

McStas-MCNP interface solutions

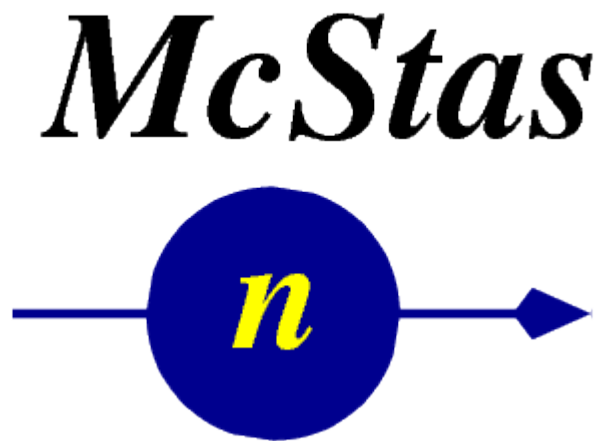
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²ESS Data Management & Software Center, Denmark

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- Monte Carlo neutron ray tracing engine
- Release 1.1 (1.2 beta available for linux)
- Portable code (Unix/Linux/Mac/Windows, 32 and 64 bit support)
Has run on all from iPhone to 1000+ node clusters (including FERMI)



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

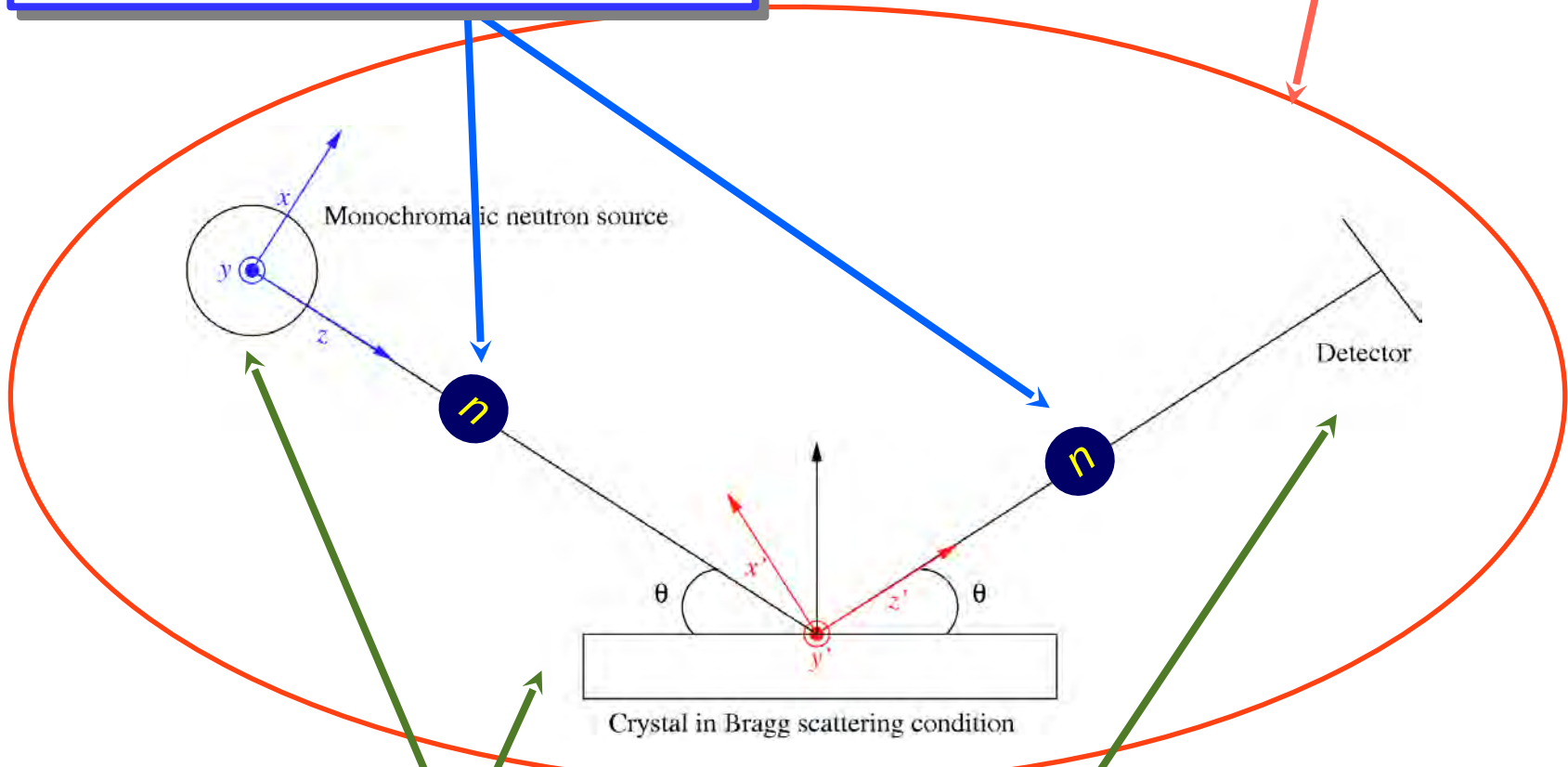
Project mailing list at
mcstas-users@mcxtrace.org

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

McStas overview

Neutron ray/package
 Weight (p): # neutrons (left) in the package
 Coordinates (x, y, z)
 Velocity (v_x, v_y, v_z)
 Spin (s_x, s_y, s_z)

Instrument: positioning + transformations
 between sequential component coordinate
 systems, e.g. neutron source, crystal, detector



Components: Where neutron physics happen,
 Weights adjusted according to scattering
 cross sections etc.

Independent geometrical entities with local
 Internal coordinate systems.

