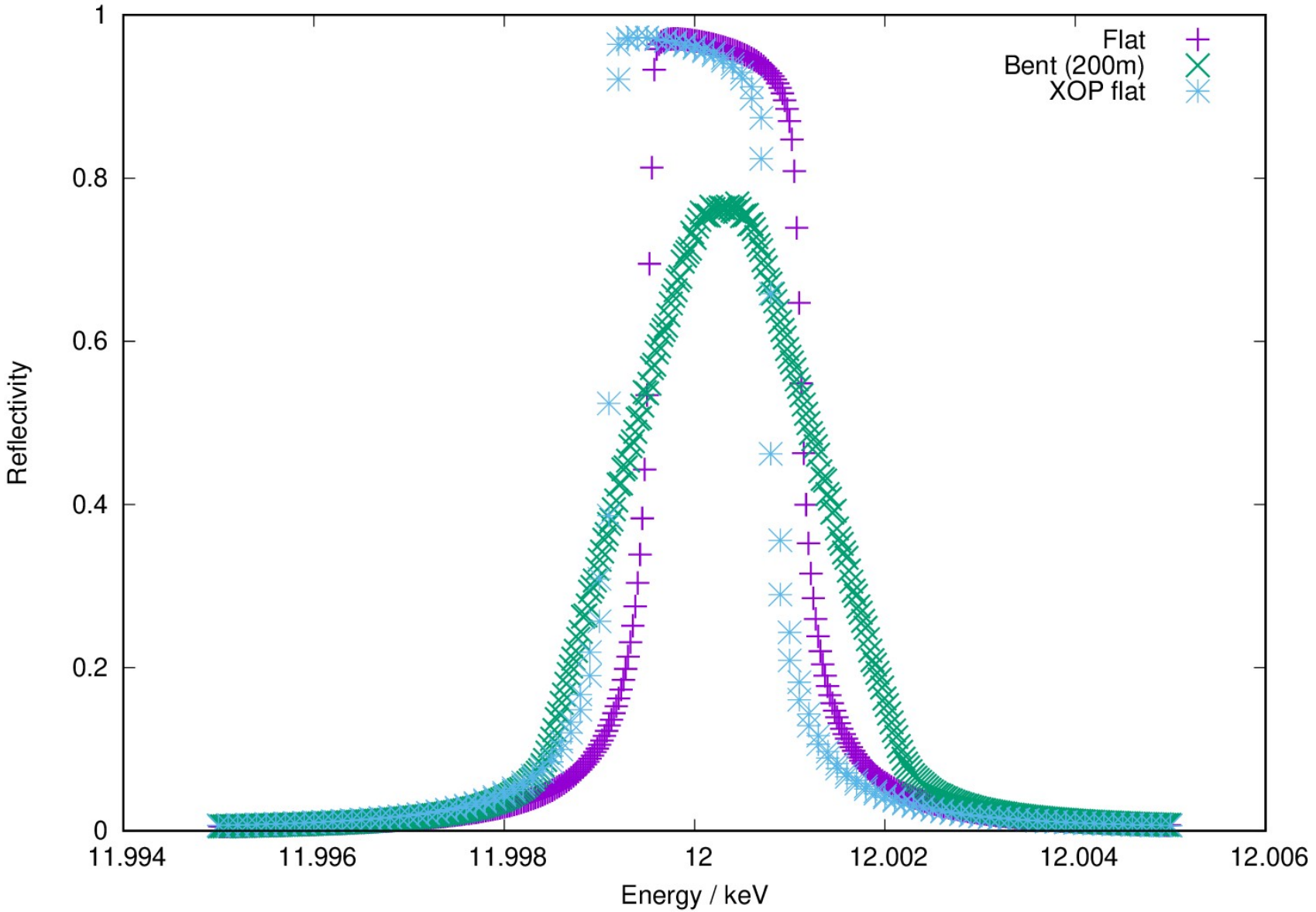
Flat



Bent (r=200m)



