Monte Carlo Simulations:

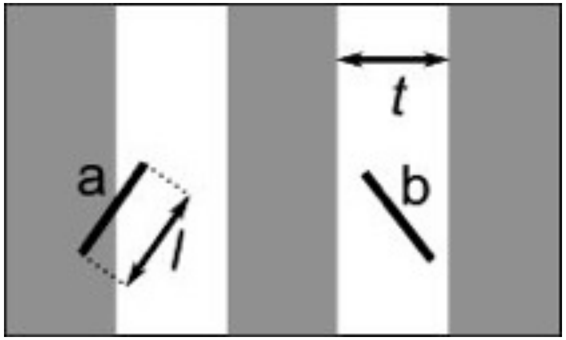
McStas and VITESS

HZB Helmholtz Zentrum Berlin

McStas	VITESS
M onte	V irtual
C arlo	I nstrumentation
S imulations of	T ool for the
T riple	E uropean
A xis	S pallation
S pectrometers	S ource

Klaus Lieutenant
Peter Willendrup

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

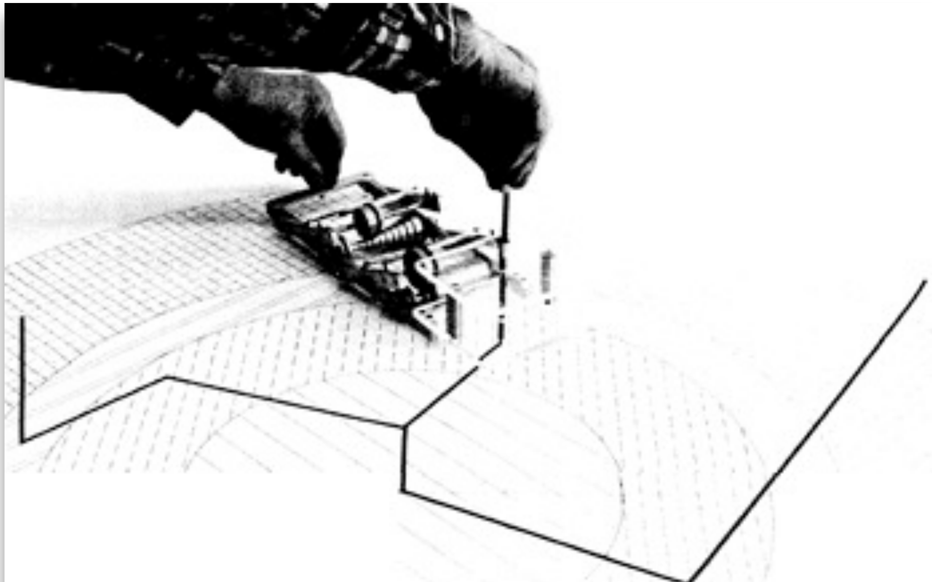
Monte Carlo techniques

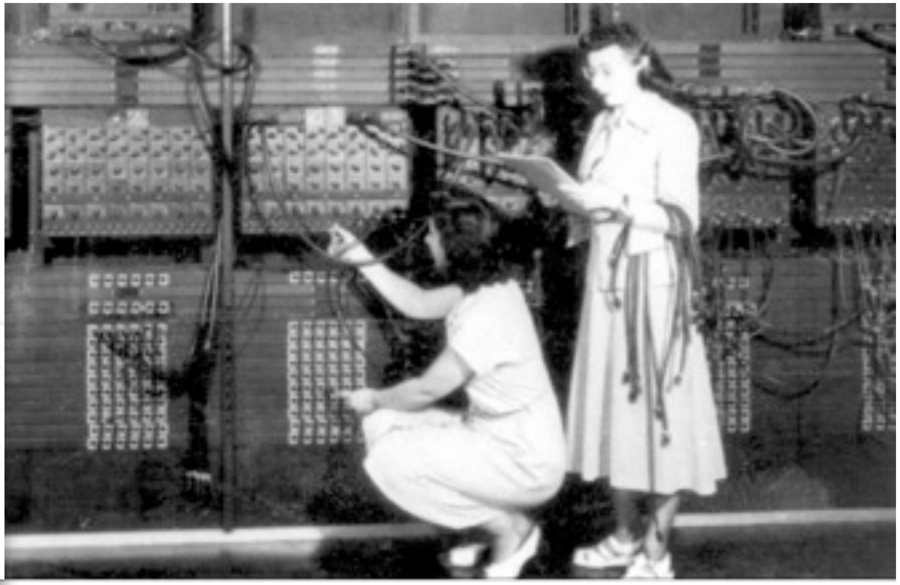
- During WW2, “numerical experiments” were applied at Los Alamos for solving mathematical complications of computing fission, criticality, neutronics, hydrodynamics, thermonuclear detonation etc.