NEUTRON STATE ($x, y, z, v_x, v_y, v_z, t, s_x, s_y, s_z, p$)

- ONLY neutrons
- Validity determined by the code in the components.
- (Epi)Thermal to cold neutrons
 - No high energy stuff
- Structured materials

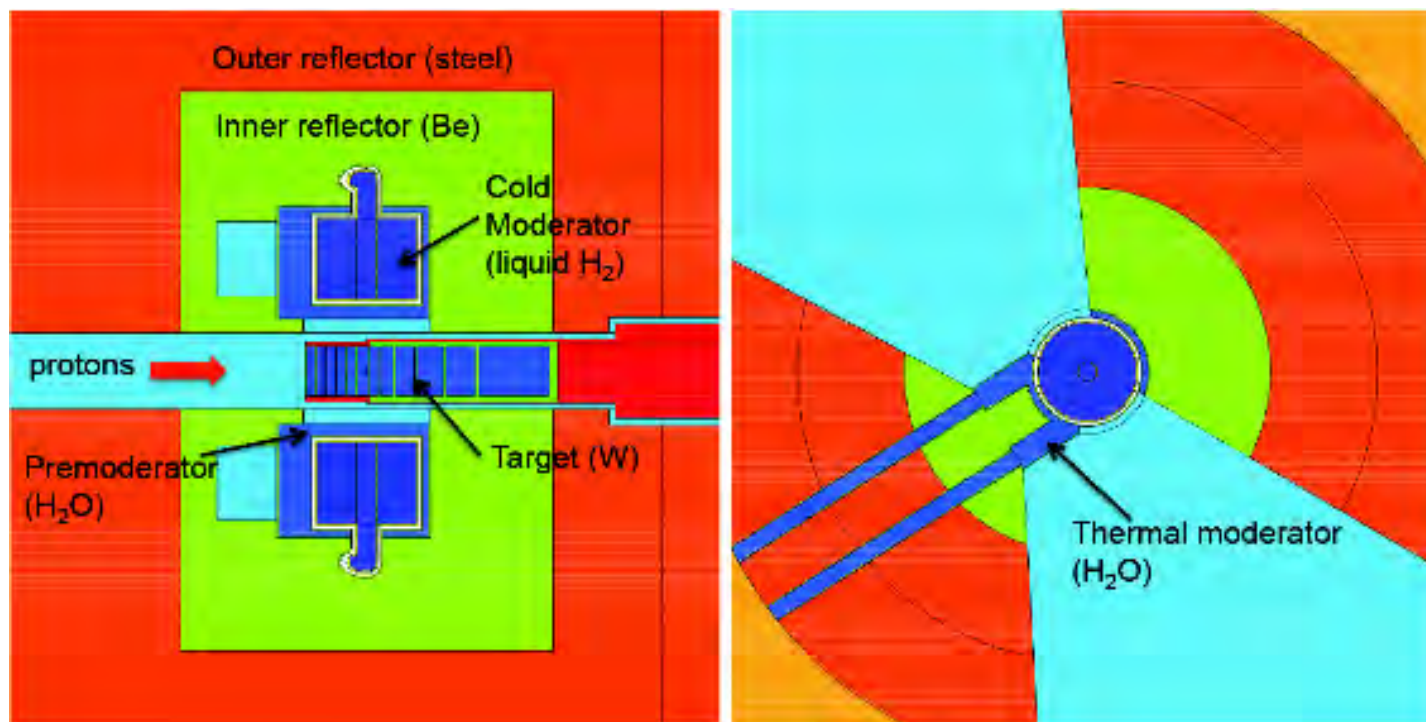
- Distributed “Freely” by RSICC.
- Source code available.
- Restrictive licensing-terms.
- Parallelism through MPI: MCNP6/MCNPx (most functionality)