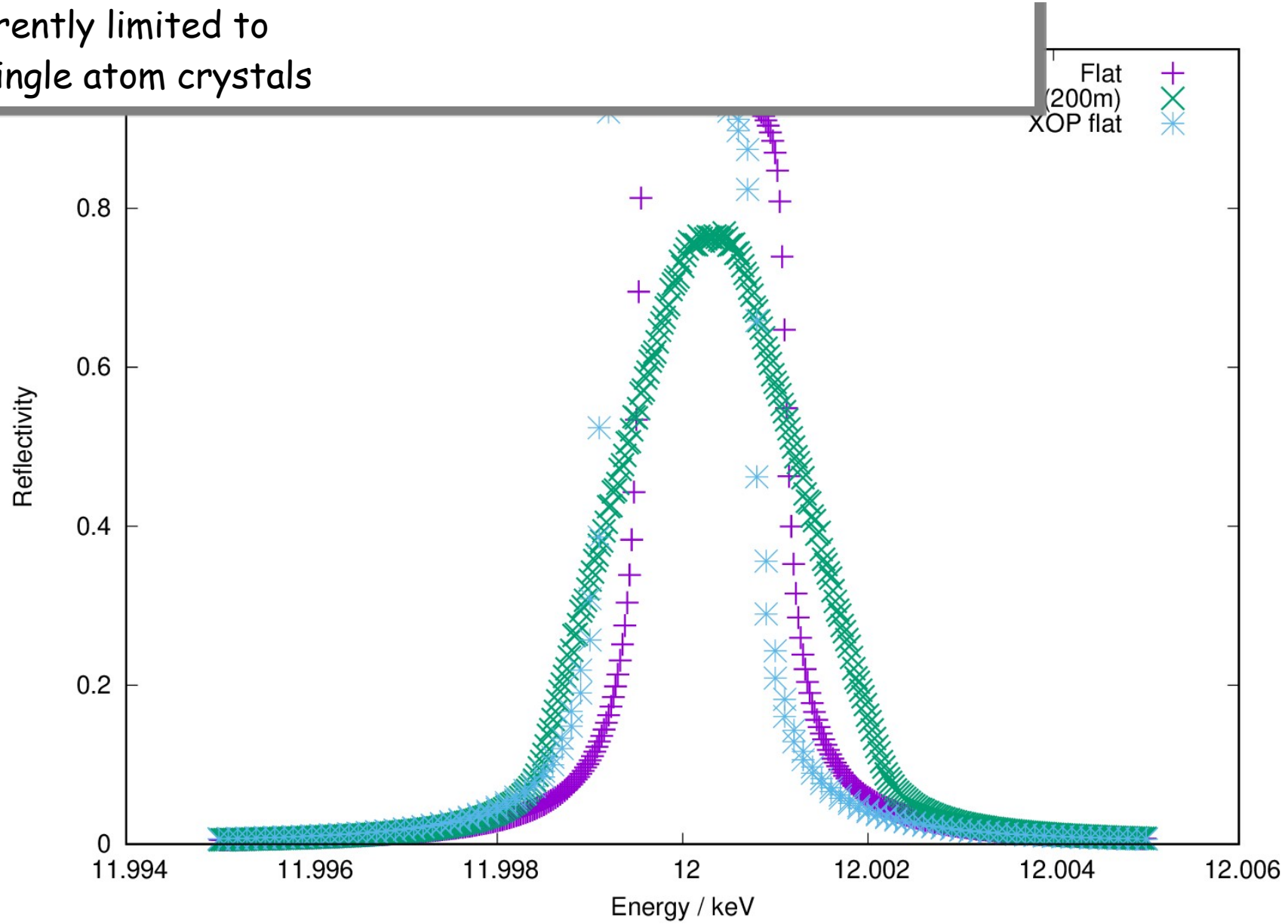
Monochromator Crystals



Monochromator Crystals

Currently limited to

- Single atom crystals



DanMAX simulation effort

