

McStas and other codes for neutron delivery and full instrument simulations

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McStas



PAUL SCHERRER INSTITUT

PSI

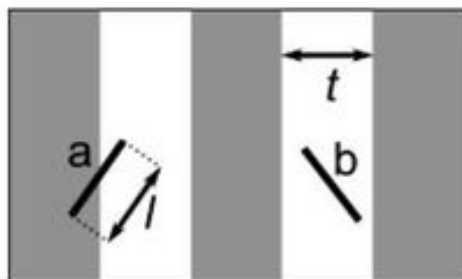


EUROPEAN
SPALLATION
SOURCE

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

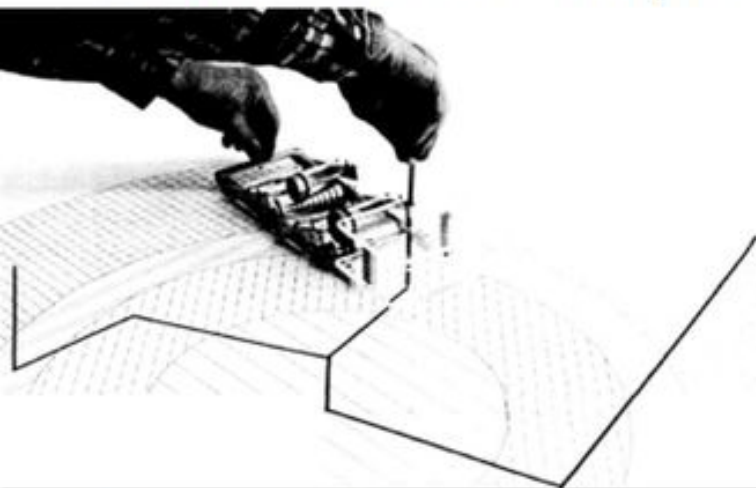
Monte Carlo techniques

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

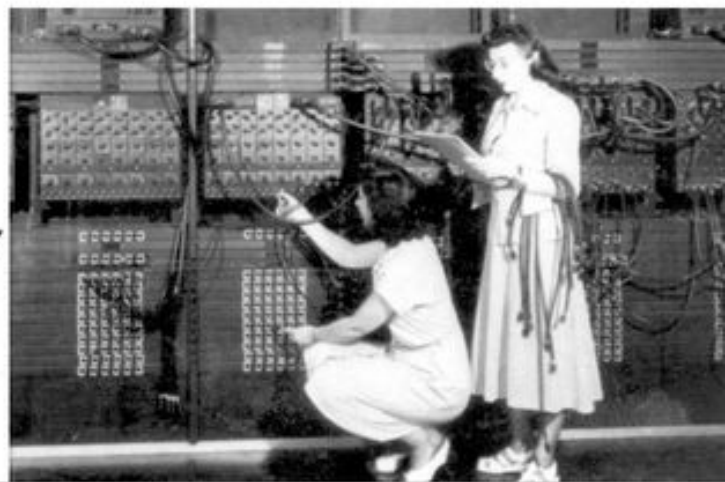


- Notable fathers: John v. Neumann Stanislaw Ulam Nicholas Metropolis
- Named “Monte Carlo” after Ulam’s fathers frequent visits to the Monte Carlo casino in Las Vegas
- Initially “implemented” by letting large numbers of women use tabularized random numbers and hand calculators for individual particle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

Monte Carlo techniques



• FERMIAAC



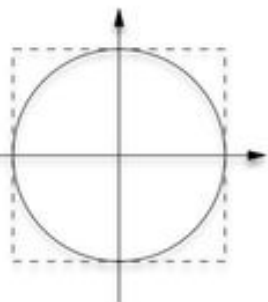
ENIAC

Monte Carlo techniques

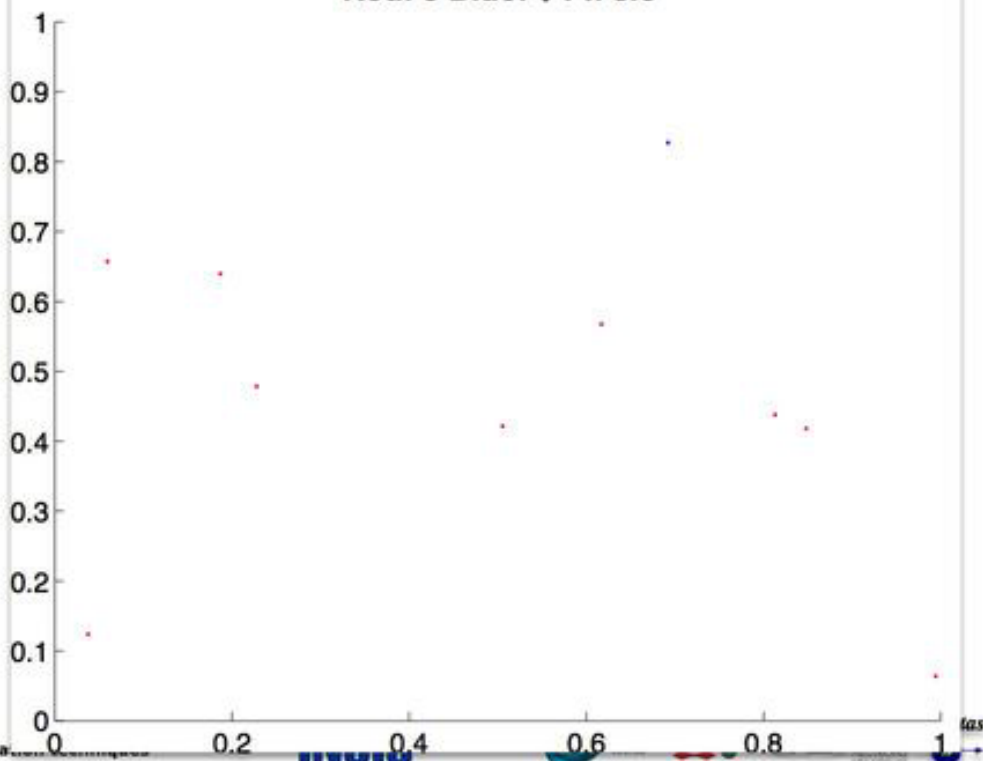
- Estimating Pi:

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

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

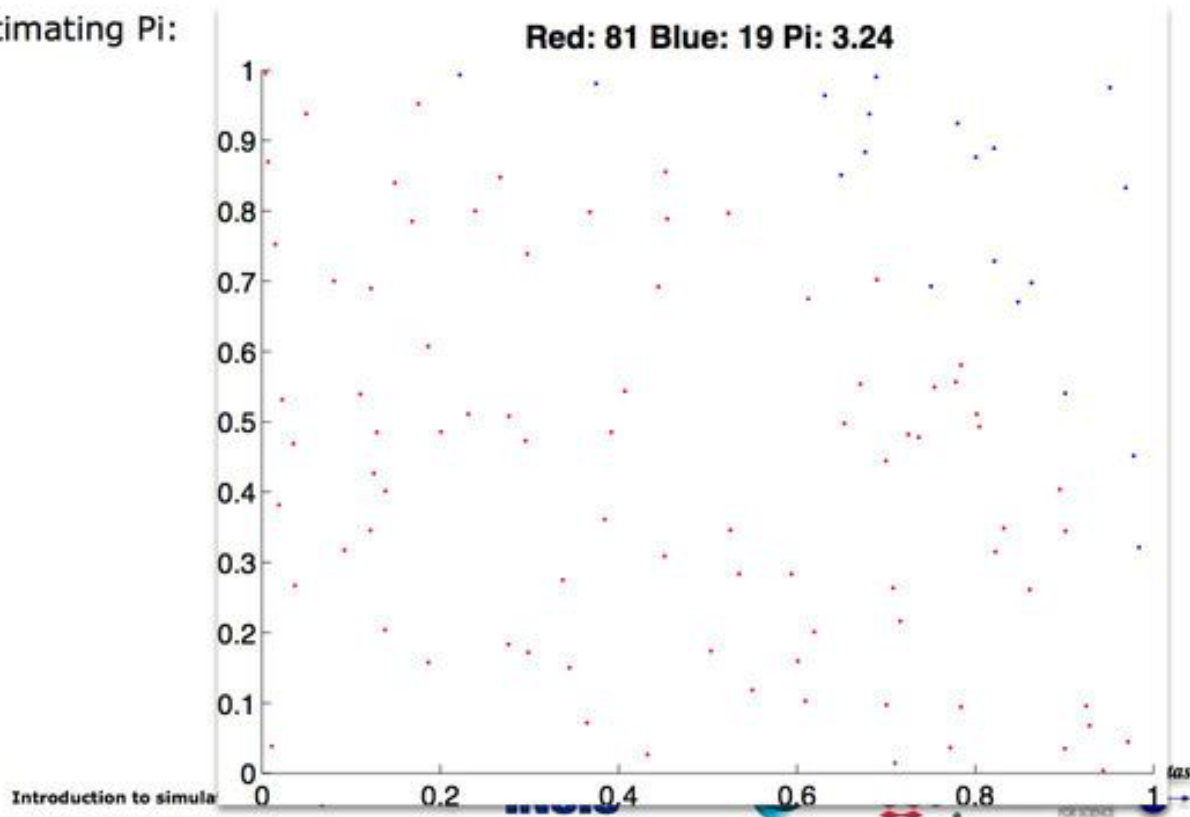


Red: 9 Blue: 1 Pi: 3.6



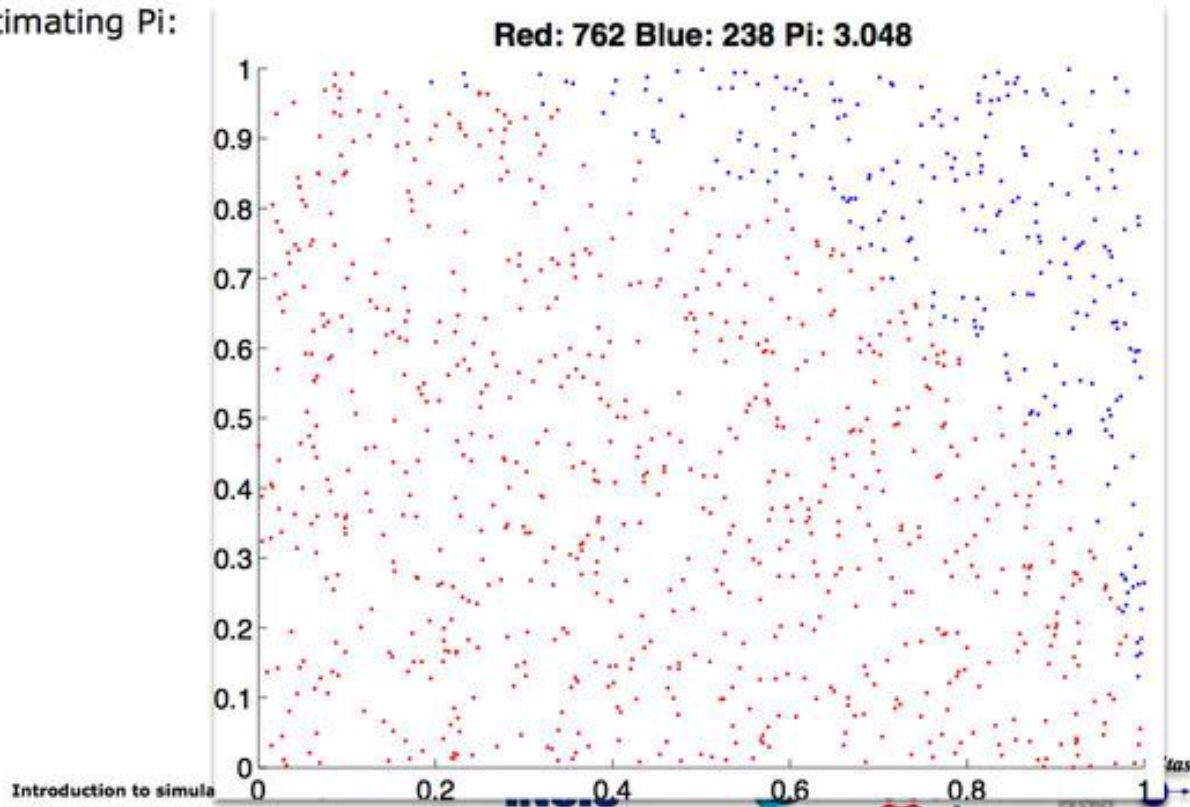
Monte Carlo techniques

- Estimating Pi:



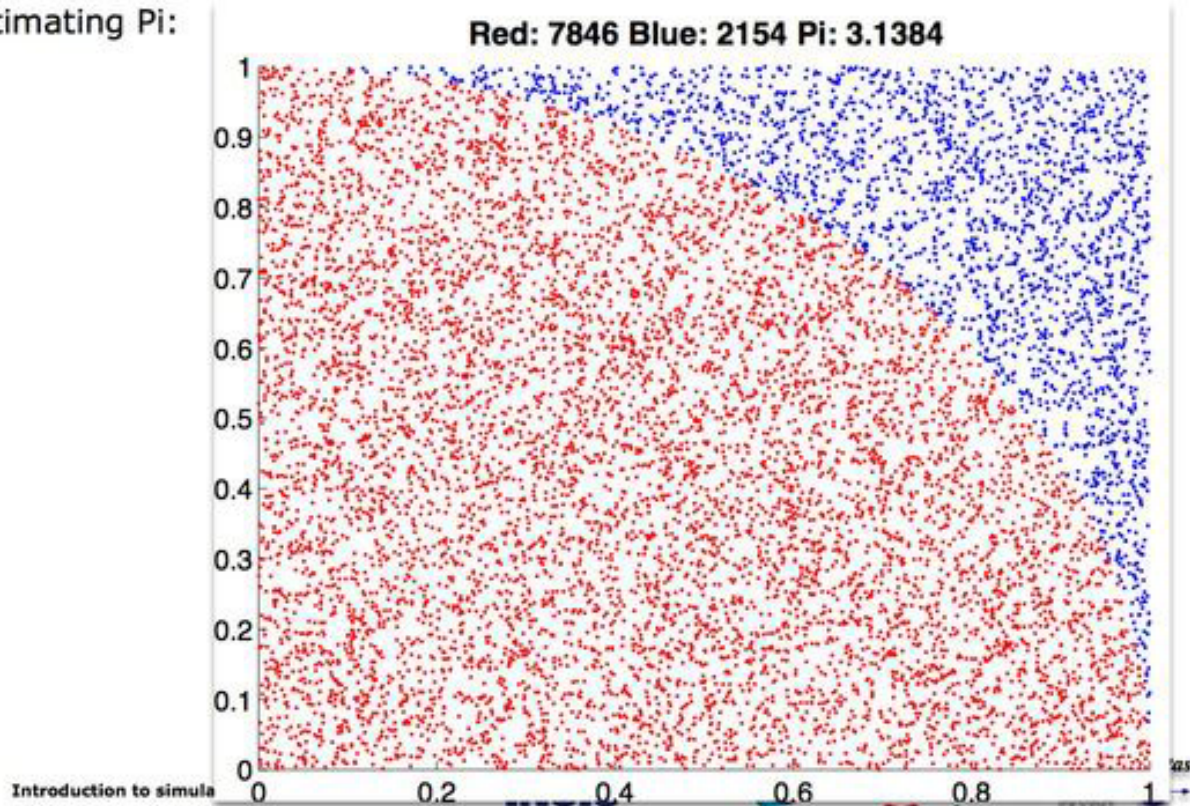
Monte Carlo techniques

- Estimating Pi:



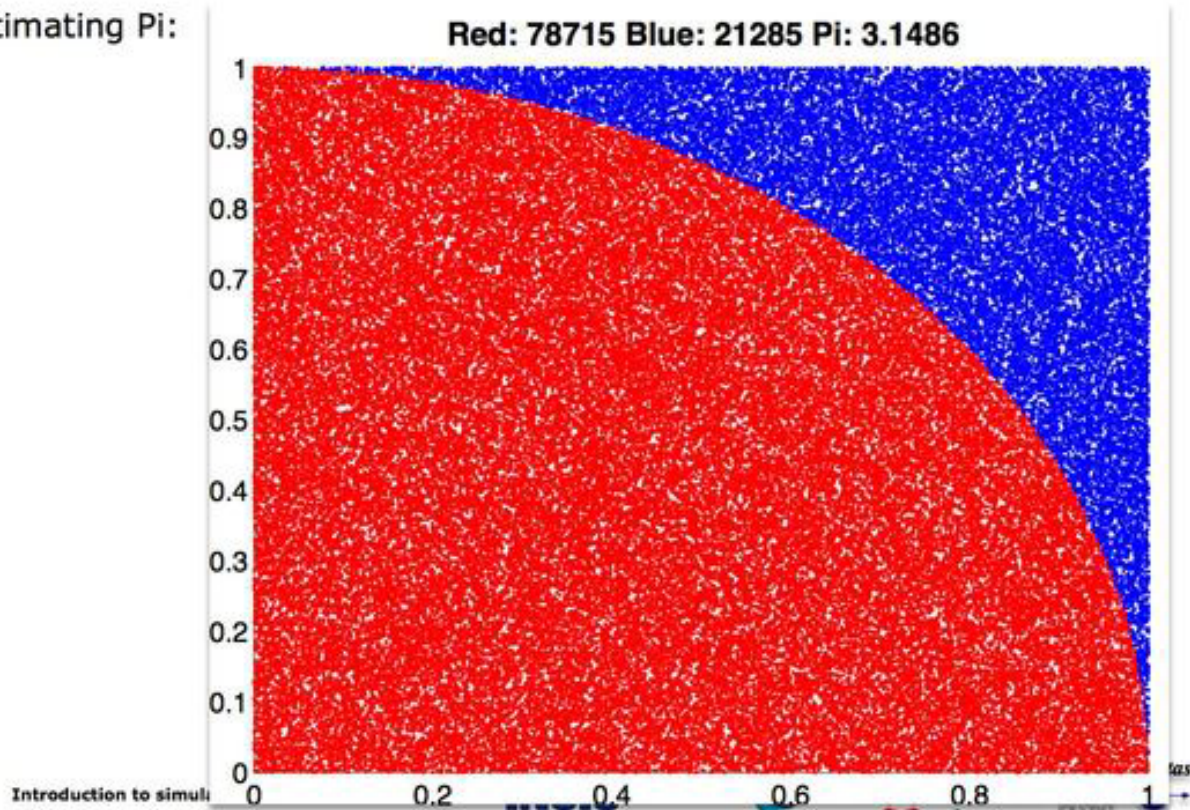
Monte Carlo techniques

- Estimating Pi:



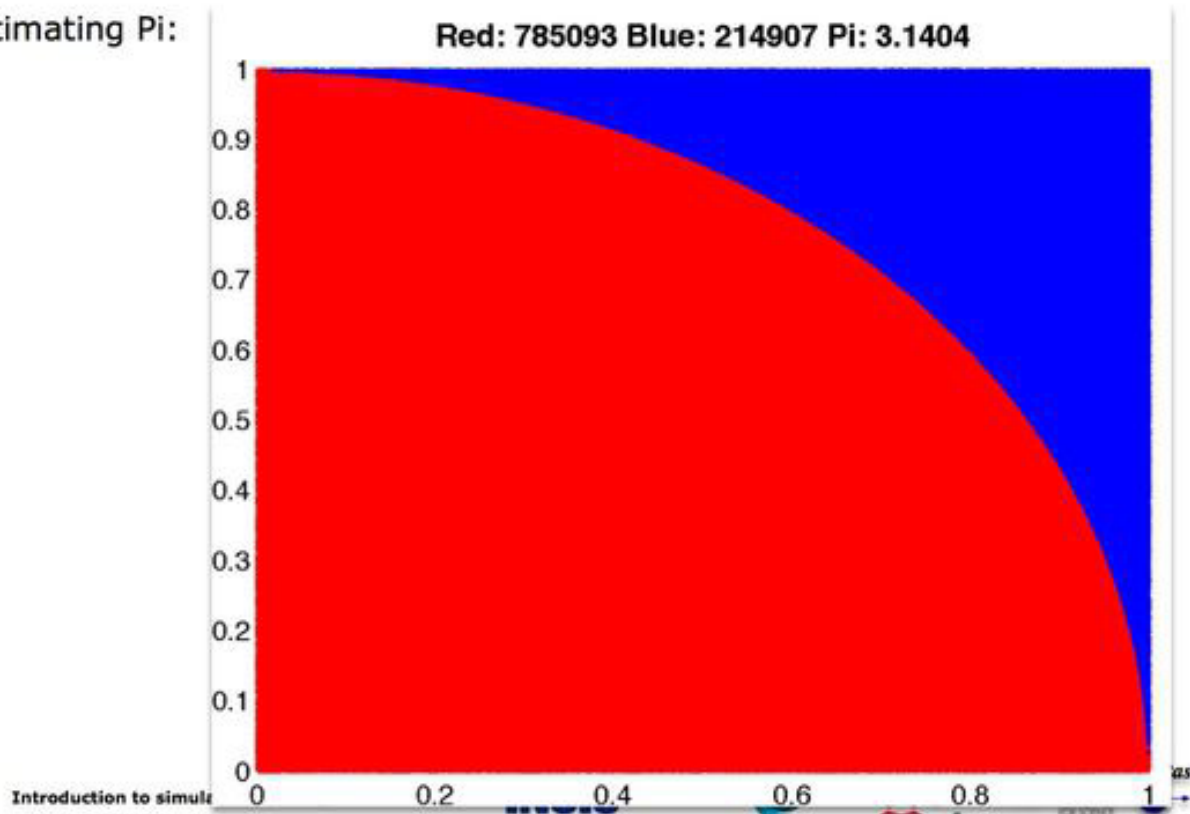
Monte Carlo techniques

- Estimating Pi:



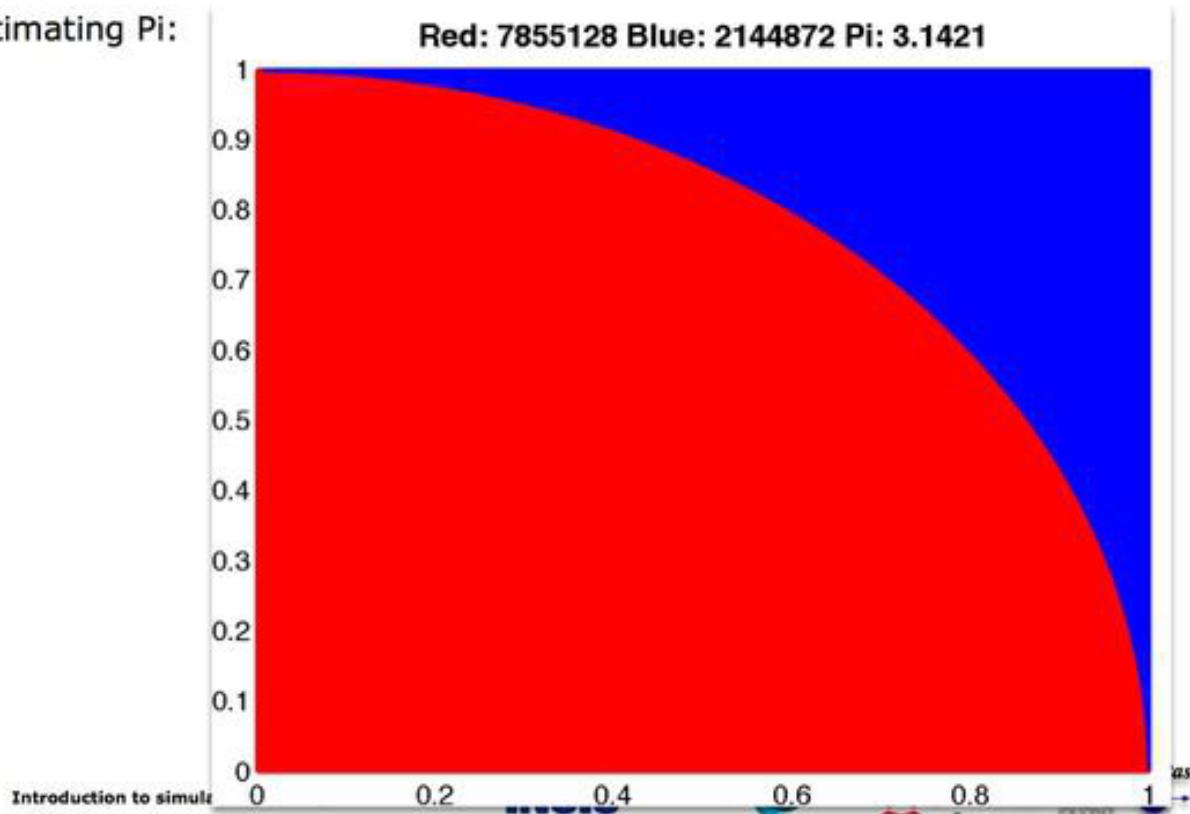
Monte Carlo techniques

- Estimating Pi:



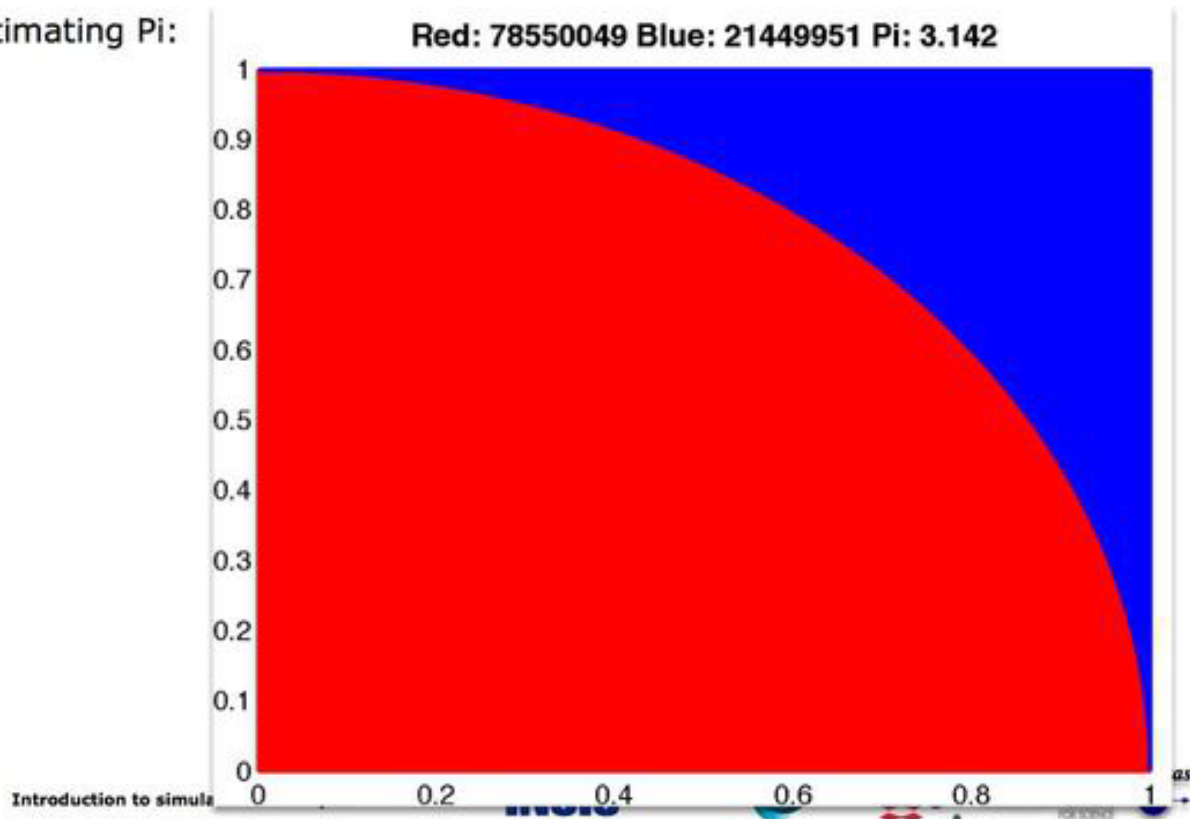
Monte Carlo techniques

- Estimating Pi:



Monte Carlo techniques

- Estimating Pi:

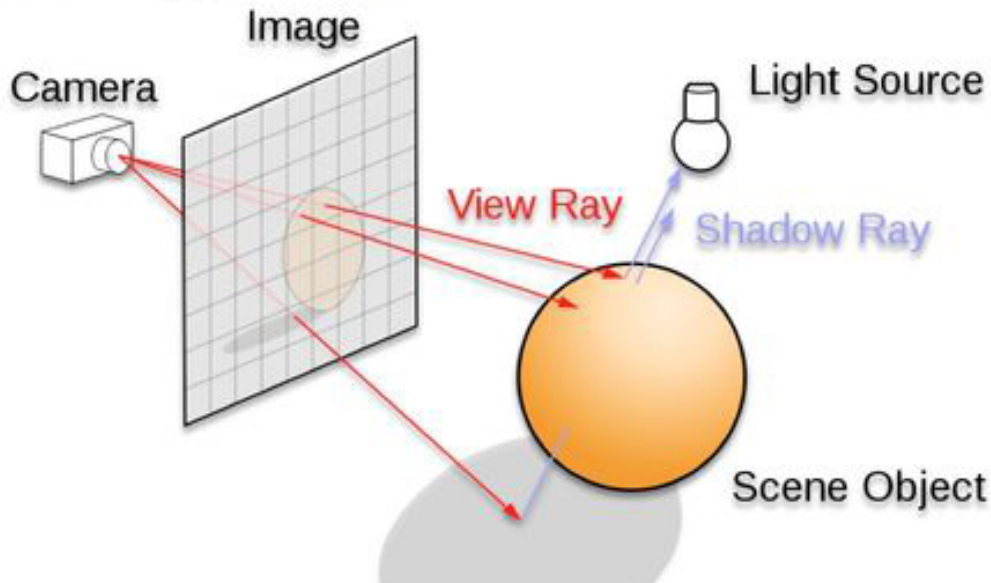


Monte Carlo techniques

- 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



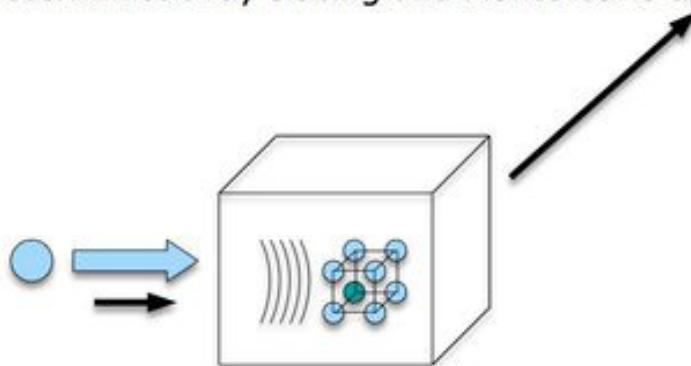
Ray-tracing methods



- 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 used 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?)
 - Unknown 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
- Unknown 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” platform 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
 - Excellent 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 intrinsically 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

- Flexible, general simulation utility for neutron scattering experiments.
- Original design for Monte carlo Simulation of triple axis spectrometers
- Developed at DTU Physics, ILL, PSI, Uni CPH
- V. 1.0 by K Nielsen & K Lefmann (1998) RISØ
- Currently 2.5+1 people full time plus students