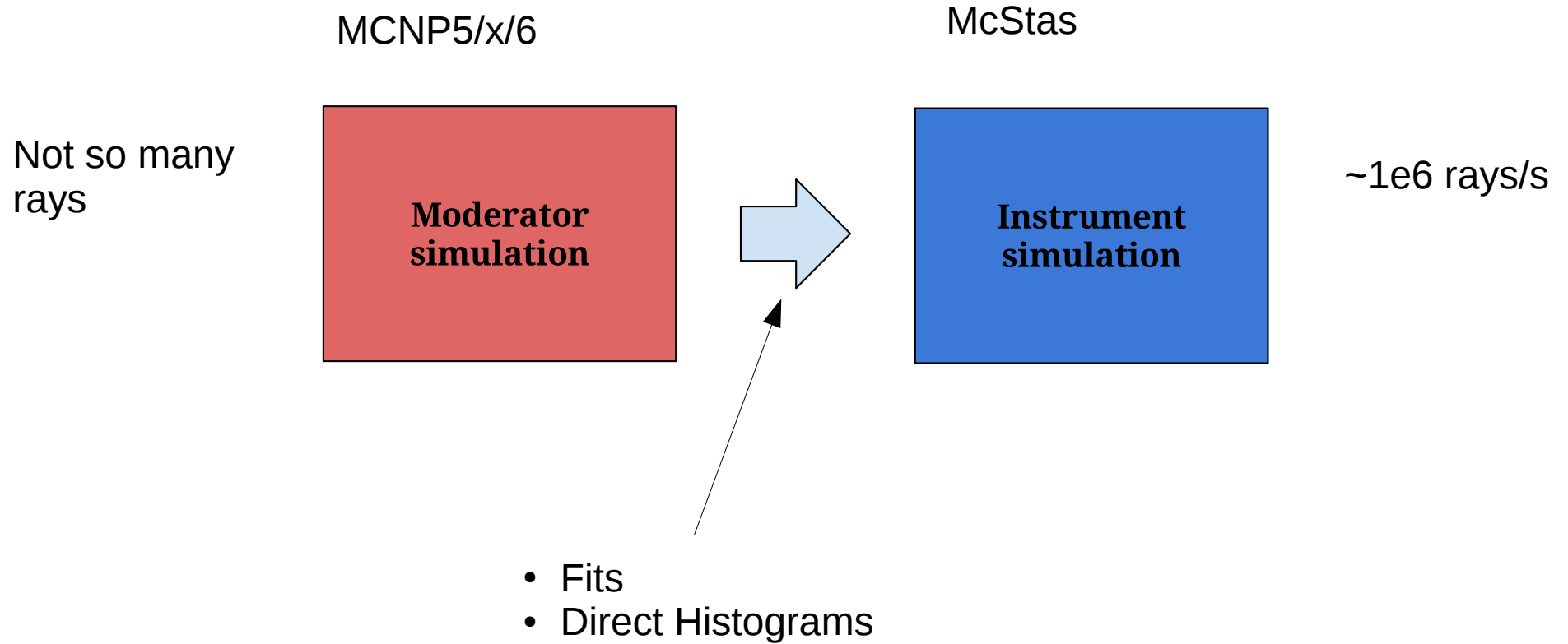


- Not restricted to neutrons (MCNPx / MCNP6)

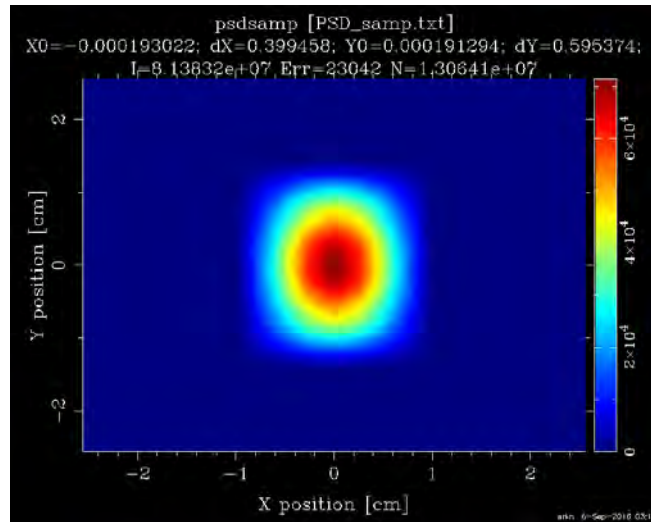
NEUTRON STATE ($x, y, z, v_x, v_y, v_z, t, p$)

- Materials: Everything is a gas
- $E < 150$ MeV
- Sense of p slightly different: $p < 1$
- Particle conversions possible

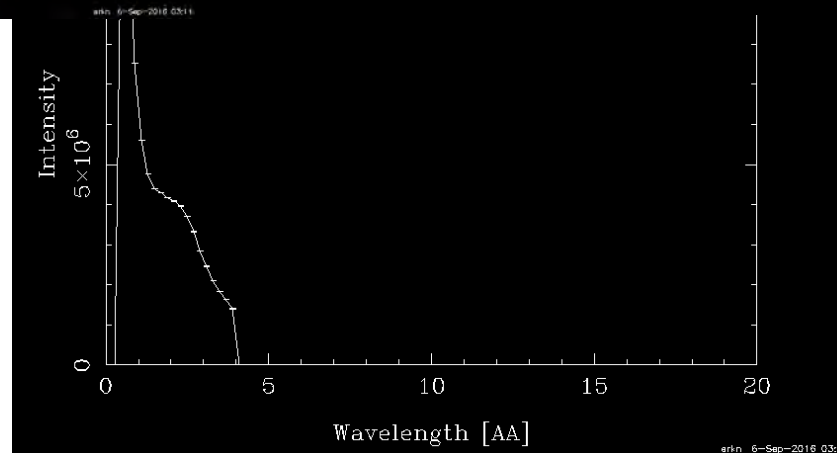
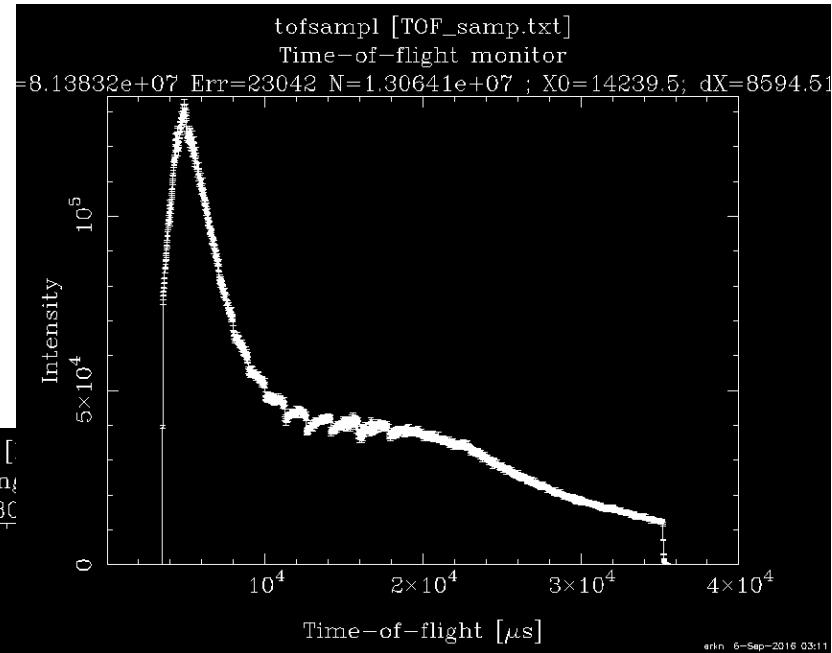




