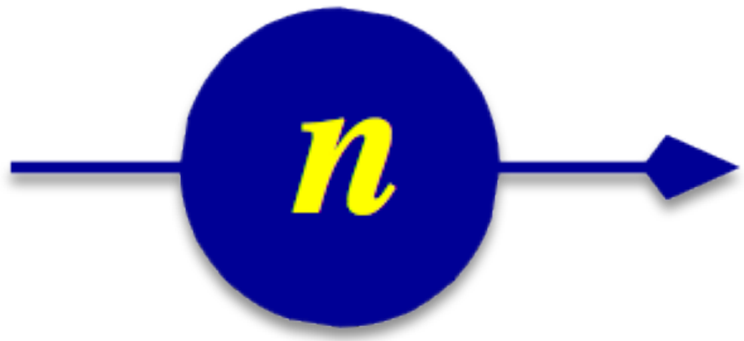
McStas and other codes for neutron delivery and full instrument simulations

Peter Willendrup[1,5], Emmanuel Farhi[2], Erik Knudsen[1,5], Uwe Filges[3,6], Linda Udby[4,5], Kim Lefmann[4,5]

[1]Physics Department, Technical University of Denmark, Denmark
[2]Calcul Scientifique, Institut Laue-Langevin, France
[3]Laboratory for Developments and Methods, Paul Scherrer Institute, Switzerland
[4]Niels Bohr Institute, University of Copenhagen, Denmark
[5]ESS design update programme, Denmark
[6]ESS design update programme, Switzerland

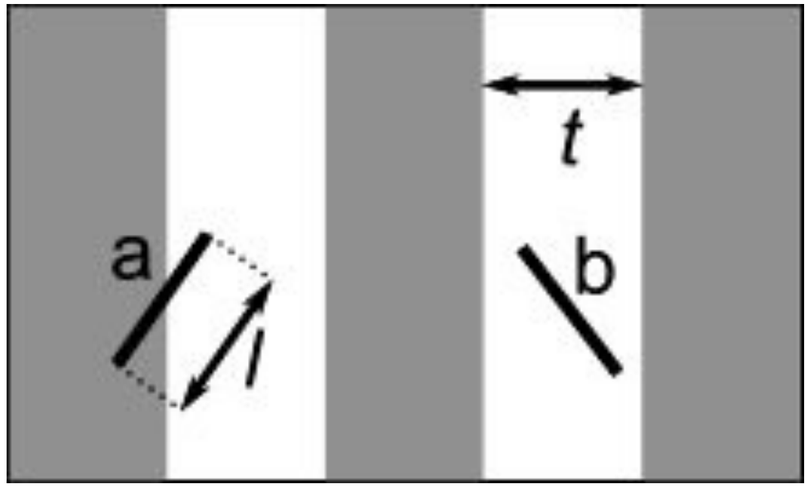


INSIS School, Frascati 2012

Agenda

- An introduction Monte Carlo & raytracing techniques
- An overview of the available packages
- An introduction to McStas
- A tour of the example suite
- Build-along exercises

Numerical experiments before Los Alamos



- In 1777 Georges-Louis Leclerc, comte de Buffon was the first to “numerical experiments” for solving a problem of geometrical probability.
- The experiment involves dropping a needle on a lined surface and can be used to estimate π

- In the 1930’s, Fermi used sampling methods to estimate quantities involved in controlled fission

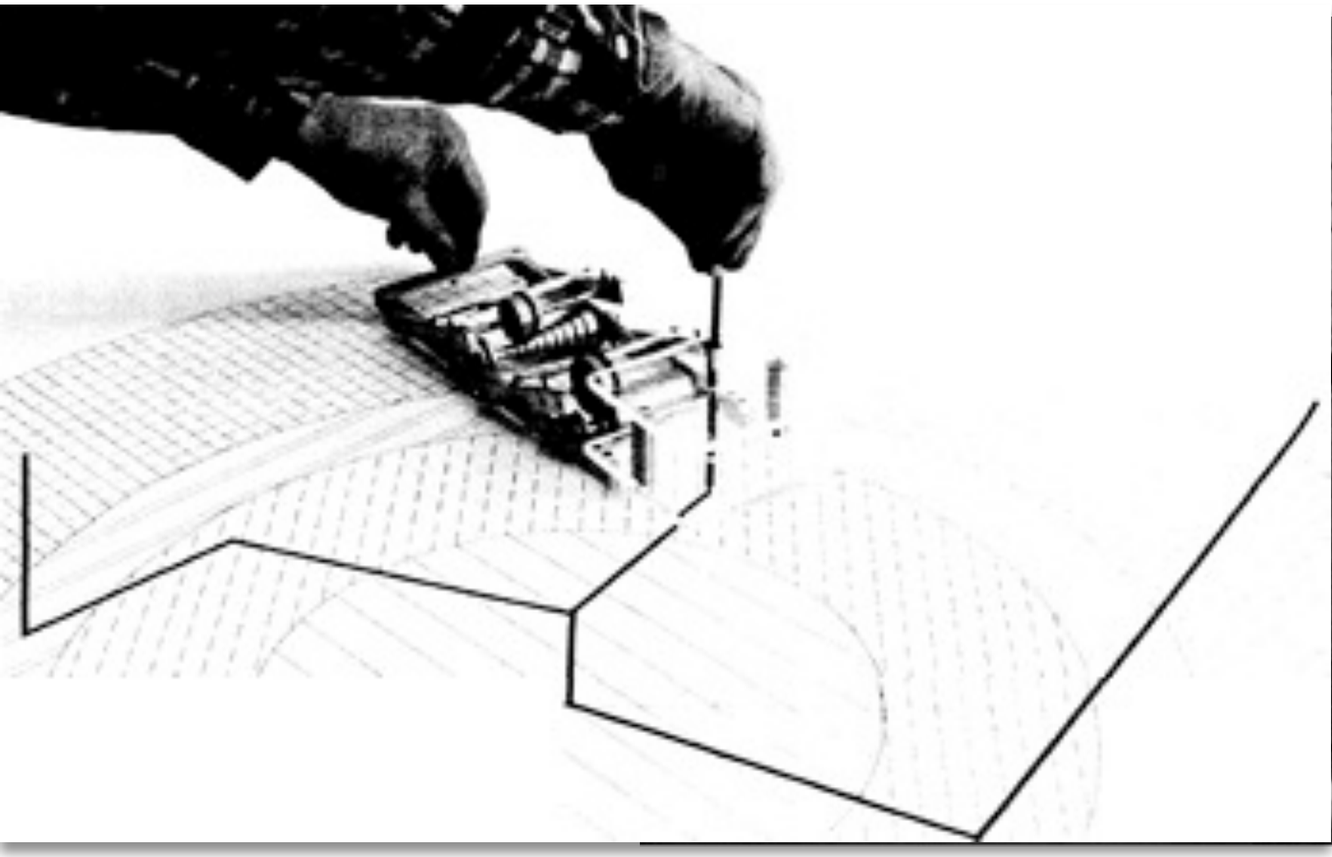
Monte Carlo techniques

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

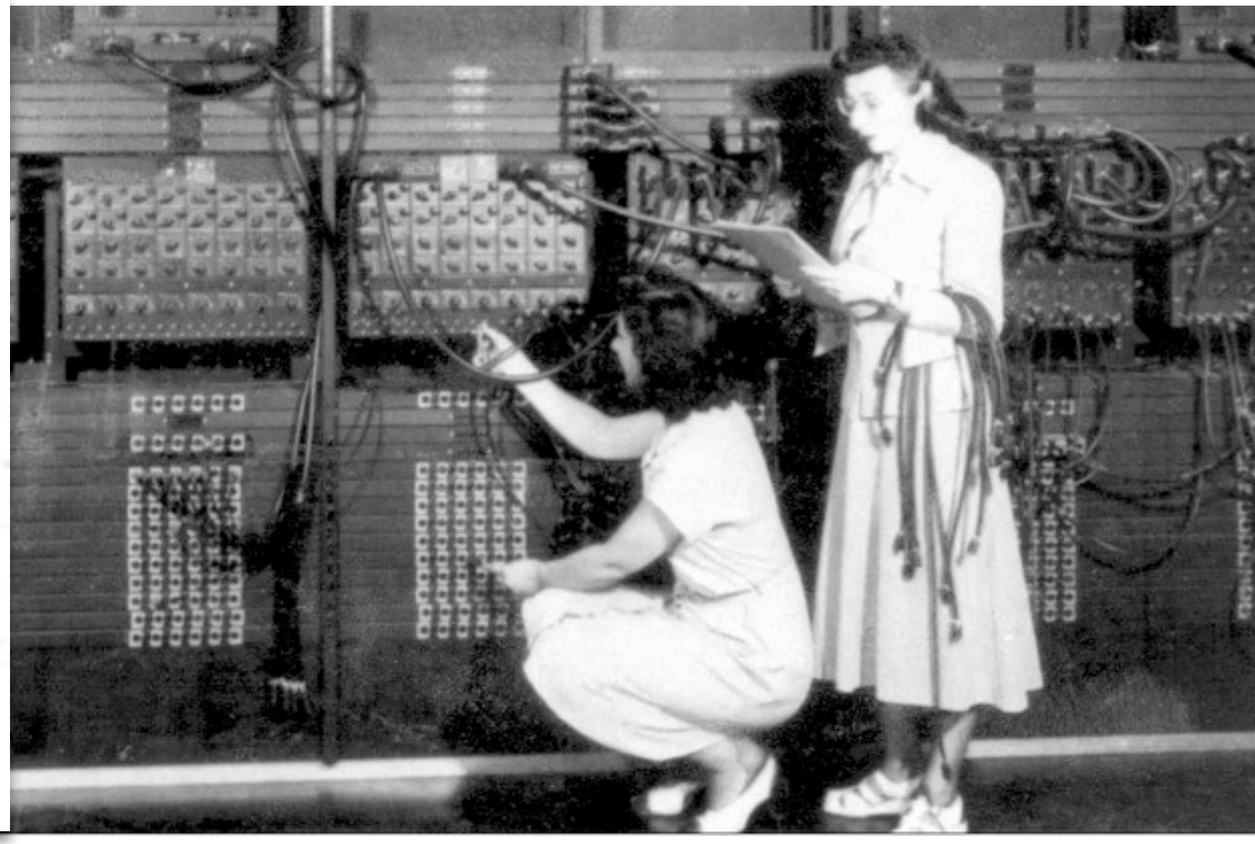


- Notable fathers: John v. Neumann Stanislav Ulam Nicholas Metropolis
- Named “Monte Carlo” after Ulam’s fathers frequent visits to the Monte Carlo casino in Las Vegas
- Initially “implemented” by letting large numbers of women use tabularized random numbers and hand calculators for individual particle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

Monte Carlo techniques



- FERMIAC



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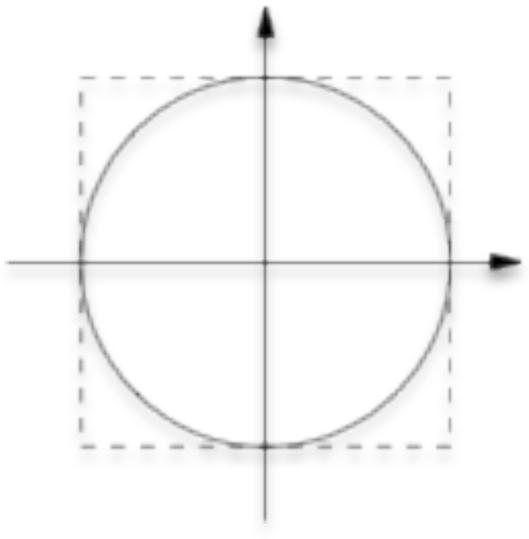
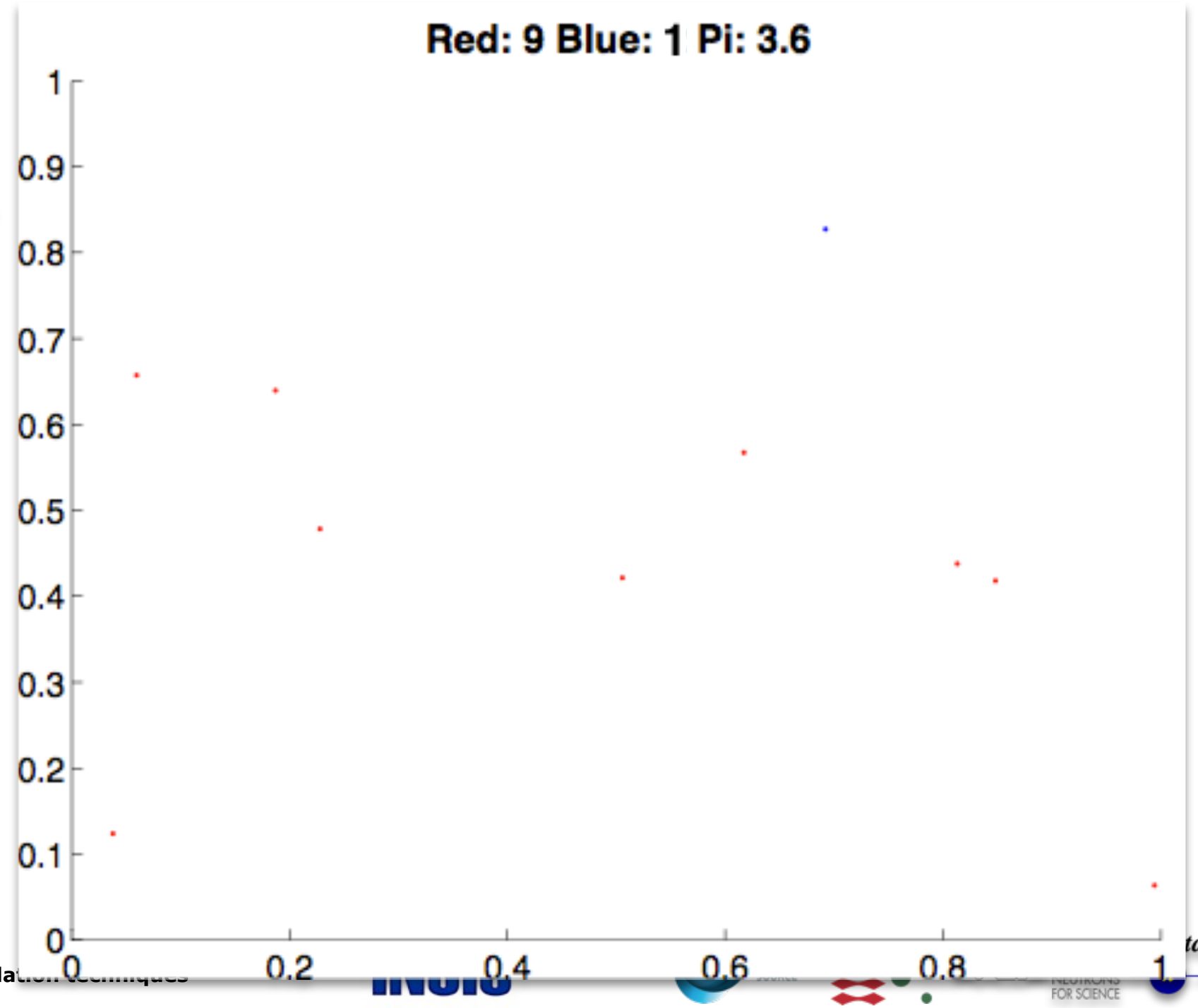
Monte Carlo techniques

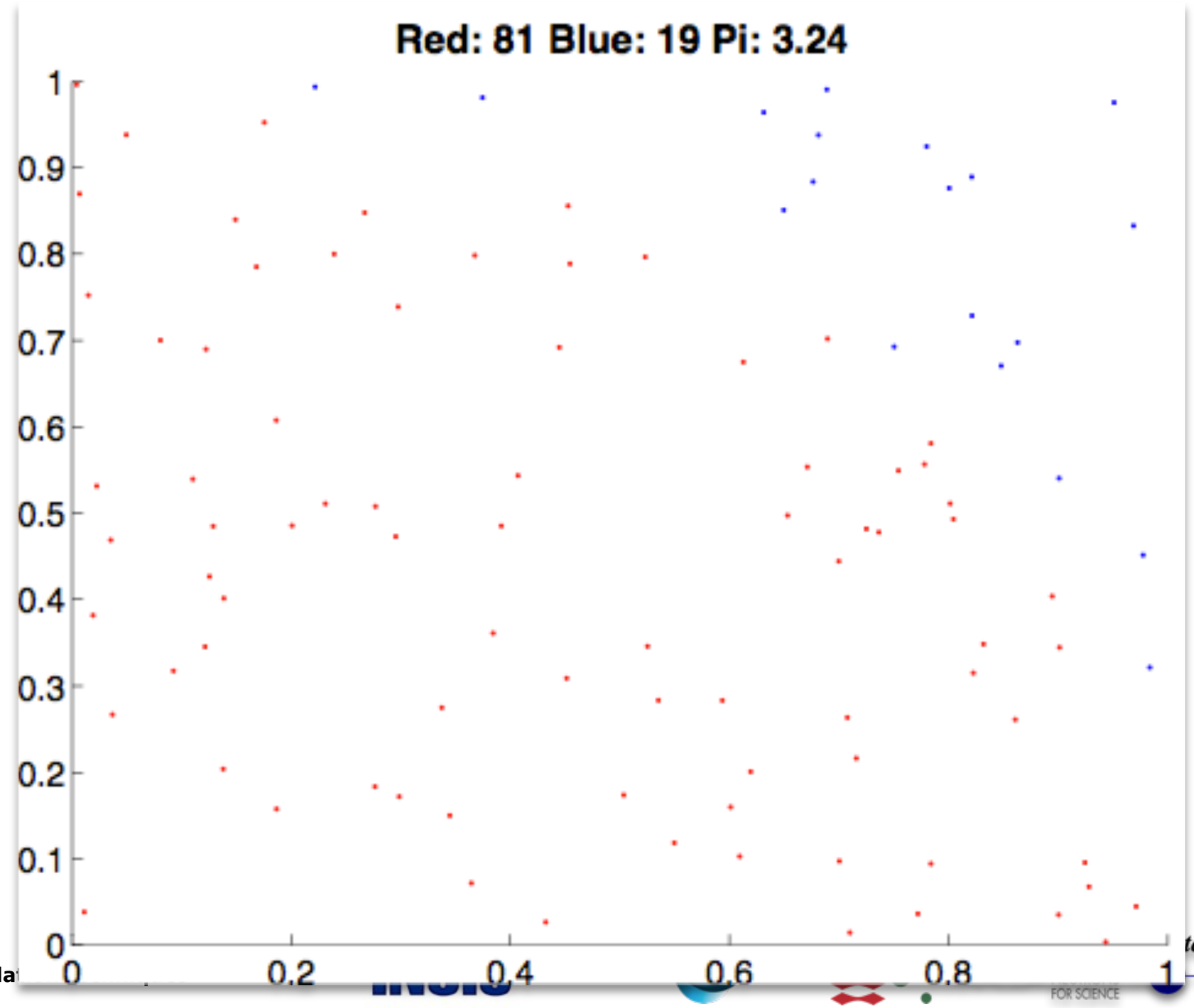
$$\pi = \frac{A_{circ}}{A_{sqr}} = \frac{\pi r^2}{(2r)^2}$$

$$\pi \approx 4\frac{9}{9+1} = 3.6$$



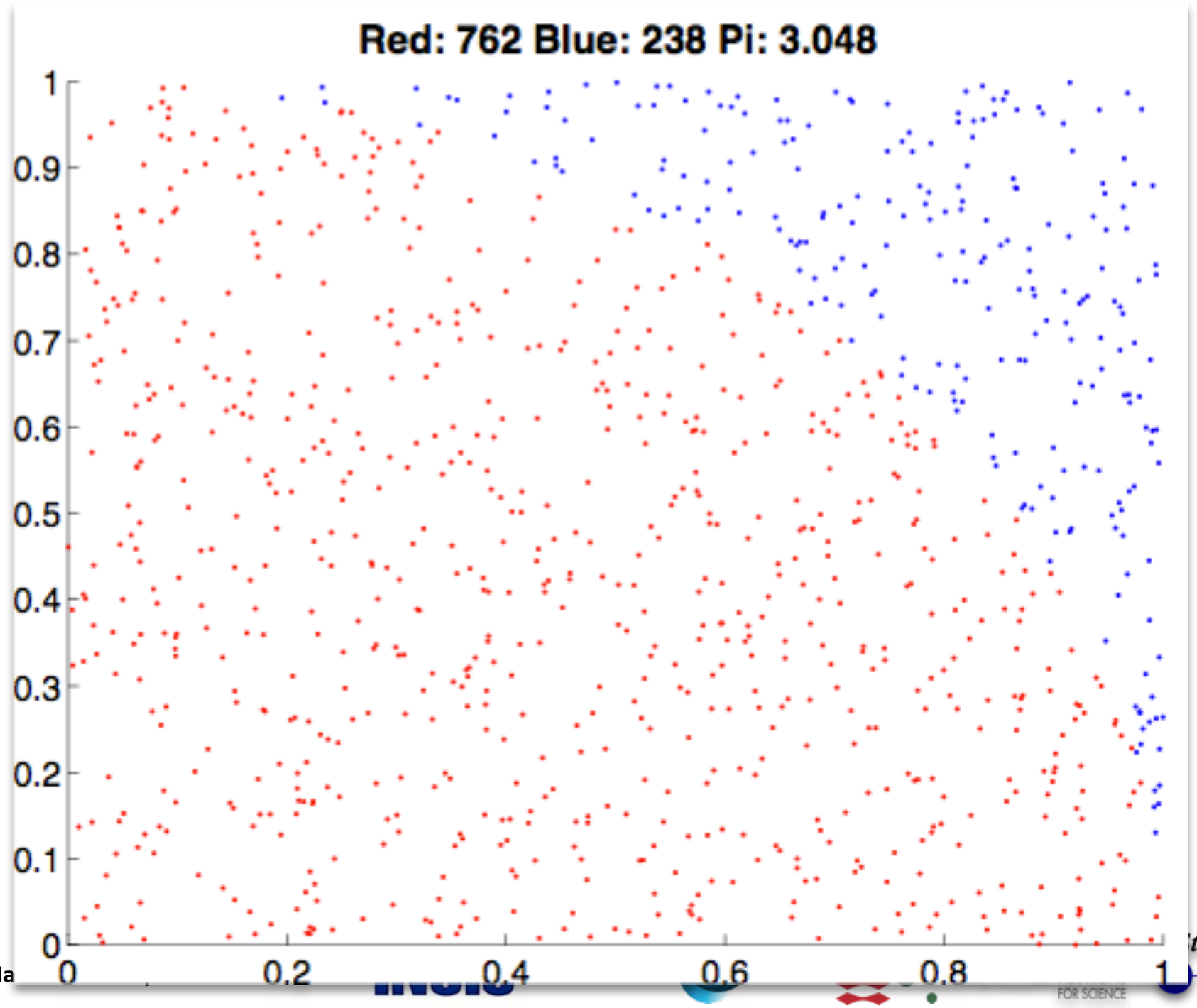


Monte Carlo techniques



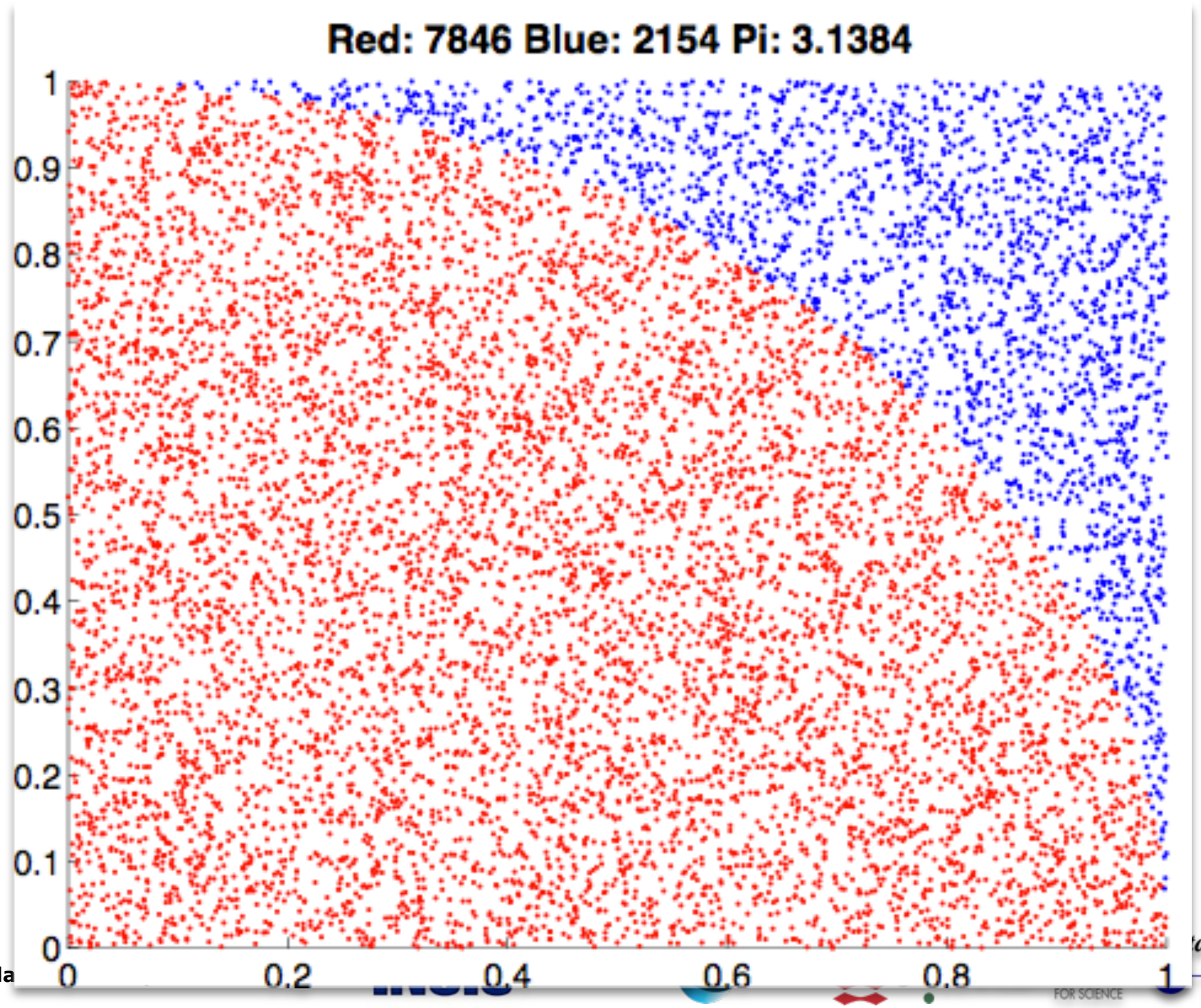
Monte Carlo techniques

- Estimating Pi:



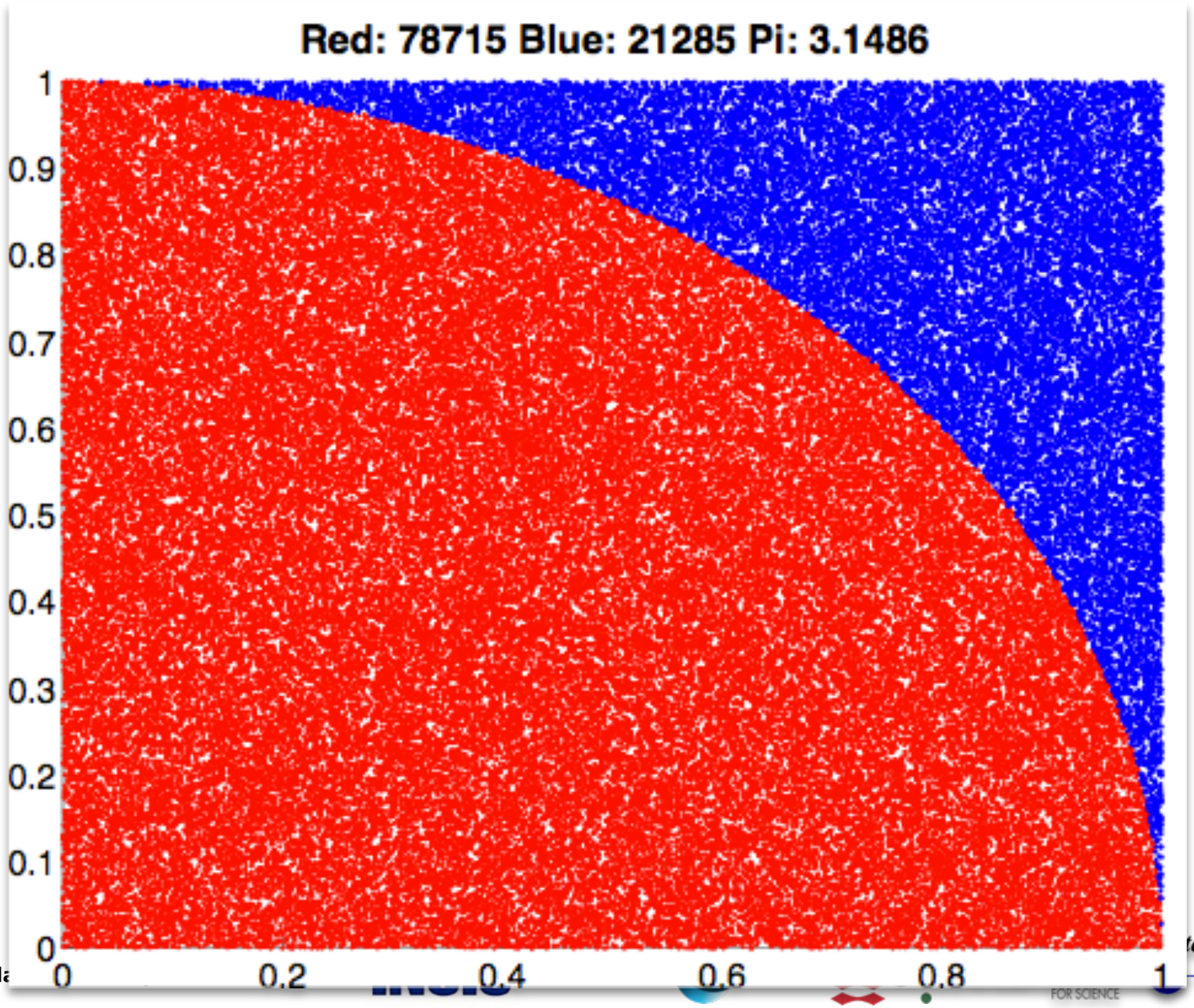
Monte Carlo techniques

- Estimating Pi:



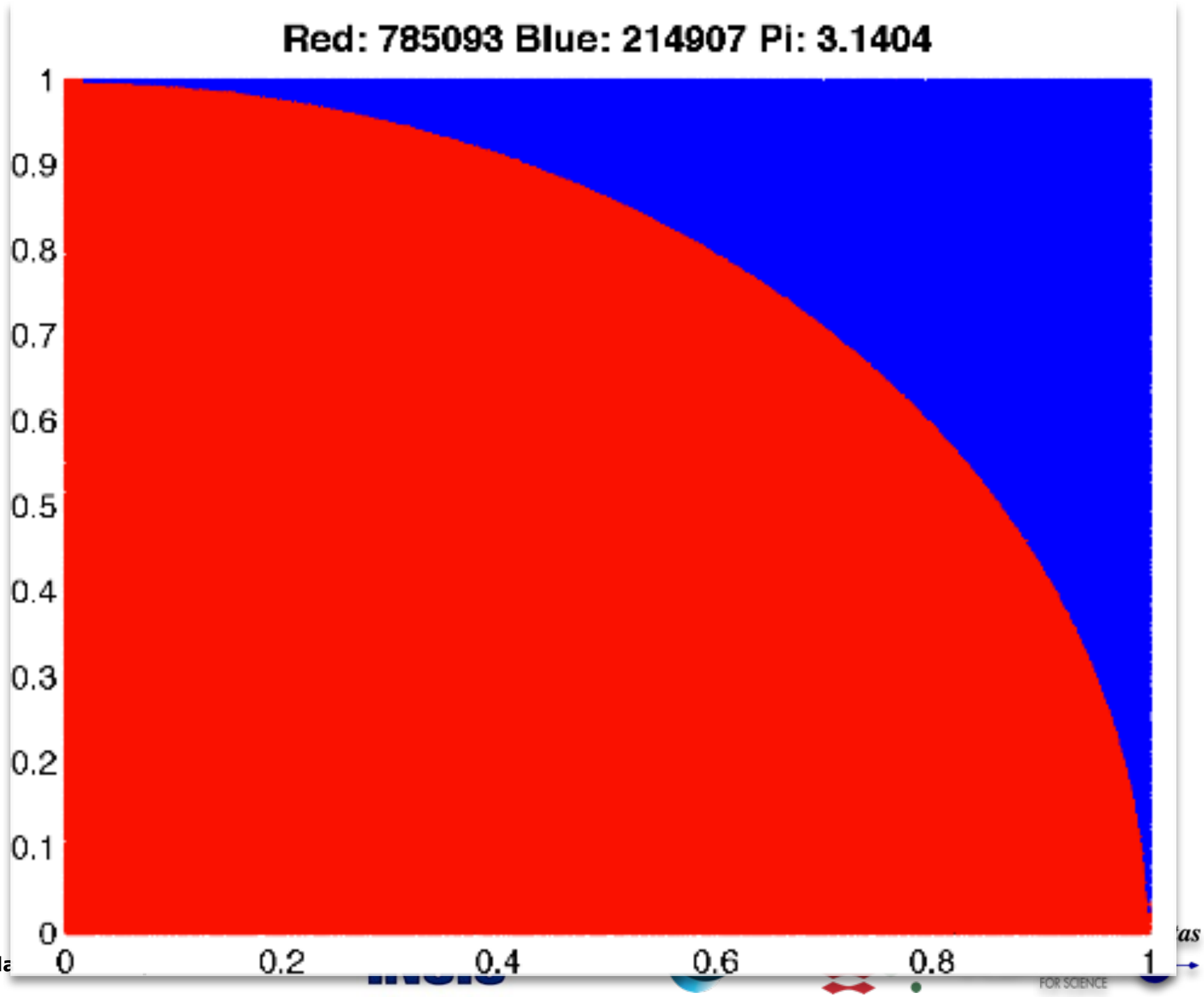
Monte Carlo techniques

- Estimating Pi:



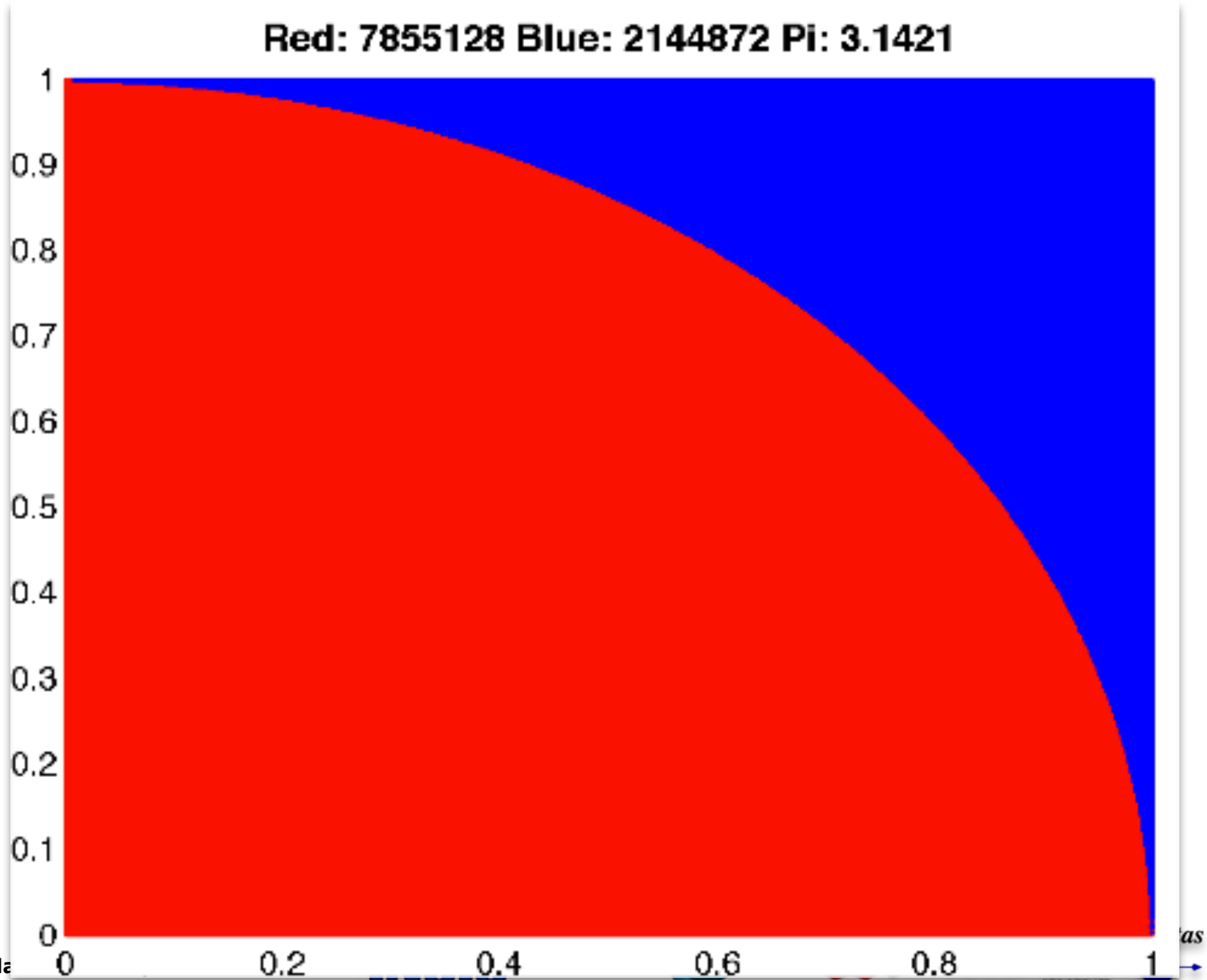
Monte Carlo techniques

- Estimating Pi:



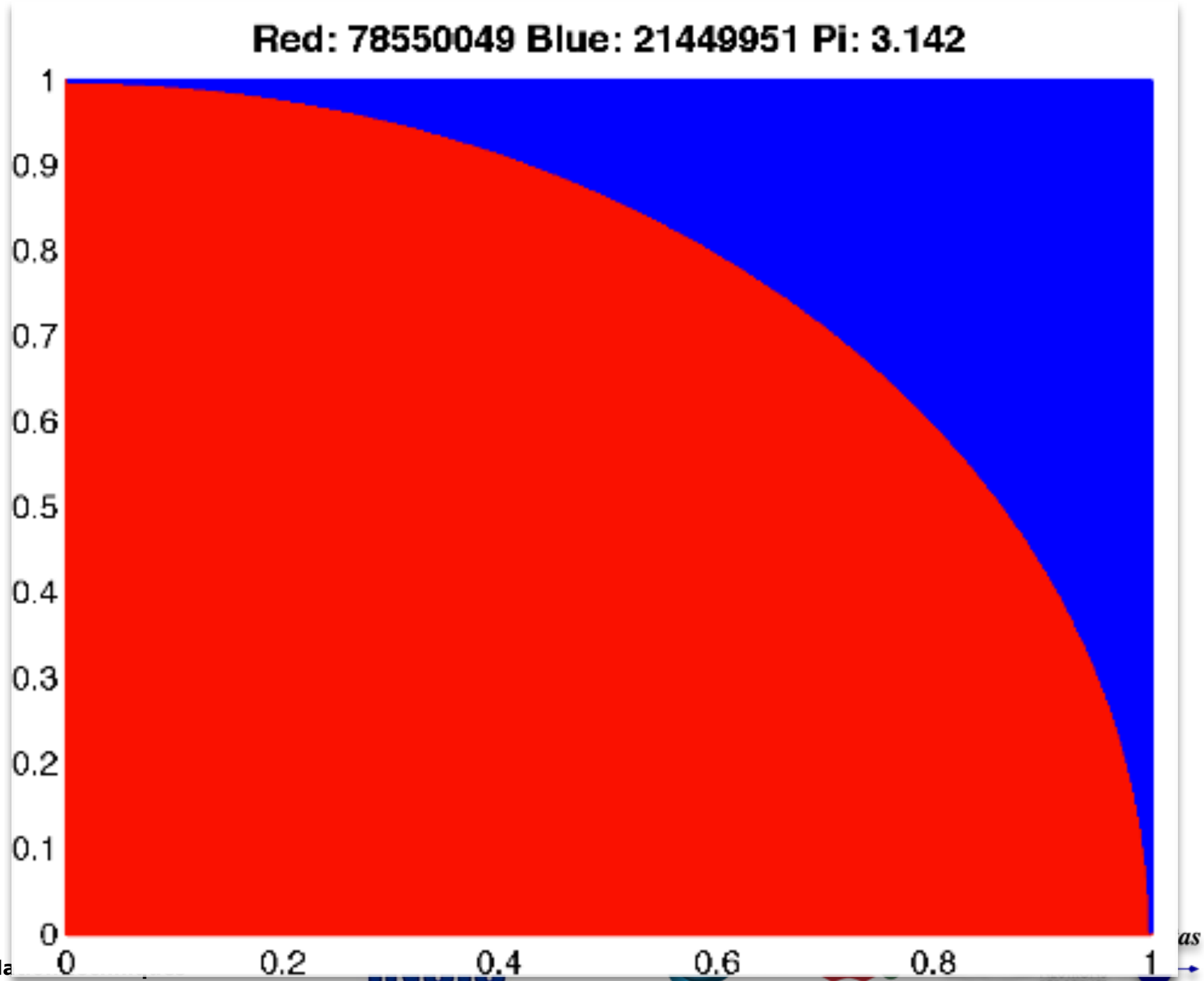
Monte Carlo techniques

- Estimating Pi:



Monte Carlo techniques

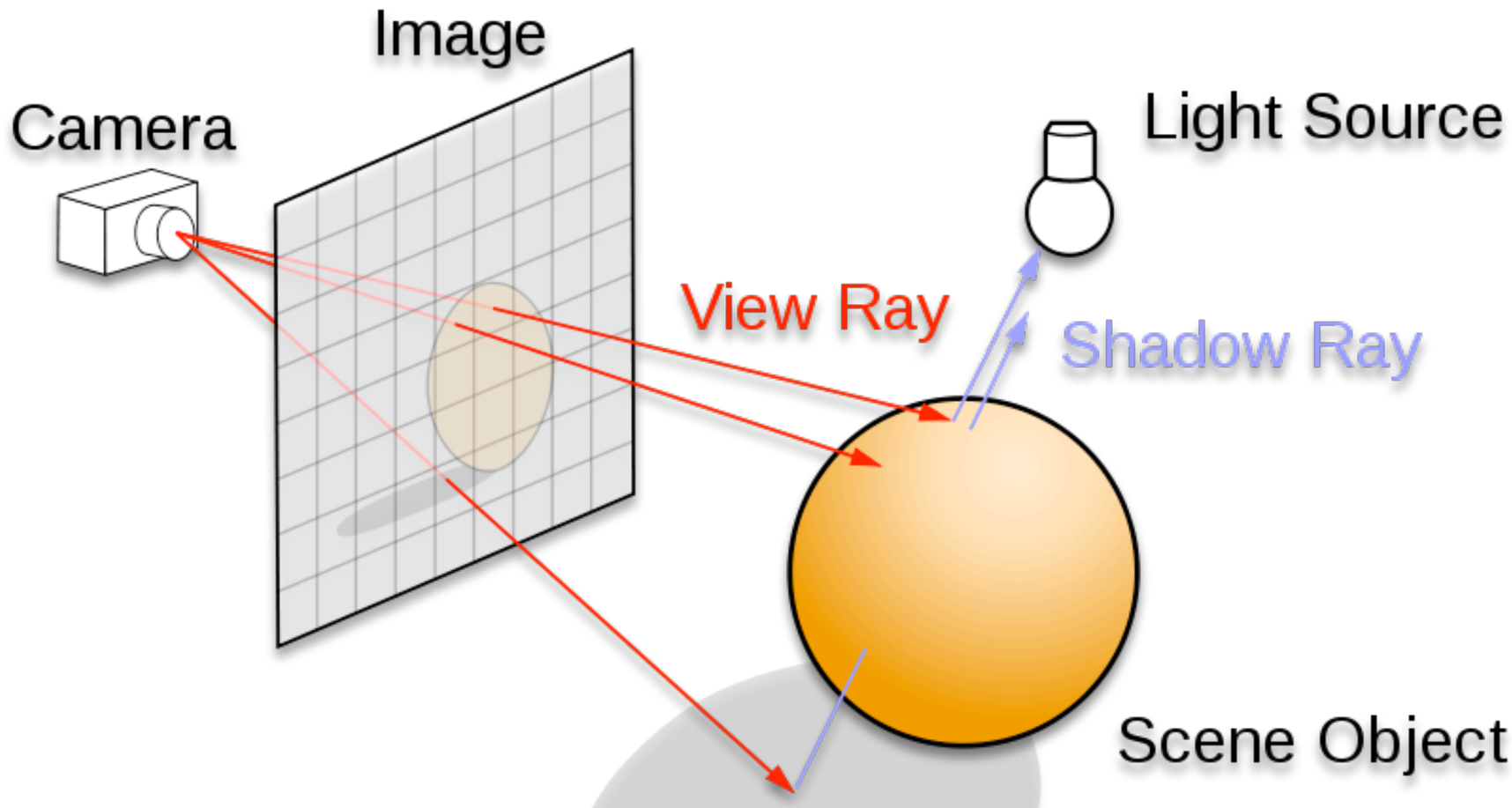
- Estimating Pi:



Monte Carlo techniques

- Los Alamos has since then developed and perfected many different monte carlo codes leading to what is today known as the codes MCNP5 and MCNPX
- State of the art is MCNPX (or soon the merged MCNP6 code) that features numerous (even exotic) particles
- MCNP was originally Monte Carlo Neutron Photon, later N-Particle
- Mainly used for high-energy particle descriptions in weapons, power reactors and routinely used for estimating dose rates and needed shielding
- Does not to date handle coherent scattering of neutrons due to the focus on high energies

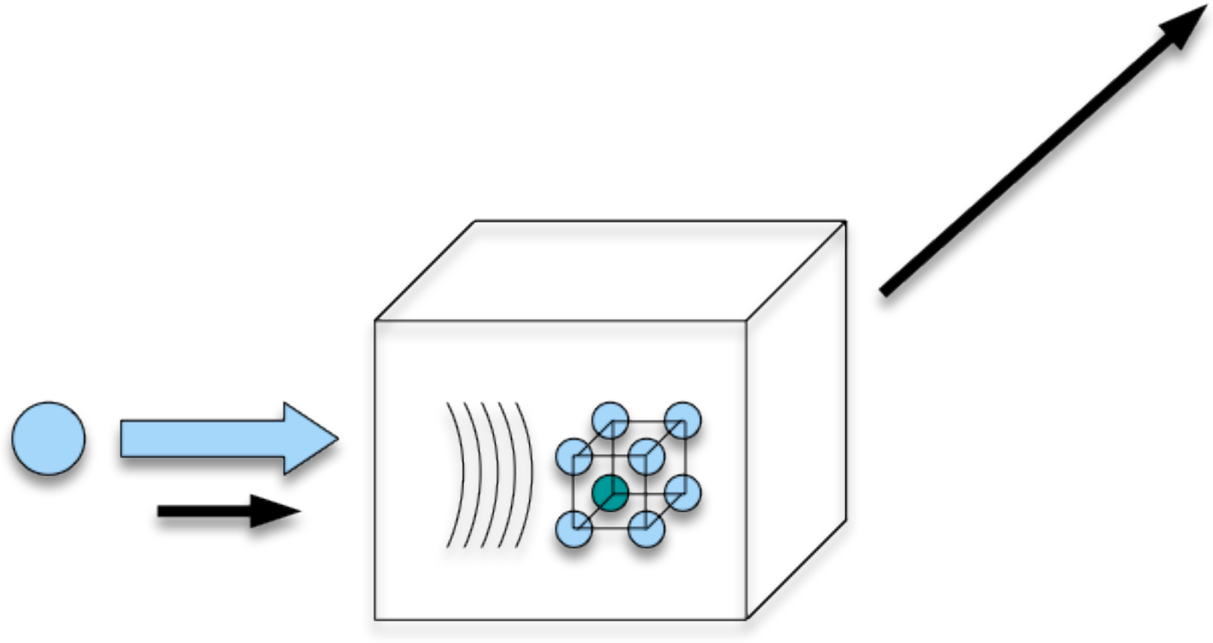
Ray-tracing methods



- When neutrons move in “free space”, we use ray-tracing - but in most cases in direction source -> detector
- Of course parabolas rather than straight lines are uses to implement gravity

Elements of Monte-Carlo raytracing

- Instrument Monte Carlo methods implement coherent scattering effects
- Uses deterministic propagation where this can be done
- Uses Monte Carlo sampling of “complicated” distributions and stochastic processes and multiple outcomes with known probabilities are involved
- - I.e. inside scattering matter
- Uses the particle-wave duality of the neutron to switch back and forward between deterministic ray tracing and Monte Carlo approach



- Result: A realistic and efficient transport of neutrons in the thermal and cold range

Simulation codes for Monte Carlo ray-tracing of neutron instruments (incomplete?)