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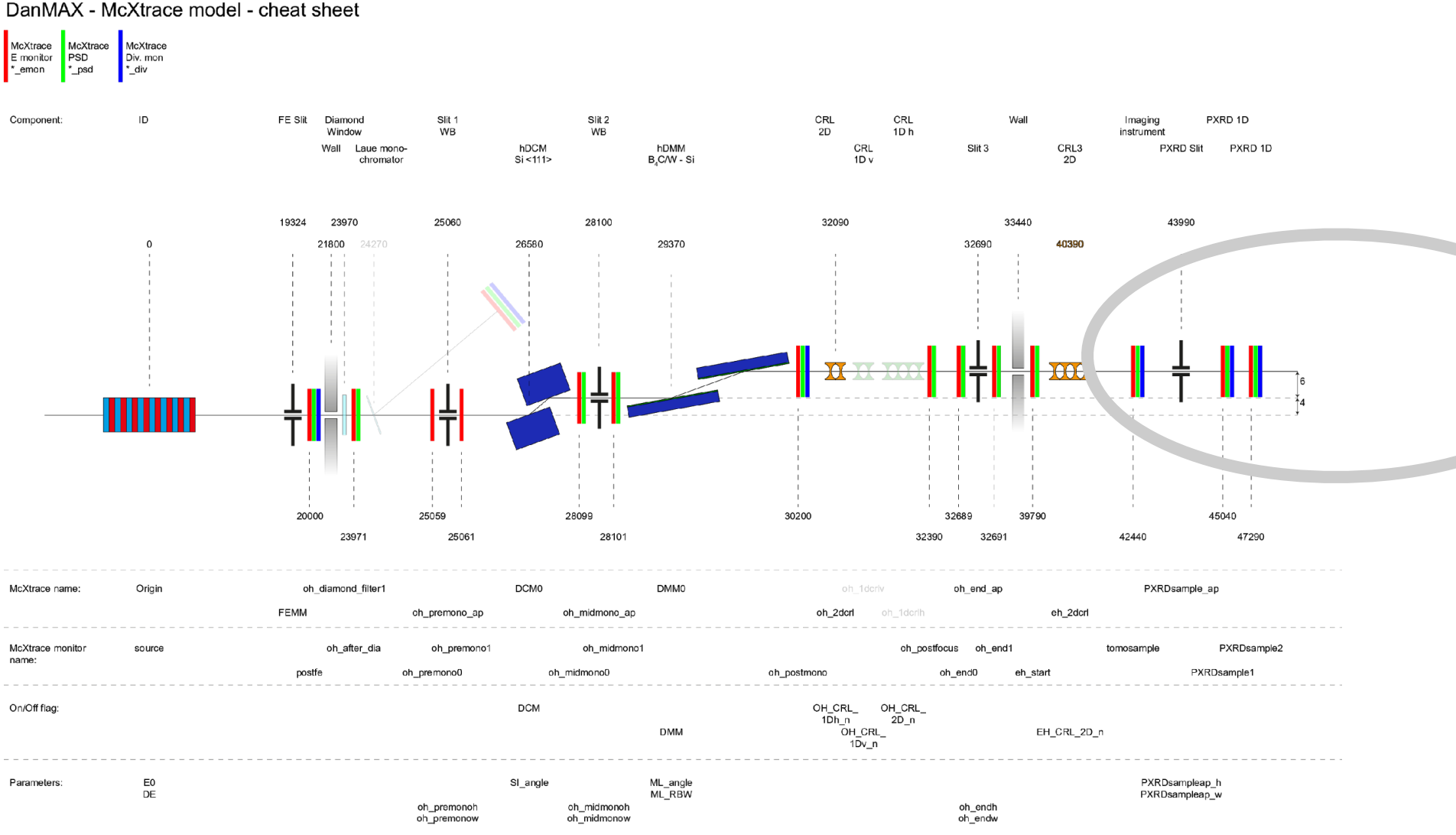
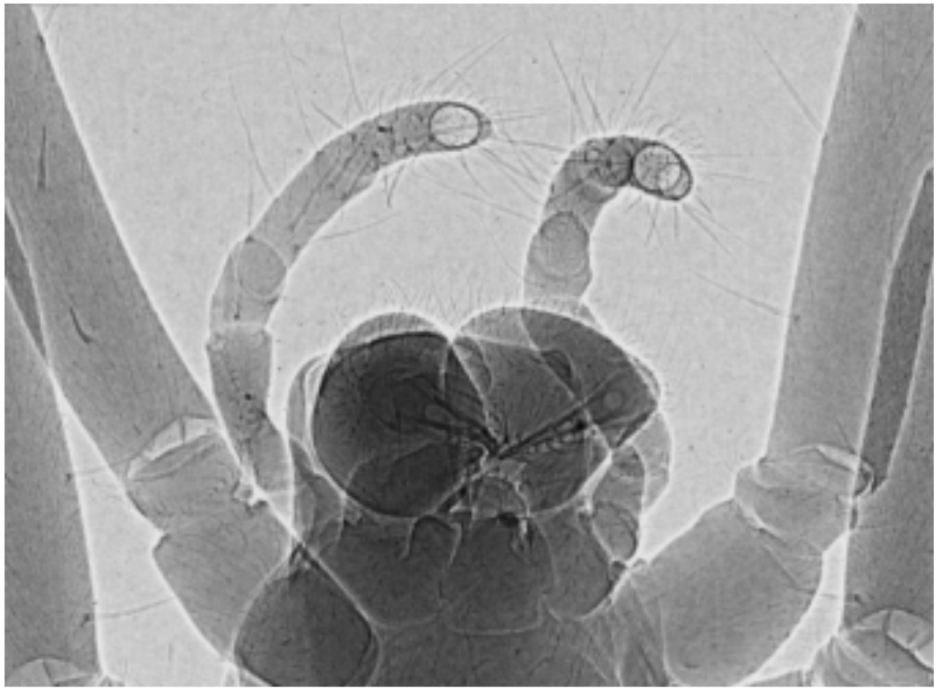
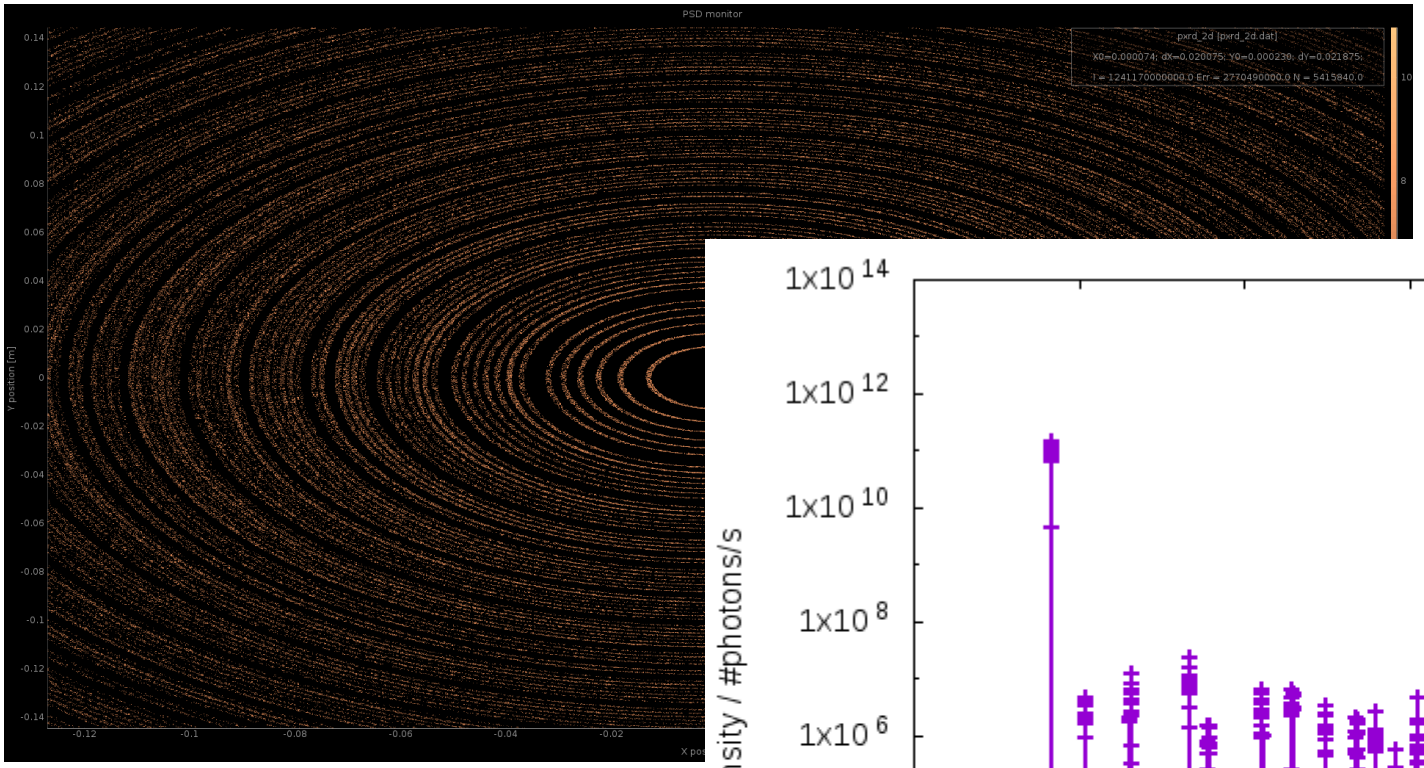