- ISIS_moderator
- SNS_source
- ESS_moderator/butterfly

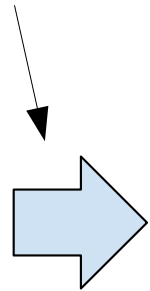
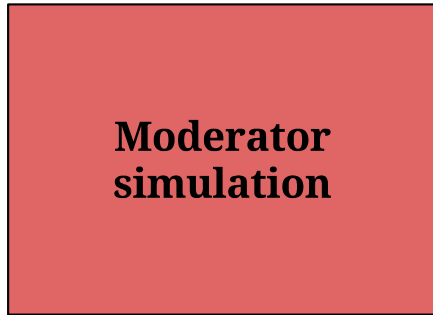


lsamp [
 Wavelen
 Err=23042 N=1.30



- Fits
- Direct Histograms

MCNP5/x/6



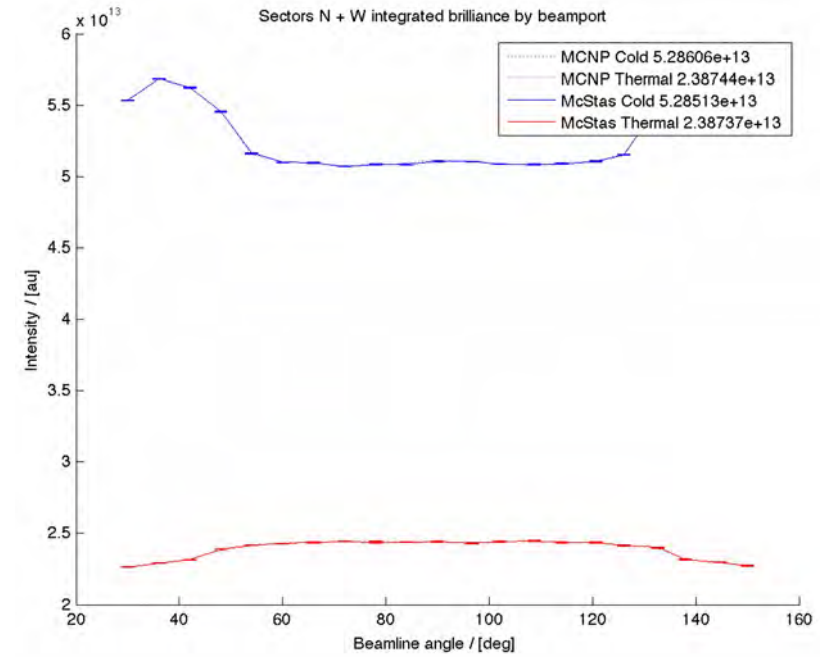
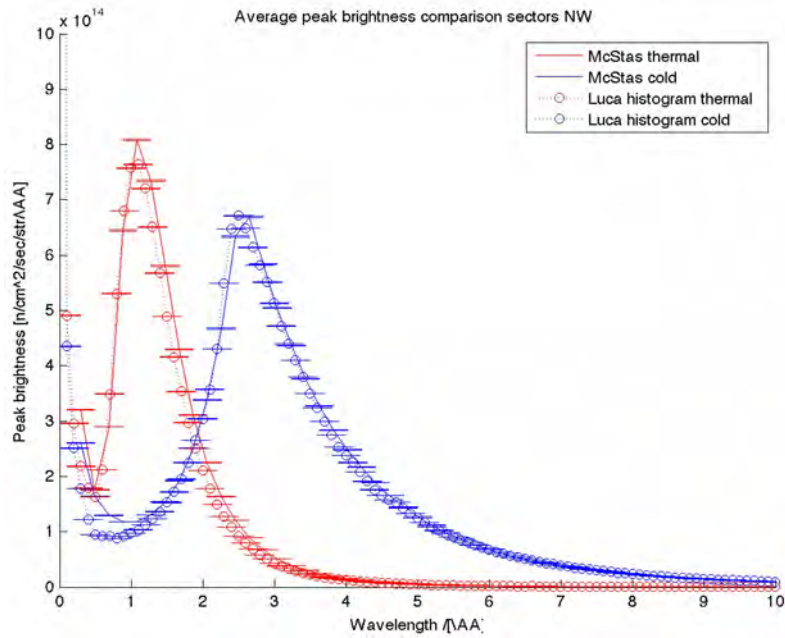
McStas



Scatter_logger / SSR/W
Using escaped neutrons

MCNP5/x/6

- 1) Tallys and Fits (traditional, typically uniform emission same spectrum everywhere)
- 2) Ptrac-files
- 3) Combined compilation
- 4) SSW/SSR
- 5)



- Fast
- Robust



- No reentry
- Highly dependent on quality of documentaion



- MCNPx outputs an ascii file containing neutron states.
- This file may be read by McStas
MCNP_virtual_input

- Fast



- No reentry
- No MPI
- Large ascii files ~.2kB/event
- Only 1 ptrac surface allowed



Ptrac format

```

-----
3000      2      10      179
100       2       0
0.00000E+00 0.28640E+00
0.43531E+00 -0.10000E+01
0.00000E+00 0.00000E+00
0.10000E+00 0.10000E+01
0.33356E-02
      3000      3      110      179
10        2       0
-0.20000E+00 0.28640E+00
0.43531E+00 -0.10000E+01
0.00000E+00 0.00000E+00
0.10000E+00 0.10000E+01
0.40028E-02
      3000      4      120      179
100       2       0
-0.40000E+00 0.28640E+00
0.43531E+00 -0.10000E+01
0.00000E+00 0.00000E+00
0.10000E+00 0.10000E+01
0.46699E-02
      3000      5      130      179
-----

```

Source Surface Write/Read in MCNP stops/starts simulations at a given logical point.