- 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





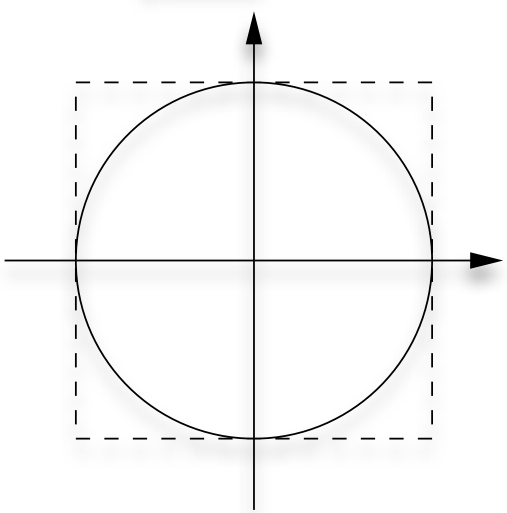
- FERMIAC ENIAC

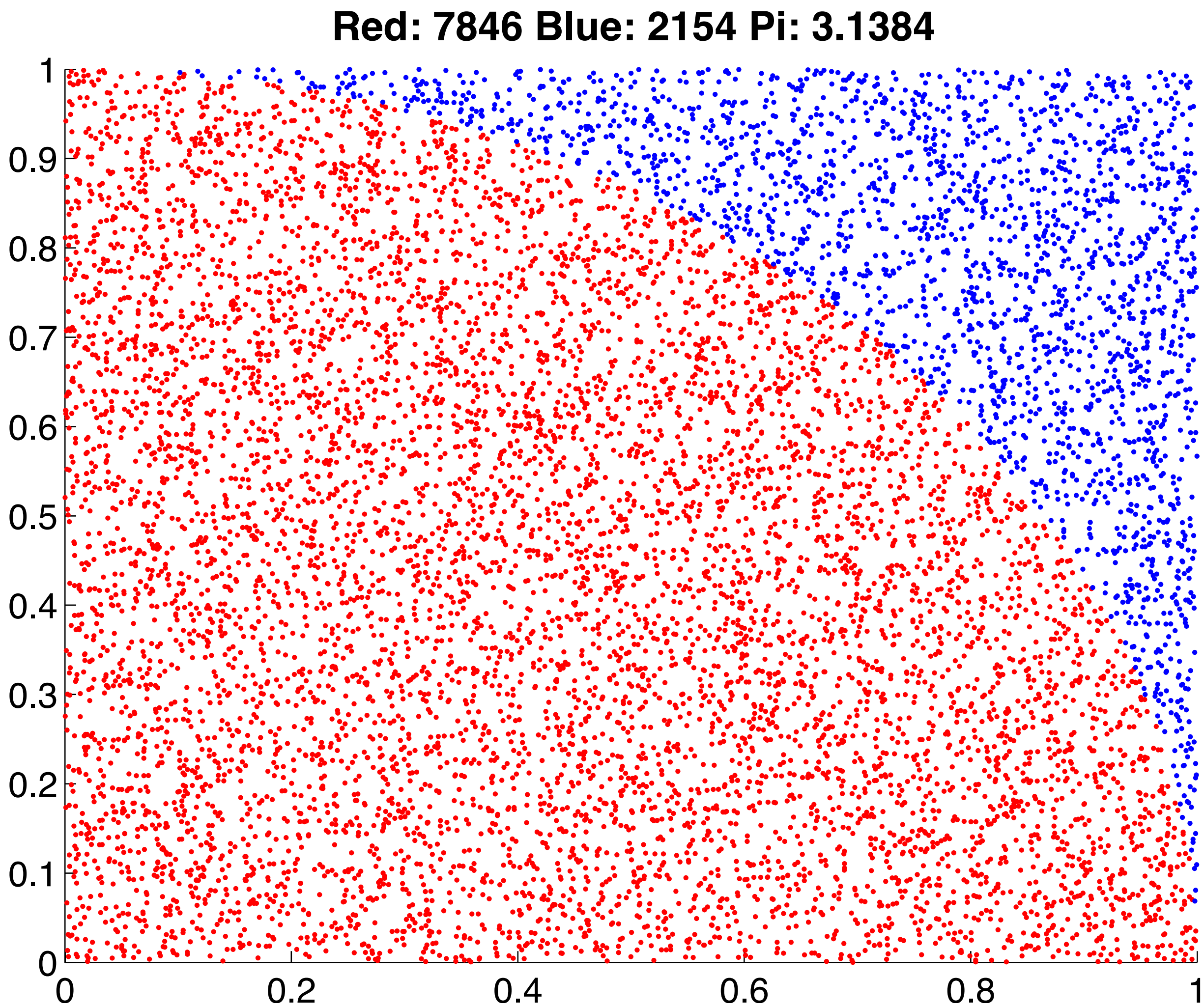
Monte Carlo techniques

- Estimating Pi:

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

$$\pi \approx 4\frac{7846}{10000} = 3.1384$$

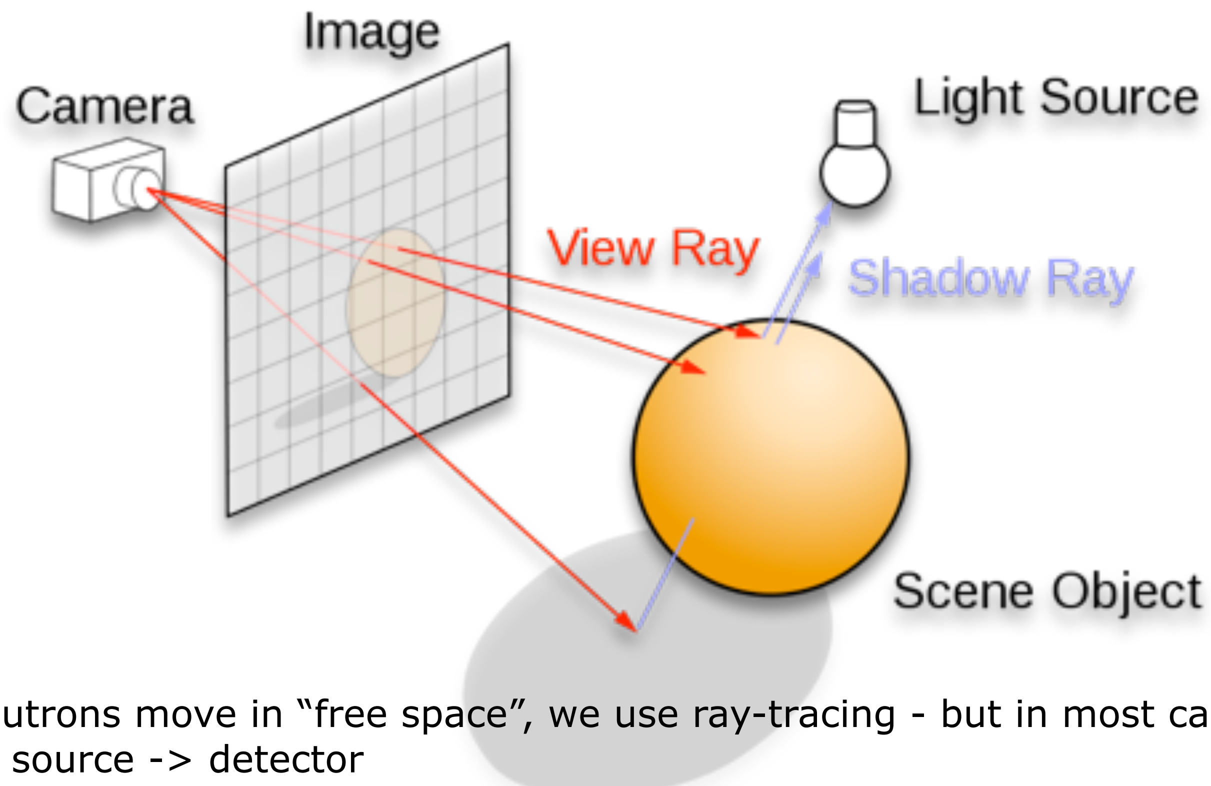




Monte Carlo techniques

- 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**

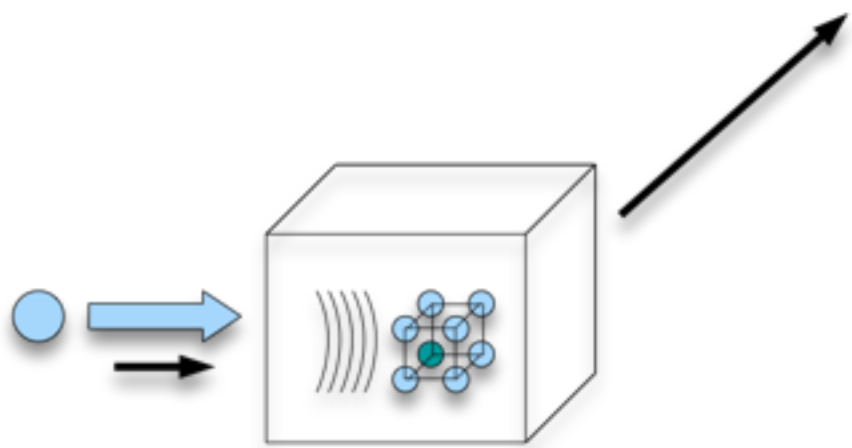
Ray-tracing methods



- 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?)