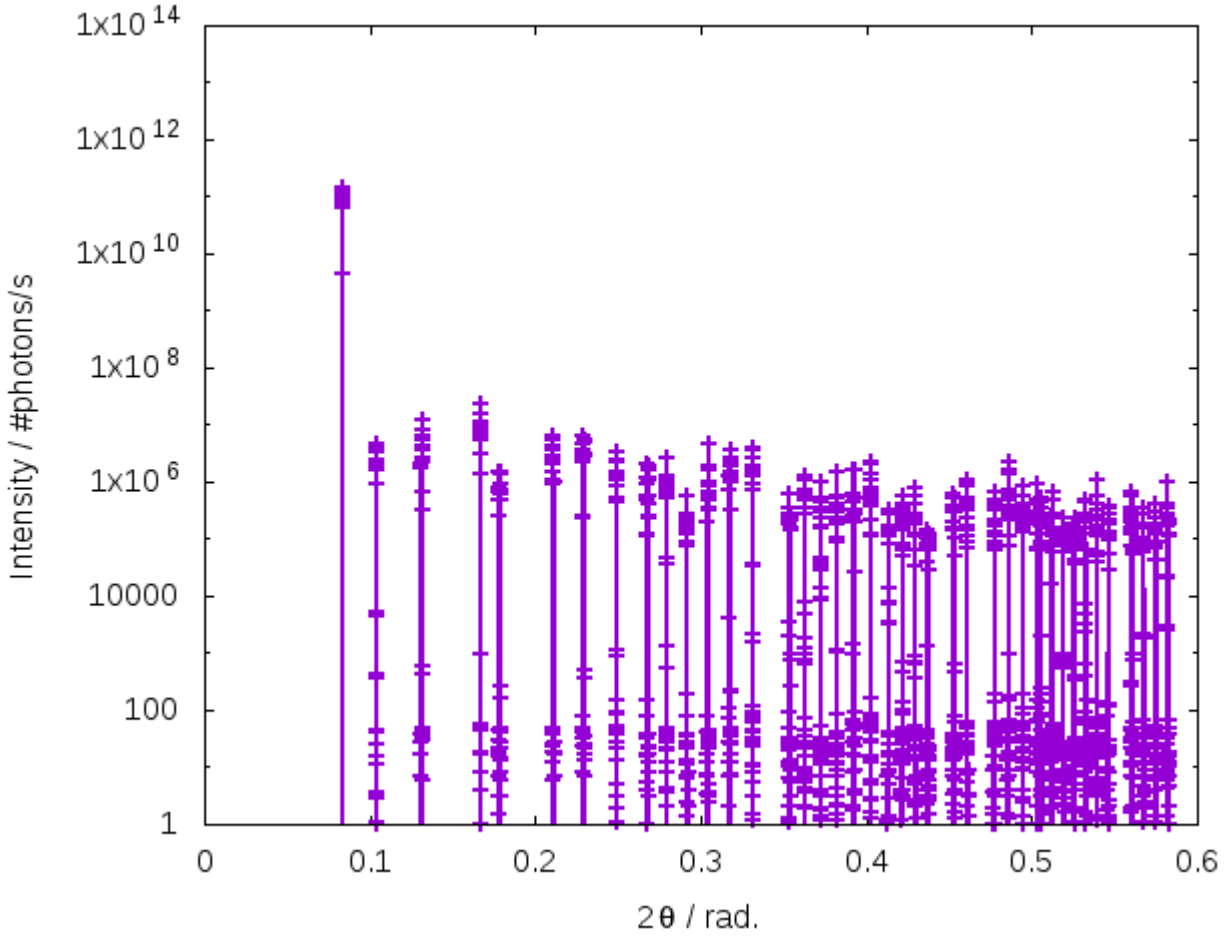
DanMAX virtual data



[I. Kantor]