- US codes:
  - NISP (P Seeger & L Daemen, LANL)
  - IDEAS (X-L Wang ORNL, originally H Lee ORNL)
  - Instrument Builder (JK Zhao ORNL)
  - McVine (engine of the DANSE vnf project) (J Lin Caltech)

- European codes:
  - RESTRAX/SIMRES (J Šaroun, NPI & J Kulda, ILL)
  - VITESS (K Lieutenant et al. HZB plus S Manoshin JINR)
  - McStas (P Willendrup & E Knudsen DTU, K Lefmann KU, E Farhi ILL, U Filges PSI)
  - [NADS (P Bentley ESS)]

- Japanese code:
  - PHITS (MCNP-like) has a few features for instrument beam transport

- There may be others I do not know of...

NISP

- "The mother of all neutron MC-raytracing"
- Builds on MCLIB which was derived from MCNP
- Does almost "anything", i.e. quadratic form geometries of material, has ability to scatter from any region to any region of the instrument
- Defined the de-facto implementation standard for polarized neutron scattering
- Website at http://www.paseeger.com
- Developed by P Seeger (consultant) & L Daemen, LANL
- Windows only (32 bit?)
- License conditions undefined, but a kind of public domain code
- Underlying legacy fortran code run via UI

- My 0.02$: Good stuff, but a limited audience expert code

IDEAS

- Developed for instrumentation work at SNS
- Was used for roughly half the instruments, the other half was mostly McStas and a little VITESS
- Was always a side-activity of the authors
- Website currently gone?
- Developed by H Lee (was ORNL now ANSTO) & X-L Wang, ORNL
- Windows only (32 bit?)
- Unkown license

- My 0.02$: Dead / sleeping project?

Instrument Builder

- Developed by single SNS employee for own project?
- Partial implementation but looks OK
- C++ and PVM/MPI for parallelization
- Website http://neutrons.ornl.gov/instruments/SNS/EQ-SANS/software/ib/doc/
- Developed by JK Zhao (ORNL)
- Windows & Linux
- Unkown license but source code provided

- My 0.02$: Sleeping project?

McVine (in vnf, DANSE)

- Developed for the “virtual neutron facility” which is a part of the DANSE project
- Uses Python “pyre” wraps to create Python versions of the McStas components
- Python script defines the instrument setup
- Allows to use e.g. bvk phonon simulations with instrument simulation
- Websites https://vnf.caltech.edu/vnf/1/ and http://docs.danse.us/MCViNE/1.0-beta/index.html
- Developed by J Lin and B Fultz (Caltech)
- Build to “any” platfrom from source code
- BSD license

- My 0.02$: vnf is really nice but so far implement only a few instruments

RESTRAX & SIMRES

- Builds on RESCAL and TRAX codes for triple axis resolution estimates (Popovici)
- RESTRAX is TAS-only but SIMRES has certain TOF components also
- Has very efficient “detector to source” propagation method
- Exellent monochromator descriptions, including bent Si
- Legacy fortran code with Java UI that lowers the learning curve
- Website http://neutron.ujf.cas.cz/restrax/
- Developed by J Šaroun (NPI) and J Kulda (ILL)
- Windows & Linux
- GPL License

- My 0.02$: RESTRAX is probably the best bet for a TAS code. Milage may vary in other areas.

VITESS

- Virtual Instrumentation Tool for the ESS
- Originally only TOF type instruments but now cover all types
- Had early implementation of polarized neutron techniques
- Is intrisically parallelized by running a set of single executables that talks via pipes, but efficiency can drop somewhat along beamline (now includes options for system-level parallelization via “helper threads”
- Easy to use GUI and no compilation
- Hard(er) to include your own developments
- C-code with little overlap between individually developed modules
- Website http://www.helmholtz-berlin.de/vitess
- Developed by K Lieutenant and his team (HZB) and Sergei Manoshin (JINR)
- Windows, Linux, Mac OS X
- GPL License

- My 0.02$: VITESS has a low learning curve and works very well. Can be hard to do more complex things. Full visualization of the instrument is being developed.

NADS

- Not a Monte Carlo raytracer - uses very quick acceptance diagram techniques instead
- So far decoupled simulation of vertical vs. horizontal beam
- Optics only
- Website http://code.google.com/p/jnads/
- Developed by P Benley (ESS, formerly ANSTO, ILL, HMI)
- "Any" system (java implementation)
- GPL License

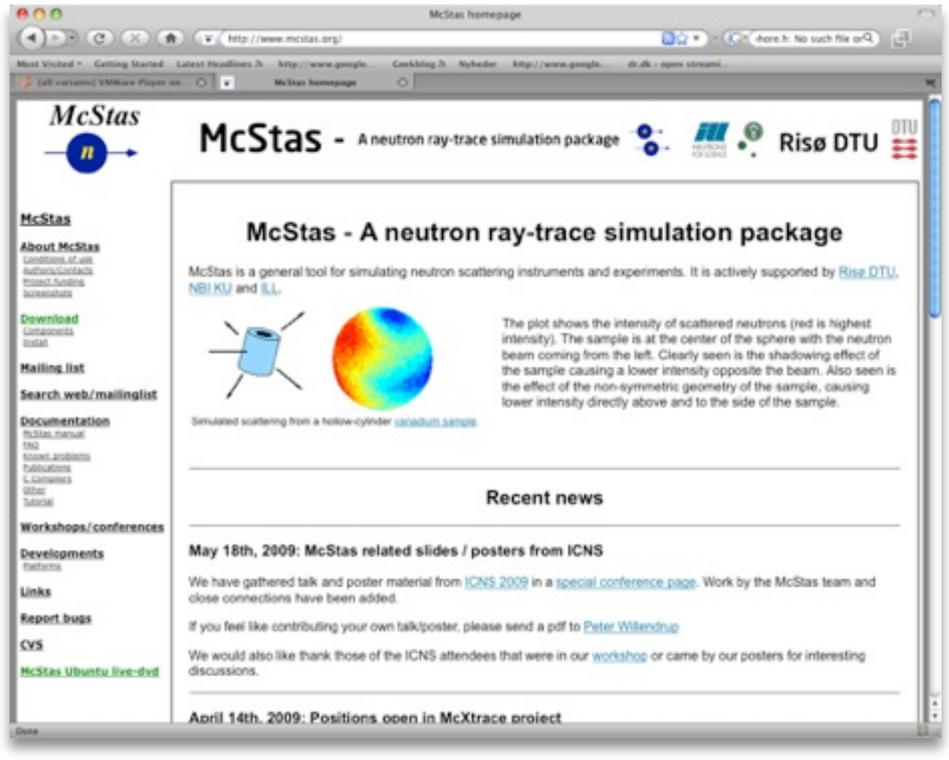
- My 0.02$: Has clear potential but is currently not an all-round package.

McStas

- The code that I develop.... :)

- Will now progress to discuss that and its features

McStas Introduction



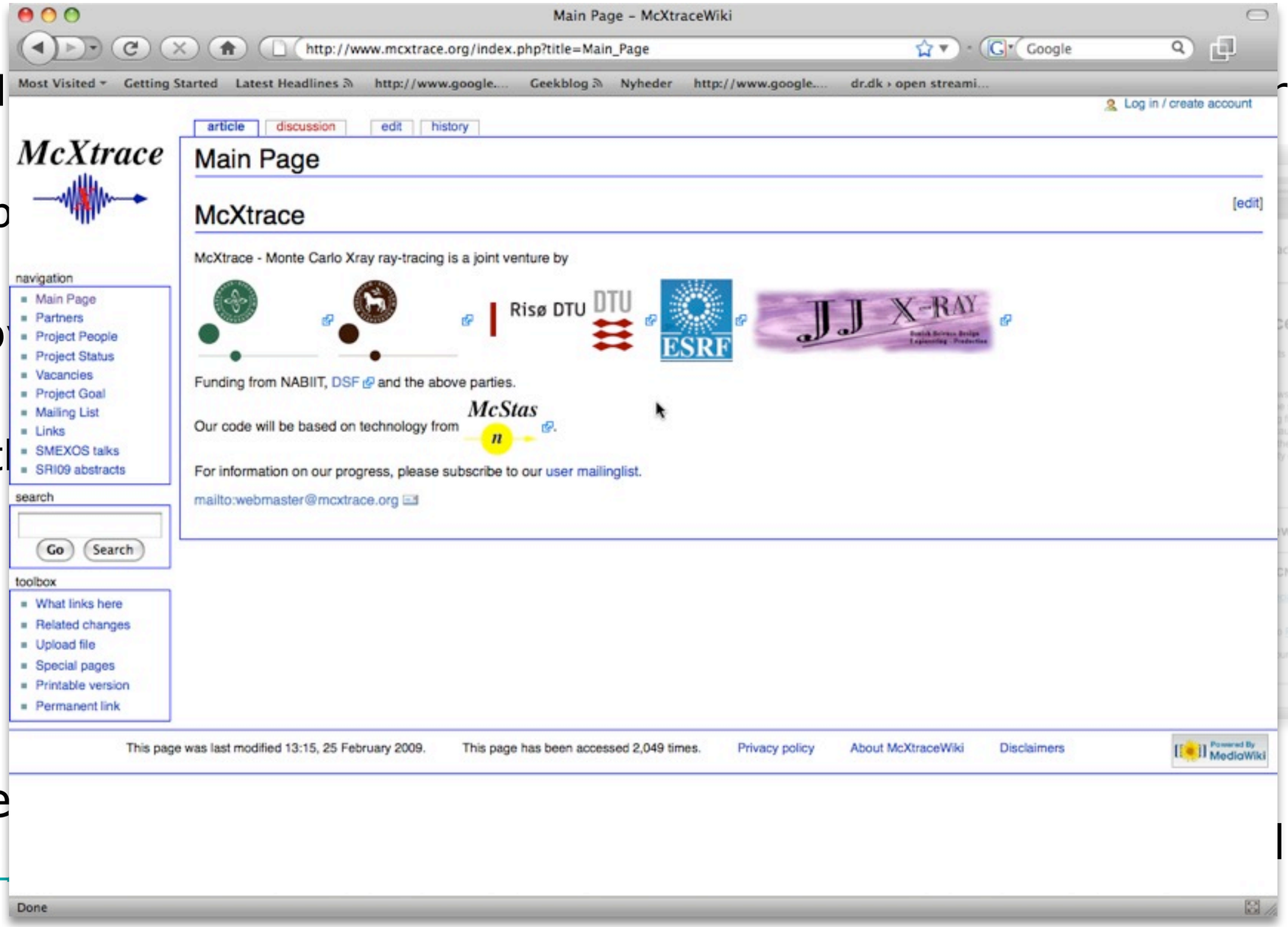
GNU GPL license
Open Source

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

mcstas-users@mcstas.org mailinglist

McStas Introduction
McXtrace - since jan 2009 similar in X-rays

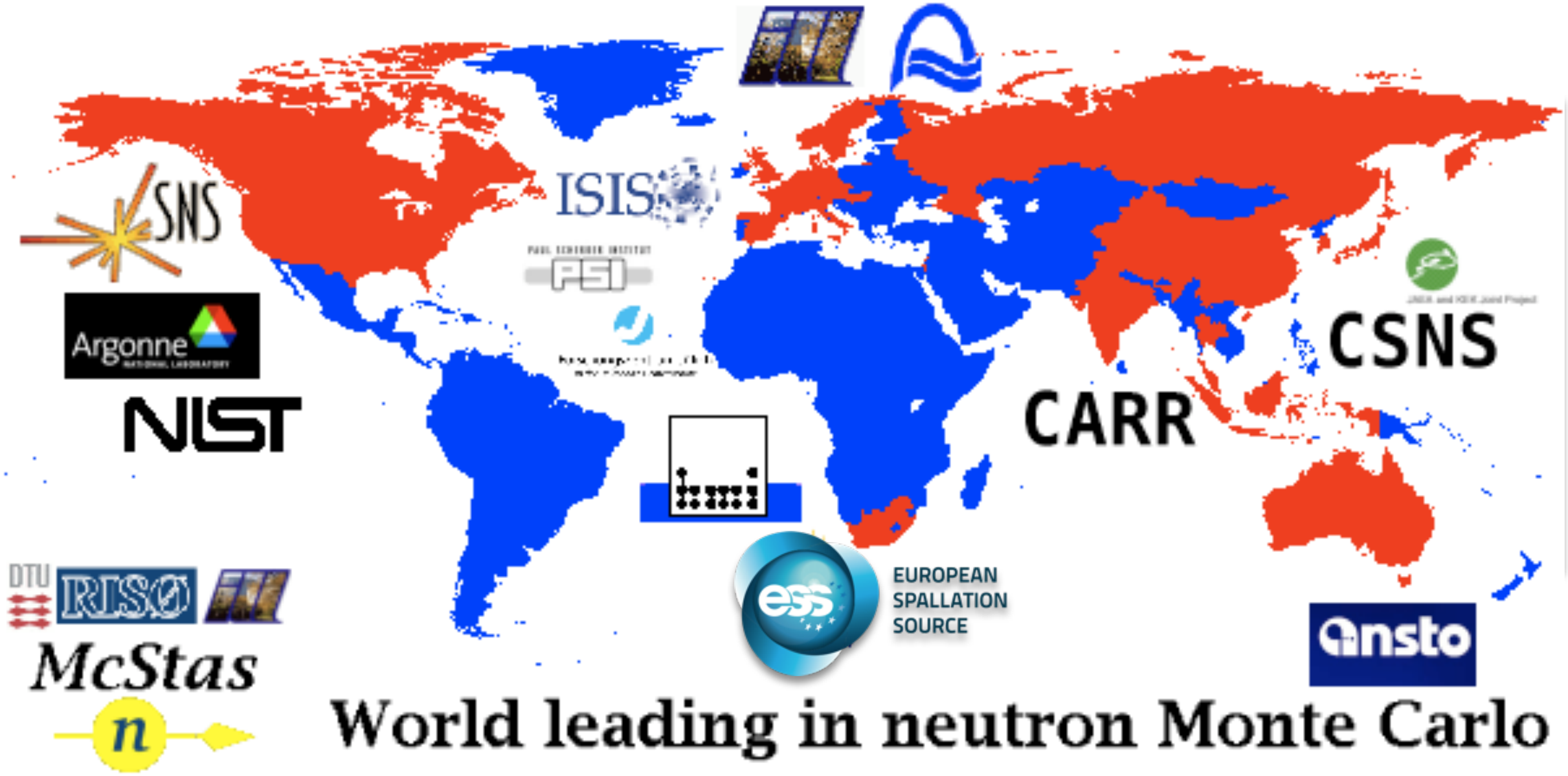
- Flexible, general simulation utility for neutron scattering experiments.
- Original
- Develop
- V. 1.0 b
- Current



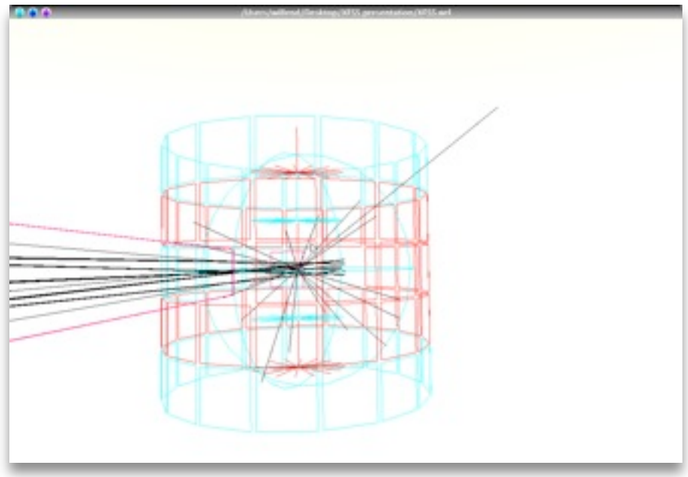
Proje
http:
list

- Synergy, knowledge transfer, shared infrastructure

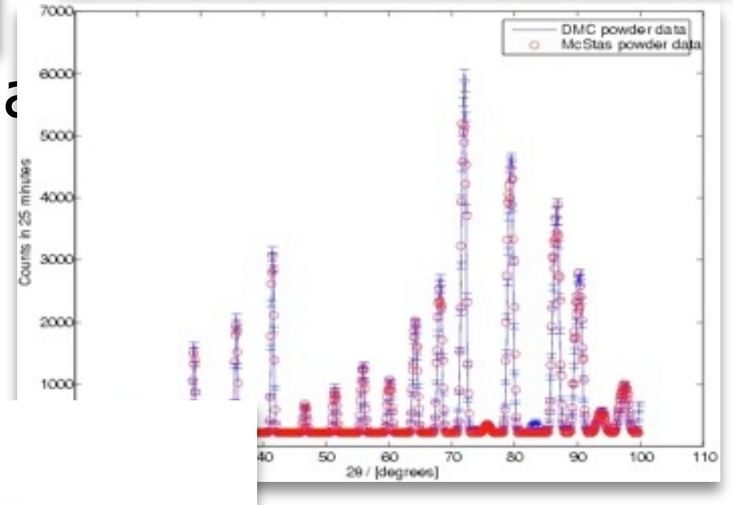
McStas Introduction



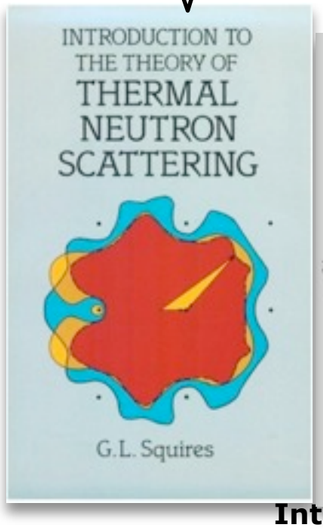
What is McStas used for?

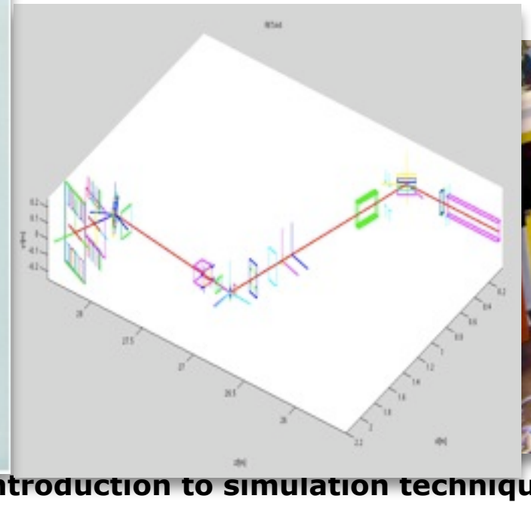


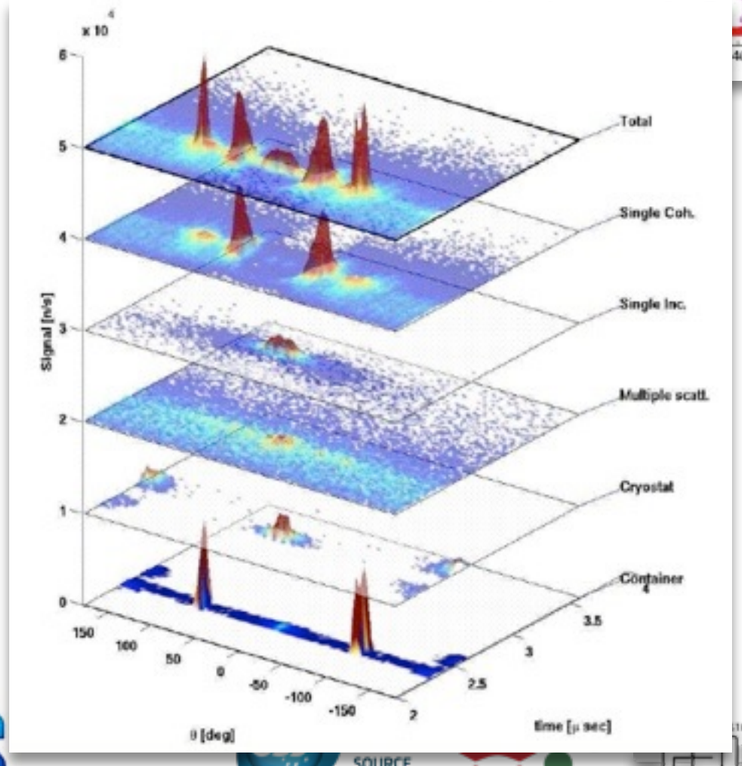
- InstrumentationVirtual experimentsData anTea



(KU, DTU)