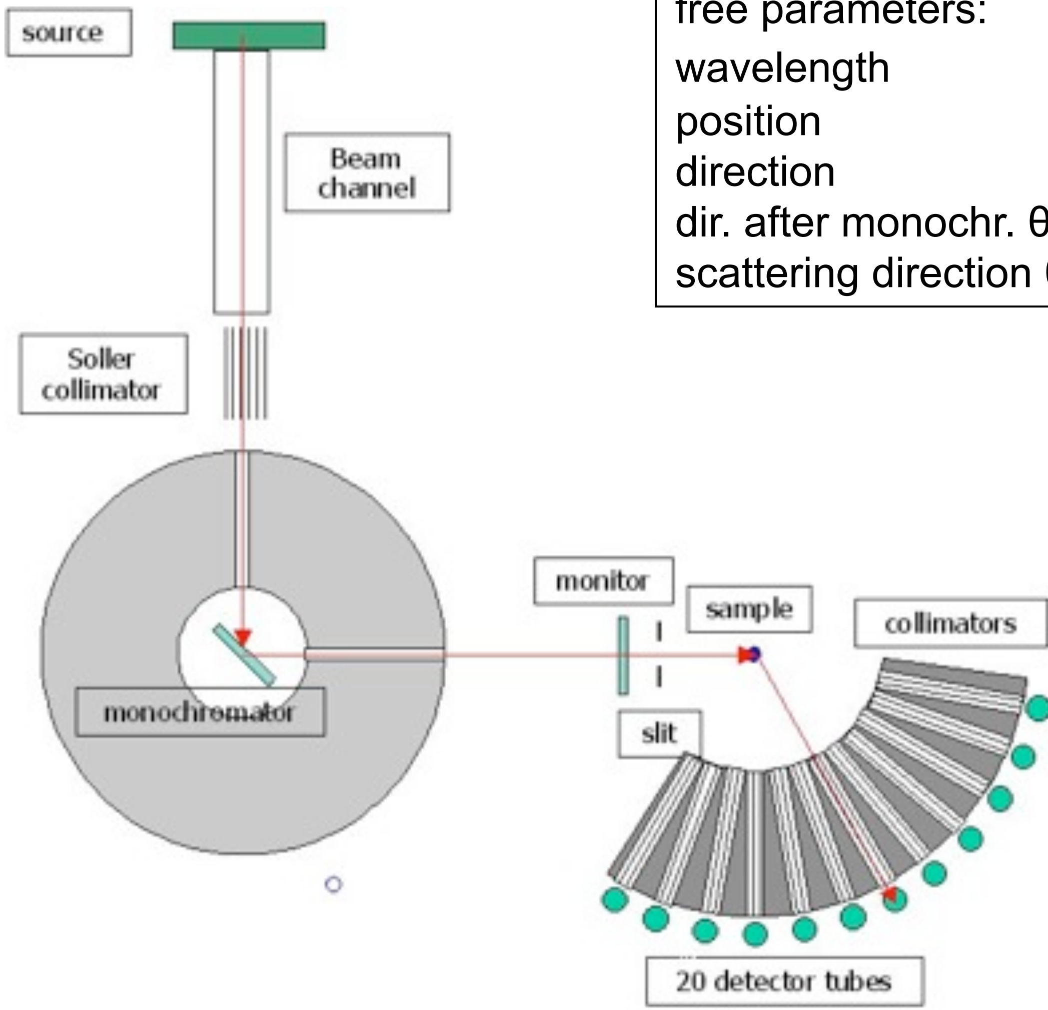
- US codes:
  - NISP (P Seeger & L Daemen, LANL)
  - IDEAS (X-L Wang ORNL, originally H Lee ORNL)
  - Instrument Builder (JK Zhao ORNL)
  - McVine (engine of the DANSE vnf project) (J Lin Caltech)

- 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...

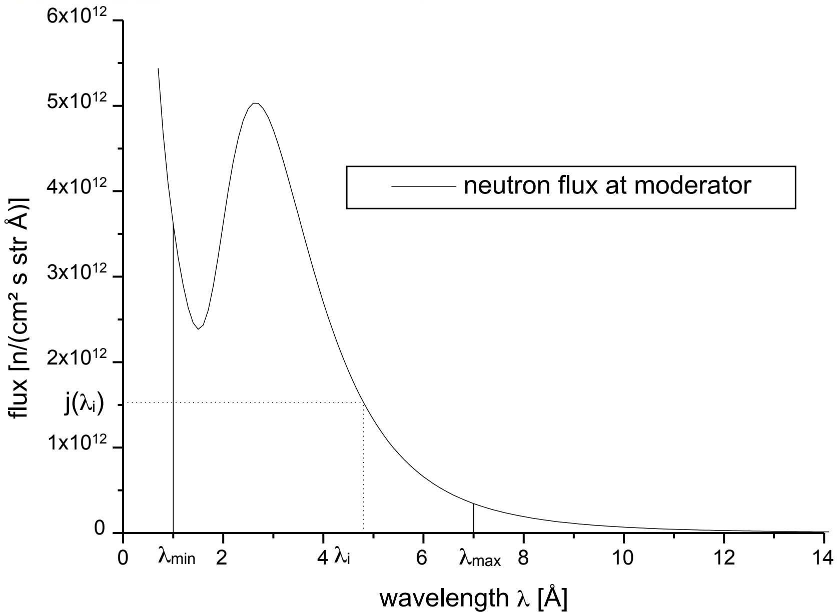
Example: Instrument simulation of R2D2



free parameters:

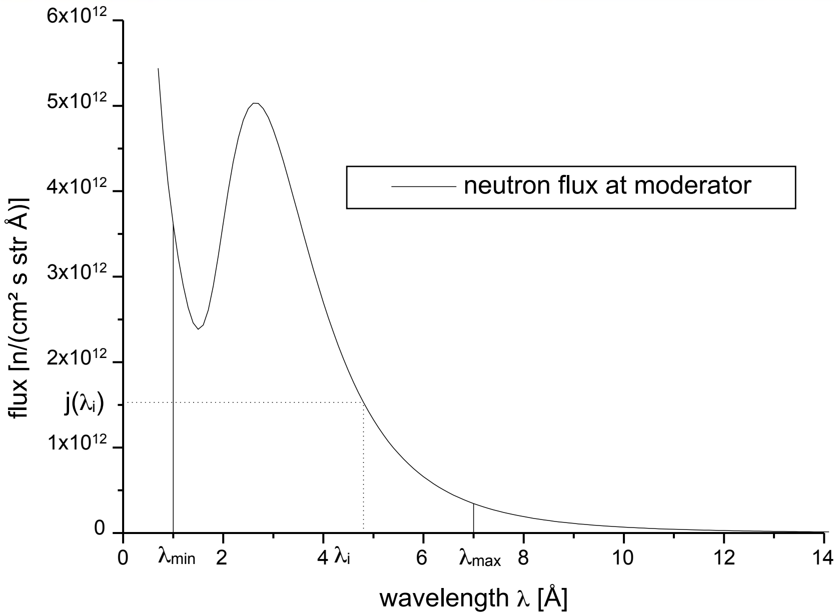
wavelength	λ initial
position	x,y initial
direction	v_{hor}/v, v_{vert}/v
dir. after monochr.	θ_m, φ_m
scattering direction	θ_s, φ_s

The 'Weight' Parameter



- The trajectories are calculated for single neutrons
- A highly unequal distribution of a parameter is a challenge
  - Choosing most events around the peak(s) and only few in the tails shows poor convergence
    - The method of choice is therefore: weighting the events (according to the distribution)
- The weight parameter can also be used to treat events like reflection
- Weighting is a numerical trick, not the treatment of an ensemble average

Absolute Flux values



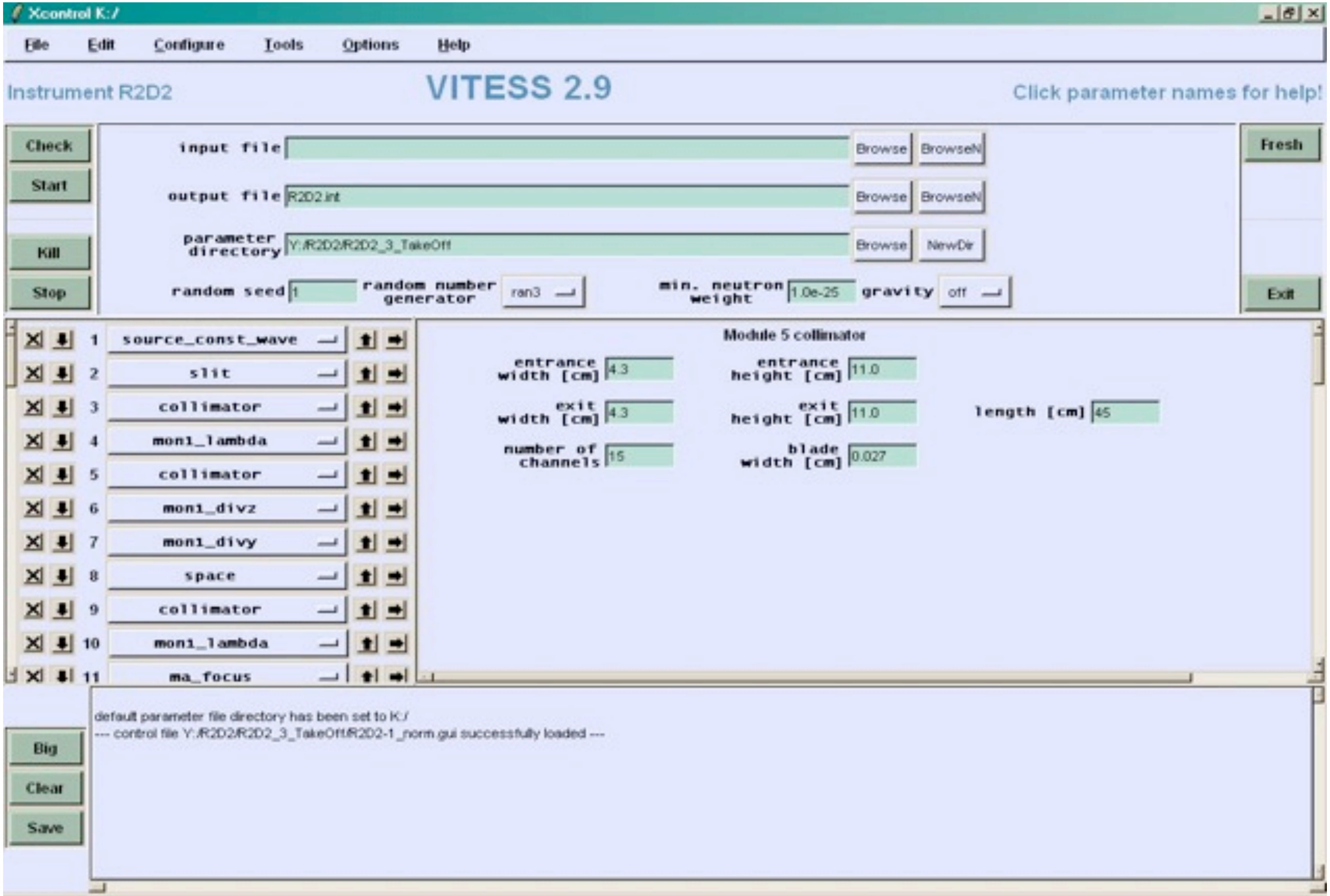
- By proper normalization, the weight can be expressed as a neutron current (or intensity) [n/s]
- Summing of the weights of all trajectories gives the neutron current at any point of the instrument
- By processes like reflection the intensity decreases, while the number of trajectories remains unchanged
- The trajectories are the events of the statistical experiment