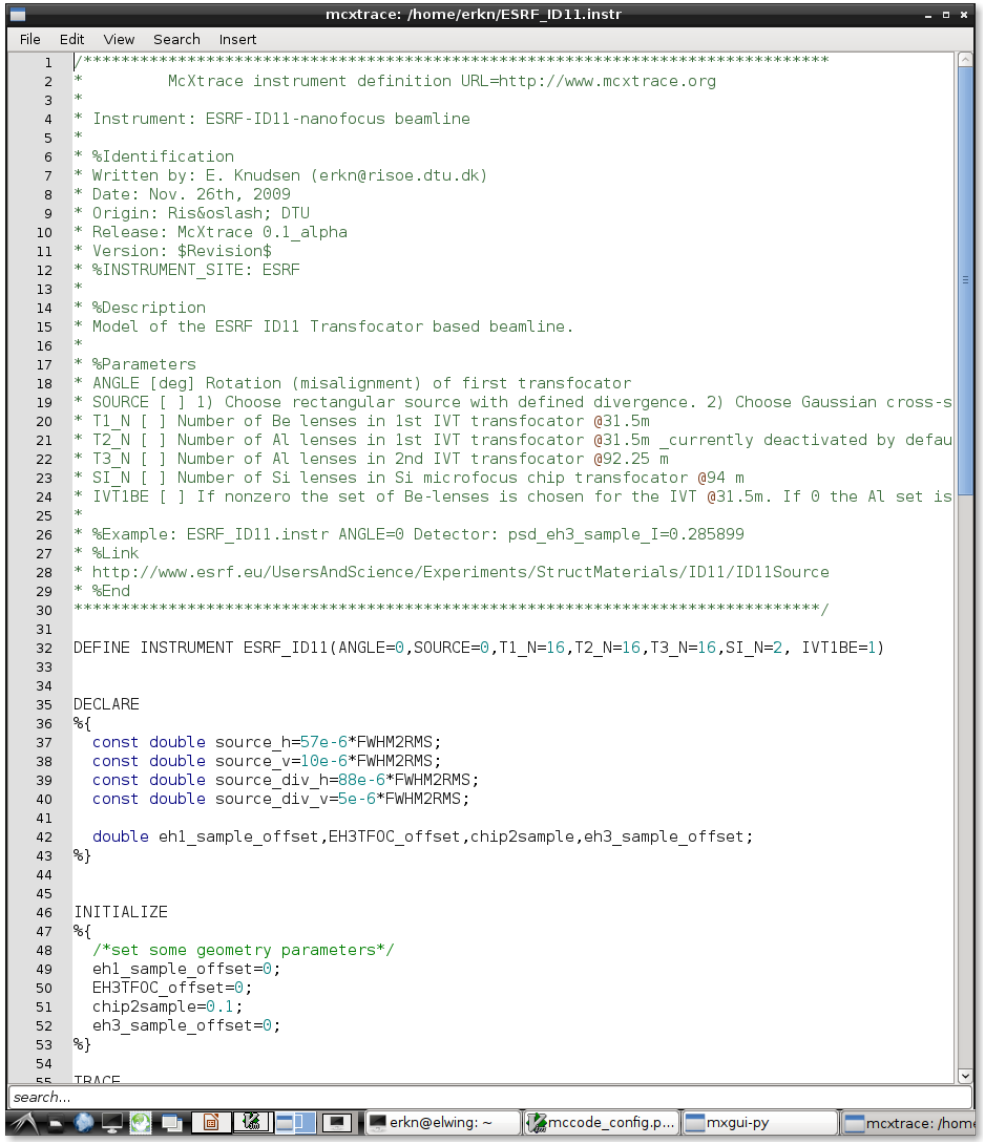
DanMAX virtual data

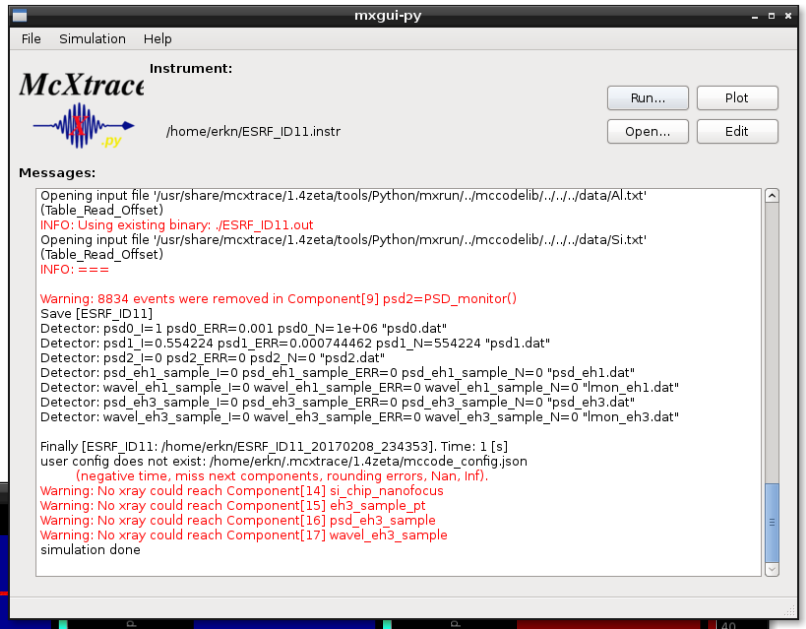




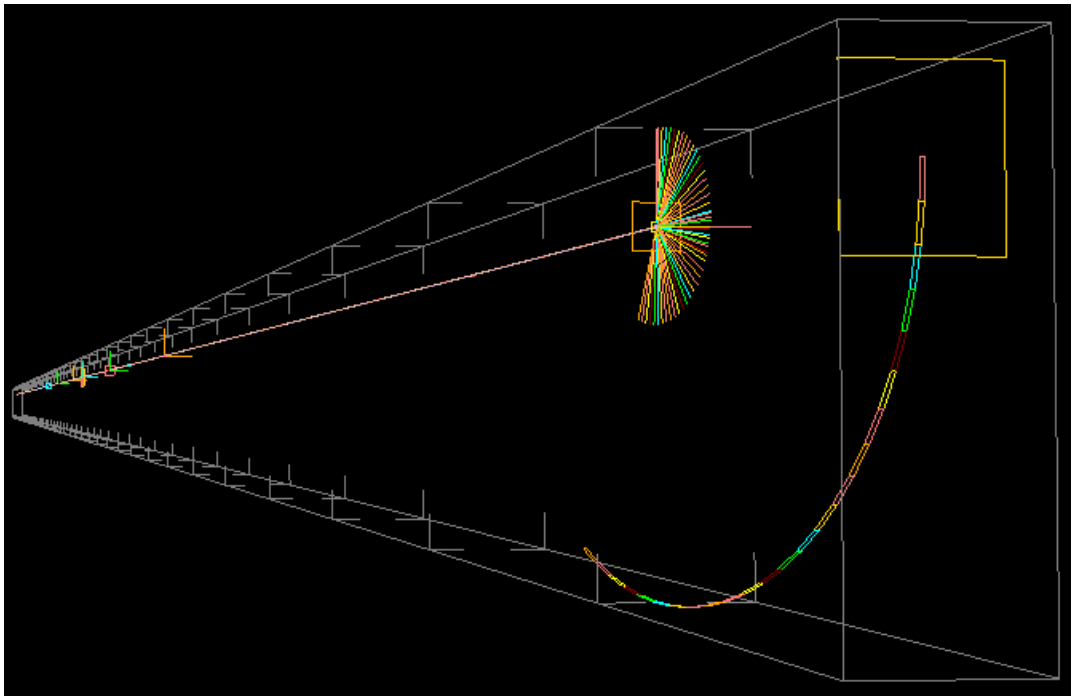
GUI

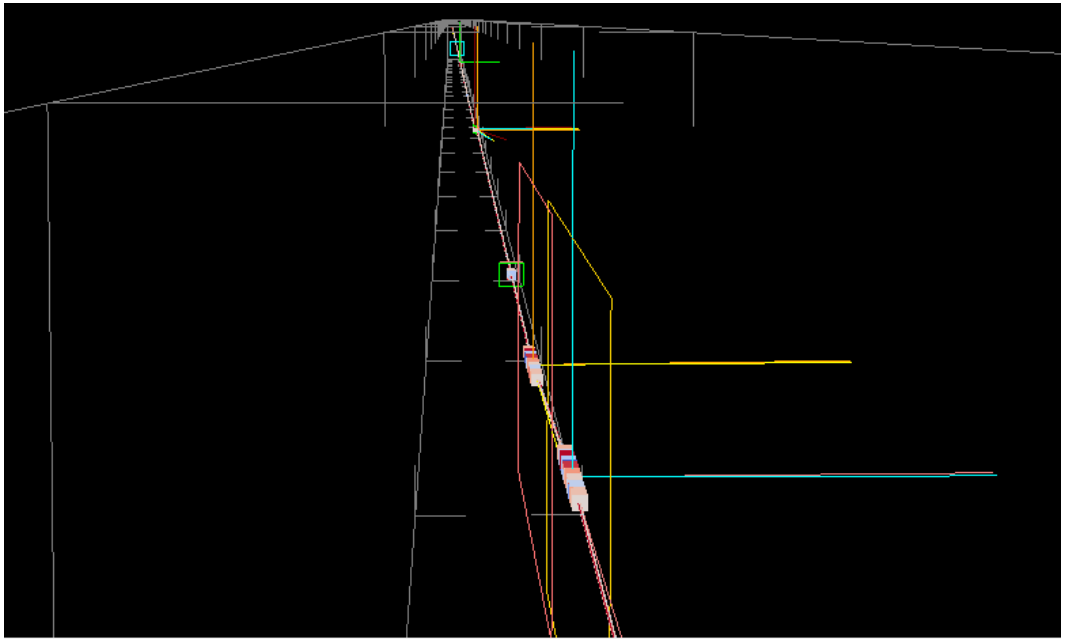