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

• Development

• V. 1.0 b

• Current



- Synergy, knowledge transfer, shared infrastructure

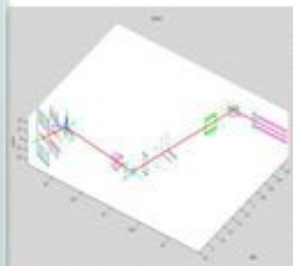
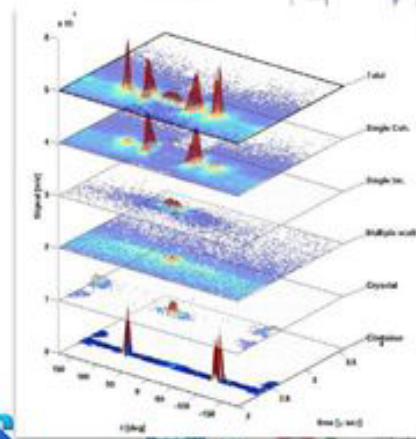
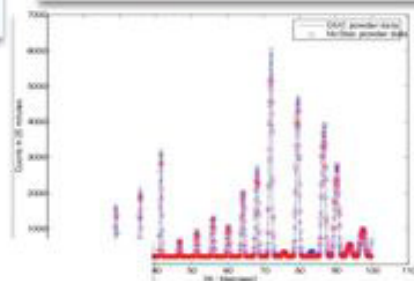
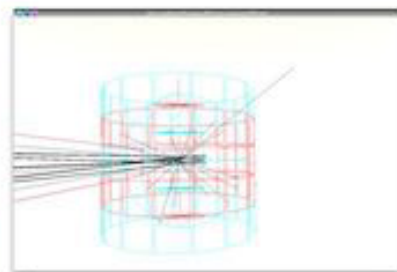
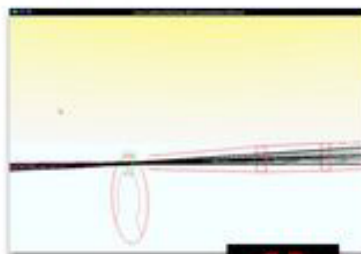
McStas Introduction



What is McStas used for?

- Instrumentation
- Virtual experiments
- Data analysis
- Teaching

(KU, DTU)

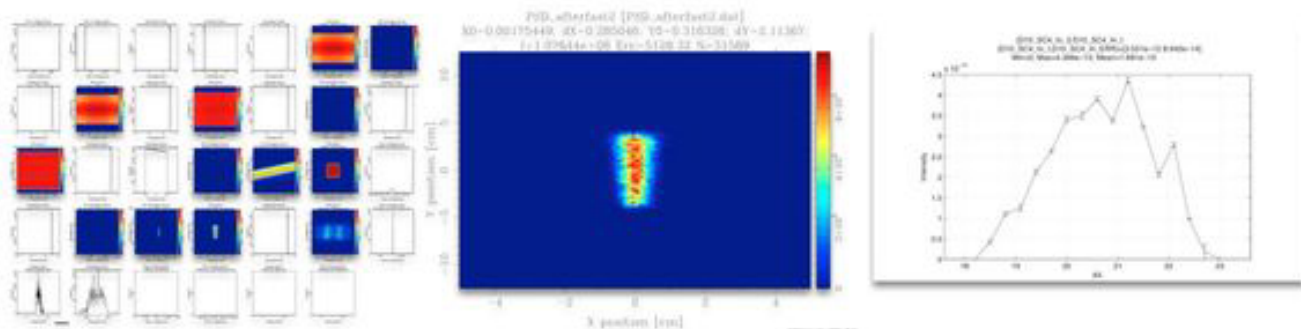
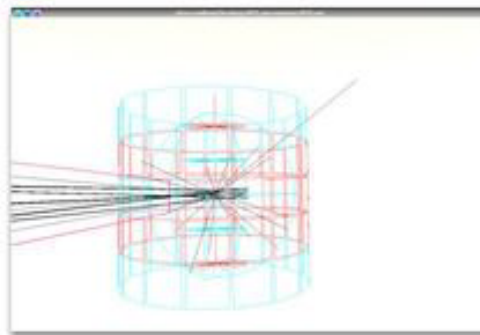
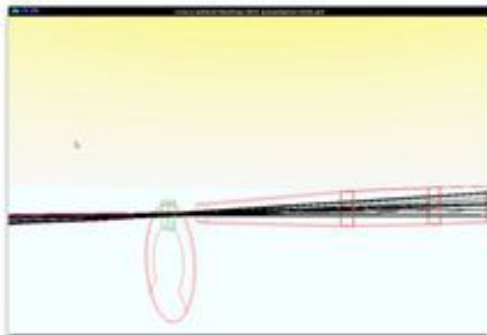


INSIS



Instrumentation

- Design and optimization of instruments



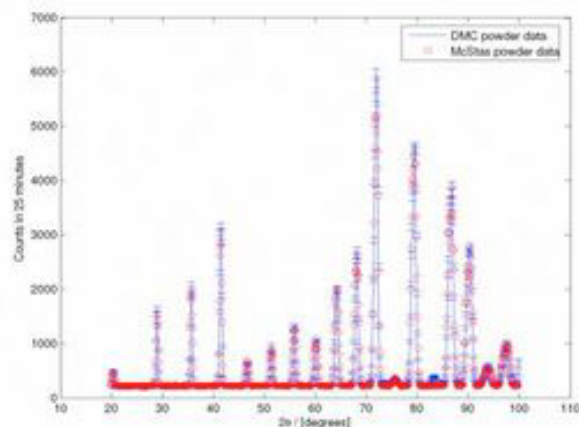
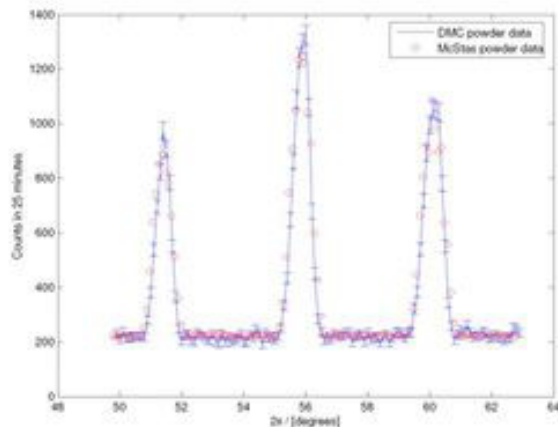
Virtual experiments (VE)

(definition:)

- Simulation of a complete experiment
- ... from source to detector
- Ideally controlled like real experiment.
- Data analysed by "real" analysis programs



A. Daud-Aladine, ISIS

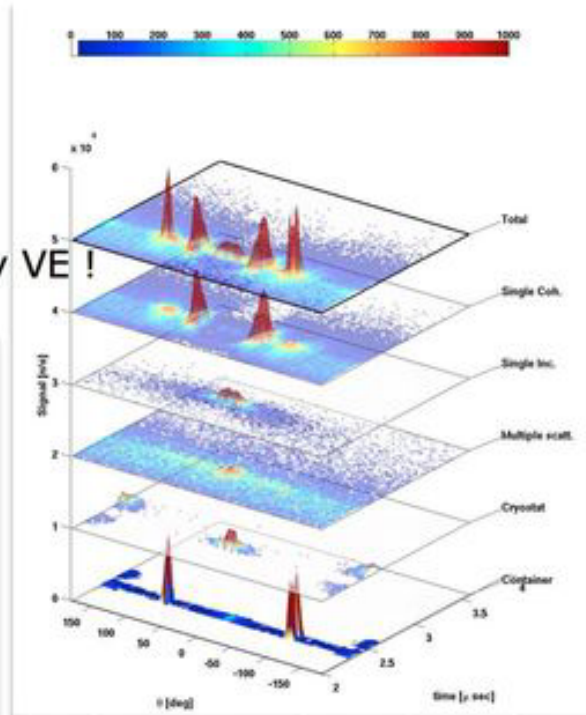
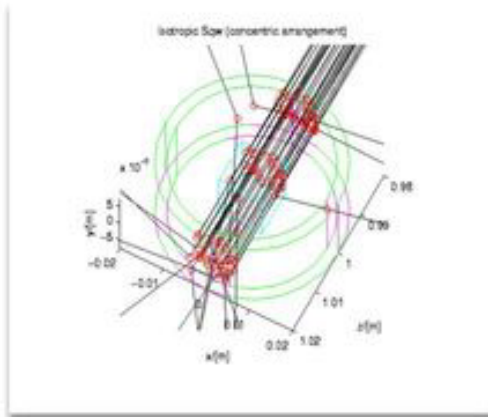


P. Willendrup, Risø DTU; Uwe Filges, L. Keller, PSI

Data analysis (1)

(using VE techniques)

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



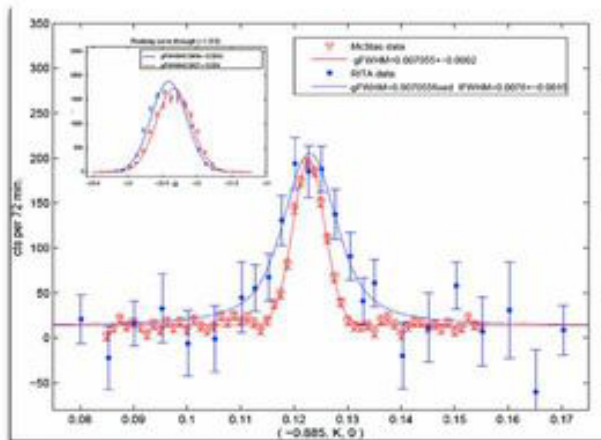
E. Farhi-ILL

INSIS

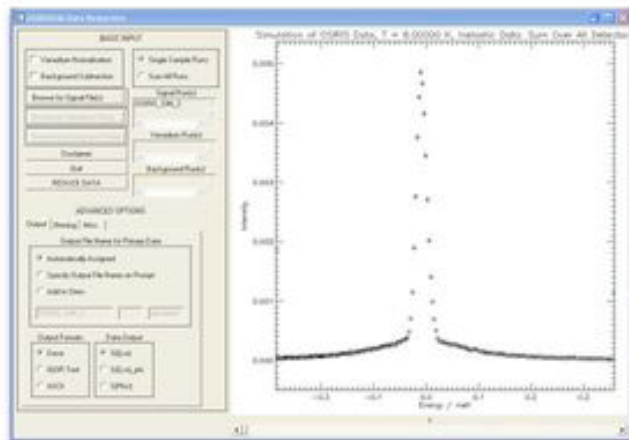
Data Analysis (2)

(using VE techniques)