- $I_{CW} = \int j(\lambda)\, d\lambda$

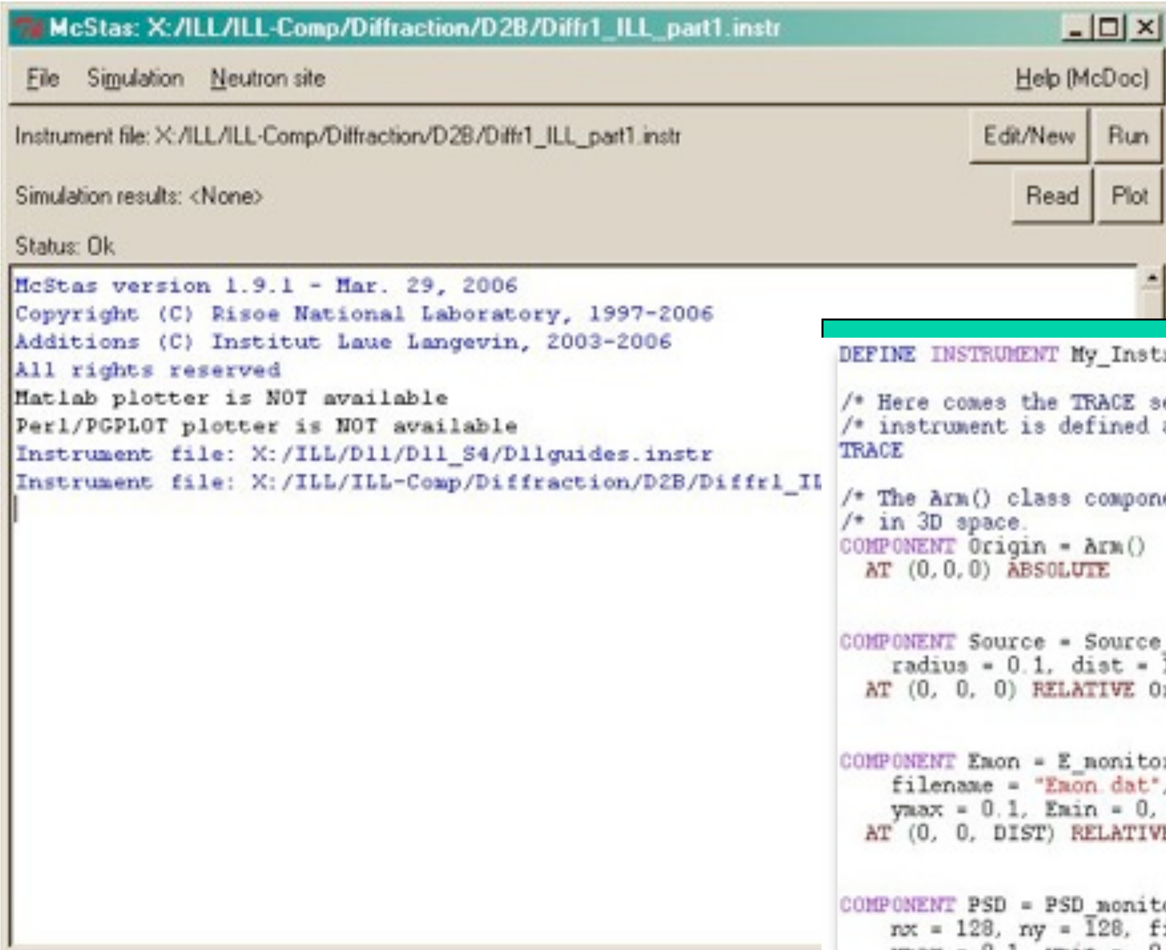
$$\approx (\lambda_{max}-\lambda_{min})/N \sum_i j(\lambda_i)$$

- $I_{SS} \approx (\lambda_{max}-\lambda_{min})(t_{max}-t_{min})/N \sum j(\lambda_i, t_i)$

VITESS GUI (after loading an instrument)