Python based



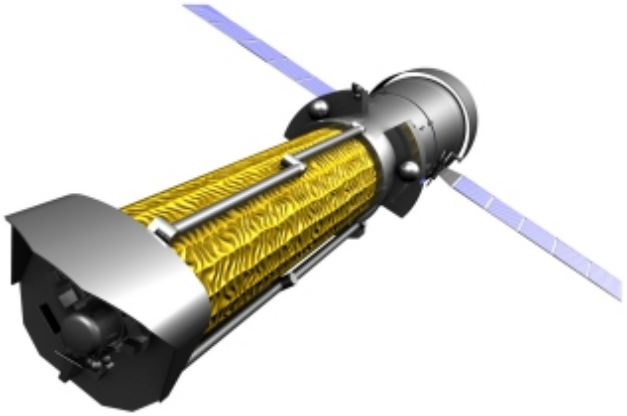


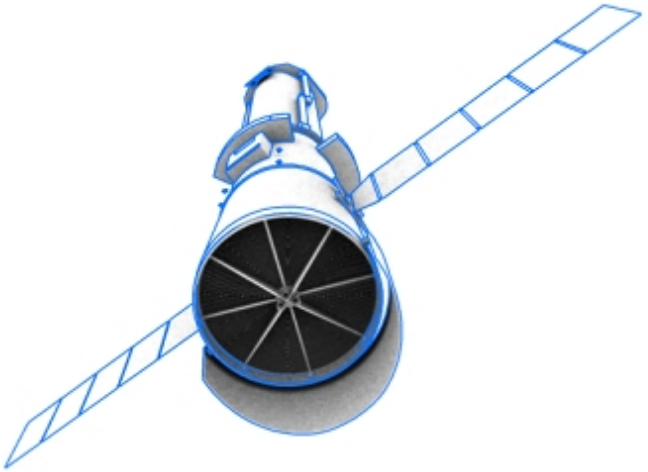
DanMAX visual ray tracing





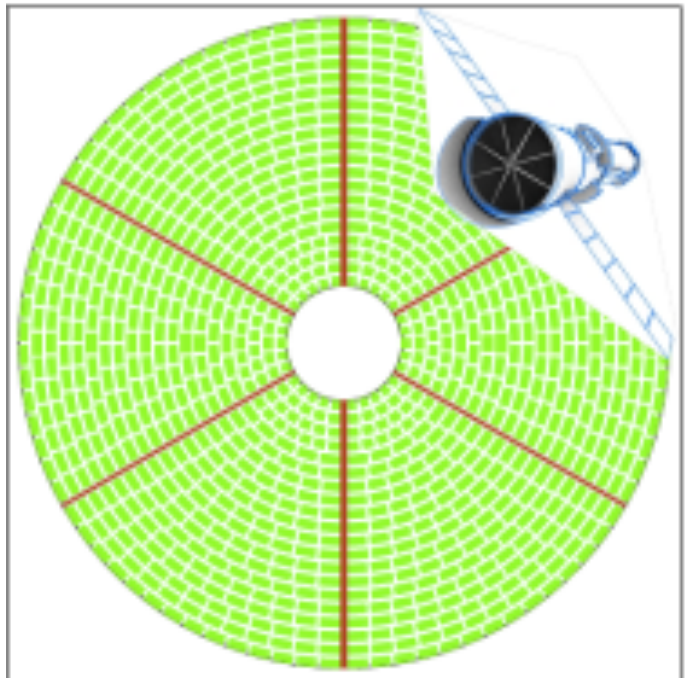