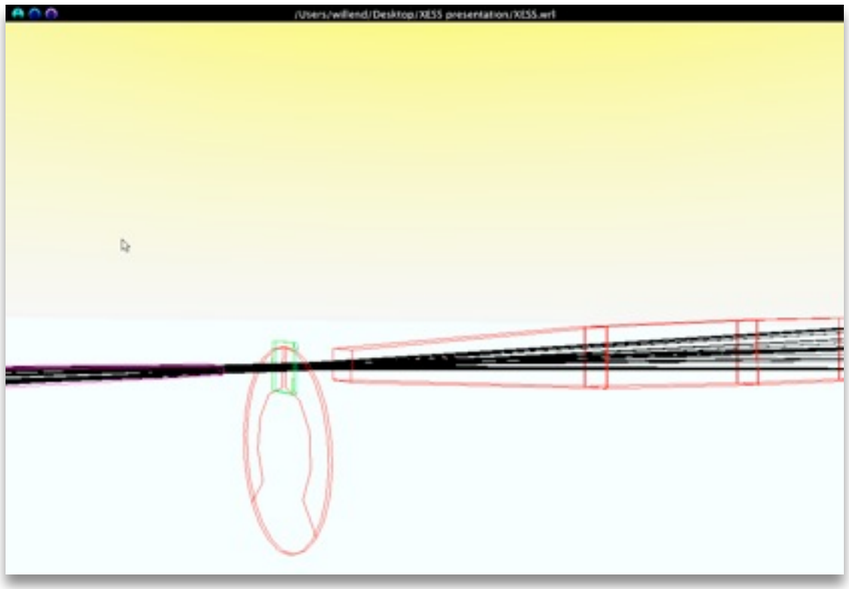


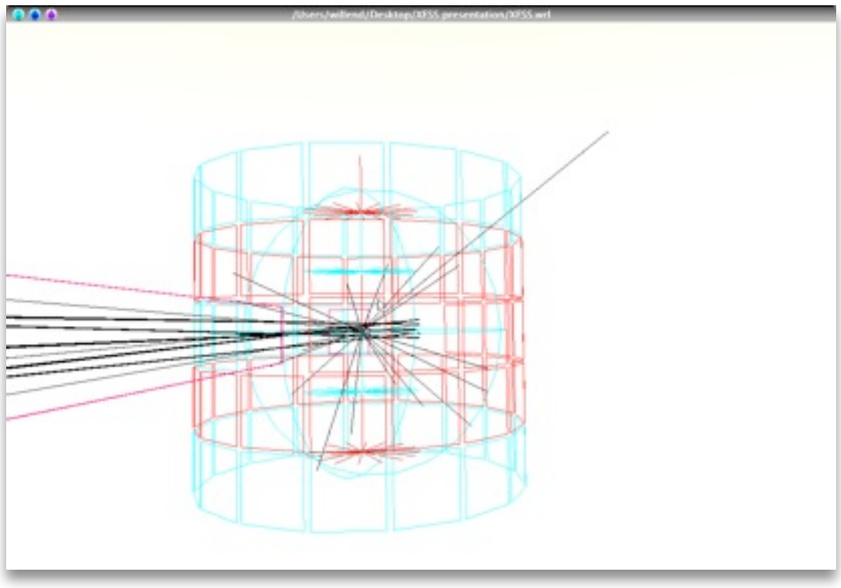


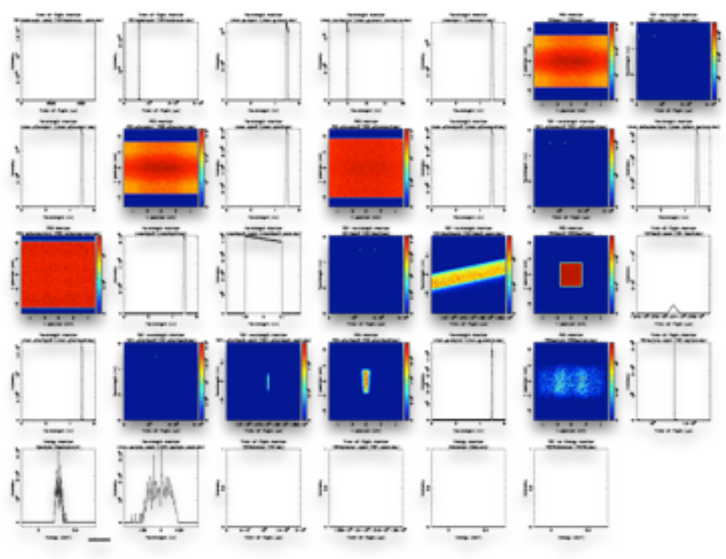


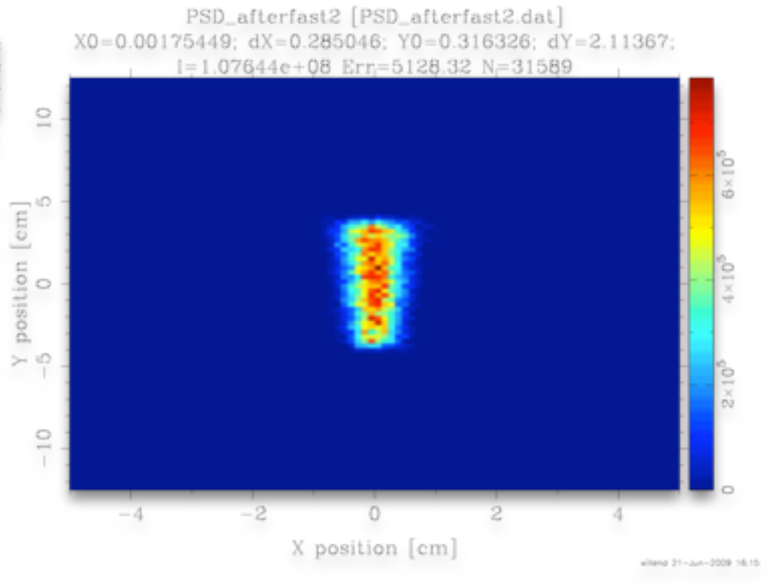
Instrumentation

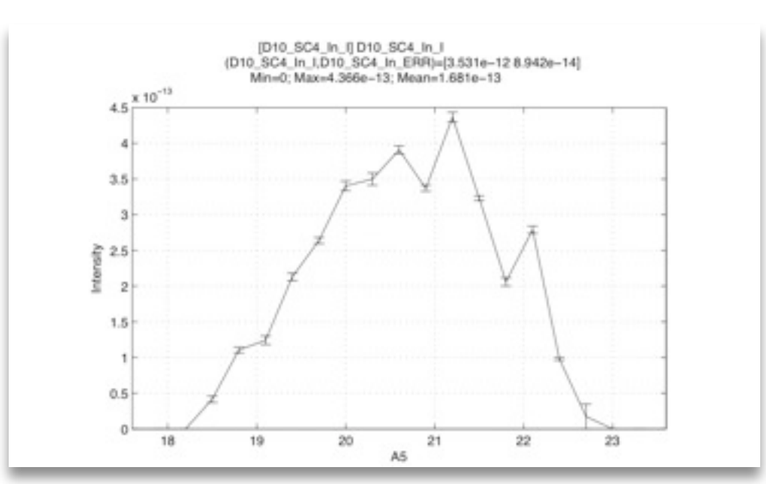
- Design and optimization of instruments



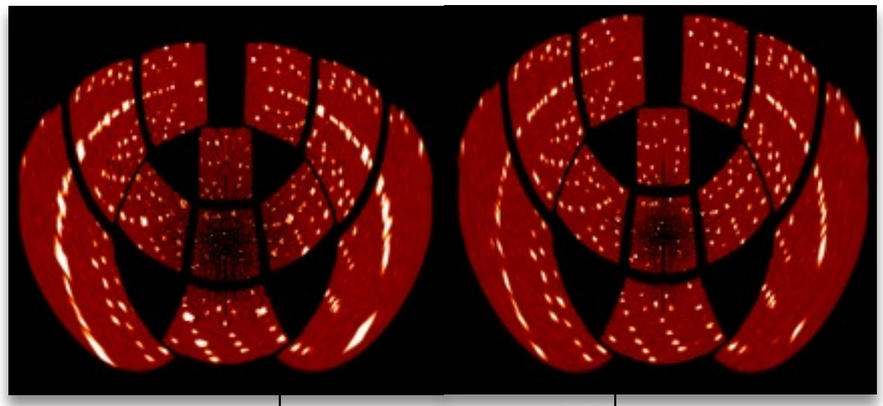




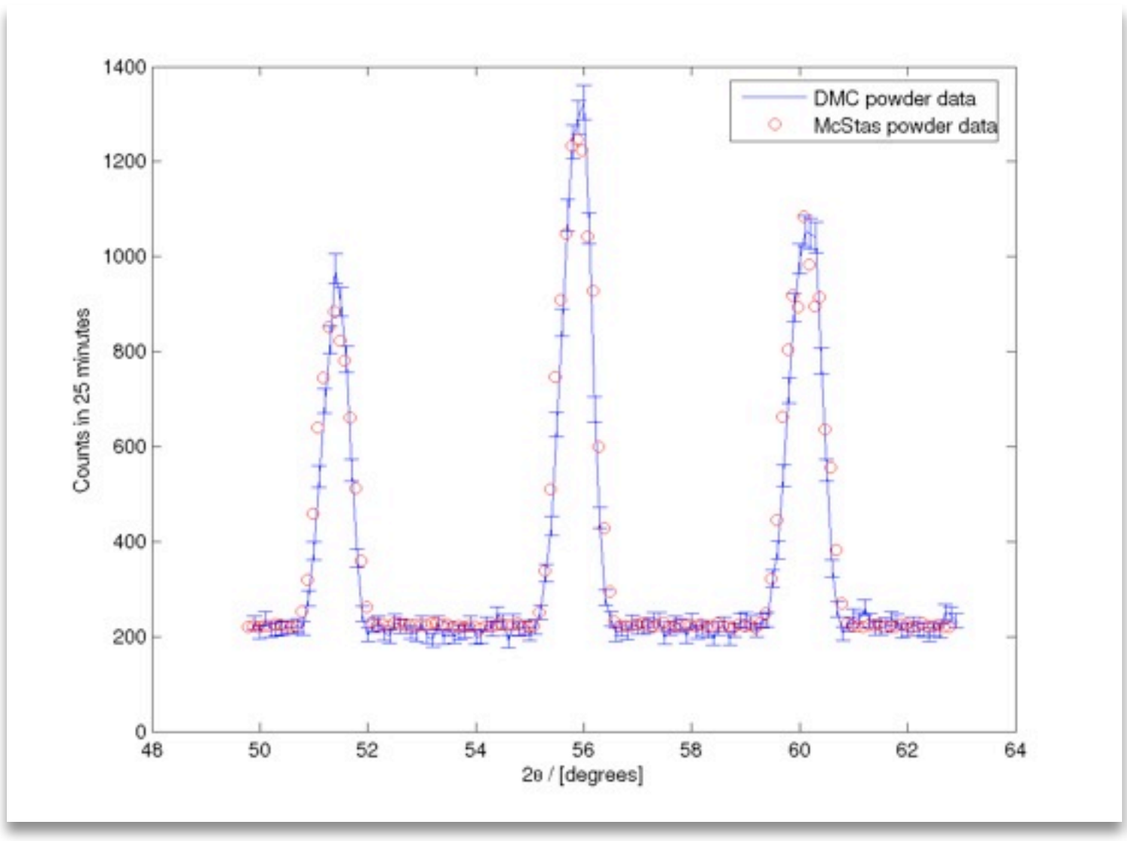


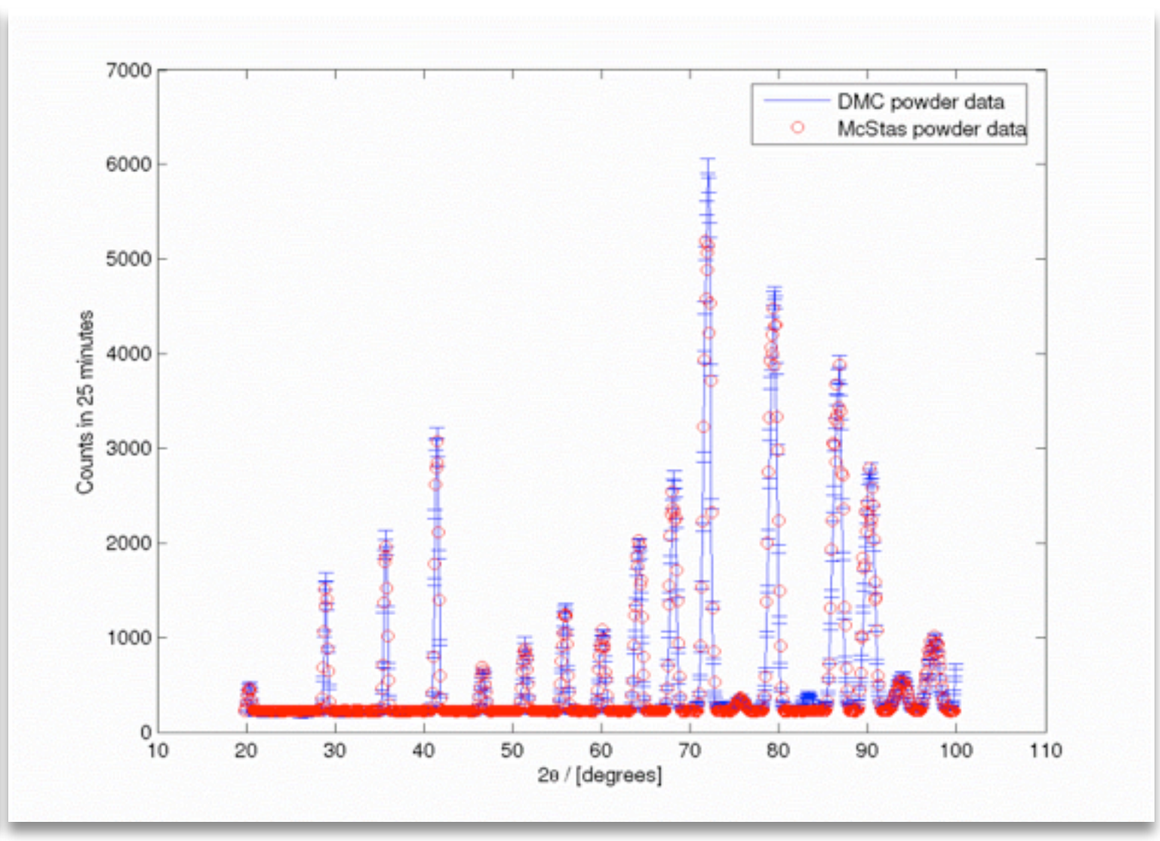


Virtual experiments (VE)
(definition:)



A. Daud-Aladine, ISIS

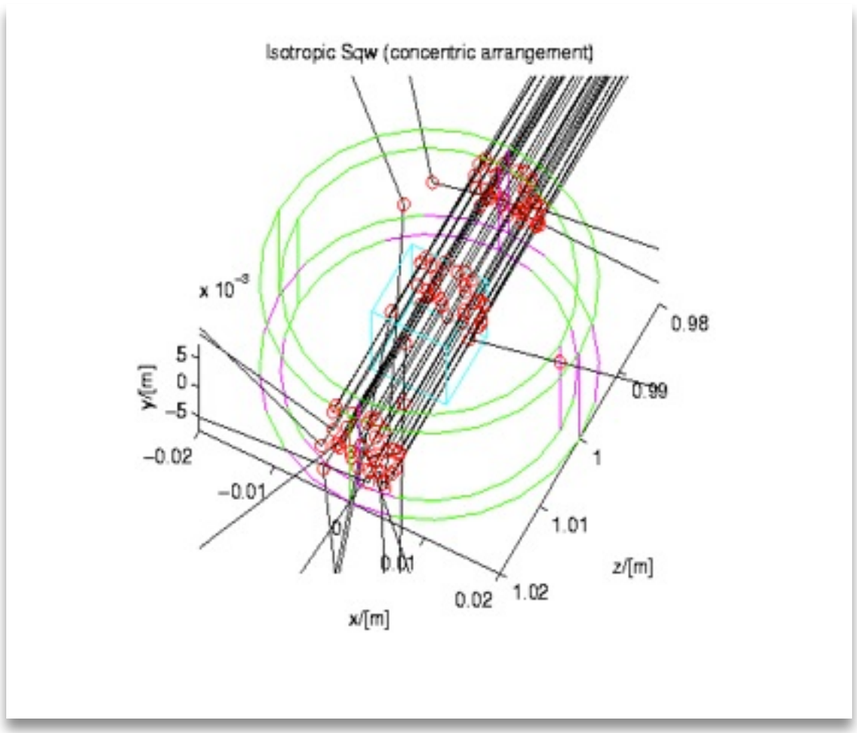


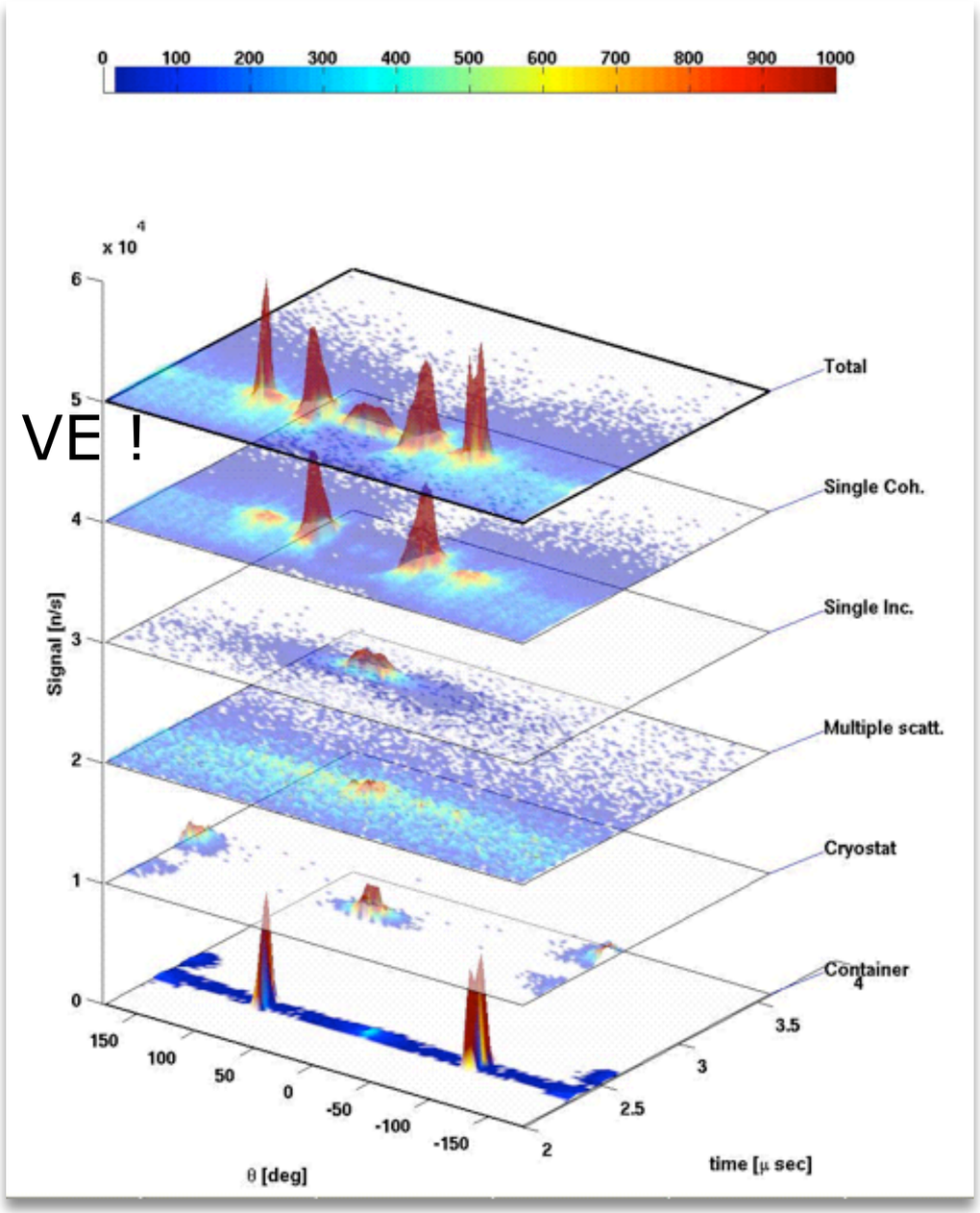


P. Willendrup, Risø DTU; Uwe Filges, L. Keller, PSI

Data analysis (1)
(using VE techiques)

- Virtual TOF exp. at IN6, ILL
- Liquid Ge sample
- Coherent / incoherent
- Multiple scattering
- And sample environment
- All contributions can be separated by VE !

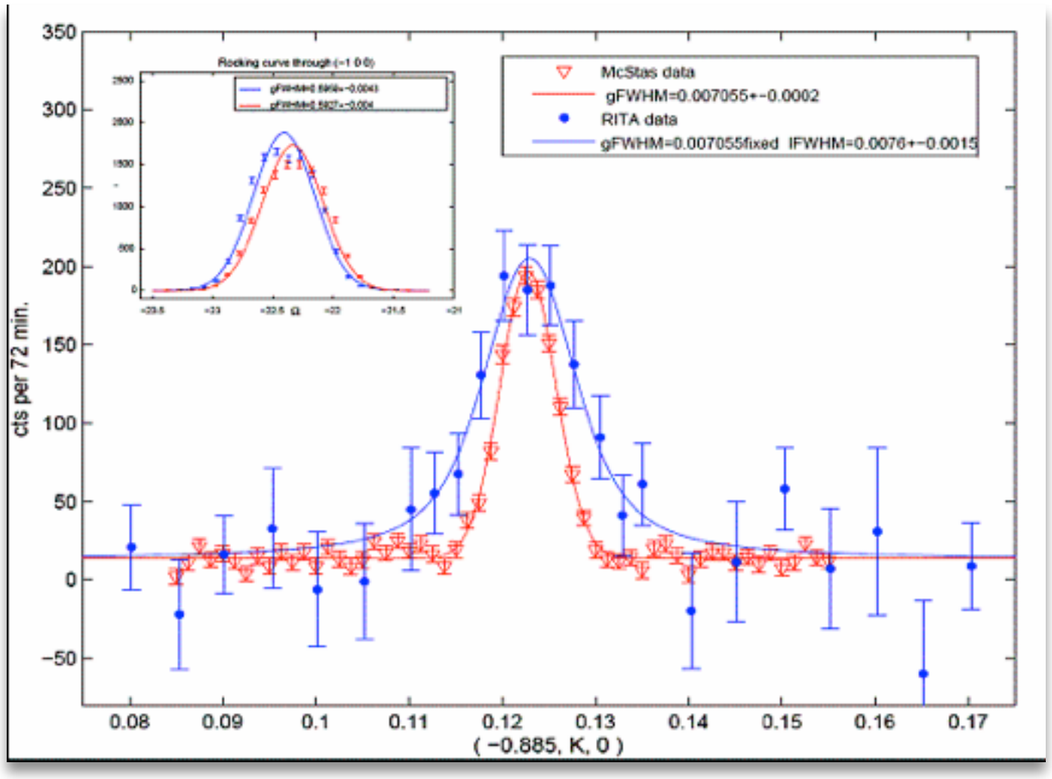




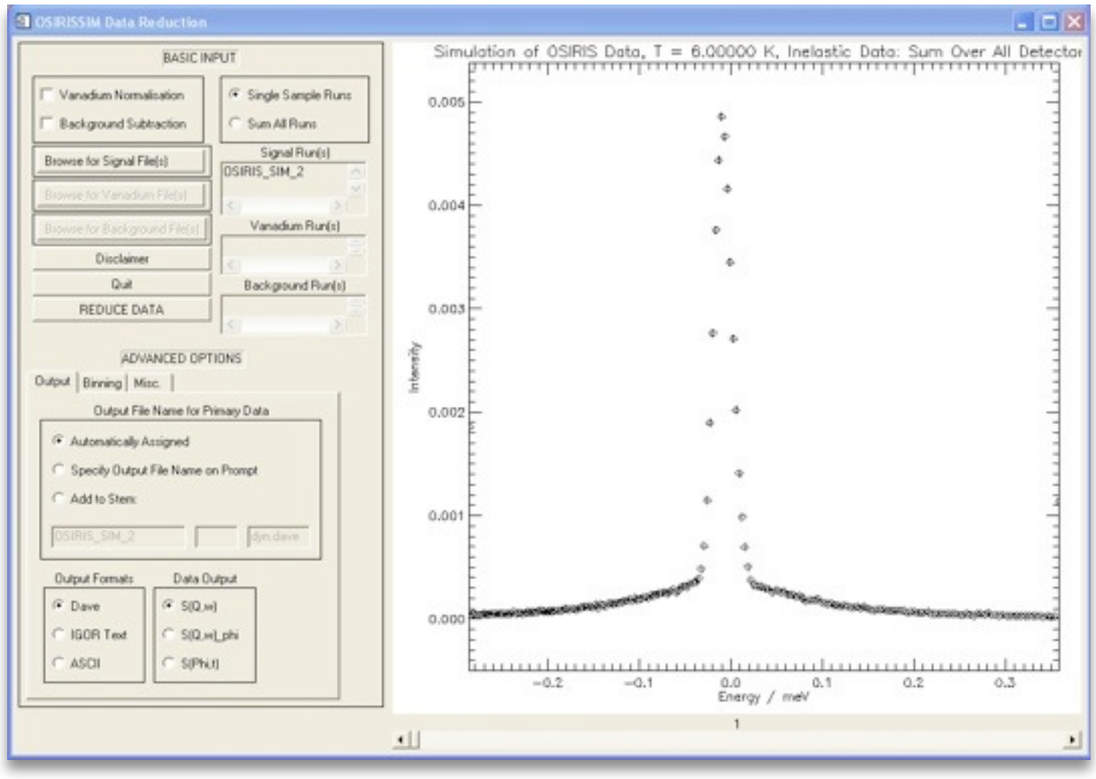
E. Farhi, ILL

Data Analysis (2)
(using VE techniques)

- VE data has been used to test data analysis programs
- … and to check resolution effects