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



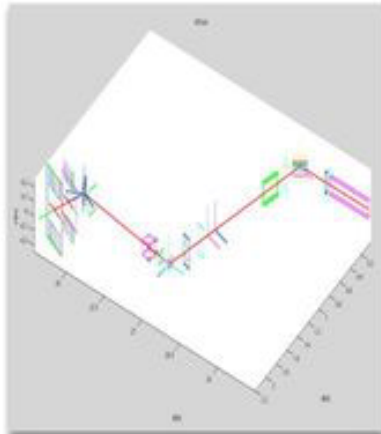
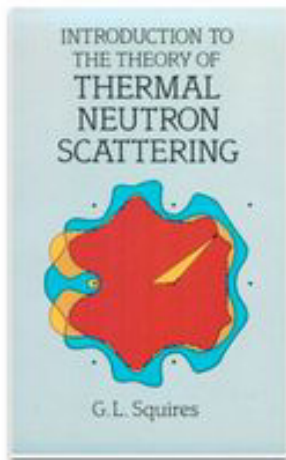
L. Udby, Risø-DTU



P. Tregenna-Piggott, PSI

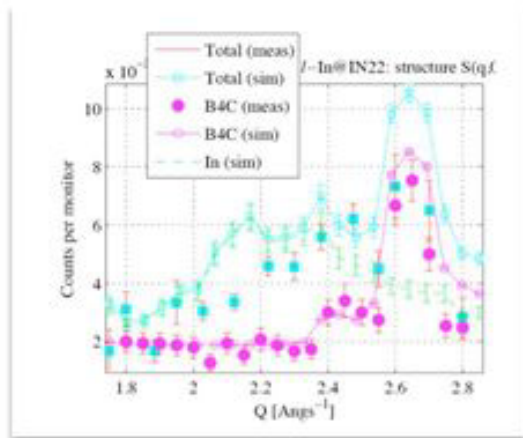
Teaching / training purposes

- Workshops
- Teaching
 - University of Copenhagen course on Neutron Scattering

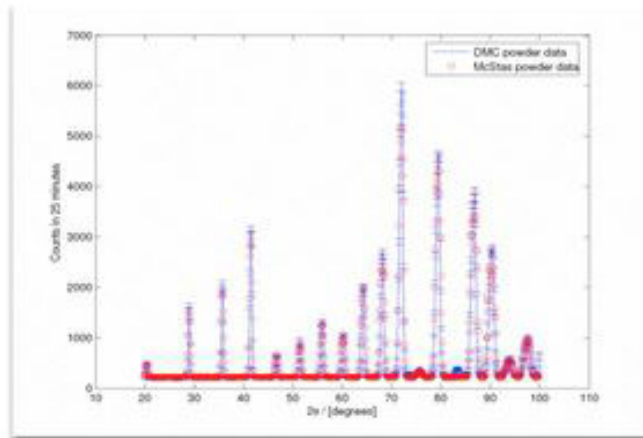


Reliability - cross comparisons

- Much effort has gone into this
- Here: simulations vs. exp. at powder diffract. DMC, PSI
- The bottom line is
- McStas agree very well with other packages (NISP, Vitess, IDEAS, RESTRAX, ...)
- Experimental line shapes are within 5%
- Absolute intensities are within 10%
- Common understanding: McStas and similar codes are reliable