Neutron state is written to a binary file

McStas Components:

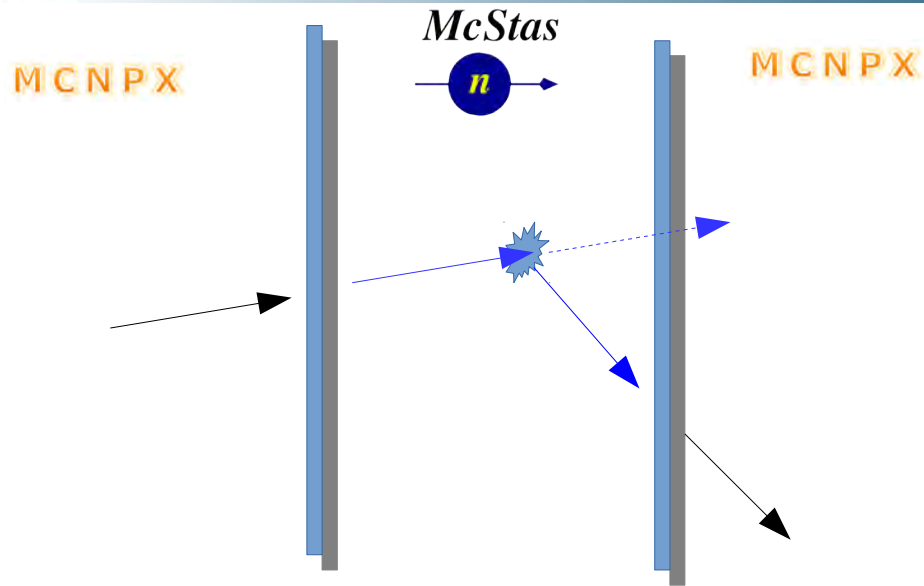
MCNP_Virtual_ss_Input & MCNP_Virtual_ss_Output

- Flexible
 - Access to full McStas functionality
 - Access to full MCNPx functionality
- Reentrant (but limited)



- Big files ~.1kB/event
- Proprietary binary format (diff. MCNPx & MCNP6)





Prototype exists for MCNPx

- McStas entry surface defined in MCNPx
- Neutrons crossing the surface trigger a McStas simulation.
- Upon reentry the neutron state is updated.
-

- Flexible
 - Access to full McStas functionality
 - Access to full MCNPx functionality
- Reentrant



- Slow
- Requires MCNP source code
- Licensing Issues
- Not all user-friendly

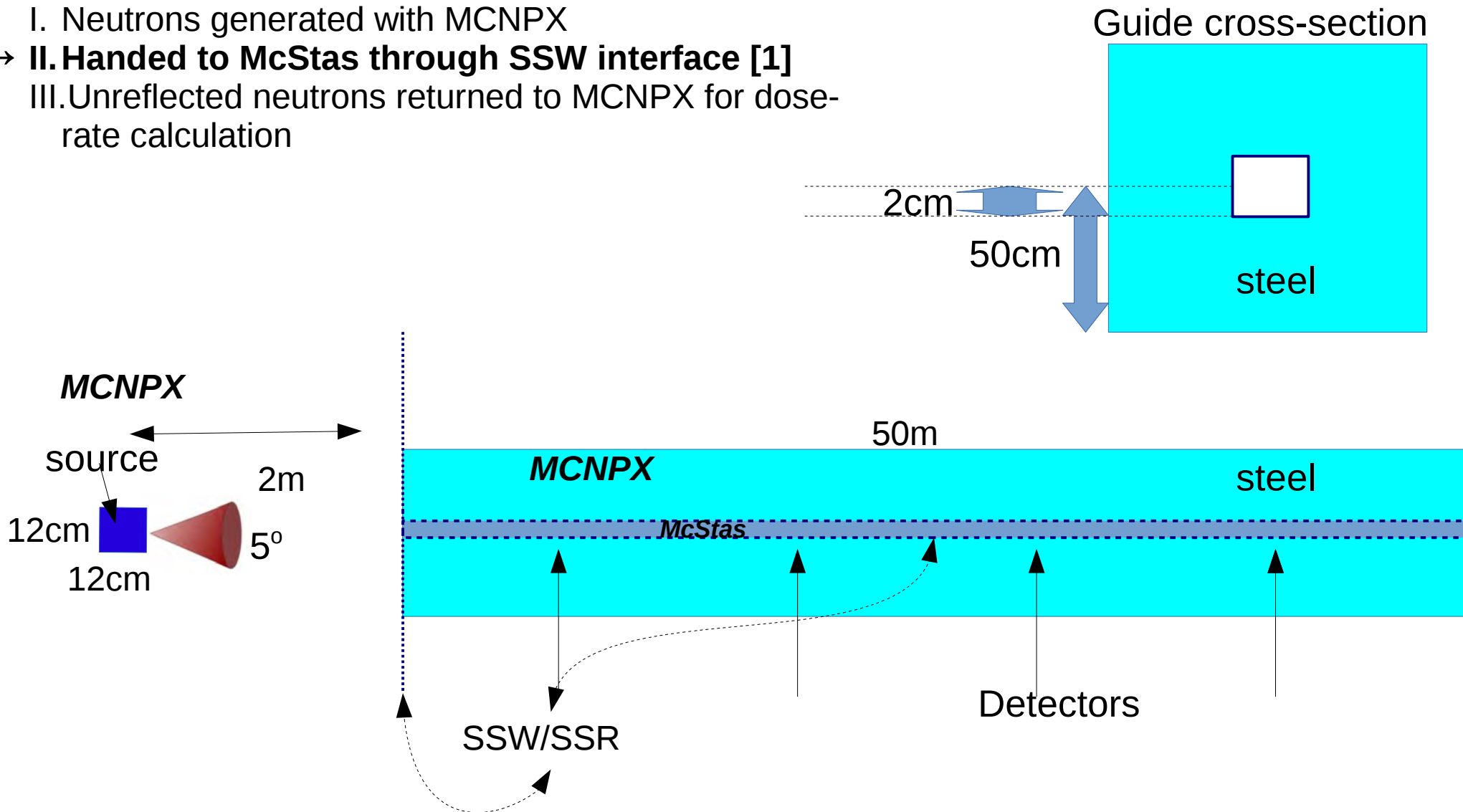


PROTOTYPE Exists for MCNPx

I. Neutrons generated with MCNPX

→ II. Handed to McStas through SSW interface [1]