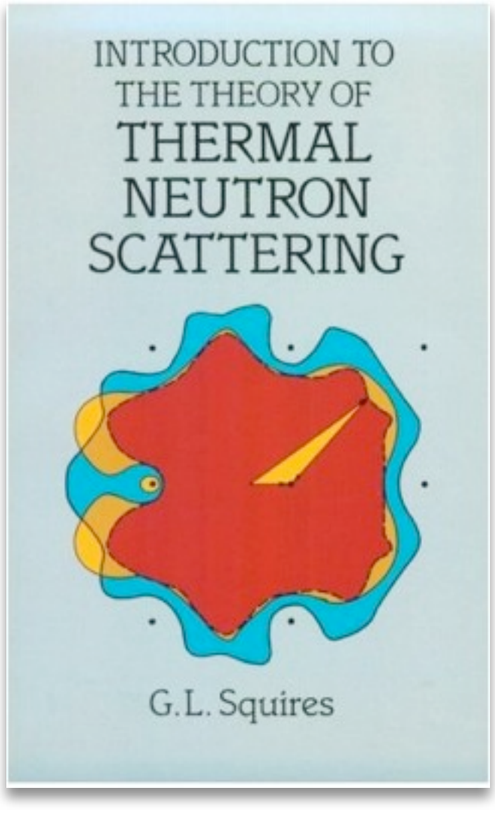
L. Udby, Risø-DTU

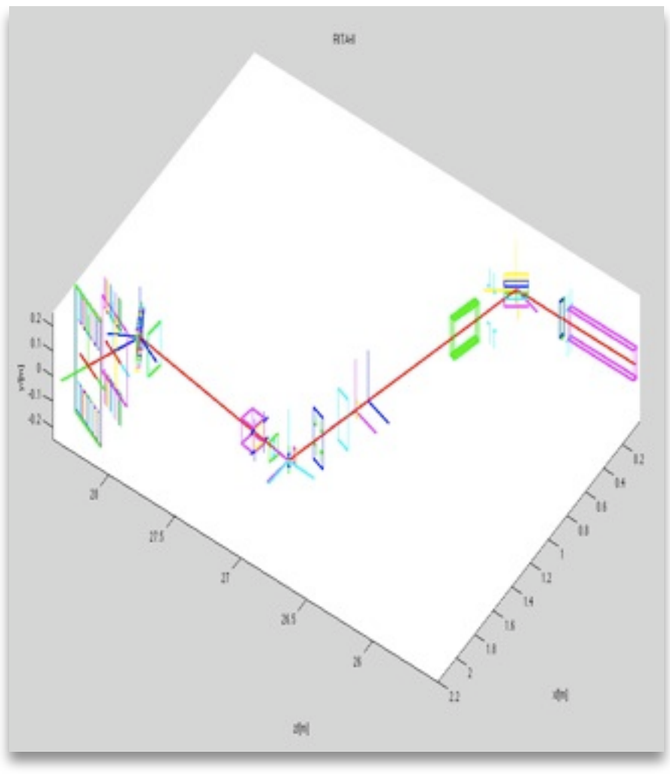


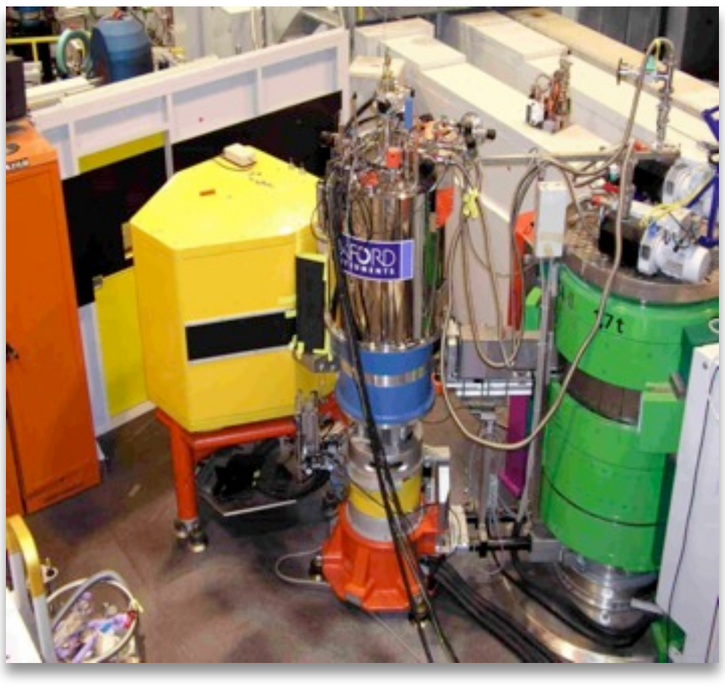
P. Tregenna-Piggott, PSI

Teaching / training purposes

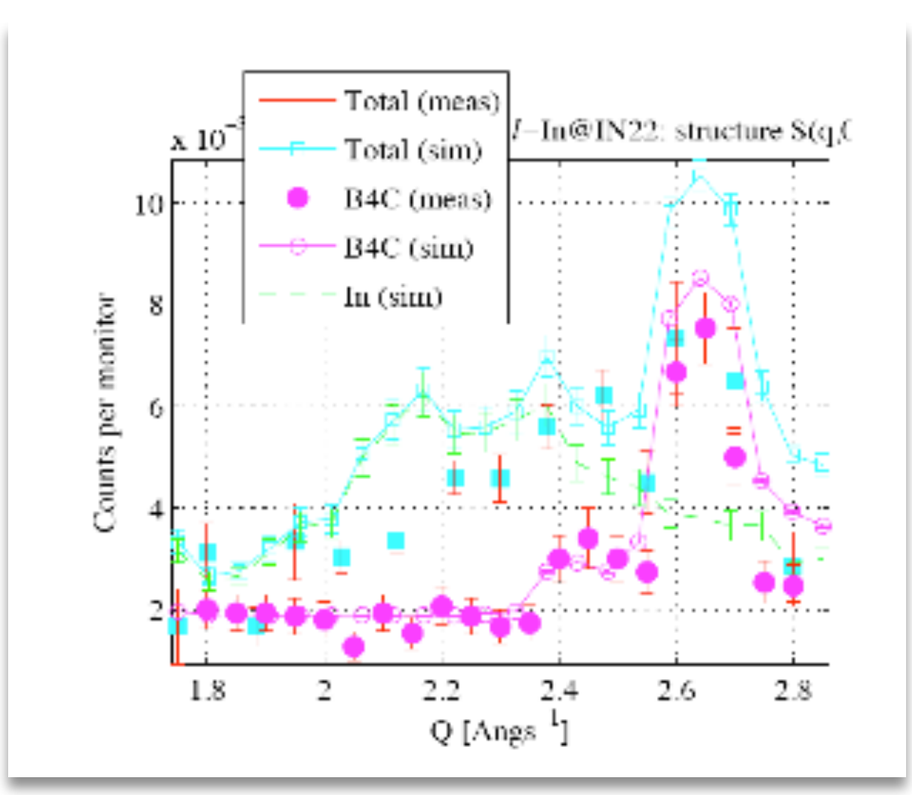
- WorkshopsTeaching
  - University of Copenhagen course on Neutron Scattering



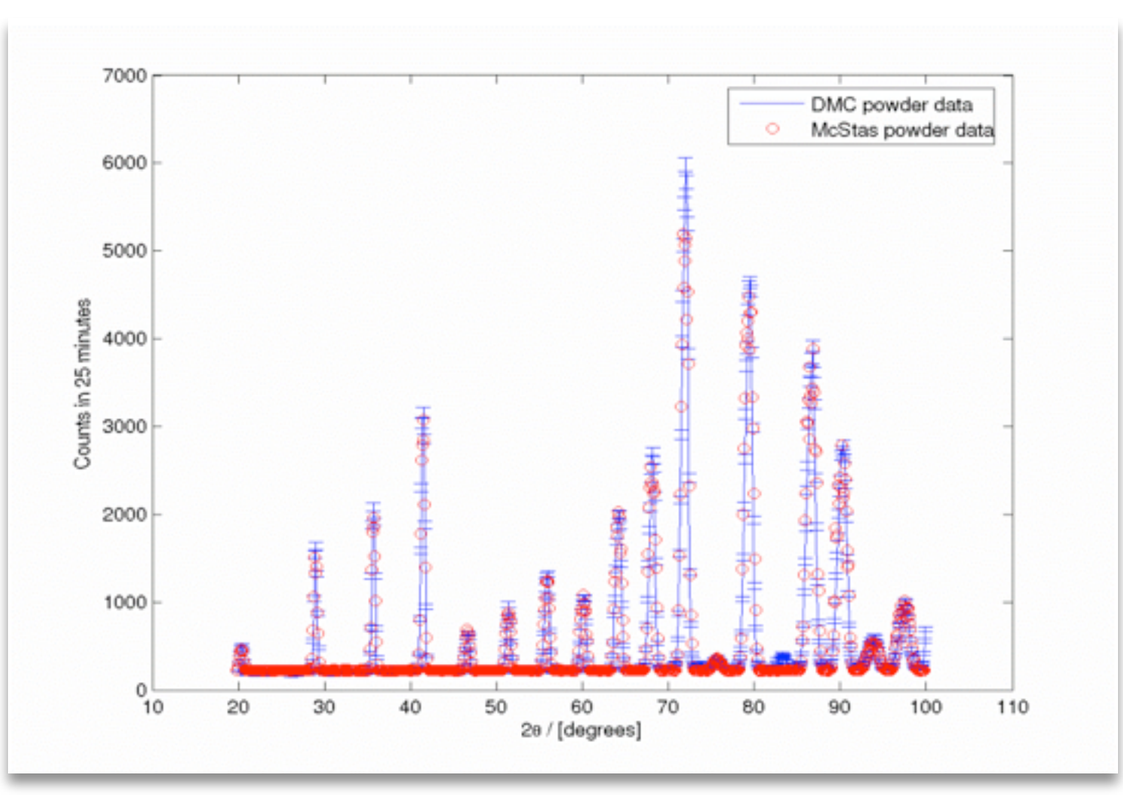




Reliability - cross comparisons

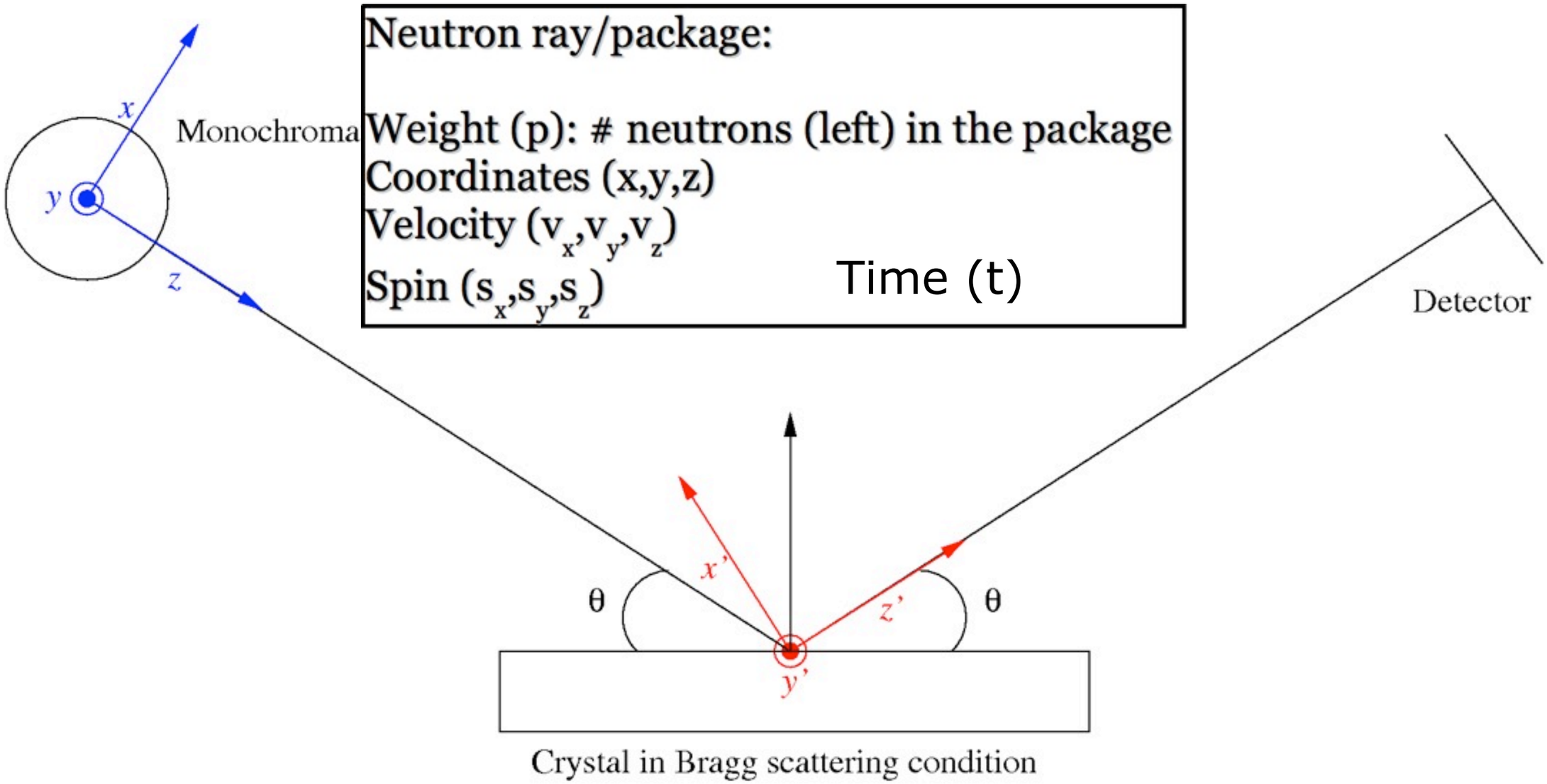


E. Farhi, P. Willendrup et al., in preparation



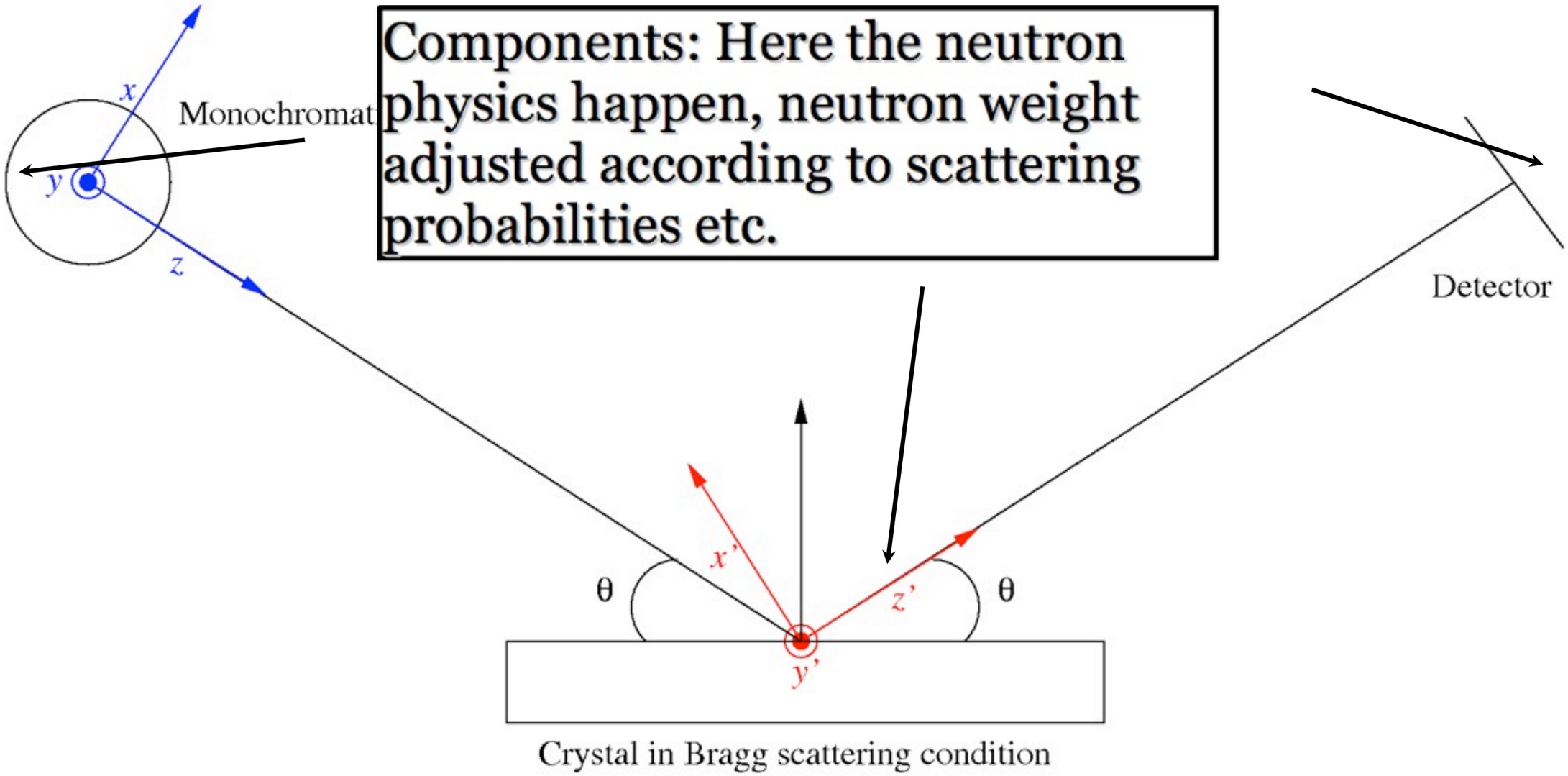
P. Willendrup et al., Physica B, 386, (2006), 1032.