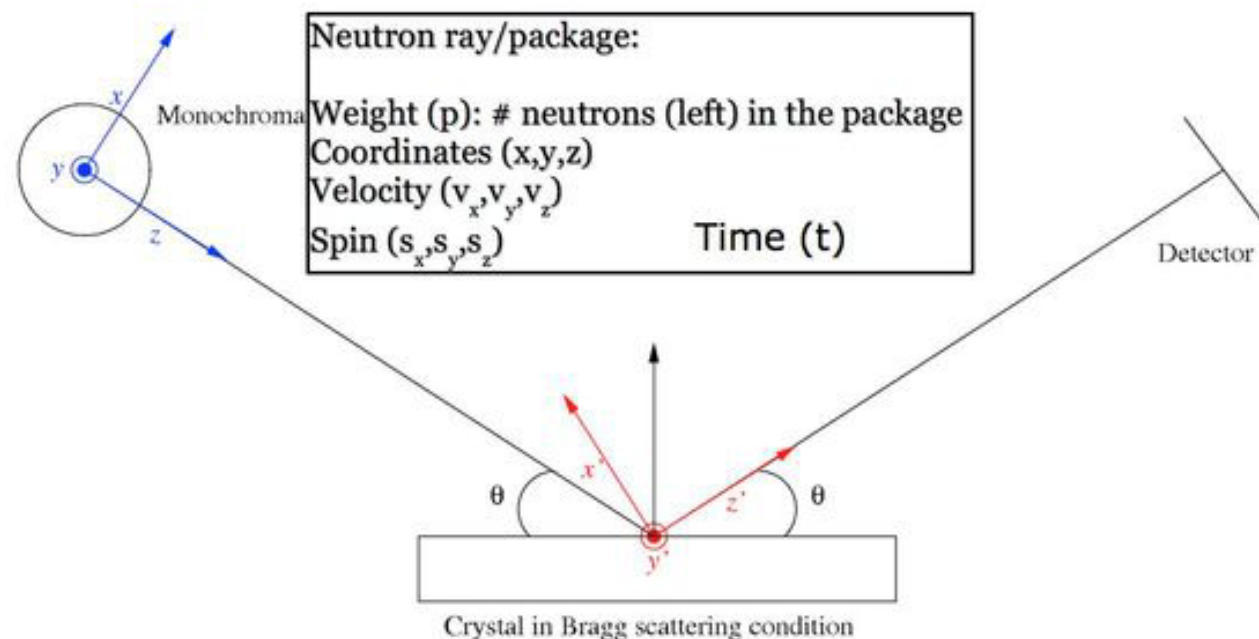


E. Farhi, P. Willendrup et al., in preparation

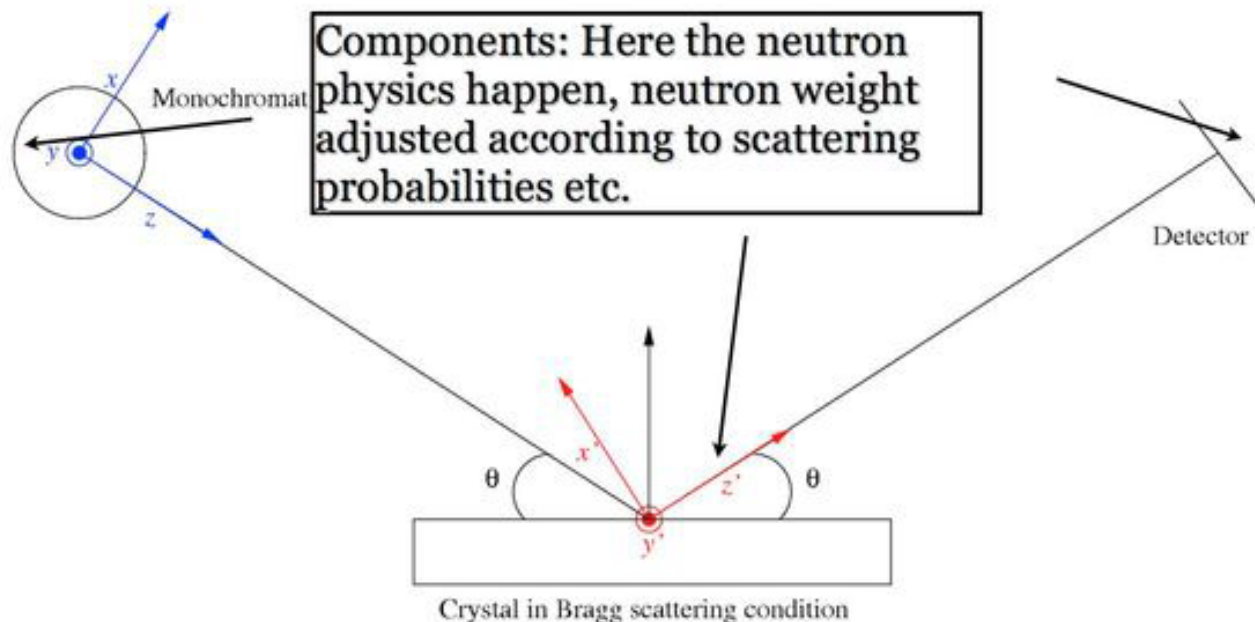


P. Willendrup et al., Physica B, 386, (2006), 1032.

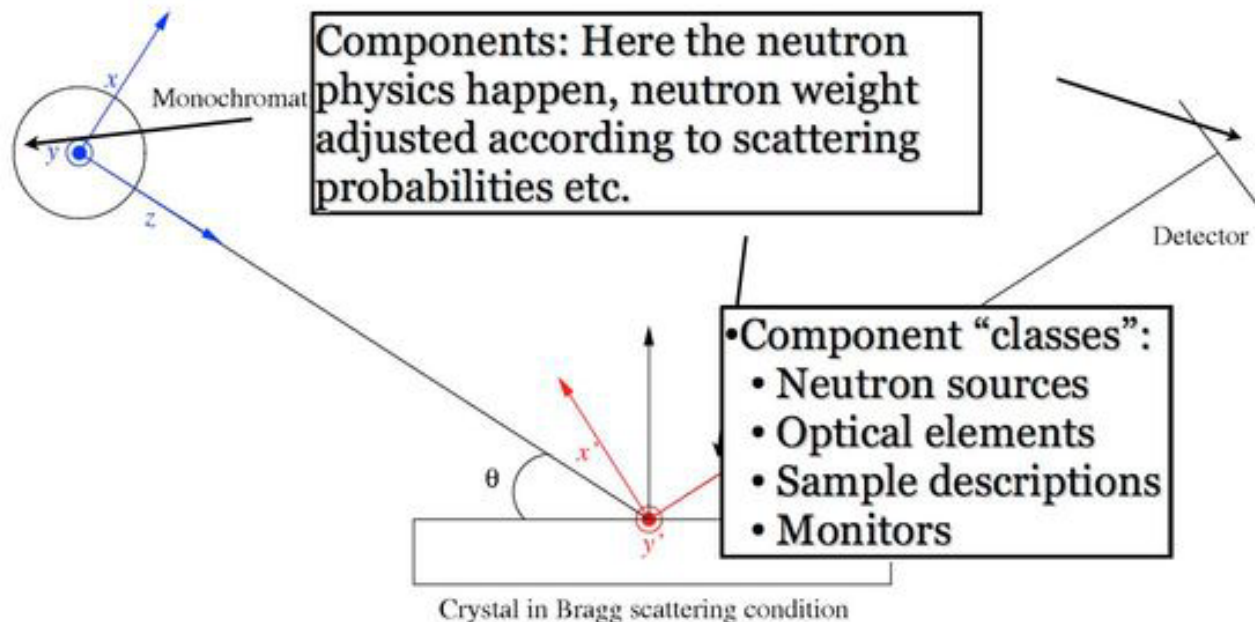
McStas: key concepts



McStas: key concepts

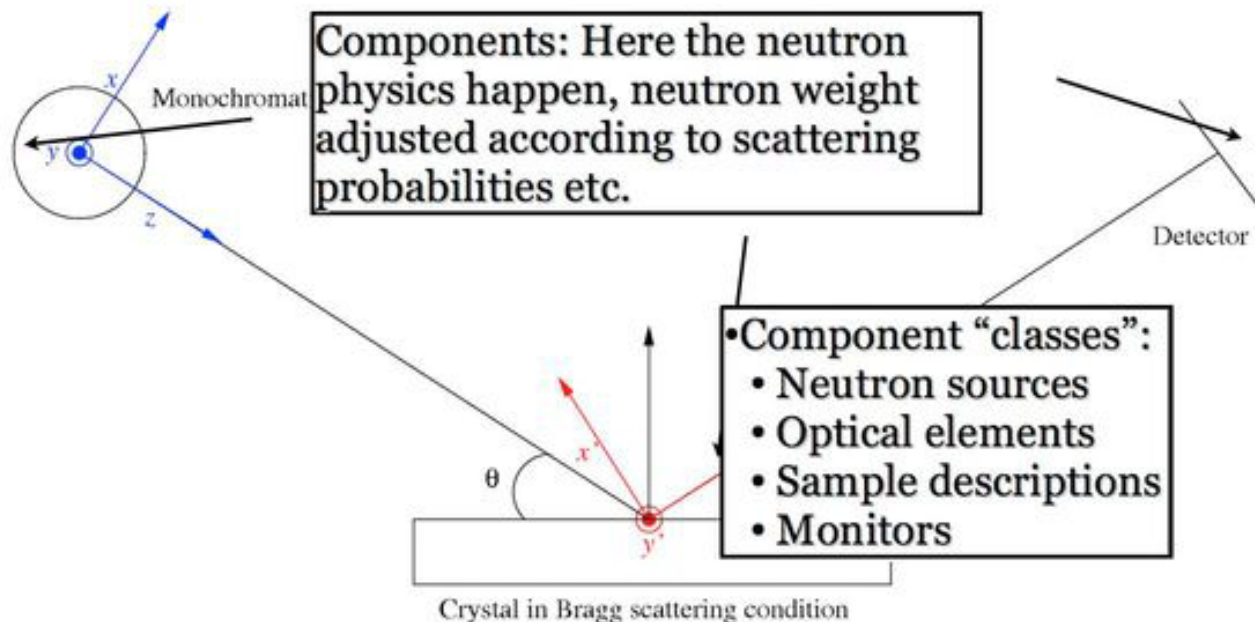


McStas: key concepts

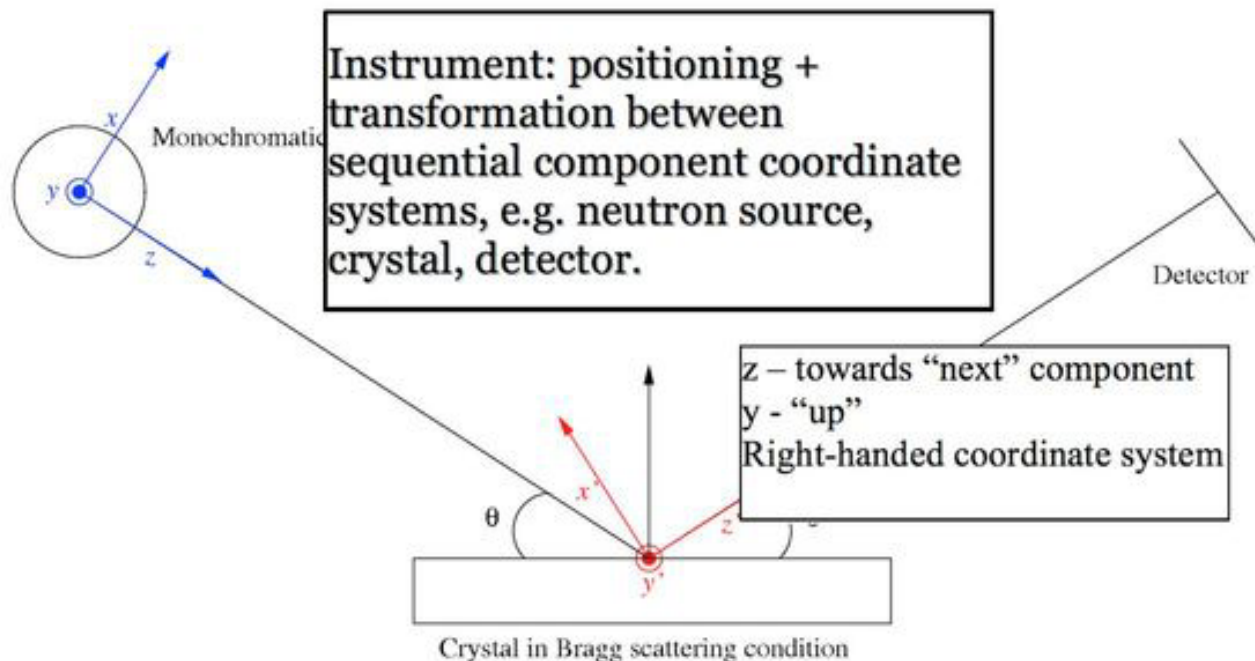


McStas: key concepts

Local, internal coordinate system!



McStas: key concepts

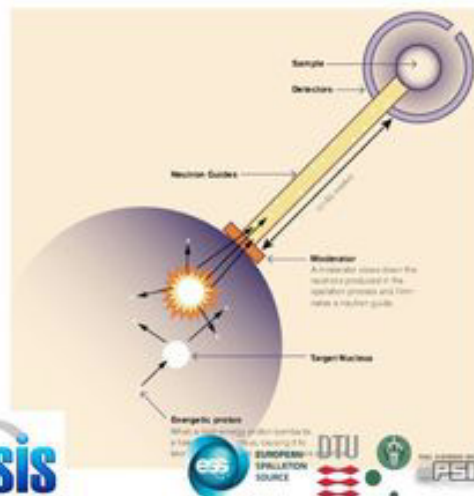


McStas overview

- Portable code (Unix/Linux/Mac/Windows)



- Ran on everything from iPhone to 1000+ node cluster!
- 'Component' files (~100) inserted from library
 - Sources
 - Optics
 - Samples
 - Monitors
 - If needed, write your own comps
- DSL + ISO-C code gen.



Under-the-hood / inner workings

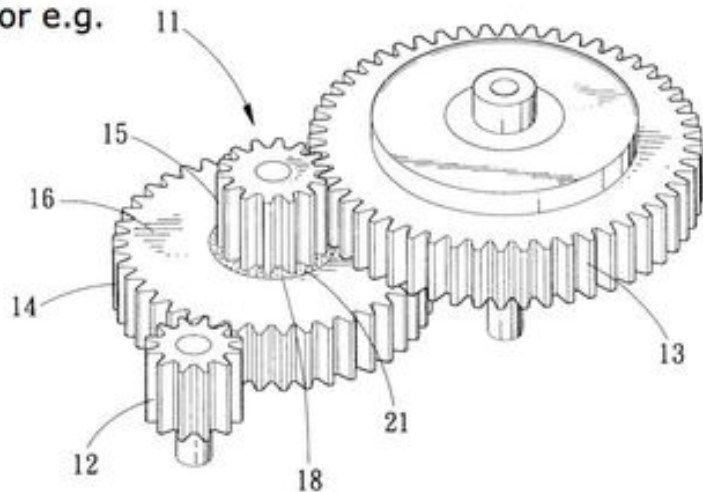
- Domain-specific-language (DSL) based on compiler technology (LeX+Yacc)

• Simple Instrument language $\xrightarrow{\text{Code generation}}$ ISO C

- Component codes realizing beamline parts (including user contribs)

- Library of common functions for e.g.

- I/O
- Random numbers
- Physical constants
- Propagation
- Precession in fields
- ...



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, xv = 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

```

*****
* Mistao: neutron ray-tracing package
* Copyright 1997-2002. All rights reserved.
* Risoe National Laboratory, Roskilde, Denmark
* Institut Louis Langevin, Grenoble, France
*
* Component: Source_flat
*
* AI
* Written by: Kim Leifmann
* Date: October 30, 1997
* Modified by: IL, 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
*
* US
* 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, xv=1, yb=1, E0=14, dE=2)
*
* UP
* radius: (m) Radius of circle in (x,y,0) plane where neutrons
* are generated.
* dist: (m) Distance to target along z axis
* xv: (m) Width(x) of target
* yb: (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/(cm**2*st)) Energy integrated flux
*
* AE
*****

DEFINE COMPONENT Source_flat
DEFINITION PARAMETERS {
  SETTING PARAMETERS (radius, dist, xv, yb, E0=0, dE=0, Lambda0=0, dLambda=0, flux=1)
  OUTPUT PARAMETERS {}
  STATE PARAMETERS (x, y, z, vx, vy, vz, t, s1, s2, p)
}
DECLASS
{
  double poul, pdir;
}
INITIALISE
{
  poul=flux*PI*1e4*radius*radius/4096*count();
}

```

```

TRACE
{
  double chi,E,Lambda,v,x, 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(sxf, syf, srf, spdir,
  0, 0, dist, xv, yb, NOT_A_CURRENT_COMP));

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

p = pdir*poul;

if (Lambda0==0) {
  E=E0+dE*rand01(); /* Choose from uniform distribution */
  v=sqrt(E)*SE2V;
} else {
  Lambda=Lambda0+dLambda*rand01();
  v = SE2V*(1+PI/Lambda);
}

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

MEDISPLAY
{
  magnify("mp");
  circle("mp",0,0,0,radius);
}

END

```

Written by developers
and possibly you!