III. Unreflected neutrons returned to MCNPX for dose-rate calculation

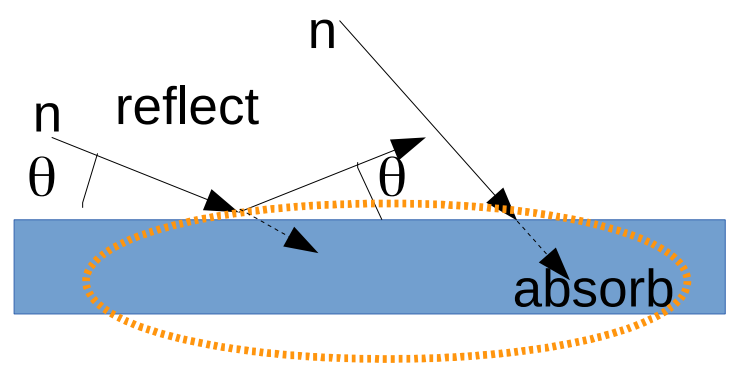


- I. Neutrons generated with MCNPX
- II. Handed to McStas through SSW interface [1]
- **III. Unreflected neutrons returned to MCNPX for dose-rate calculation**

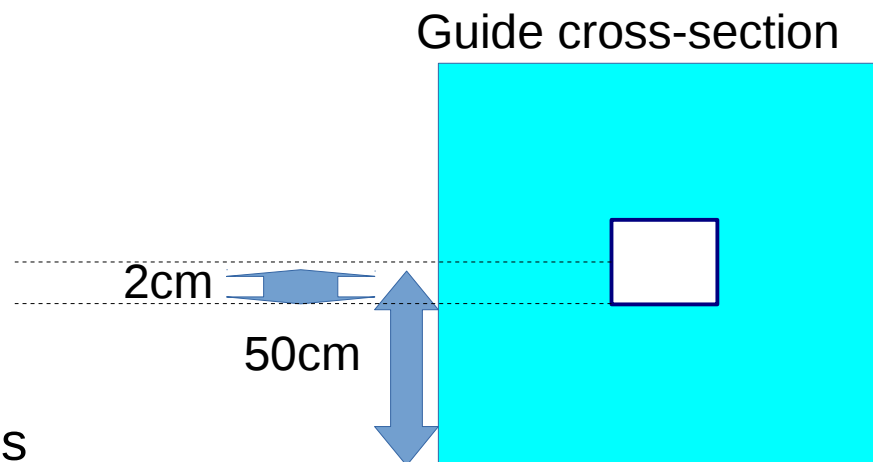
At each scattering:



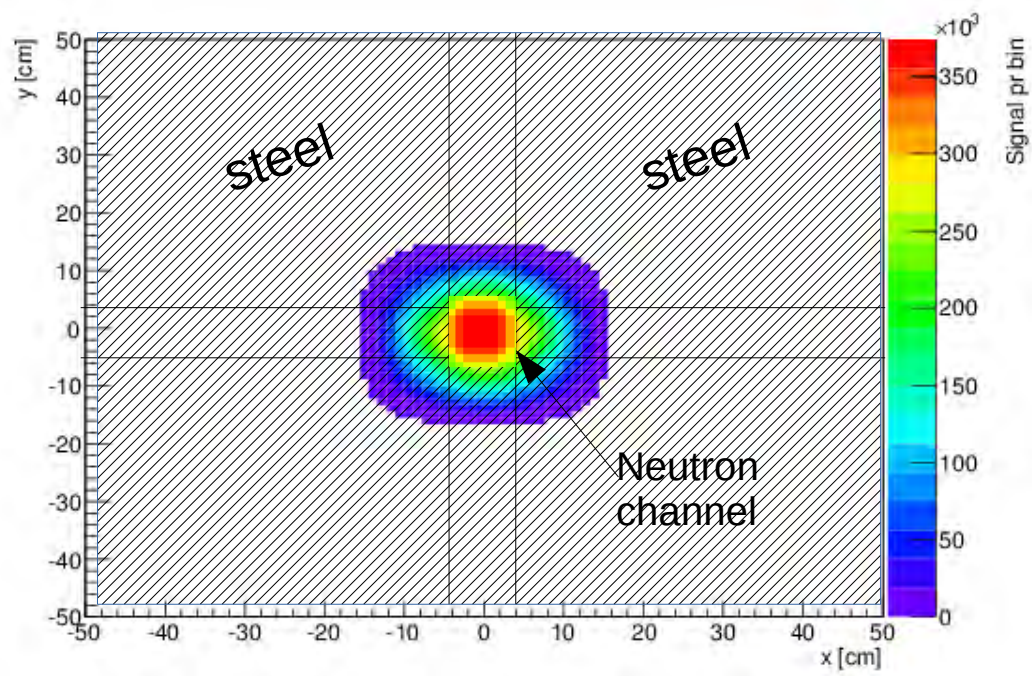
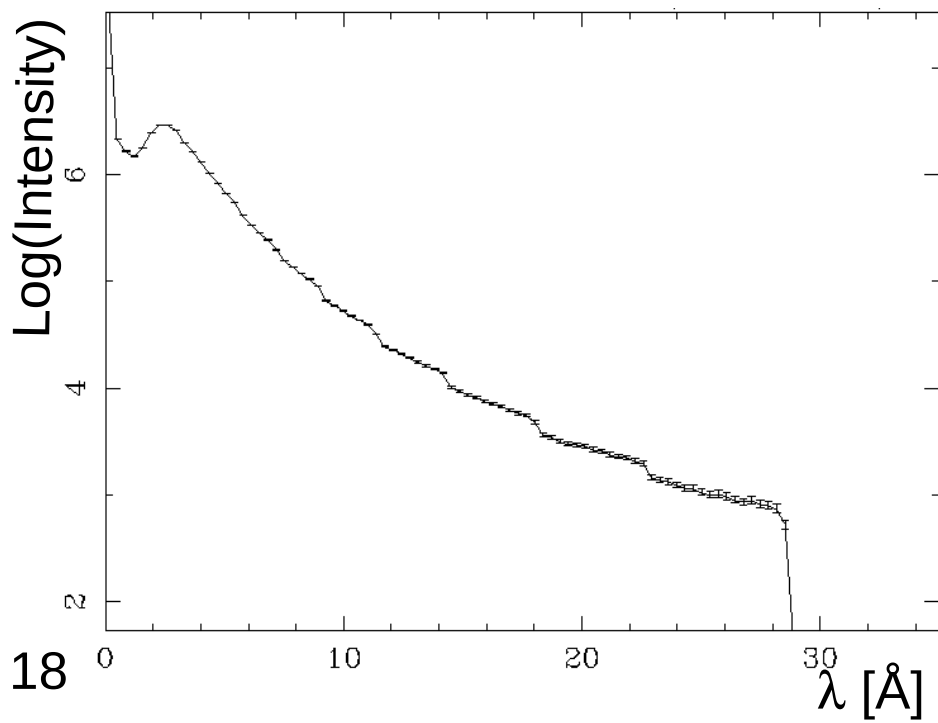
Incomming state: $n_{in} = (\mathbf{x}, \mathbf{v}_{in}, t, w_{in})$
 Transmitted state: $n_{trans} = (\mathbf{x}, \mathbf{v}_{in}, t, w_{trans})$
 Reflected state: $n_{refl} = (\mathbf{x}, \mathbf{v}_{out}, t, w_{in} - w_{itrans})$