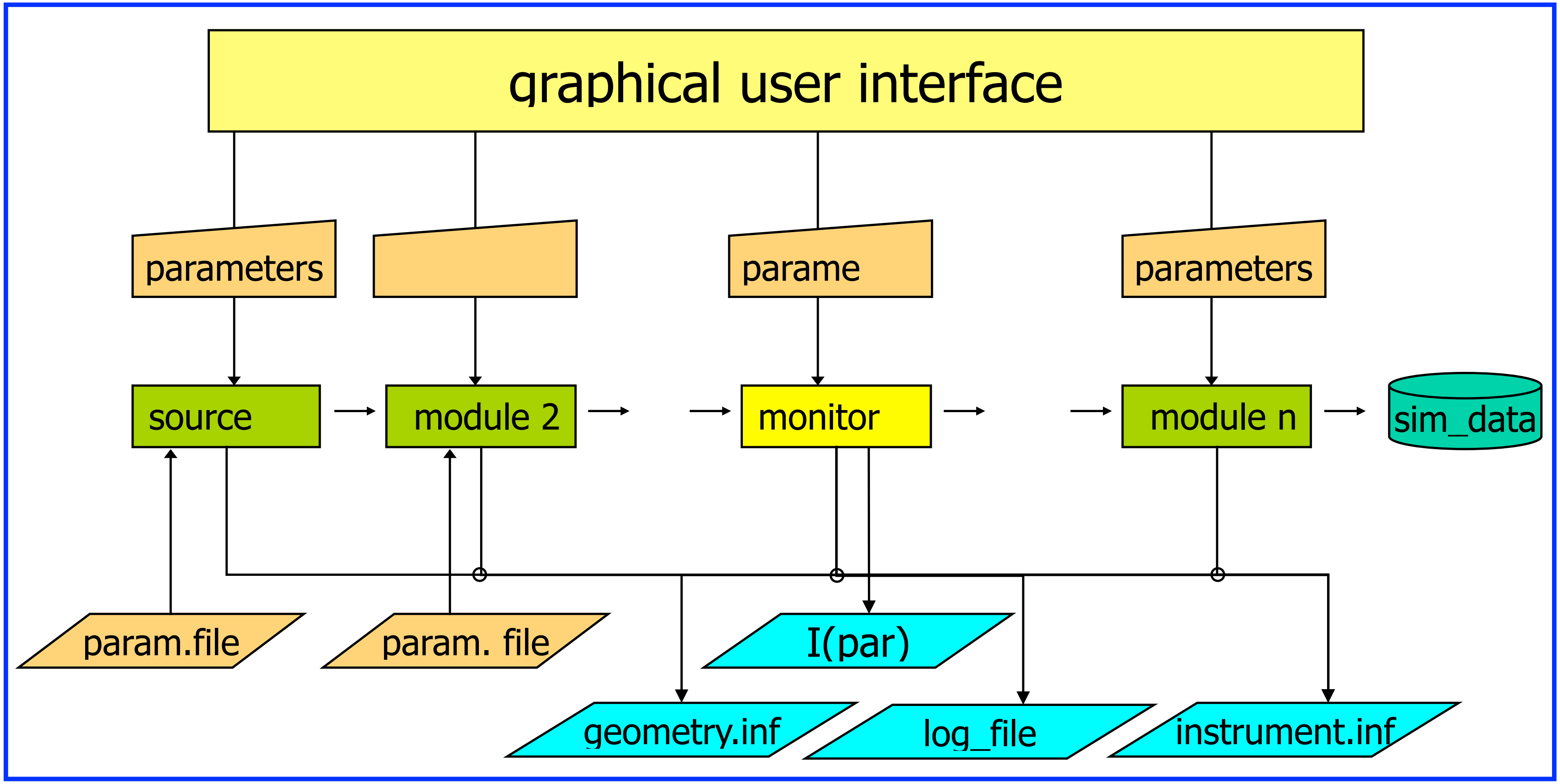


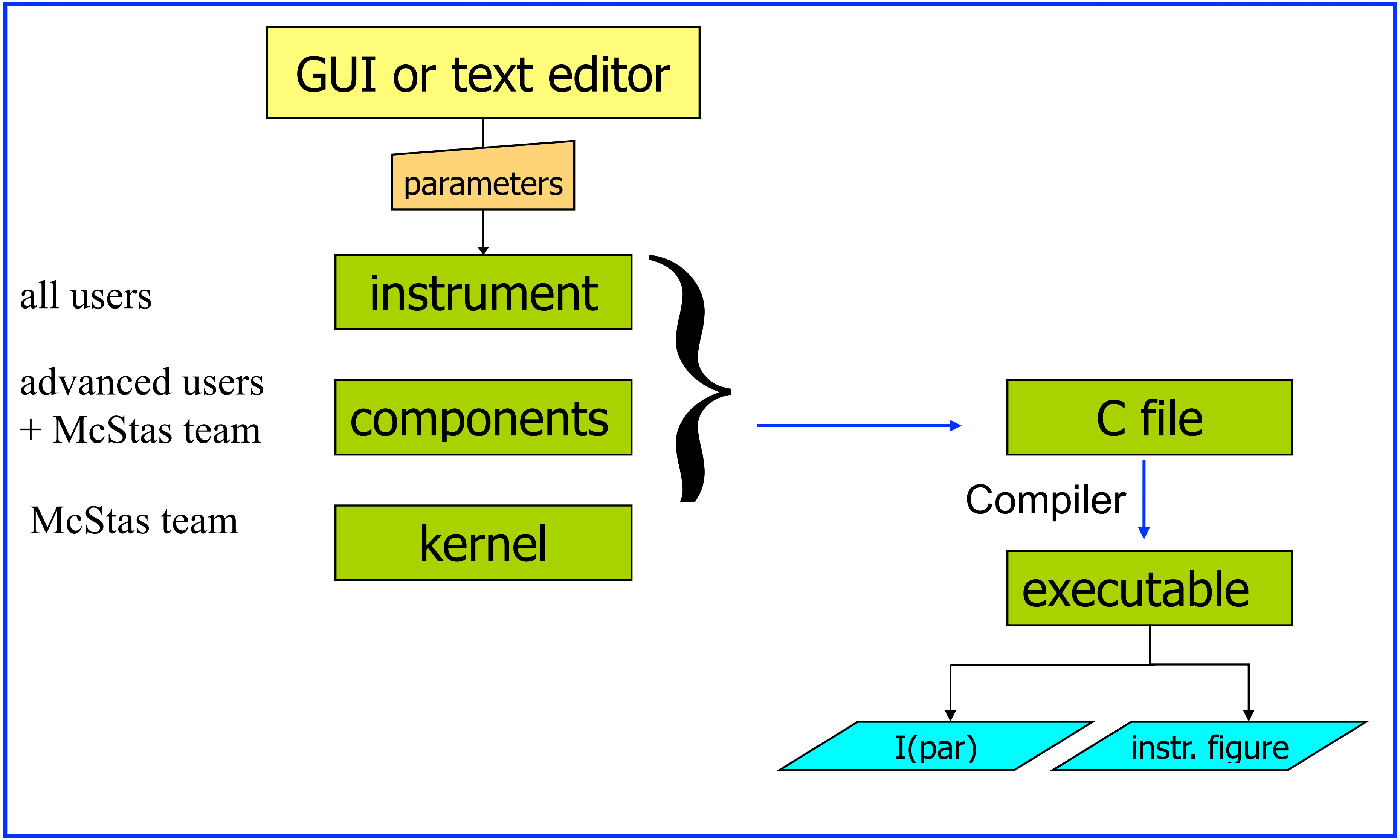
McStas GUI (after loading an instrument)




```
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
```

Concept of VITESS

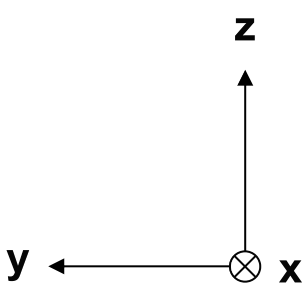


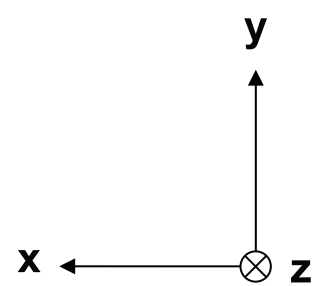

GUI or text editor
parameters
all users
instrument
advanced users
+ McStas team
components
McStas team
kernel
C file
Compiler
executable
I(par)
instr. figure

Co-ordinate Systems in VITESS and McStas

Right-handed co-ordinate systems

VITESS **McStas** **x: along**
the beamline **x: to the left** **y: to the left**
y: (vertically) up **z:**
(vertically) up **z: along the beamline**