McStas: key concepts

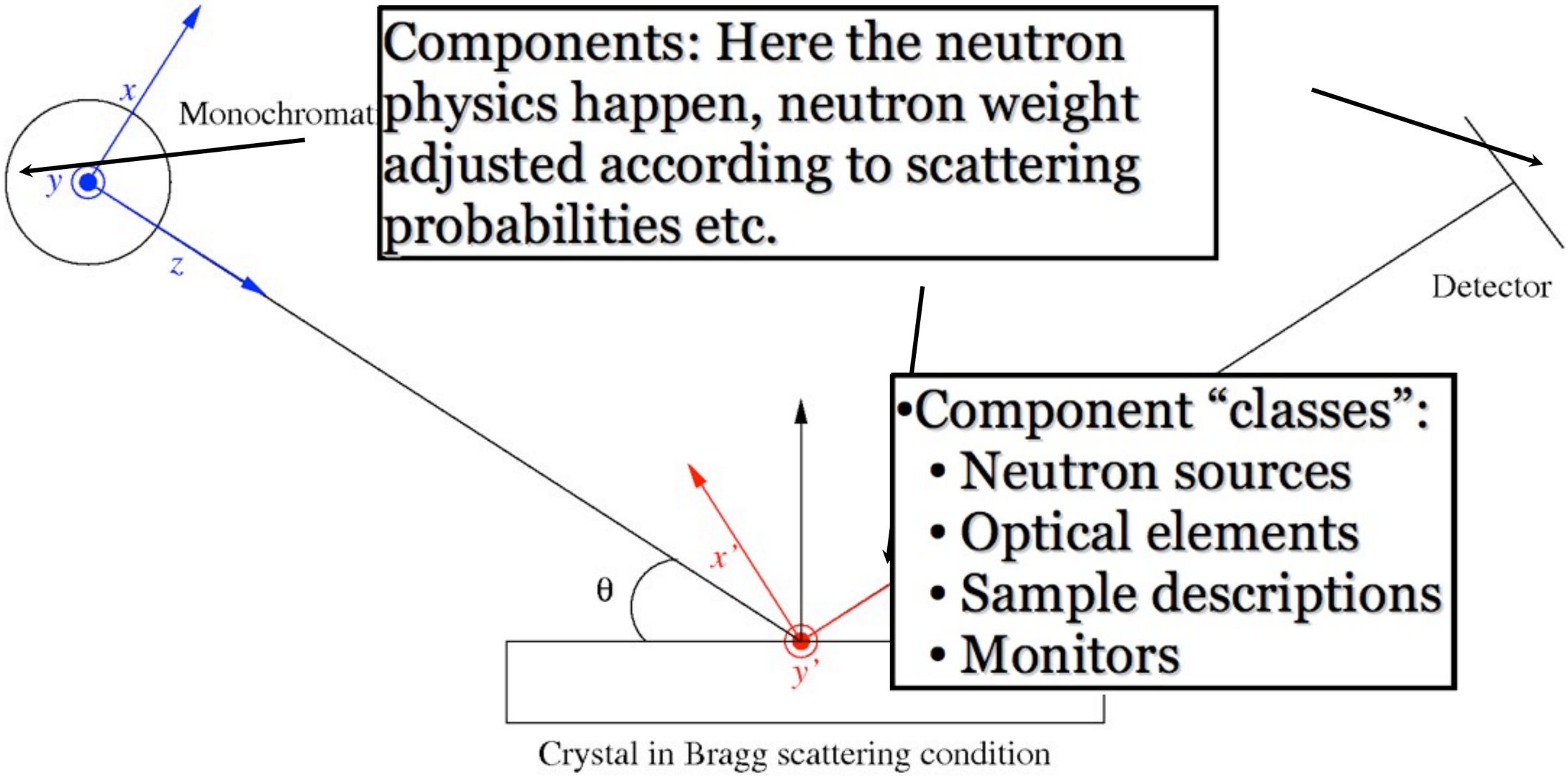


Crystal in Bragg scattering condition

McStas: key concepts

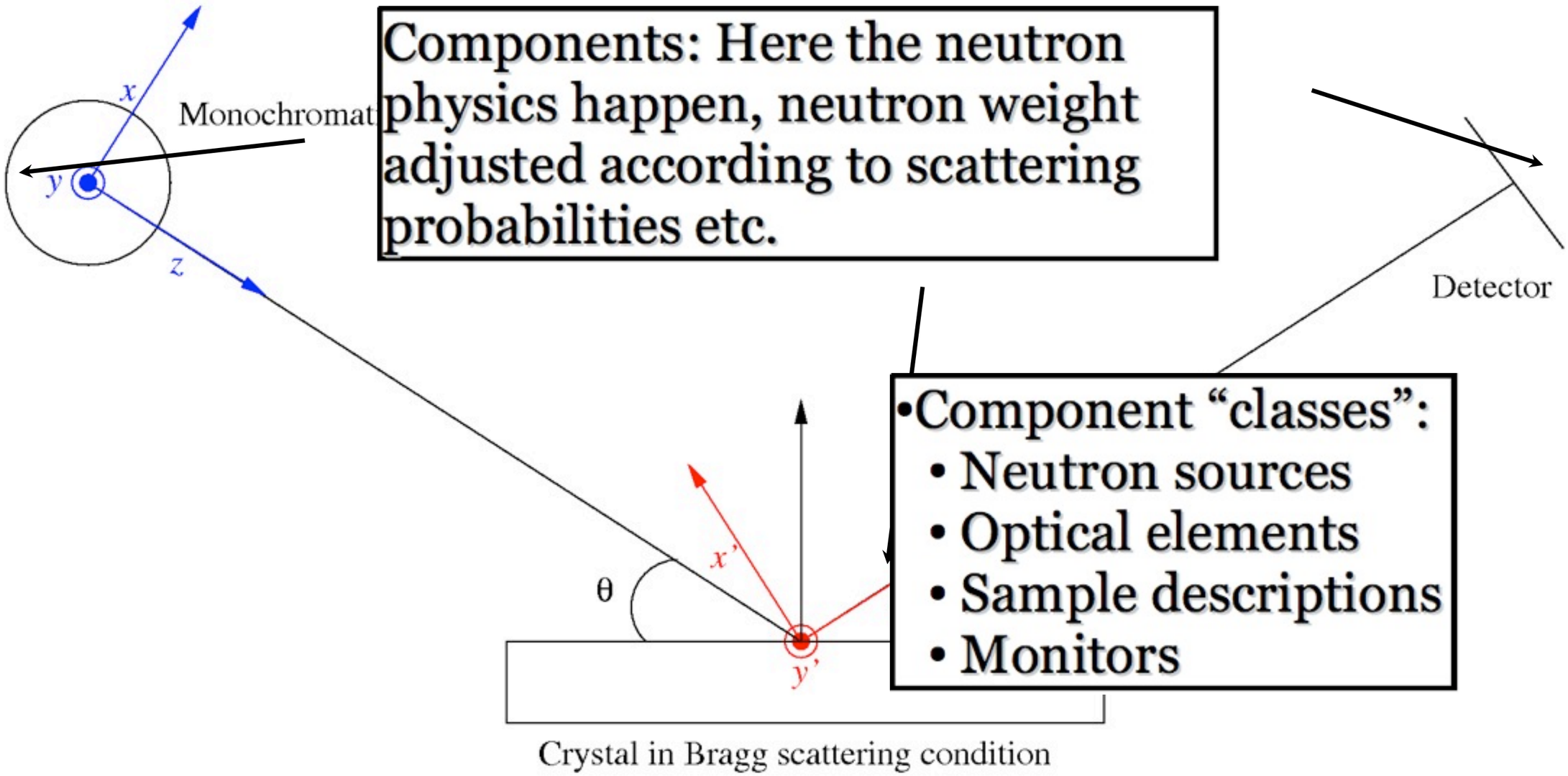


McStas: key concepts

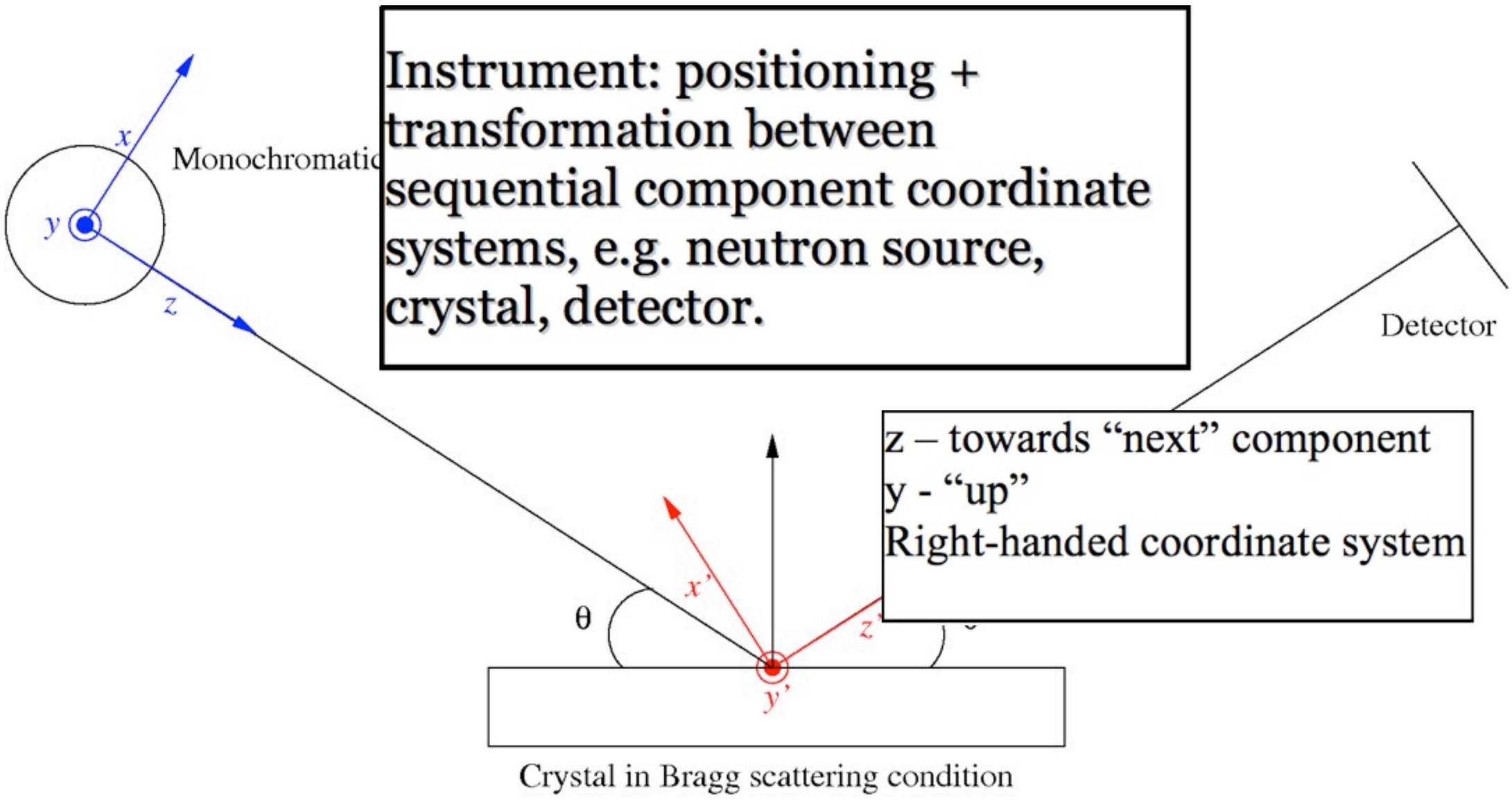


McStas: key concepts

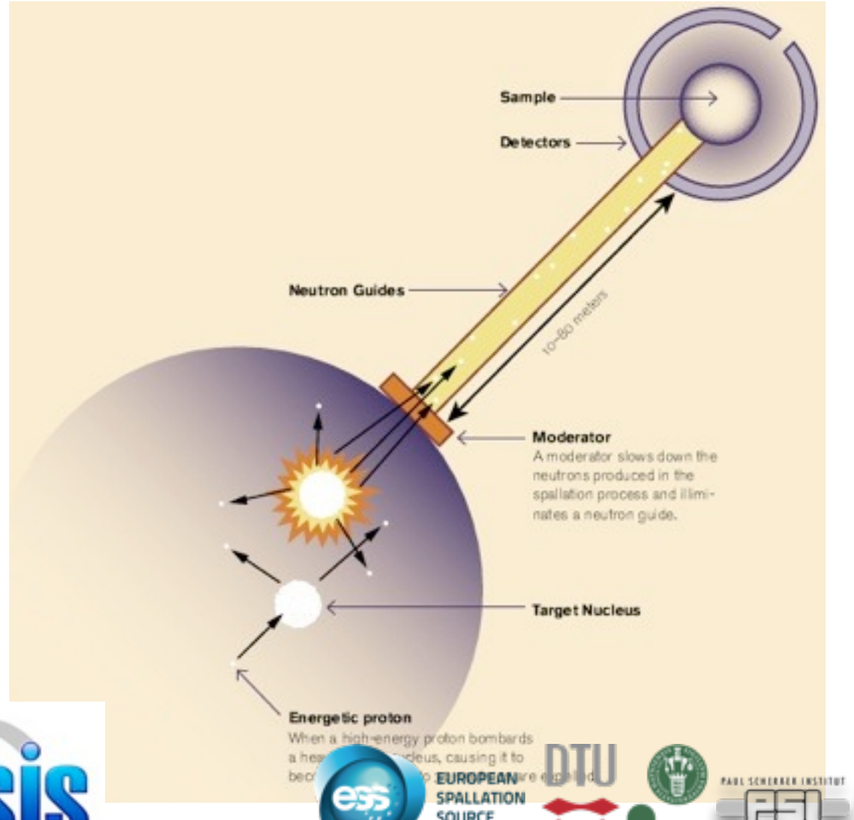
Local, internal coordinate system!



McStas: key concepts

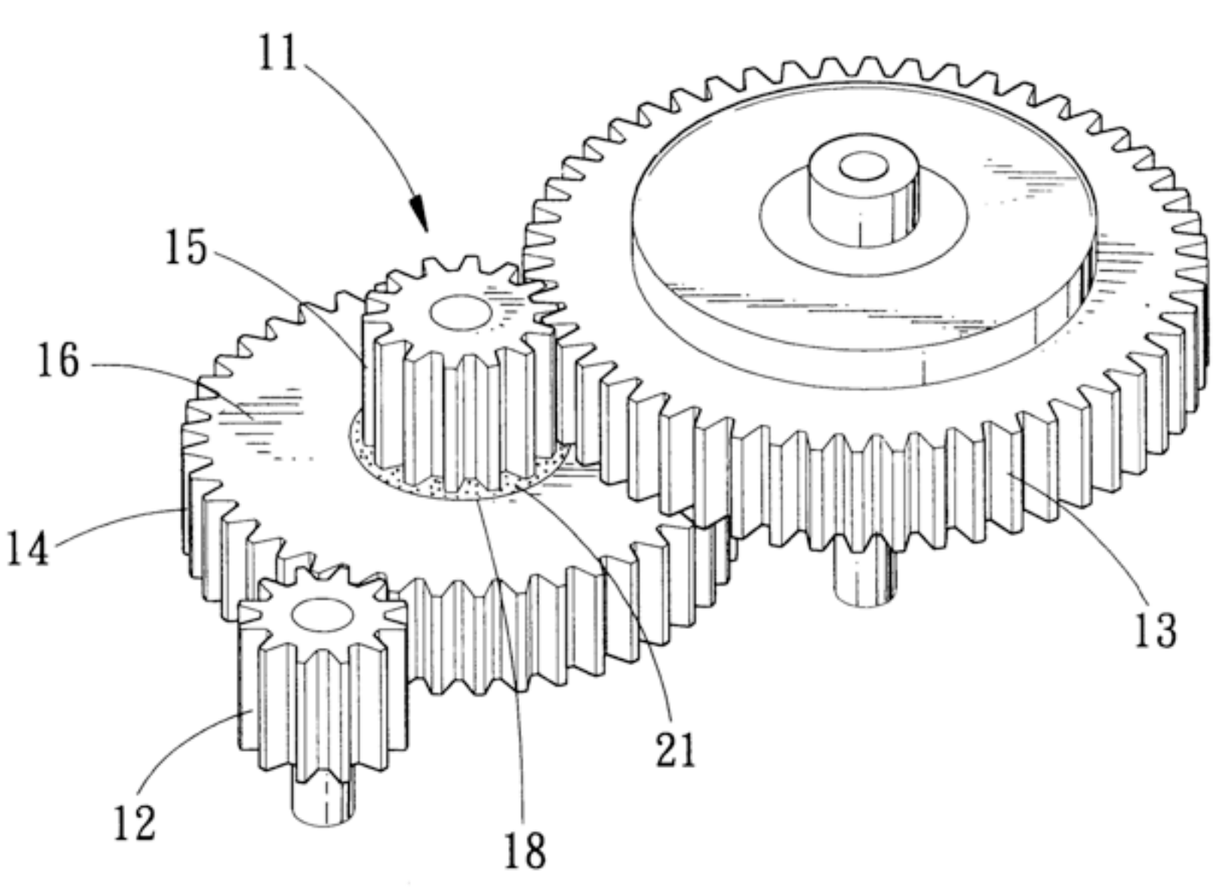


McStas overview



Under-the-hood / inner workings

Code generation



Implementation

- Three levels of source code:
- Instrument file (All users)
- Component files (Some users)
- ANSI c code (no users)

Instrument file

```
DEFINE INSTRUMENT My_Instrument(DIST=10)

/* Here comes the TRACE section, where the actual      */
/* instrument is defined as a sequence of components.  */
TRACE

/* The Arm() class component defines reference points and orientations  */
/* in 3D space.                                                         */
COMPONENT Origin = Arm()
  AT (0,0,0) ABSOLUTE


COMPONENT Source = Source_simple(
    radius = 0.1, dist = 10, xw = 0.1, yh = 0.1, E0 = 5, dE = 1)
  AT (0, 0, 0) RELATIVE Origin


COMPONENT Emon = E_monitor(
    filename = "Emon.dat", xmin = -0.1, xmax = 0.1, ymin = -0.1,
    ymax = 0.1, Emin = 0, Emax = 10)
  AT (0, 0, DIST) RELATIVE Origin


COMPONENT PSD = PSD_monitor(
    nx = 128, ny = 128, filename = "PSD.dat", xmin = -0.1,
    xmax = 0.1, ymin = -0.1, ymax = 0.1)
  AT (0, 0, 1e-10) RELATIVE Emon

/* The END token marks the instrument definition end */
END
```

Written by you!

Component file

```
/*******************************************************************************
*
* Mcstas, neutron ray-tracing package
*         Copyright 1997-2002, All rights reserved
*         Risoe National Laboratory, Roskilde, Denmark
*         Institut Laue Langevin, Grenoble, France
*
* Component: Source_flat
*
* %I
* Written by: Kim Lefmann
* Date: October 30, 1997
* Modified by: KL, October 4, 2001
* Modified by: Emmanuel Farhi, October 30, 2001. Serious bug corrected.
* Version: $Revision: 1.22 $
* Origin: Risoe
* Release: McStas 1.6
*
* A circular neutron source with flat energy spectrum and arbitrary flux
*
* %D
* The routine is a circular neutron source, which aims at a square target
* centered at the beam (in order to improve MC-acceptance rate).  The angular
* divergence is then given by the dimensions of the target.
* The neutron energy is uniformly distributed between E0-dE and E0+dE.
*
* Example: Source_flat(radius=0.1, dist=2, xw=.1, yh=.1, E0=14, dE=2)
*
* %P
* radius: (m)   Radius of circle in (x,y,0) plane where neutrons
*               are generated.
* dist:   (m)   Distance to target along z axis.
* xw:     (m)   Width(x) of target
* yh:     (m)   Height(y) of target
* E0:     (meV) Mean energy of neutrons.
* dE:     (meV) Energy spread of neutrons.
* Lambda0 (AA)  Mean wavelength of neutrons.
* dLambda (AA)  Wavelength spread of neutrons.
* flux    (1/(s*cm**2*st)) Energy integrated flux
*
* %E
*******************************************************************************/

DEFINE COMPONENT Source_simple
DEFINITION PARAMETERS ()
SETTING PARAMETERS (radius, dist, xw, yh, E0=0, dE=0, Lambda0=0, dLambda=0, flux=1)
OUTPUT PARAMETERS ()
STATE PARAMETERS (x,y,z,vx,vy,vz,t,s1,s2,p)
DECLARE
%{
  double pmul, pdir;
%}
INITIALIZE
%{
  pmul=flux*PI*1e4*radius*radius/mcget_ncount();
%}
```

```
TRACE
%{
 double chi,E,Lambda,v,r, xf, yf, rf, dx, dy;

 t=0;
 z=0;

 chi=2*PI*rand01();                          /* Choose point on source */
 r=sqrt(rand01())*radius;                    /* with uniform distribution. */
 x=r*cos(chi);
 y=r*sin(chi);

 randvec_target_rect(&xf, &yf, &rf, &pdir,
        0, 0, dist, xw, yh, ROT_A_CURRENT_COMP);

 dx = xf-x;
 dy = yf-y;
 rf = sqrt(dx*dx+dy*dy+dist*dist);

 p = pdir*pmul;

 if(Lambda0==0) {
   E=E0+dE*randpm1();                        /*  Choose from uniform distribution */
   v=sqrt(E)*SE2V;
 } else {
   Lambda=Lambda0+dLambda*randpm1();
   v = K2V*(2*PI/Lambda);
 }

 vz=v*dist/rf;
 vy=v*dy/rf;
 vx=v*dx/rf;
%}

MCDISPLAY
%{
  magnify("xy");
  circle("xy",0,0,0,radius);
%}

END
```

Written by developers and possibly you!

Generated c-code

```
/* Automatically generated file. Do not edit.
 * Format:     ANSI C source code
 * Creator:    McStas <http://neutron.risoe.dk>
 * Instrument: My_Instrument.instr (My_Instrument)
 * Date:       Sat Apr  9 15:27:56 2005
 */


/* THOUSANDS of lines removed here.... */

  /* TRACE Component Source. */
  SIG_MESSAGE("Source (Trace)");
  mcDEBUG_COMP("Source")
  mccoordschange(mcposrSource, mcrotrSource,
    &mcnlx, &mcnly, &mcnlz,
    &mcnlvx, &mcnlvy, &mcnlvz,
    &mcnlt, &mcnlsx, &mcnlsy);
  mcDEBUG_STATE(mcnlx, mcnly, mcnlz, mcnlvx, mcnlvy, mcnlvz,mcnlt,mcnlsx,mcnlsy, mcnlp)
#define x mcnlx
#define y mcnly
#define z mcnlz
#define vx mcnlvx
#define vy mcnlvy
#define vz mcnlvz
#define t mcnlt
#define s1 mcnlsx
#define s2 mcnlsy
#define p mcnlp
  STORE_NEUTRON(2,mcnlx, mcnly, mcnlz, mcnlvx,mcnlvy,mcnlvz,mcnlt,mcnlsx,mcnlsy, mcnlsz, mcnlp);
  mcScattered=0;
  mcNCounter[2]++;
#define mccompcurname Source
#define mccompcurindex 2
{   /* Declarations of SETTING parameters. */
MCNUM radius = mccSource_radius;
MCNUM dist = mccSource_dist;
MCNUM xw = mccSource_xw;
MCNUM yh = mccSource_yh;
MCNUM E0 = mccSource_E0;
MCNUM dE = mccSource_dE;
MCNUM Lambda0 = mccSource_Lambda0;
MCNUM dLambda = mccSource_dLambda;
MCNUM flux = mccSource_flux;
#line 58 "Source_simple.comp"
{
 double chi,E,Lambda,v,r, xf, yf, rf, dx, dy;

 t=0;
 z=0;

 chi=2*PI*rand01();                         /* Choose point on source */
 r=sqrt(rand01())*radius;                   /* with uniform distribution. */
 x=r*cos(chi);
 y=r*sin(chi);

 randvec_target_rect(&xf, &yf, &rf, &pdir,
       0, 0, dist, xw, yh, ROT_A_CURRENT_COMP);
```

Written by mcstas!

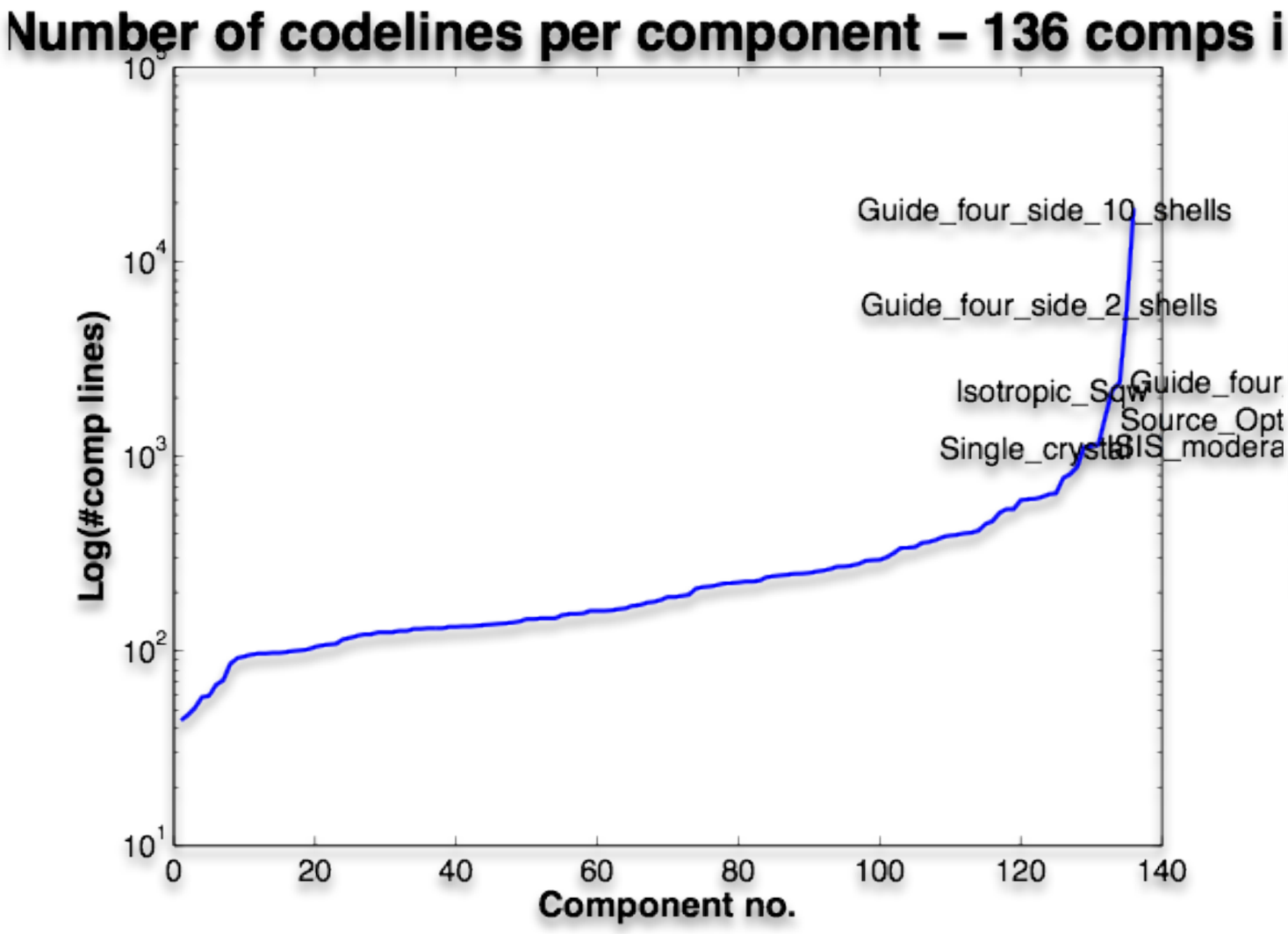
McStas is a (pre)compiler!

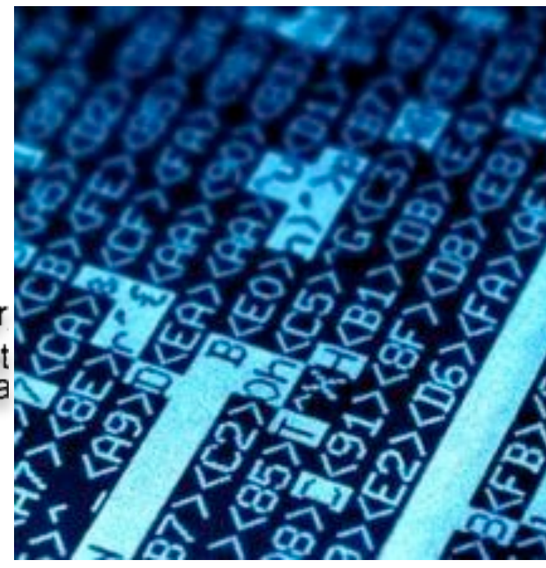
Input is .comp and .instr files + runtime functions for e.g. random numbers

Output is a single c-file, which can be compiled using e.g. gcc.

Can take input arguments if needed.

Writing new comps or understanding existing is not that complex...





Including user contribs

- Well-developed community support
  - 30-40% of existing and new additions are from users
  - No direct refereeing of the code, but these requirements:
    - At least one test-instrument
    - Meaningful documentation headers (in-code docs)
  - Contributions go in dedicated contrib/ section of library
- Natural life-cycle of contrib's
  - Bug-fixes are applied both by contributor and developers
  - If contributor becomes unavailable either:
    - Many users of comp: Promote to official components, e.g. in optics/
    - Few/no users of comp: Move to obsolete/ until next major release

Advanced language features

- Macros and tricks for your instrument...

DECLARE / INITIALIZE

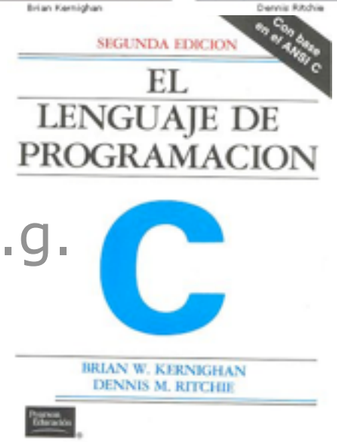
- Use the DECLARE section define user variables and functions.
  - DECLARE %{
  - double myvar;
  - %}

- Use INITIALIZE for initialization of user variables and calculations.
  - INITIALIZE %{
  - myvar = sqrt(PI*input_var)*rand01();
  - %}

- - Both use normal c-syntax.

- BEWARE: (example) What you do in the c-style areas is c-standard, e.g. trigonometric functions from math.h use radians! - McStas placement specifiers work in degrees, etc...