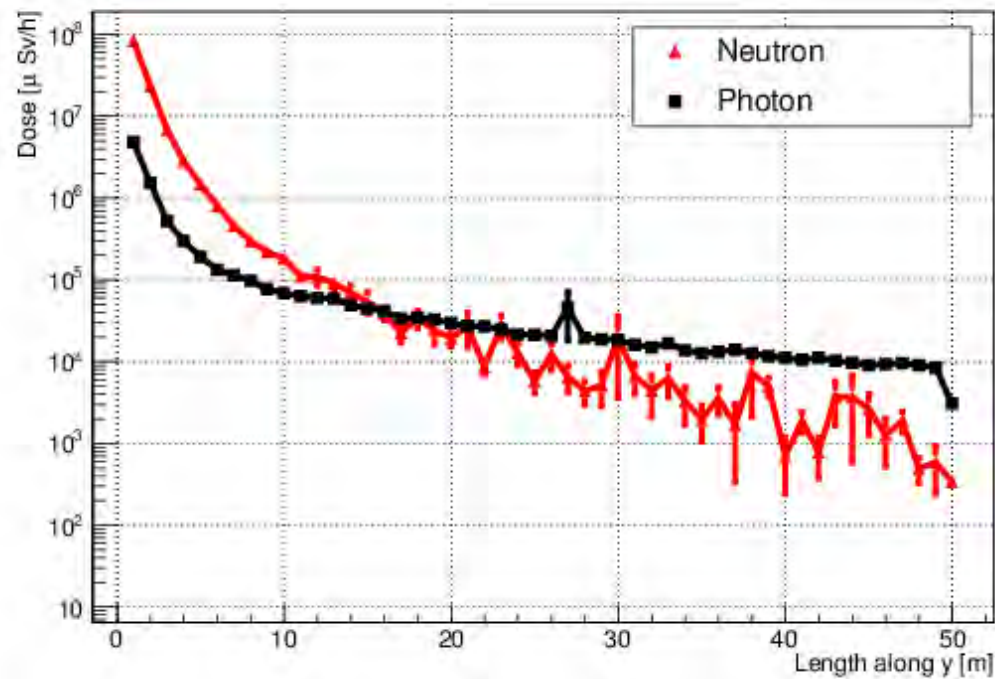
- I. Neutrons generated with MCNPX
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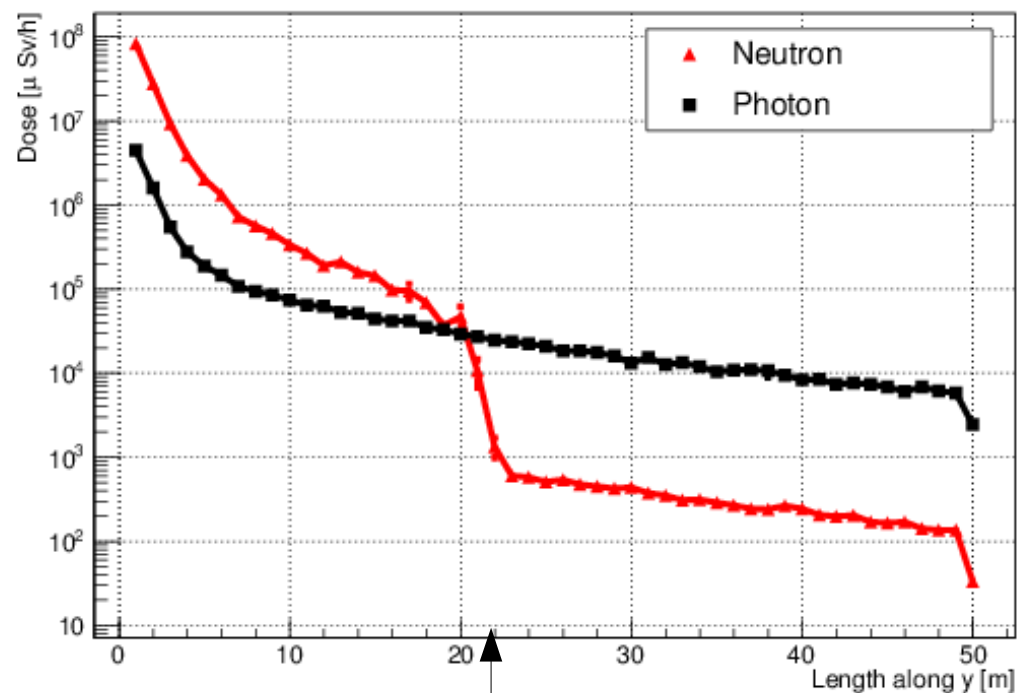
Guide end overilluminated by energetic neutrons