Generated c-code

```
/* Automatically generated file. Do not edit.
 * Format:      ASCII C source code
 * Creator:     McStas (http://neutron.rice.edu)
 * Instrument:   MyInstrument.instr (MyInstrument)
 * Date:        Sat Apr 9 15:27:56 2005
 */

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

/* TRACE Component Source. */
SIO MESSAGE("Source (Trace)");
mcDEBUG_COMP("Source");
mcCOORDSChange(mcPOSrSource, mcCTRSource,
               &mcNLX, &mcNLY, &mcNLZ,
               &mcNLVX, &mcNLVY, &mcNLVZ,
               &mcNLTX, &mcNLTX, &mcNLTY);
mcDEBUG_STRING(mcNLX, mcNLY, mcNLZ, mcNLVX, mcNLVY, mcNLVZ, mcNLTX, mcNLTX, mcNLTY, mcNLZ);

#define x mcNLX
#define y mcNLY
#define z mcNLZ
#define vx mcNLVX
#define vy mcNLVY
#define vz mcNLVZ
#define tx mcNLTX
#define ty mcNLTY
#define sz mcNLZ
#define p mcNLZ
STORE mcNLX, mcNLY, mcNLZ, mcNLVX, mcNLVY, mcNLVZ, mcNLTX, mcNLTX, mcNLTY, mcNLZ, mcNLZ);
mcScattered=0;
mcNCounter[2]++;

#define mcCOMPNAME Source
#define mcCOMPINDEX 2
{ /* Declarations of SETTING parameters. */
mcNUM radius = mcSource_radius;
mcNUM dist = mcSource_dist;
mcNUM xv = mcSource_xv;
mcNUM yb = mcSource_yb;
mcNUM ED = mcSource_ED;
mcNUM dx = mcSource_dx;
mcNUM Lambda0 = mcSource_Lambda0;
mcNUM dLambda = mcSource_dLambda;
mcNUM flux = mcSource_flux;
#line 58 "Source_single.comp"
{
double chi,E,Lambda,v,vx,vy,zz,xf,yf,zf,dx,dy;

t=0;
z=0;

chi=2*PI*rand01();
r=sqrt(rand01())*radius;
x=r*cos(chi);
y=r*sin(chi);

randvec target_vec(xf,yf,zf,xf,yf,zf);
0, 0, dist, xv, yb, 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

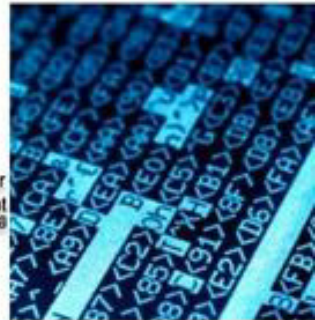
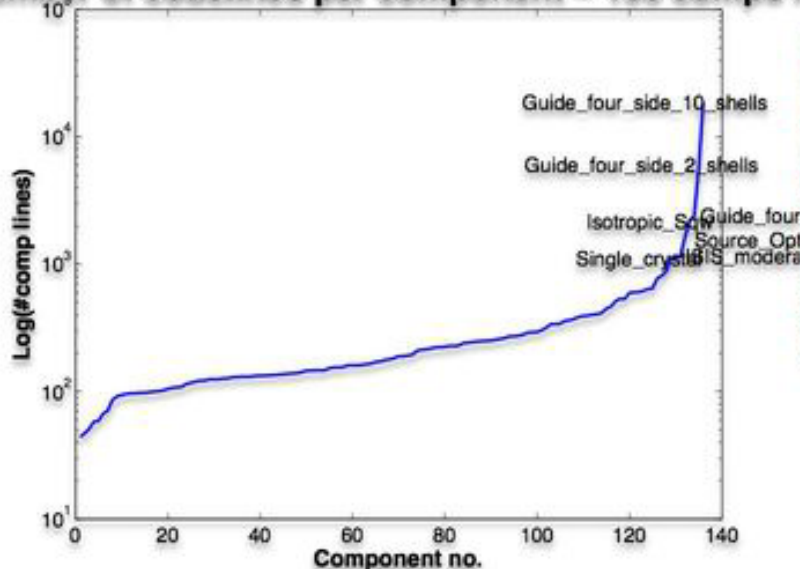
Output is a single c-file, which can
be compiled using e.g. gcc.

Can take input arguments if
needed.

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

- Check our long list of components and look inside... Most of them are quite simple and short... Statistics:

Number of codelines per component – 136 comps i



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



SEVENTH EDITION
EL
LENGUAJE DE
PROGRAMACION

C

SEVEN EDITION
FOR SCIENCE

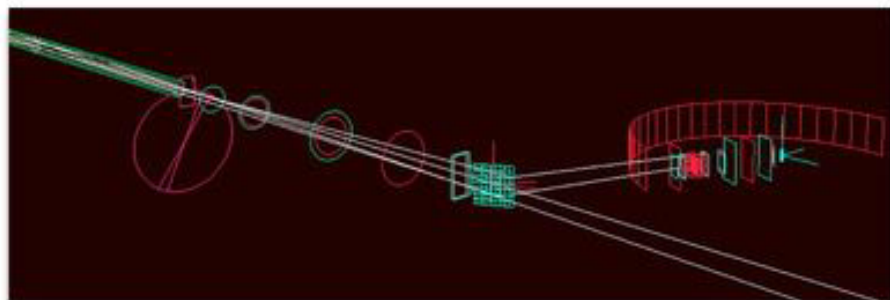
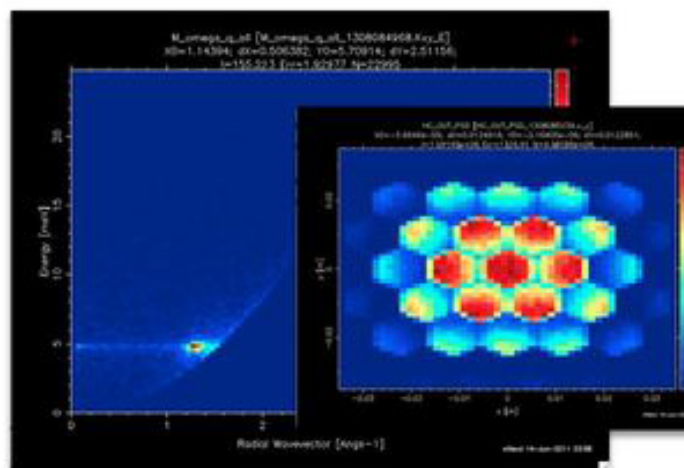
Syntax in one, complex view...