view from moderator towards sample

Parameters in VITESS and McStas

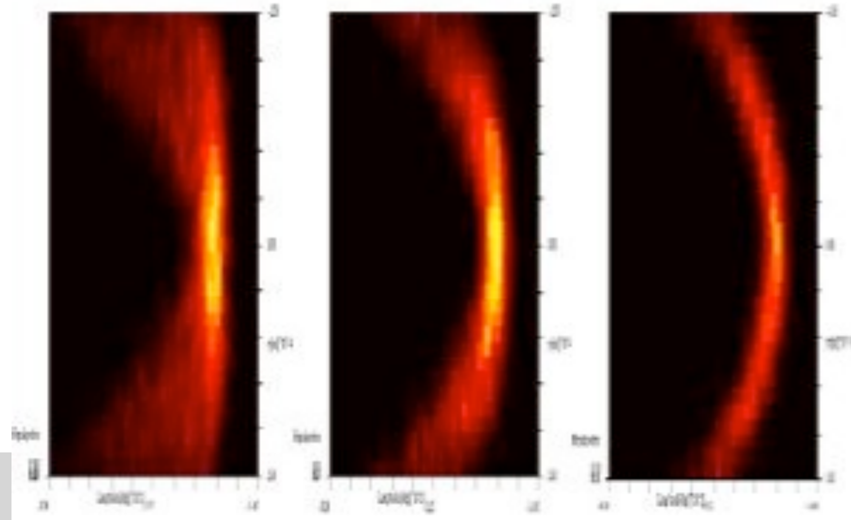
VITESS

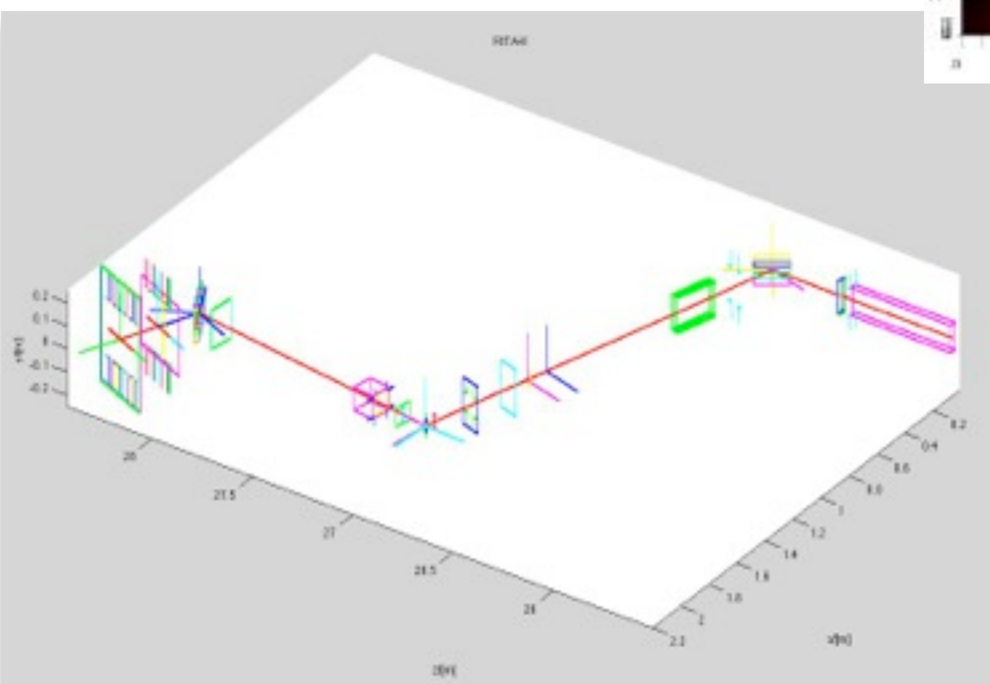
- ID
- criterion ‘ray tracing’
- ‘colour’
- time of flight [ms]
- weight [n/s]
- location of neutron x [cm]
- location of neutron y [cm]
- location of neutron y [cm]
- wavelength [Å]
- flight direction $v_x/|\underline{v}|$
- flight direction $v_y/|\underline{v}|$
- flight direction $v_z/|\underline{v}|$
- spin S_x
- spin S_y
- spin S_z

McStas

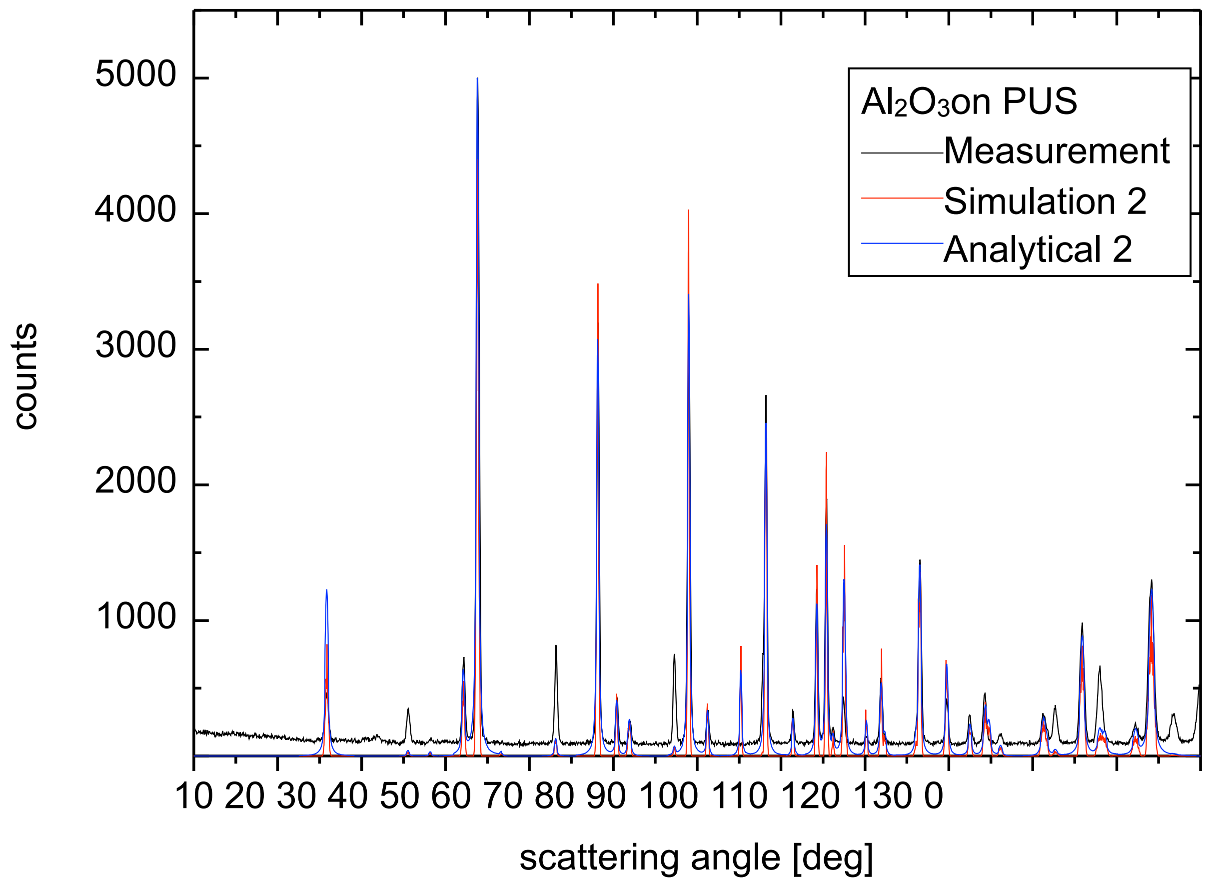
- time of flight [s]
- weight [n/s]
- location of neutron x [m]
- location of neutron y [m]
- location of neutron y [m]
- speed v_x[m/s]
- speed v_y[m/s]
- speed v_z[m/s]
- spin S_x
- spin S_y
- spin S_z