Straight guide



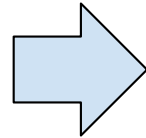
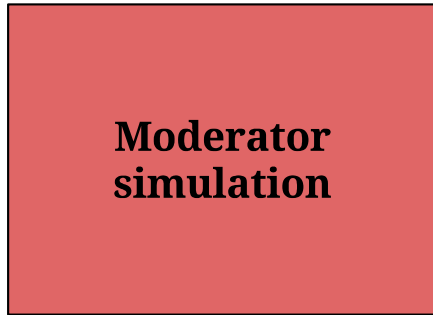
Curved guide ($r_{\text{curvature}} = 1500\text{m}$)



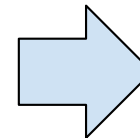
Line-of-sight lost

- Dose-rates, measured 5cm in the steel converted from flux according to official Swedish radiation protection procedures

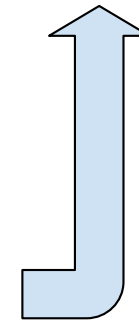
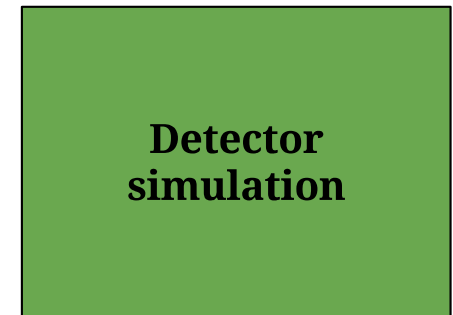
MCNP5/x/6



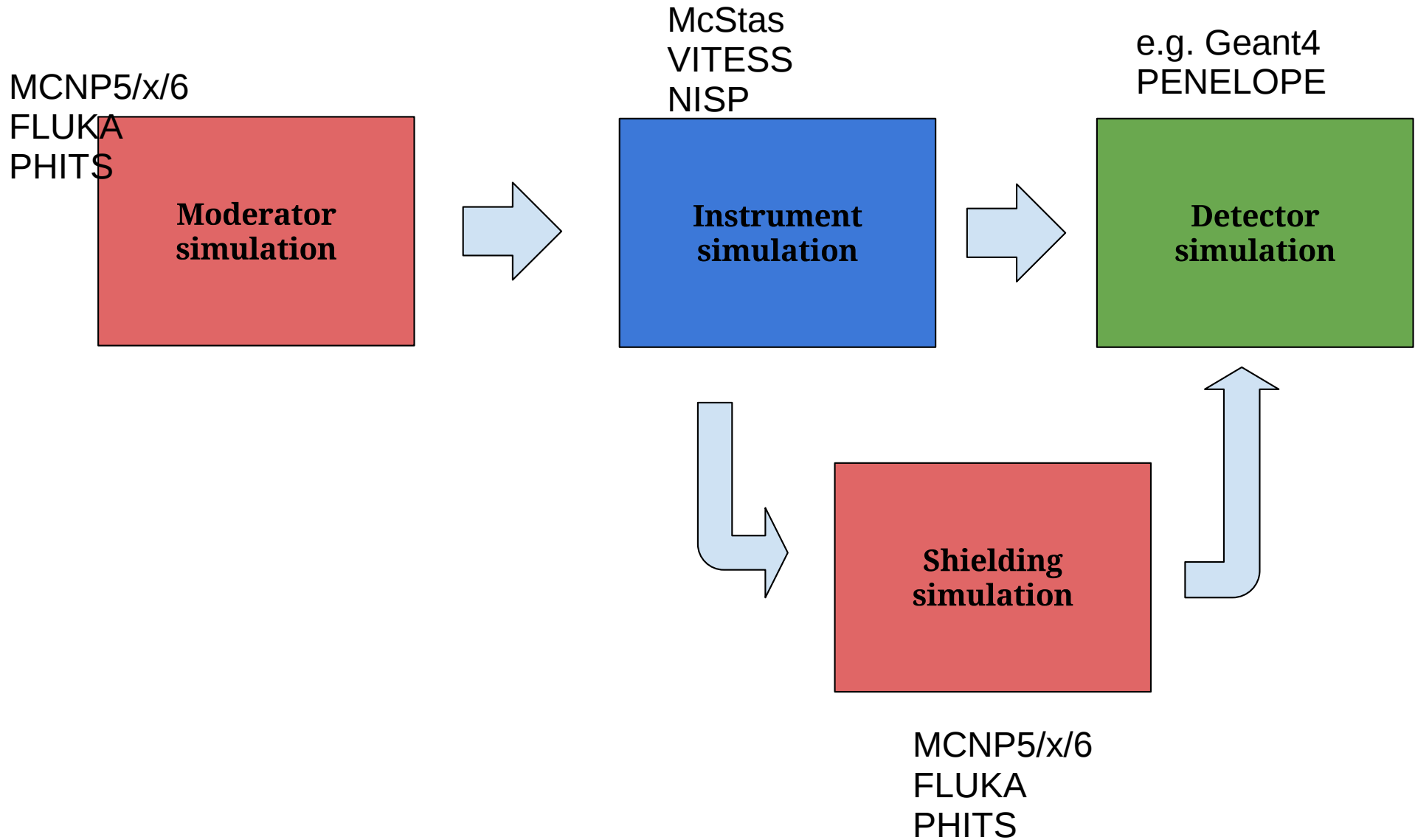
McStas



e.g. Geant4



MCNP5/x/6



NONE OF THE ABOVE

Next talk by Thomas Kittelmann