```
{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] }
```



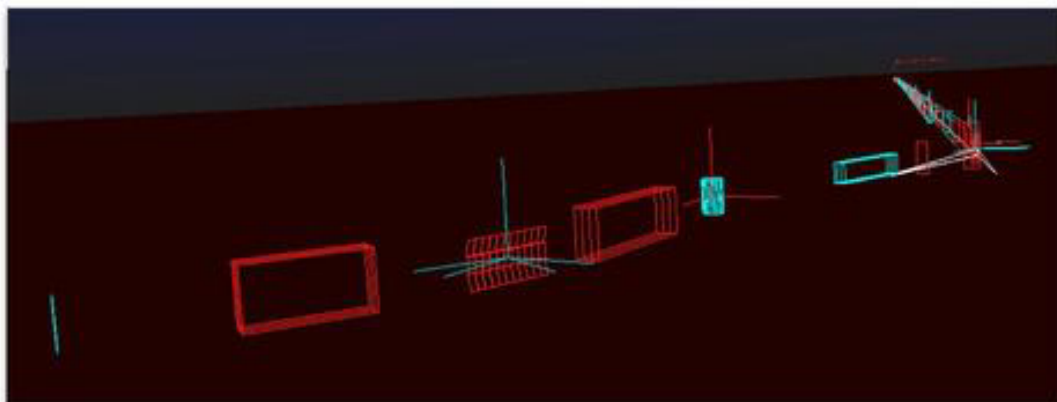
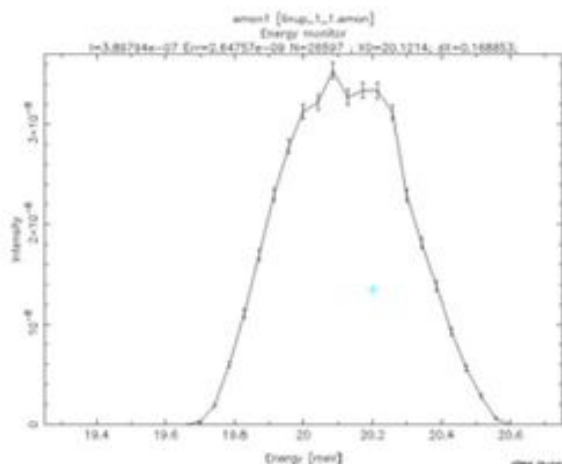
Example suite: 7 TOF spectrometers:

- 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



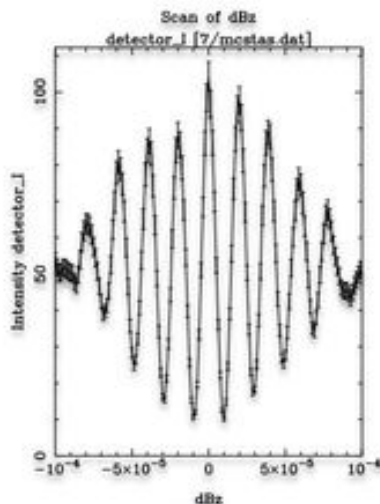
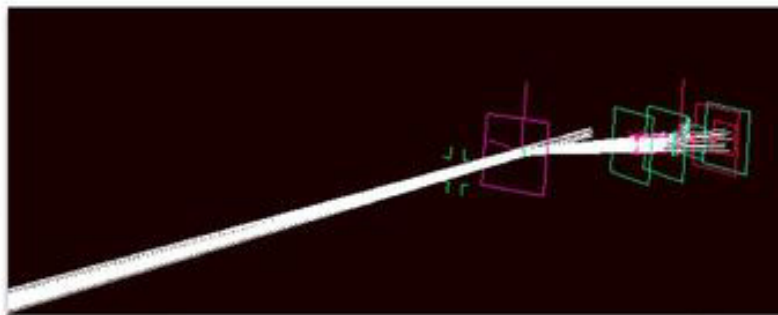
Example suite: 5 TAS

- 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



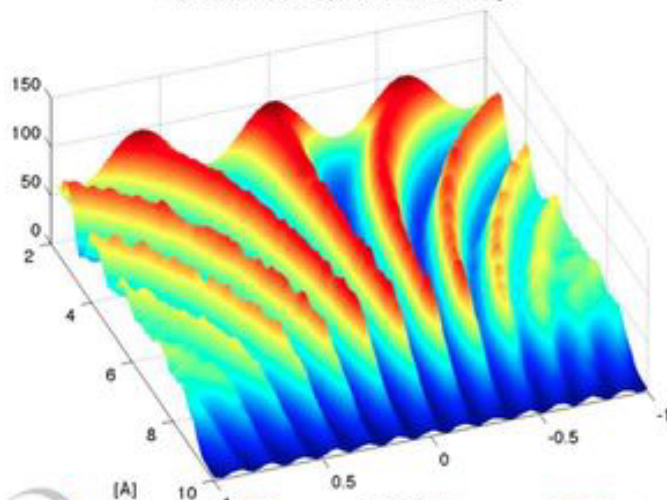
Example suite: 1 Hybrid spectrometer + 1 Spin-echo

- 1 Hybrid spectrometer:
 - prisma2.instr
- 1 Spin-echo (two implementations)
 - SE_example.instr
 - SE_example2.instr



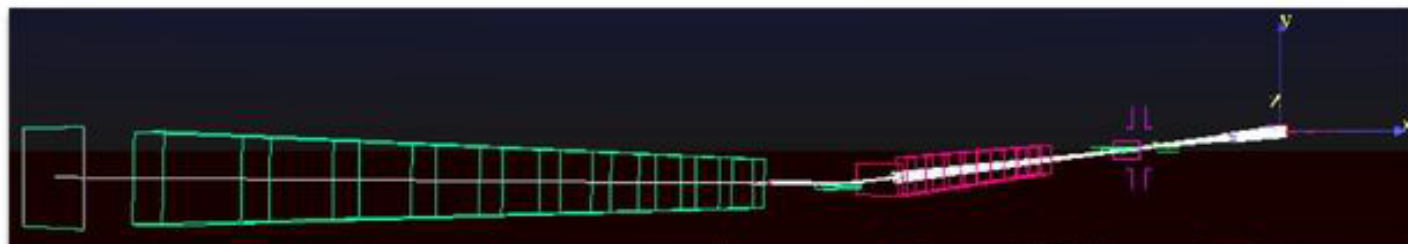
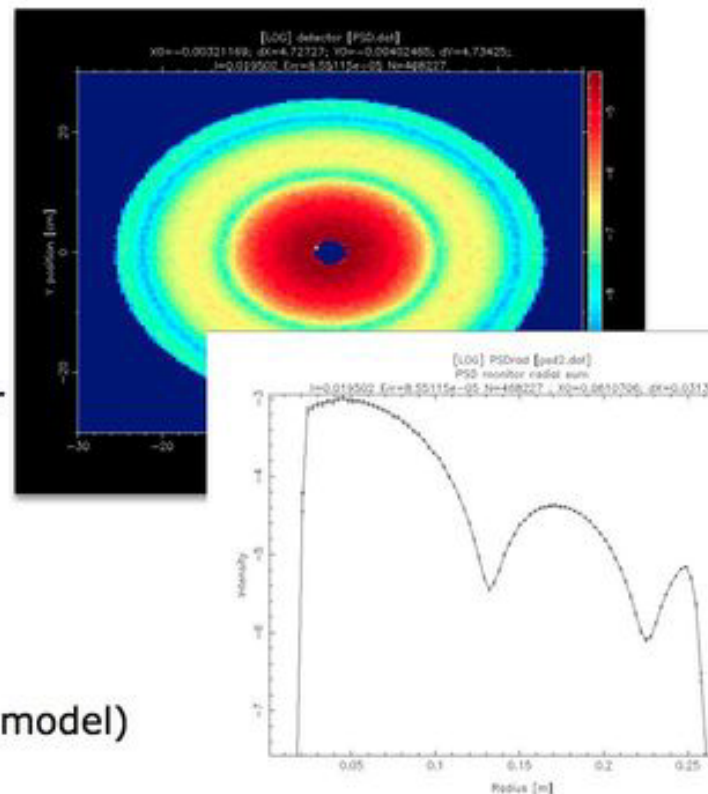
Introduction to simulation techniques

Spin-echo B scan dependence of wavelength



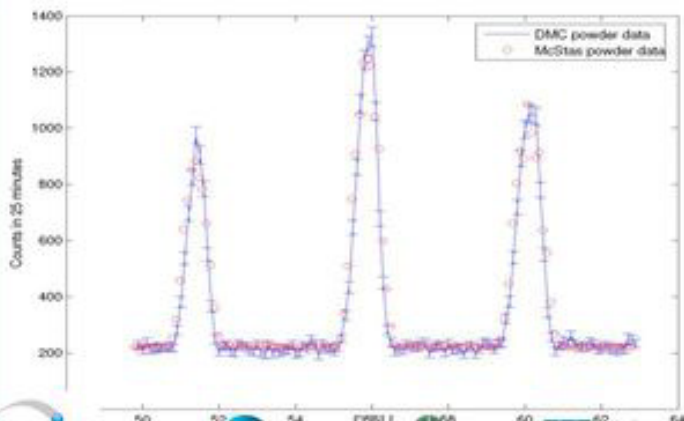
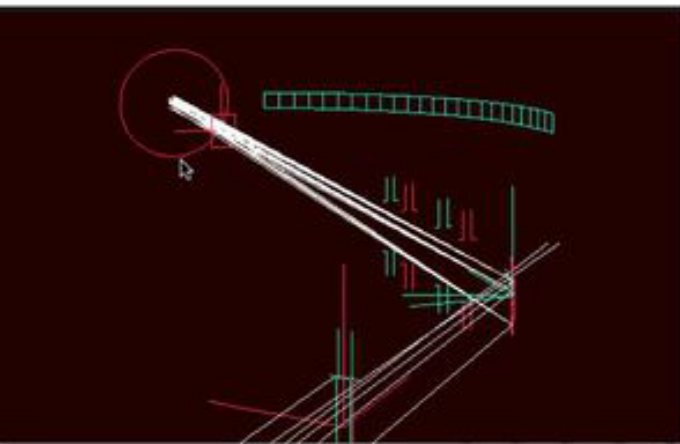
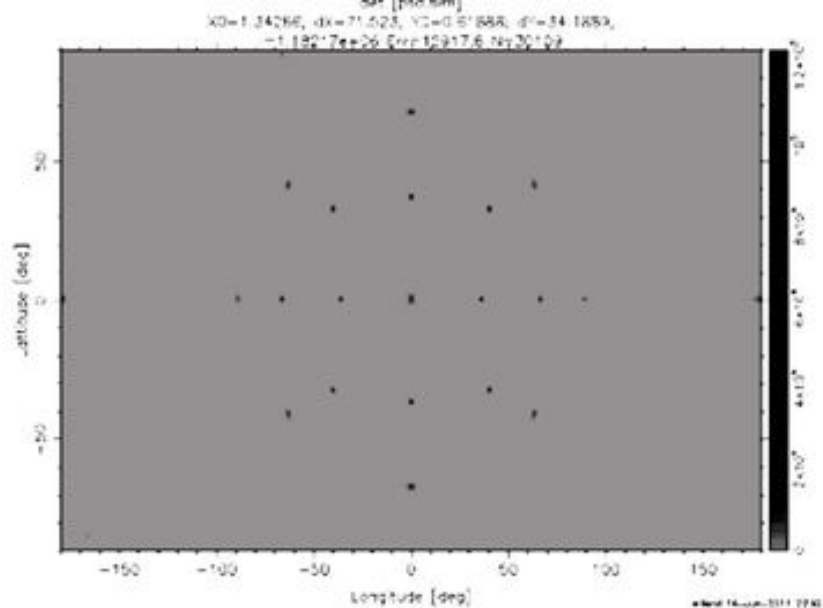
Example suite: Large scale structures

- 2 SANS:
- FZJ_KWS2_Lens.instr
- FZJ_SANS_KWS2_AnySample.instr
- FZJ_SANS_KWS2_DebyeS.instr
- FZJ_SANS_KWS2_Guinier.instr
- FZJ_SANS_KWS2_NoSample.instr
- SANS.instr
- 1 Reflectometer:
- ISIS_CRISP.instr (Not an accurate model)



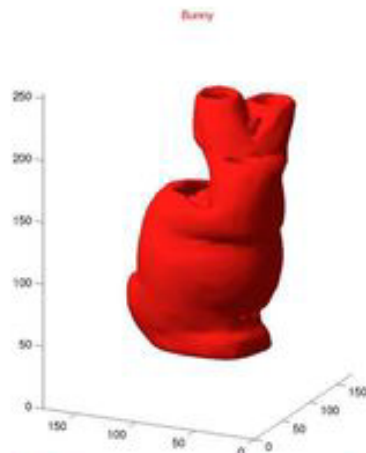
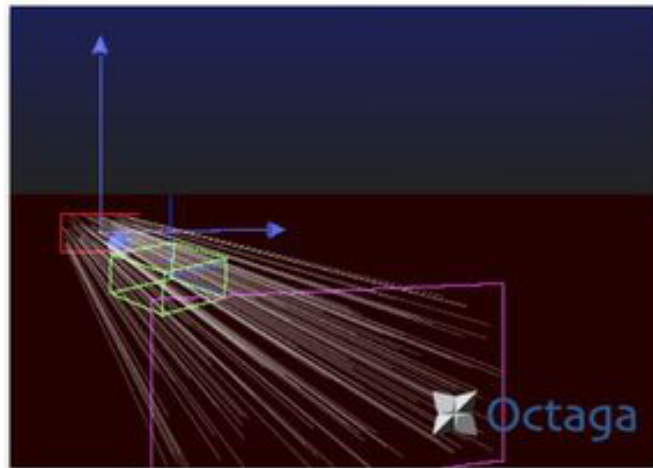
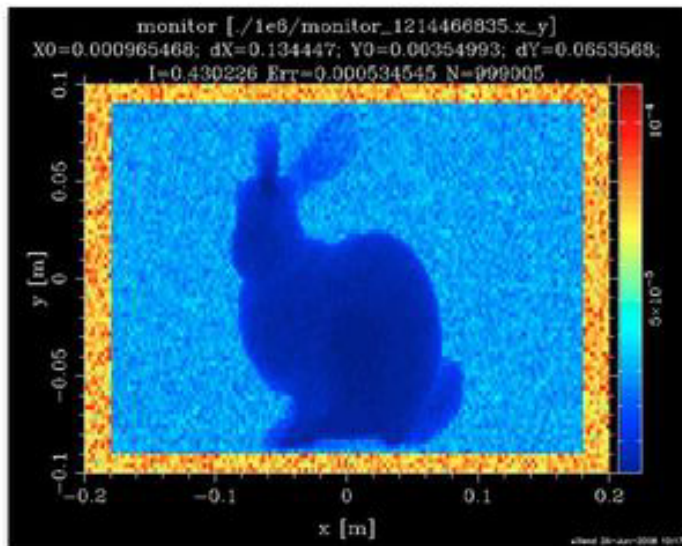
Example suite: Diffractometers

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



Example suite: Imaging

- Tomography.instr
- - comes with simple
- filtered backprojection
- reconstruction (Matlab)
-



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 spurious 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

- The success of the project is also about the people:

- Present McStas team members



• K Lefmann



E Farhi



P Willendrup



E Knudsen



U Filges

- Past McStas team members



• K Nielsen



PO Åstrand



K Lieutenant



P Christiansen



Enough Talk!

Let's see McStas run?