X-Ray satellite telescope

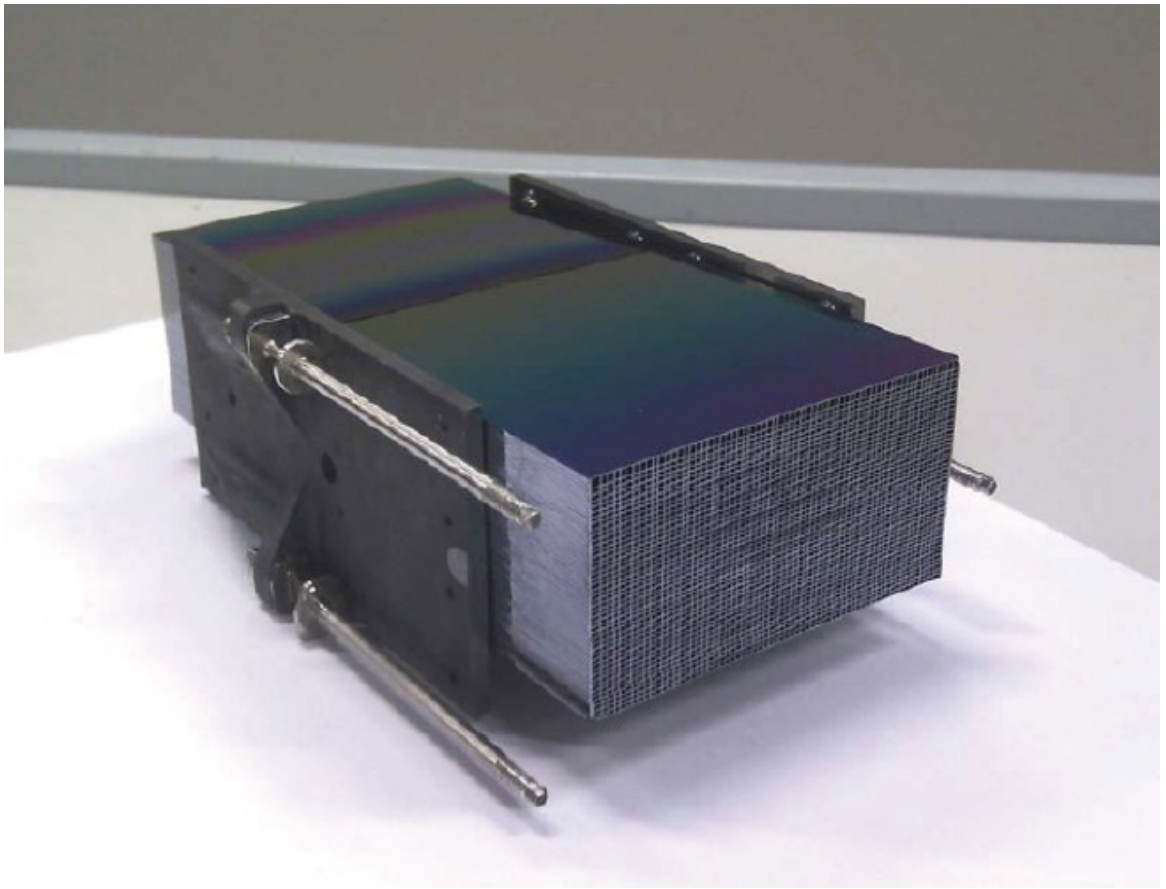




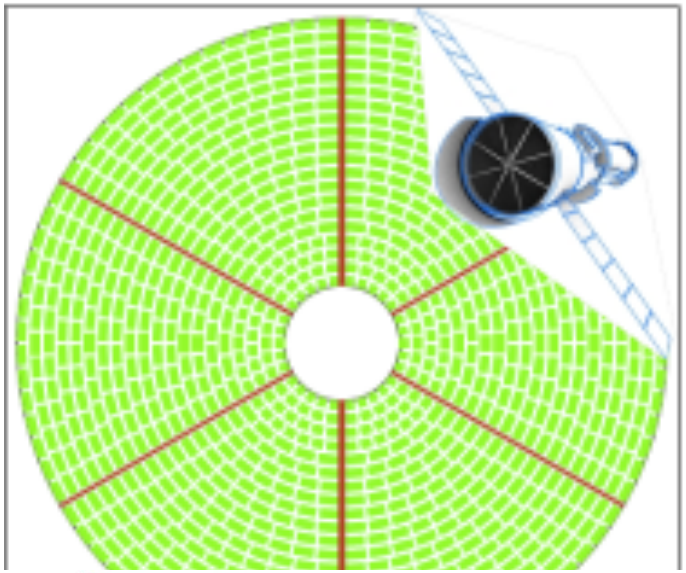
ATHENA X-ray space telescope: http://sci.esa.int/ixo/