Simulation Output

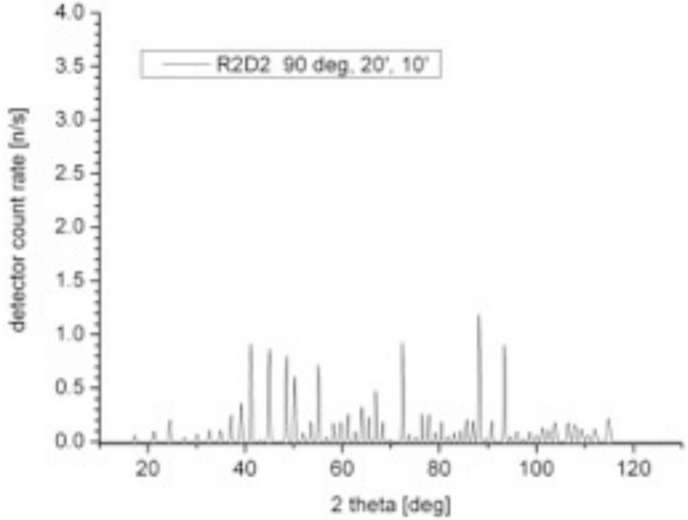


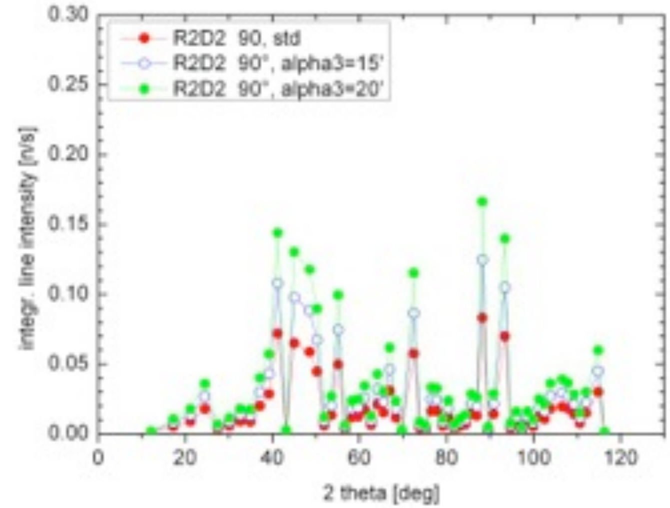


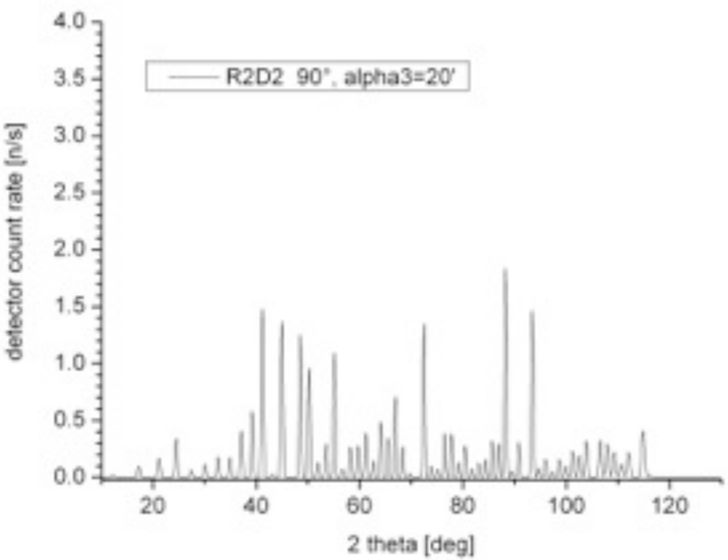
Example: Al_2O_3 on PUS

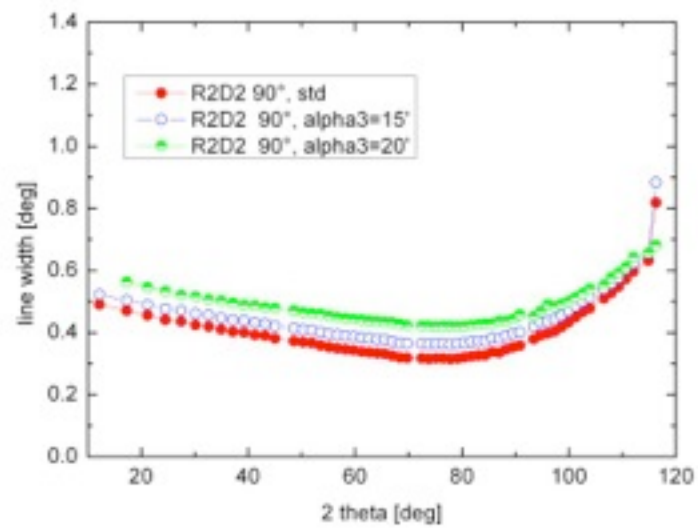


Example: Improvement of R2D2 using NAC sample



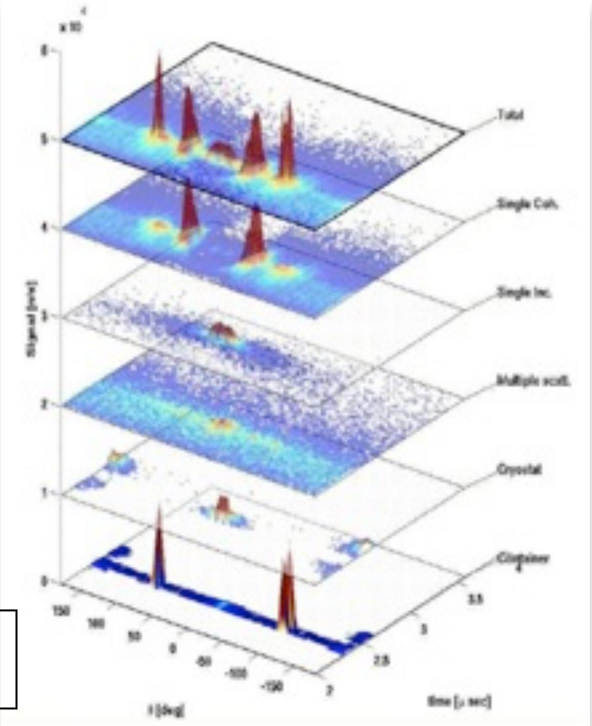






What can Monte Carlo Simulations be used for ?

- Instrument optimization
  - New ideas can be tested first in a simulation
  - Different option can be compared
  - Numerical optimization is possible
- Virtual experiments
  - If some information about the sample is available, it can be checked what time and which settings are needed for the real experiment
- Instrument and data analysis
  - Simulations provide a large amount of information on the properties of the neutrons (e.g. on correlations in phase space and spin space)
  - They allow comparing true and measured sample properties
- Teaching



E. Farhi, M. Johnson, V. Hugouvieux and W. Kob, ILL Annual Report (2006) 87.

Thank you for your attention