K & R

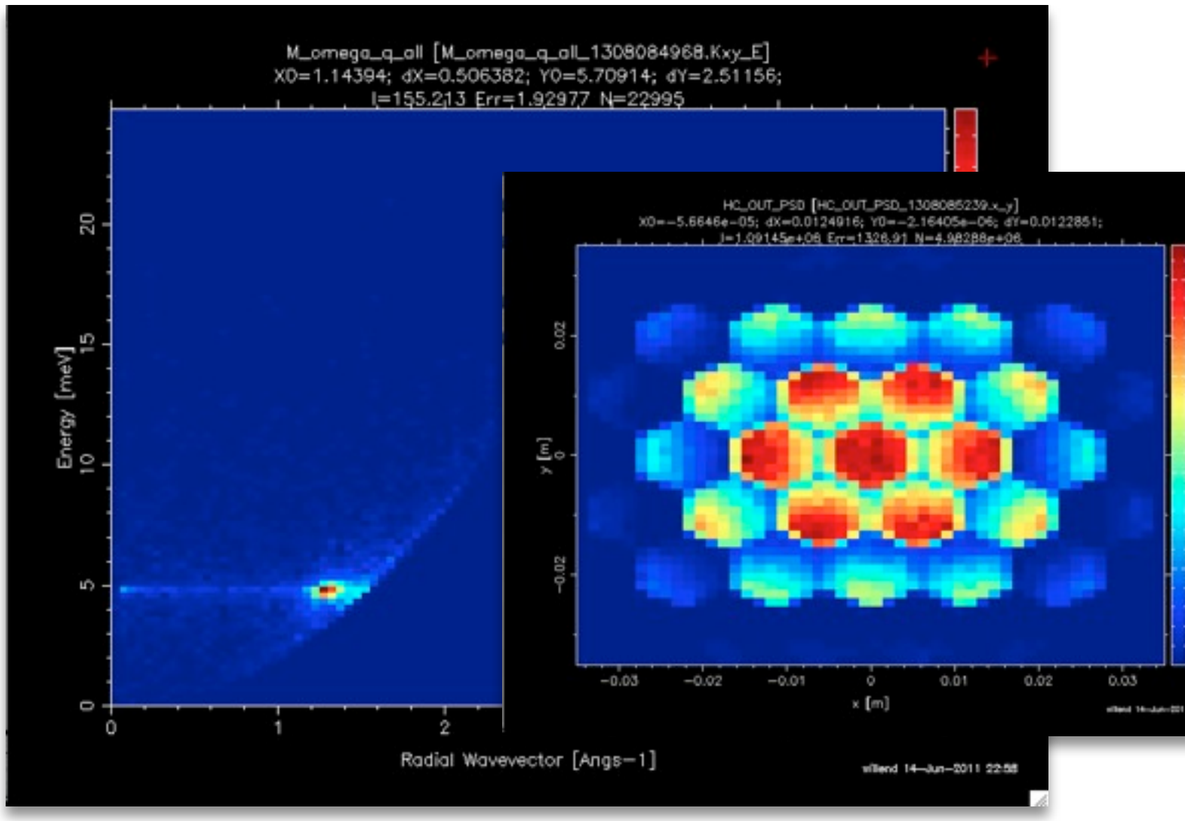


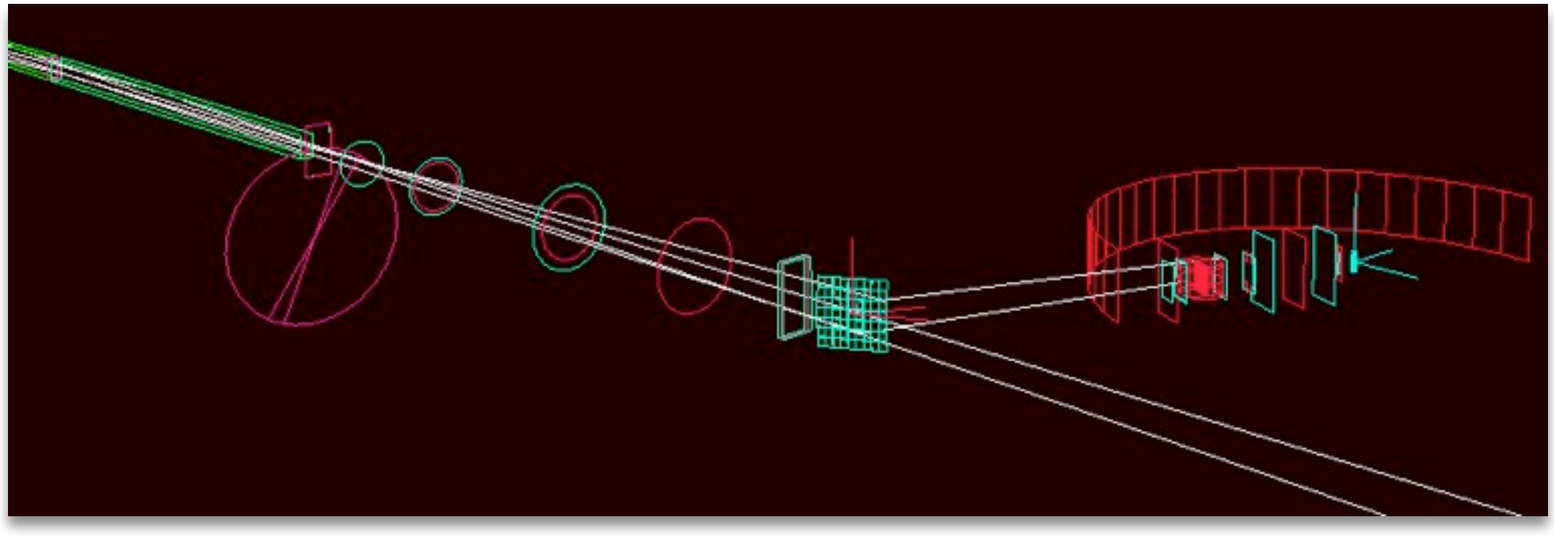
Syntax in one, complex view...

{SPLIT} COMPONENT name = comp(parameters) {WHEN condition}
 AT (...) [RELATIVE [reference|PREVIOUS] | ABSOLUTE]
 {ROTATED {RELATIVE [reference|PREVIOUS] | ABSOLUTE} }
 {GROUP group_name}
 {EXTEND C_code}
 {JUMP [reference|PREVIOUS|MYSELF|NEXT] [ITERATE number_of_times | WHEN condition] }

Example suite: 7 TOF spectrometers:

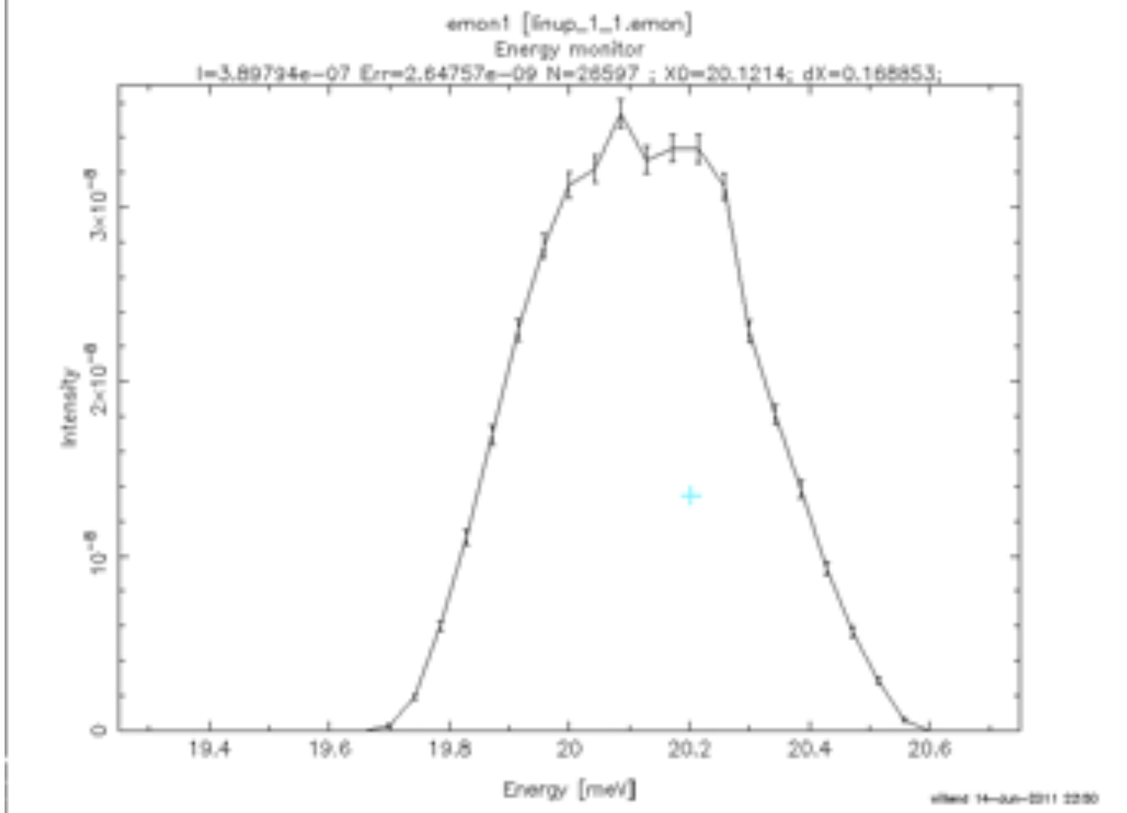
- ESS_IN5_reprate.instr
- ILL_BRISP.instr (Small-angle)
- ILL_H15_IN6.instr
- ILL_H16_IN5.instr
- ISIS_Hetfull.instr
- PSI_Focus.instr
- templateTOF.instr

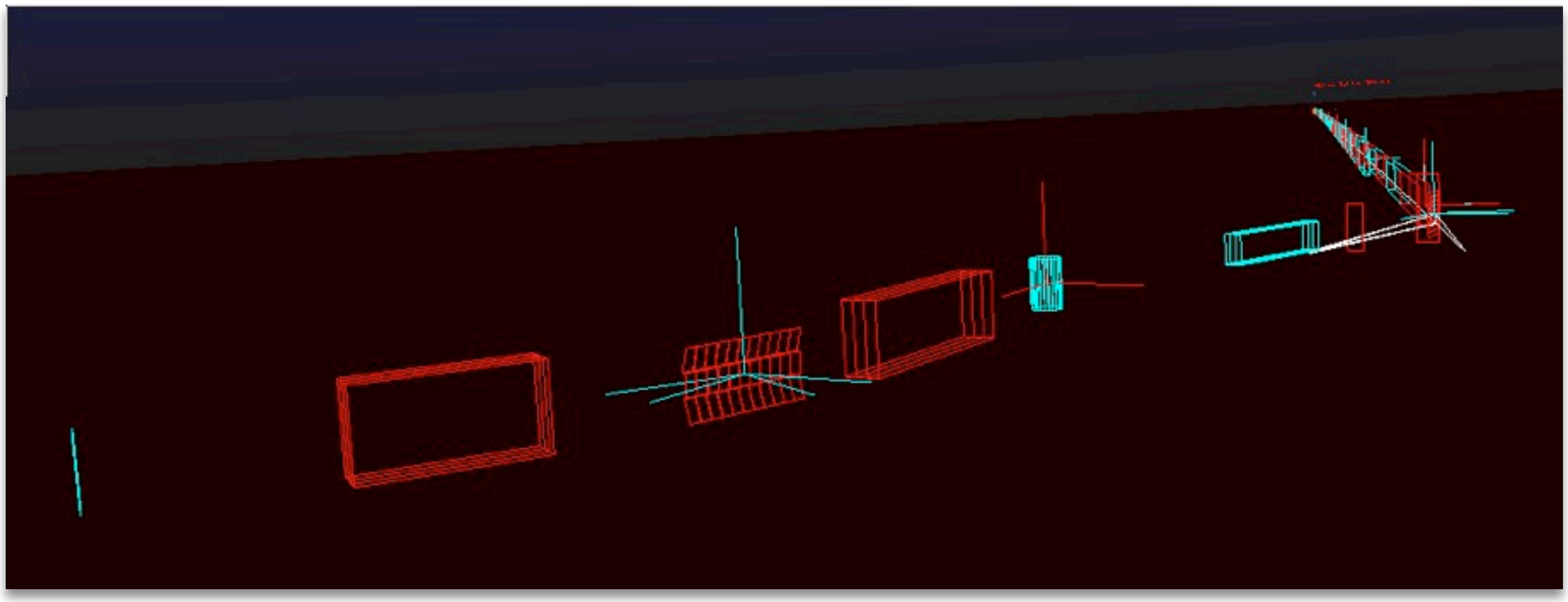




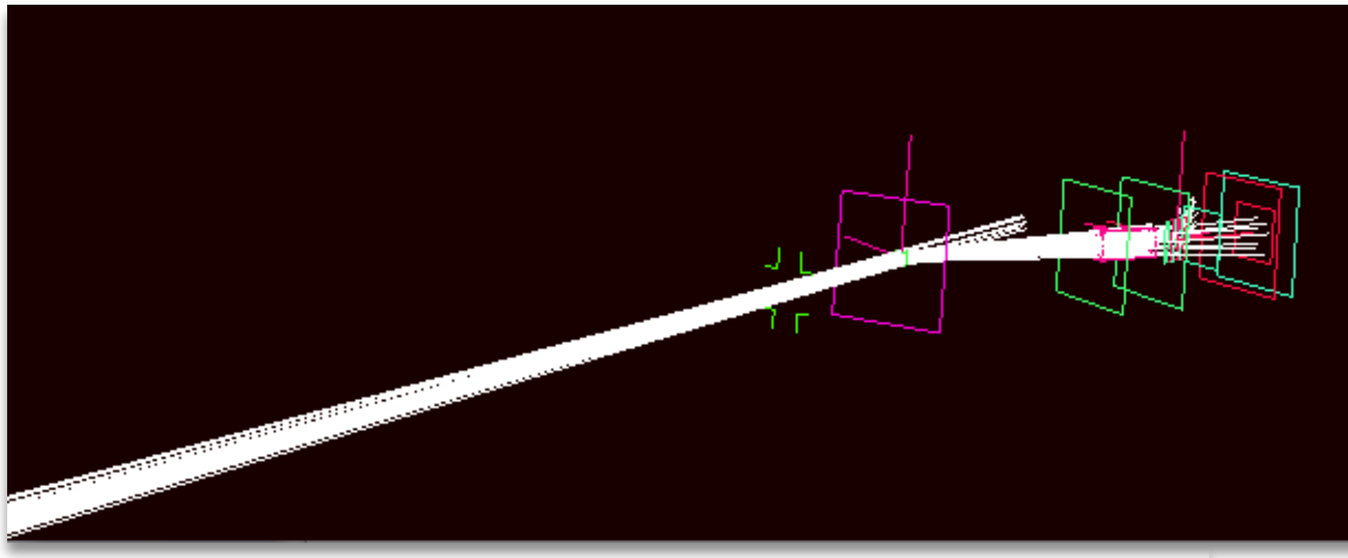
Example suite: 5 TAS

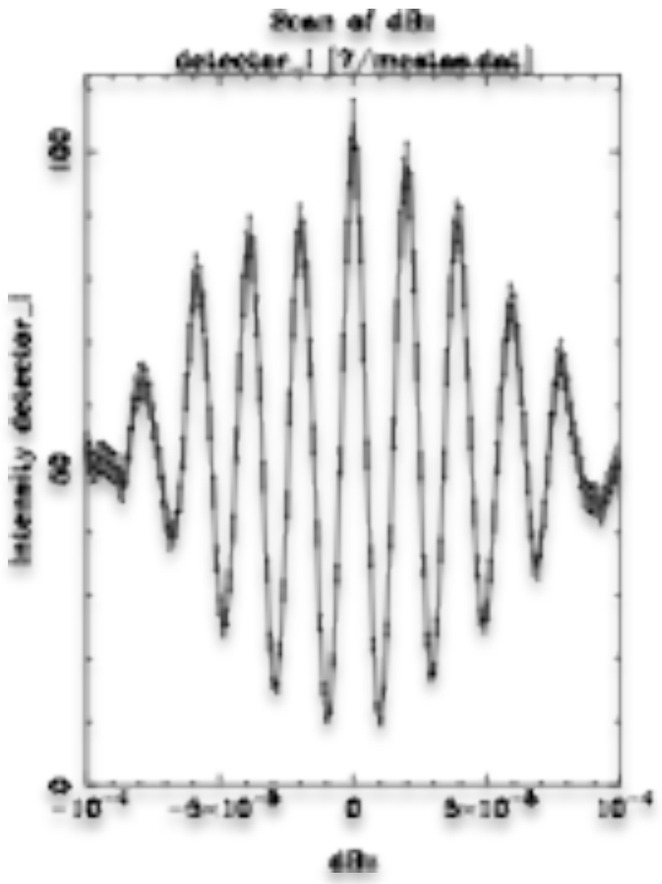
- ILL_H142_IN12.instr
- ILL_H25_IN22.instr
- h8_test.instr
- templateTAS.instr
- linup-1.instr (Risø TAS 1)
- linup-2.instr
- linup-3.instr
- linup-4.instr
- linup-5.instr
- linup-6.instr
- linup-7.instr

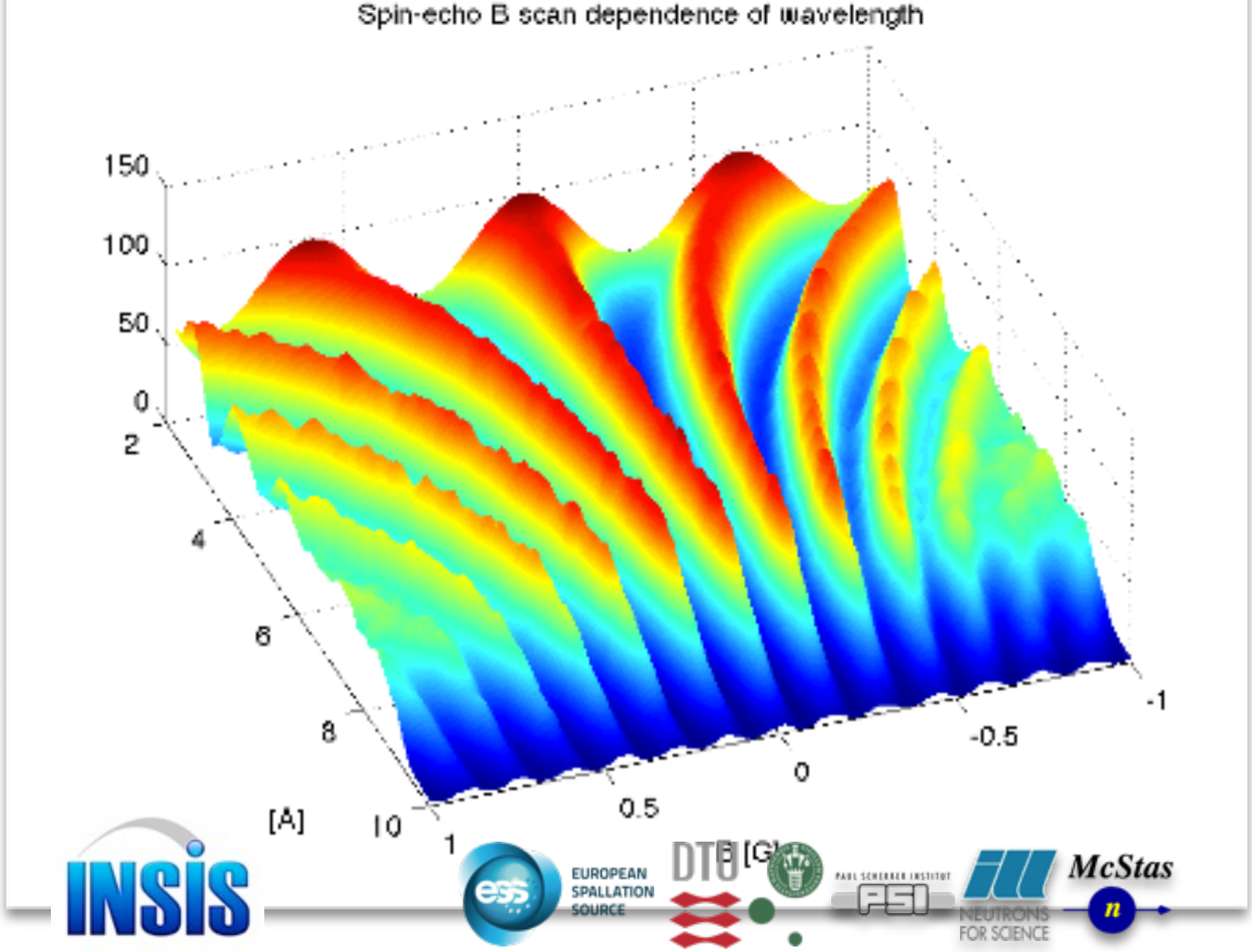




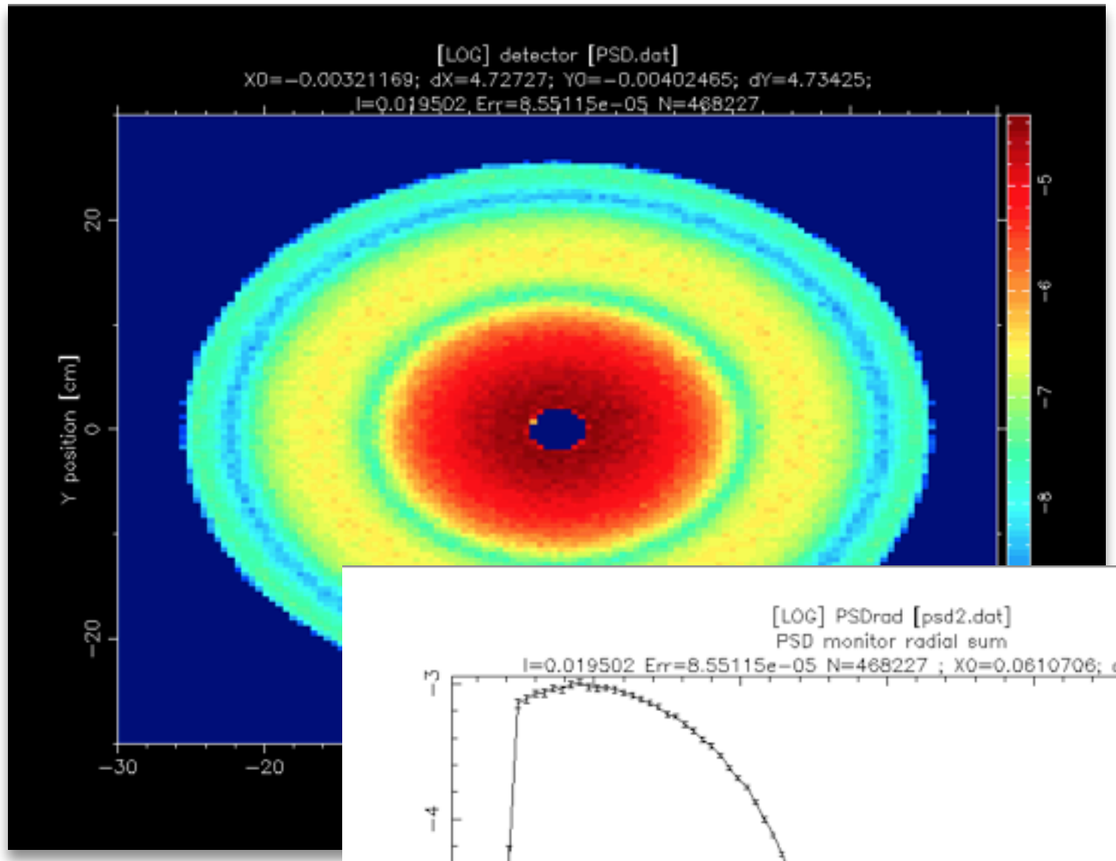
Example suite: 1 Hybrid spectrometer + 1 Spin-echo