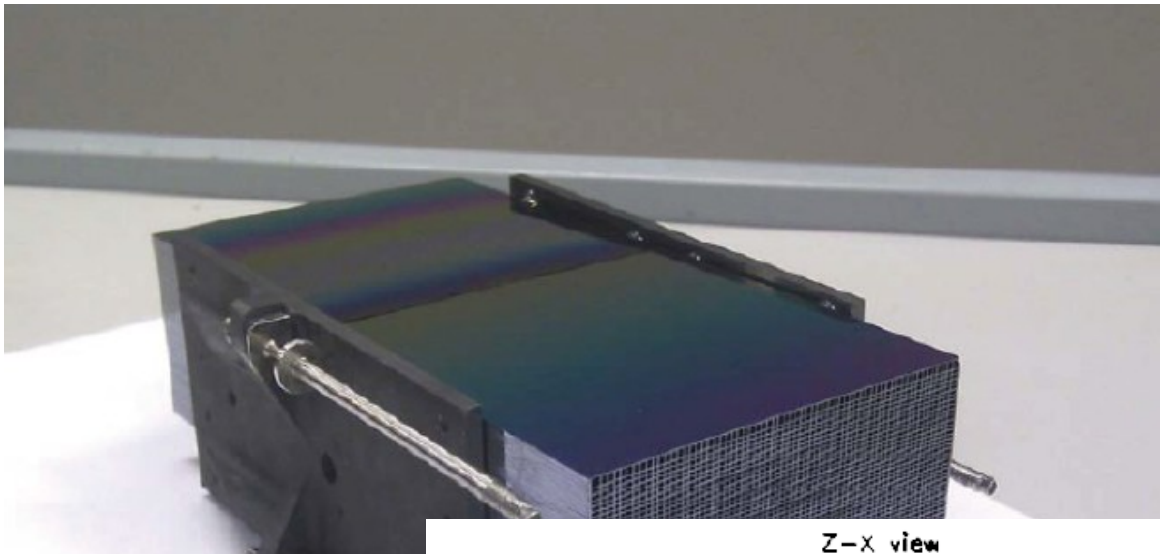
X-Ray satellite telescope



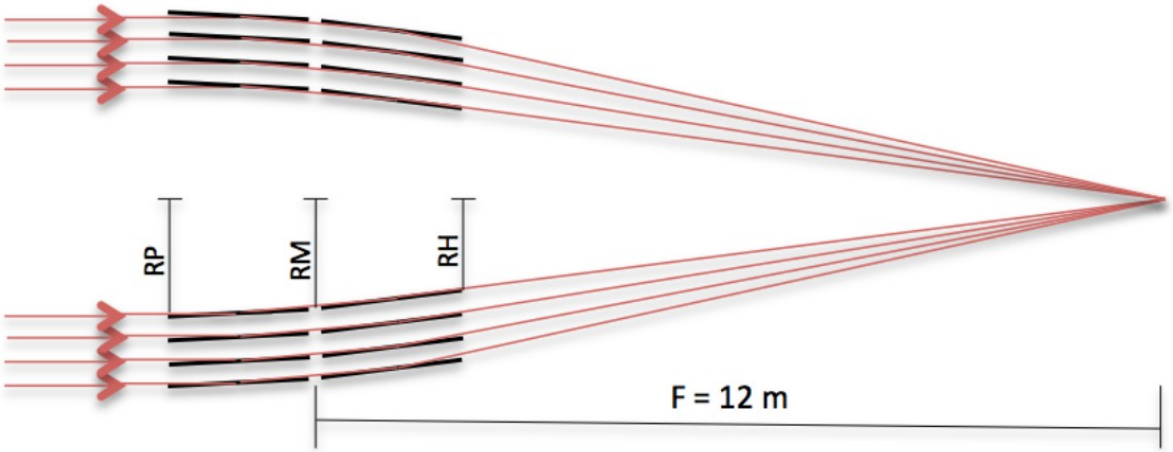


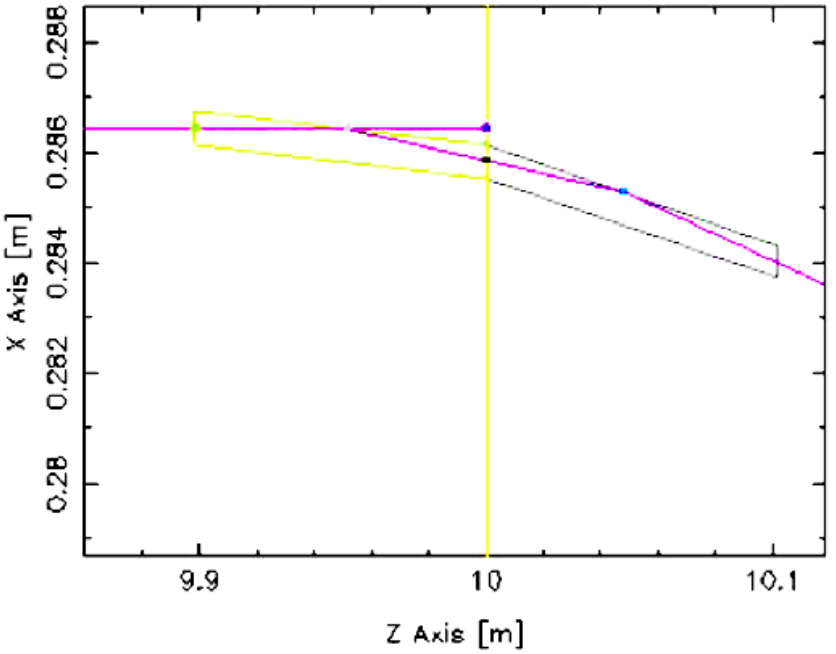
X-Ray satellite telescope





Z-X view





Thank you for your attention!

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Søren Kynde [3]
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