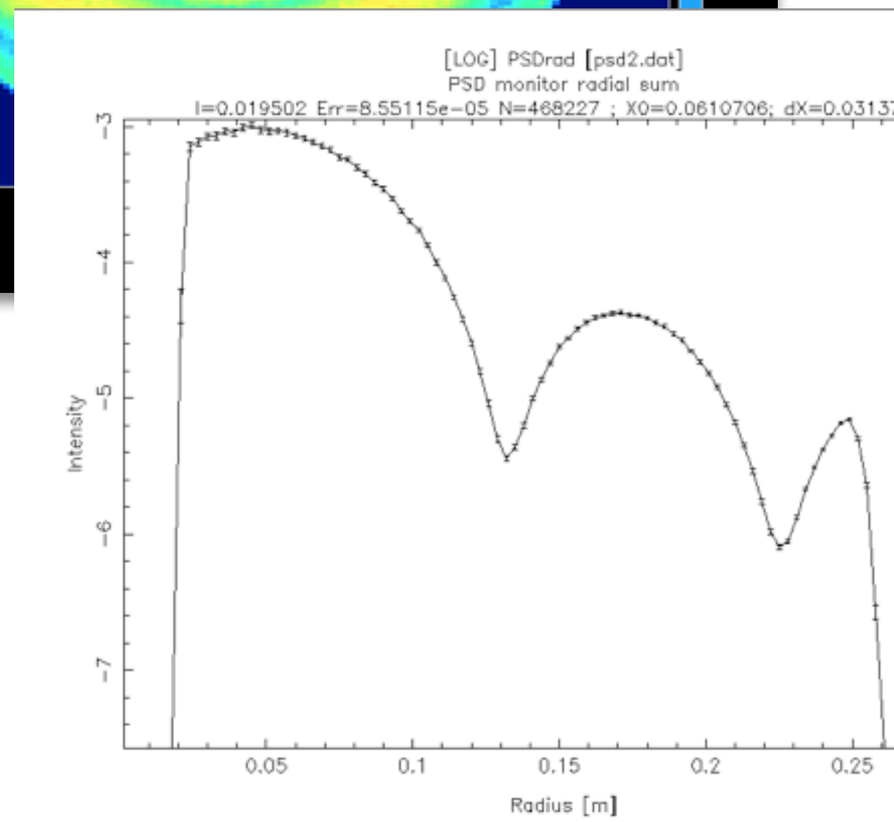


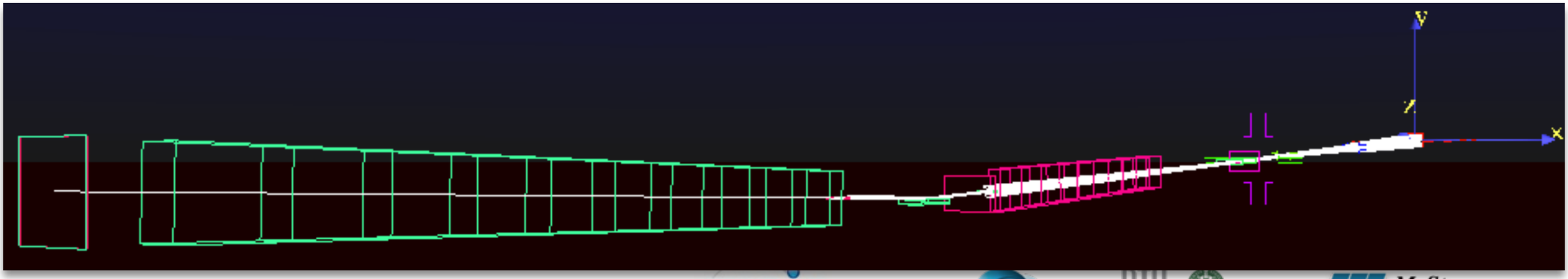




Example suite:
Large scale structures

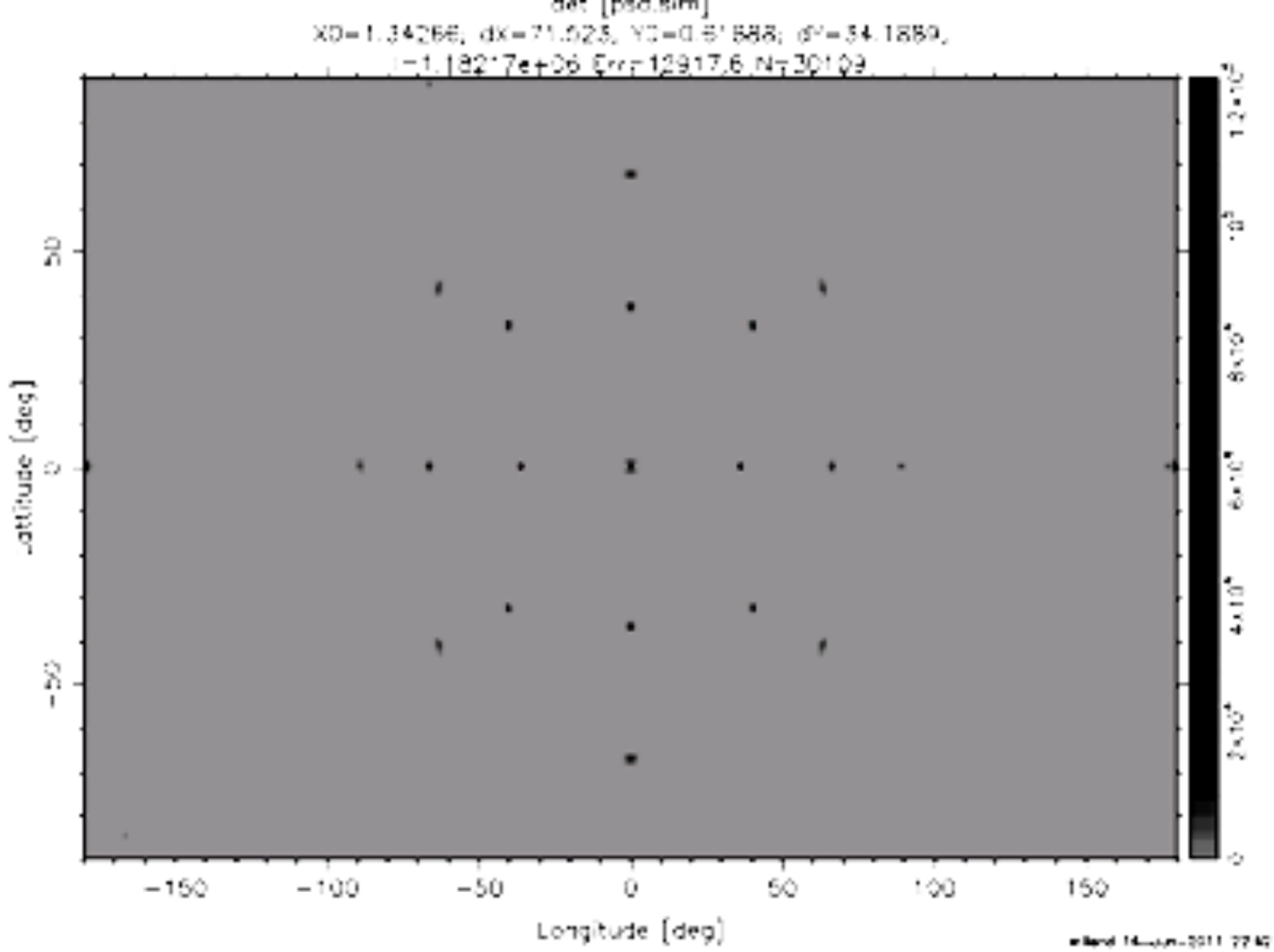


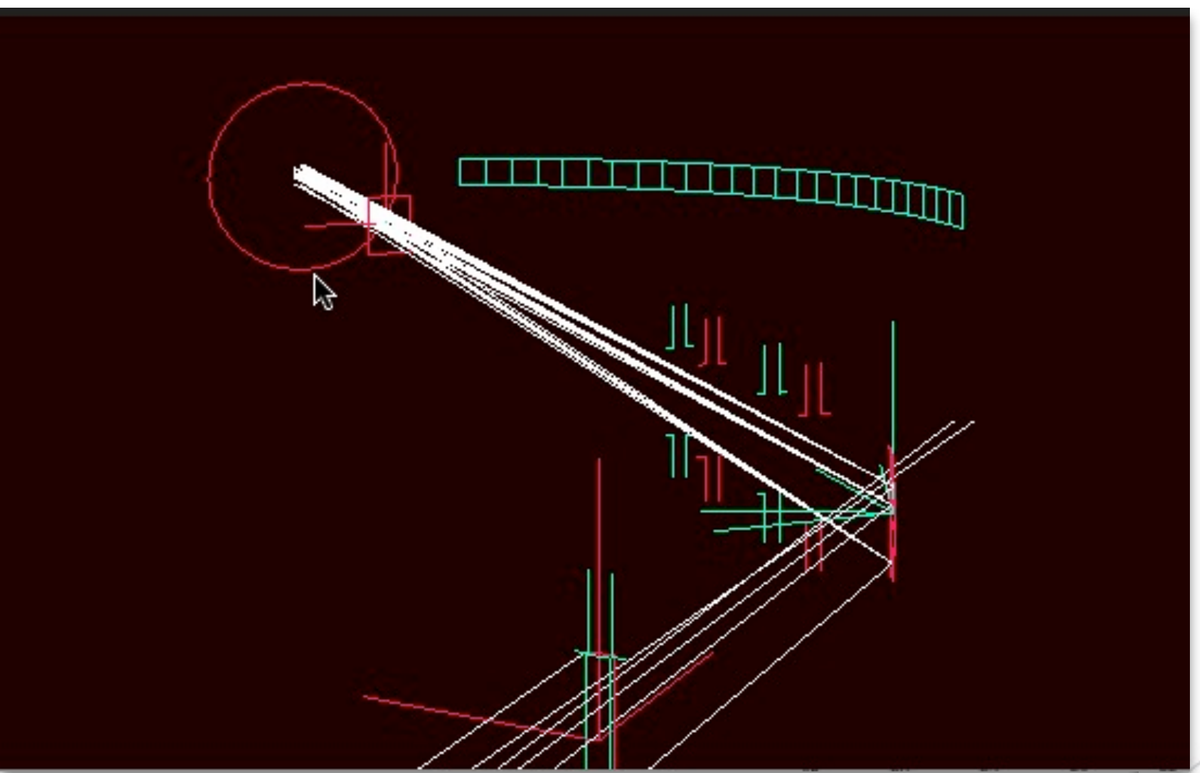


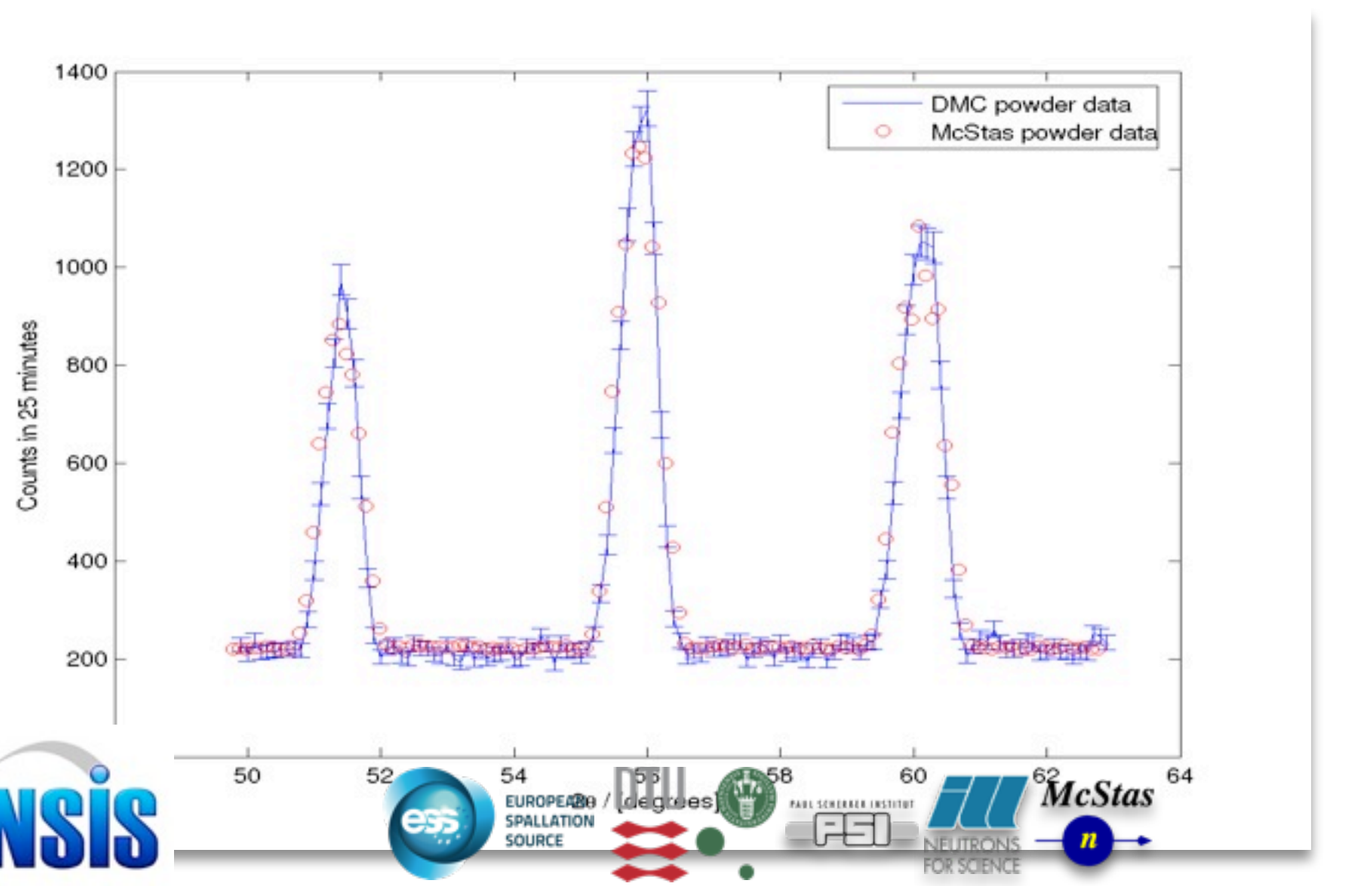


Example suite: Diffractometers

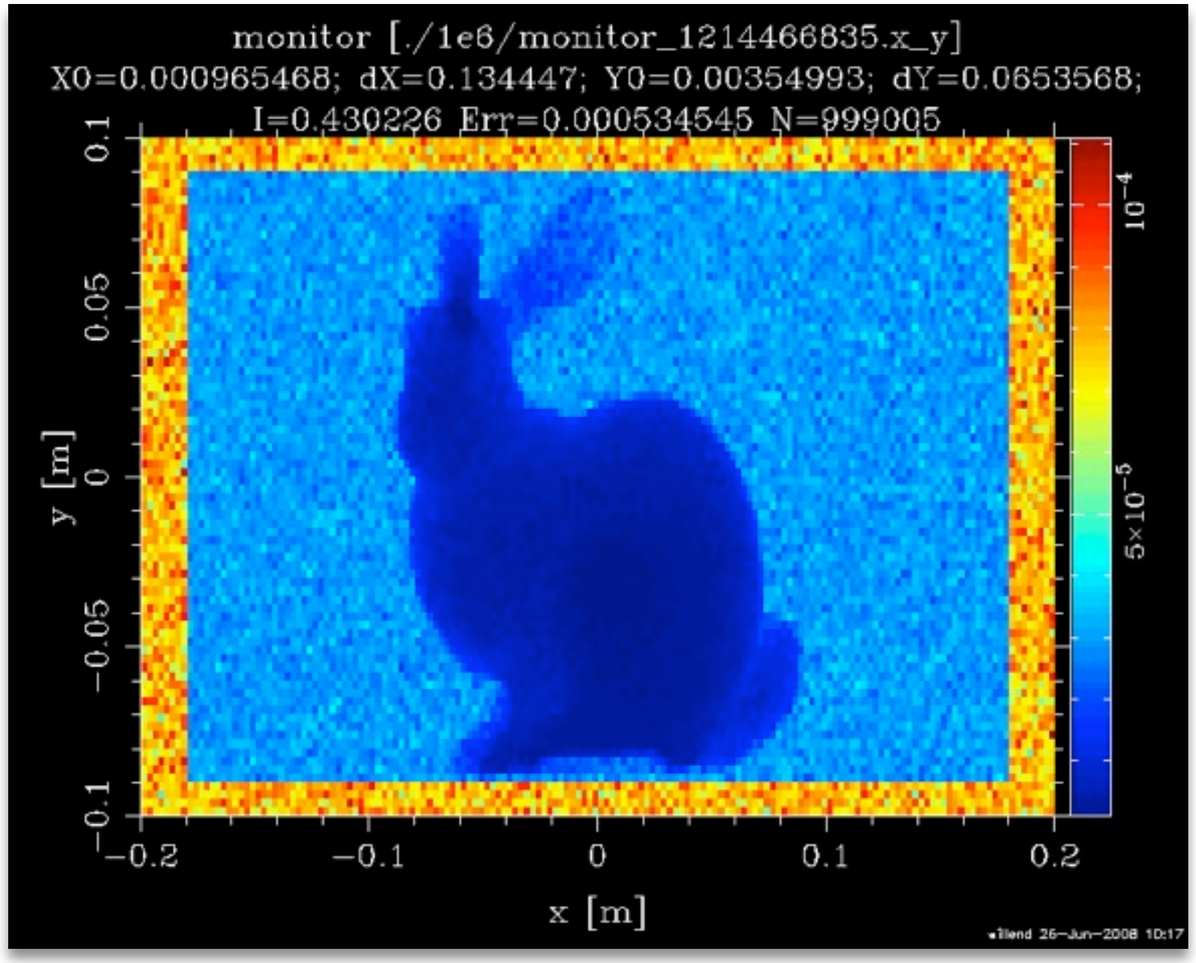
- ILL_D1A.instr
- PSI_DMC.instr
- templateDIFF.instr
- templateLaue.instr

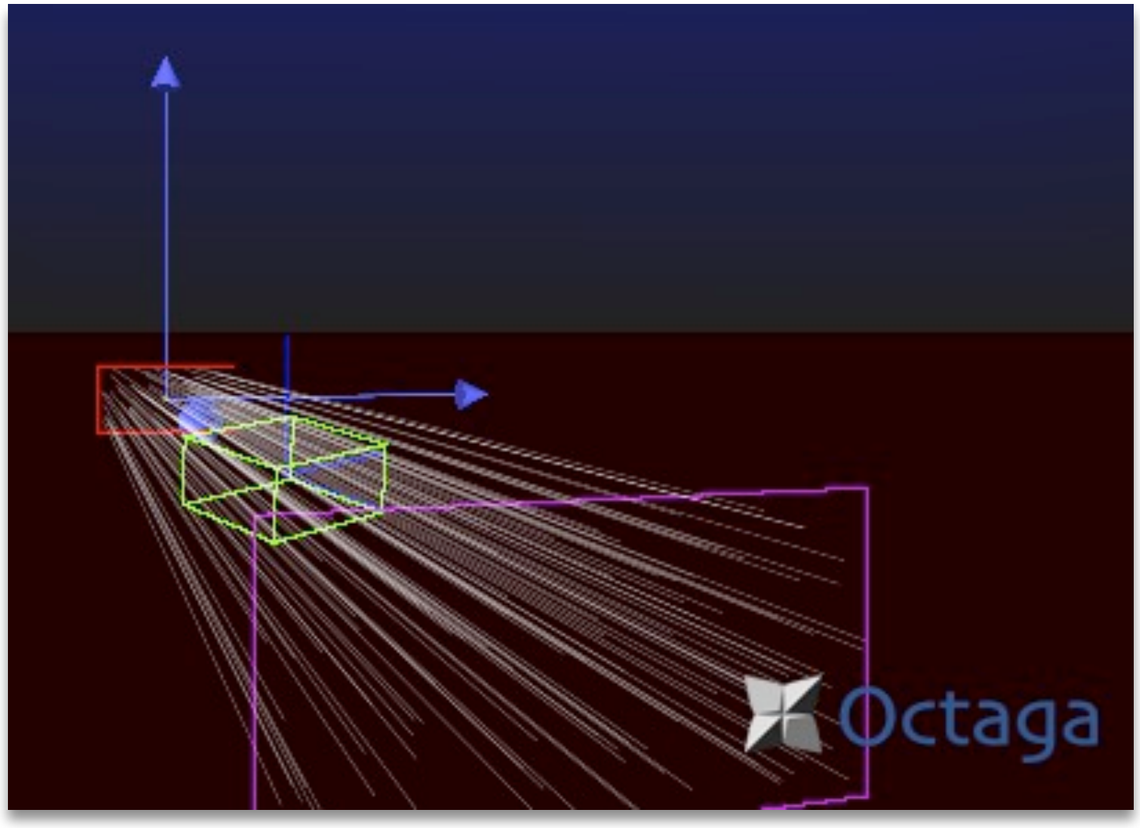


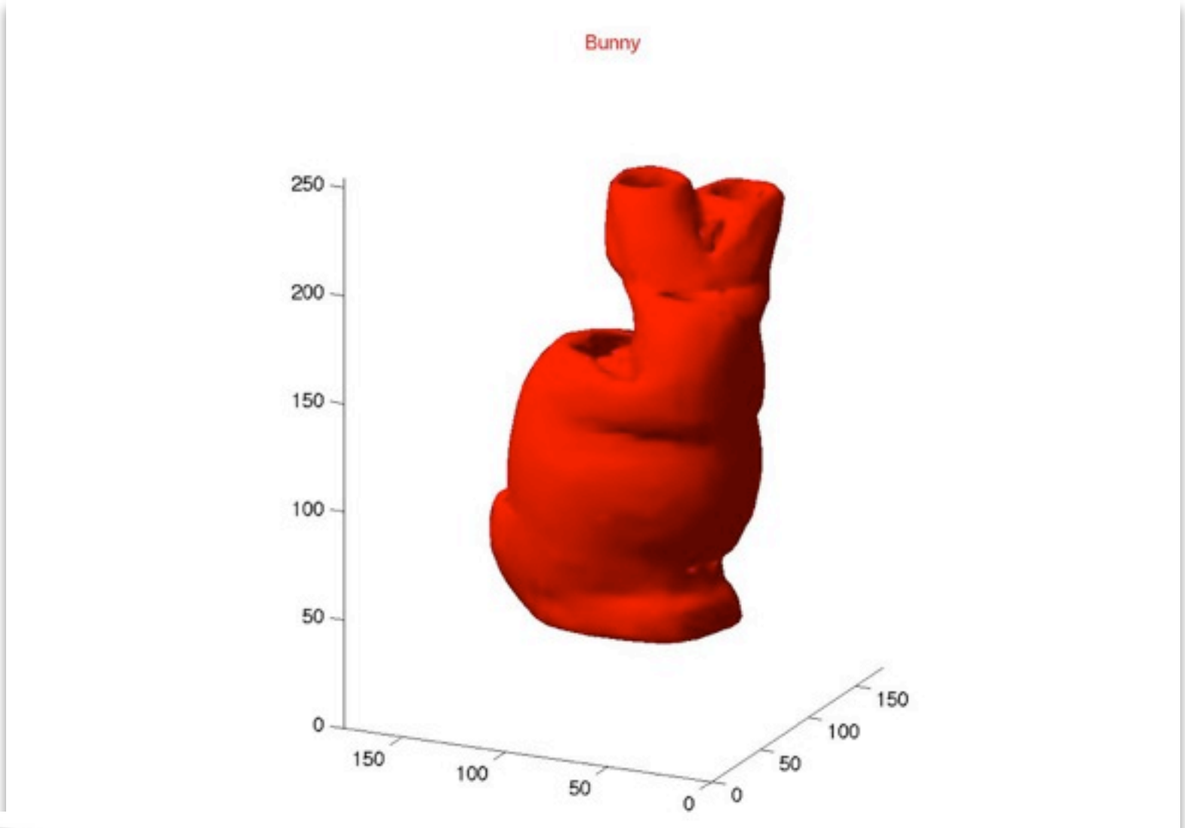




Example suite: Imaging







Documentation

- Basic use info is available inside comp & instr codes, extracted by perl to html

- 100+ page manuals documenting
  - Metalanguage
  - What is “under the hood”
  - Examples of practical use plus advanced features
  - Assumptions and algorithms applied in the components

- More than 70 example instruments

- Various tutorial and teach yourself solutions are available

Technique limitations / words of advice

- These codes all describe the “wanted” neutrons / tailor your beam
- Every code has unique features, advantages, disadvantages. If possible, choose the one where someone you trust has experience
- Less easy to discuss instrument backgrounds and spurions etc. but effort is going in this direction on the McStas team (concentric components, interfaces to the MCNPX code etc.)
- These codes can not be considered “black box” utilities, a lot of thinking / calculus required before, during, after simulation

Knowing more / continuing at home

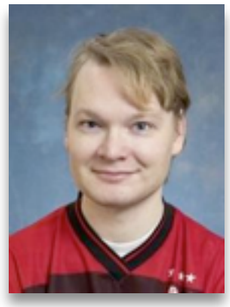
- All development teams are very dedicated and want to help, pass your problems on!

- McStas+VITESS teams often do schools/workshops together where you solve problems with one, the other or both codes. Exercises and code from a workshop in Ven 2010 is available here:
  - http://ven2010.essworkshop.org/storage/

- We will provide you with a take-home Linux Live DVD (ILL/NMI3) where several of the european codes are preinstalled

People




McStas




DTU PAUL SCHERRER INSTITUT PSI NEUTRONS FOR SCIENCE

INSIS

EUROPEAN SPALLATION SOURCE DTU PAUL SCHERRER INSTITUT PSI NEUTRONS FOR SCIENCE McStas

Enough Talk!
Let's see McStas run?