McStas-MCNP interface solutions

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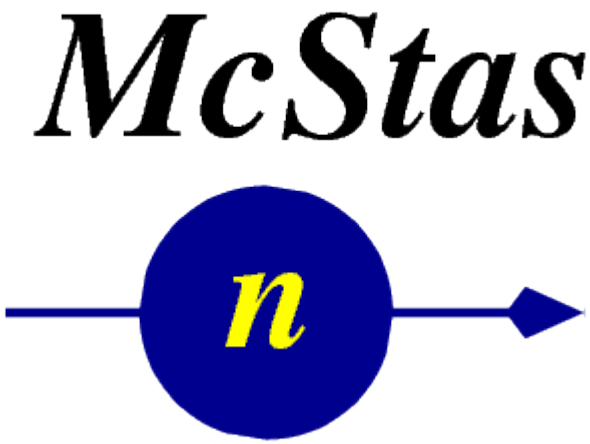
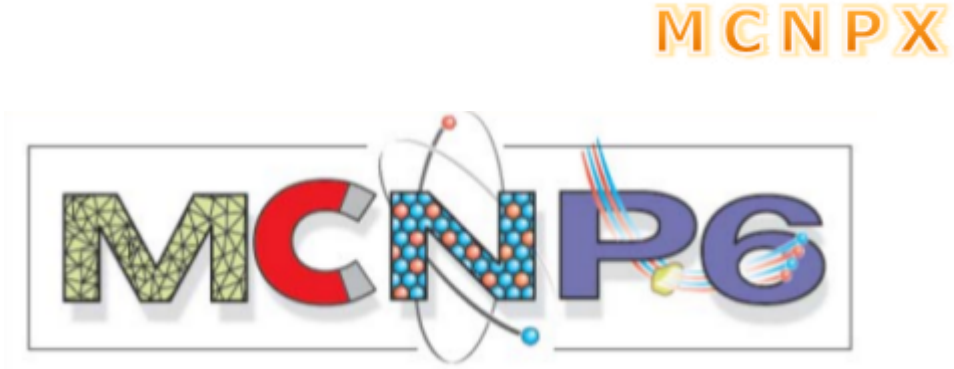




McStas overview

- 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 (inlucding FERMI)

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

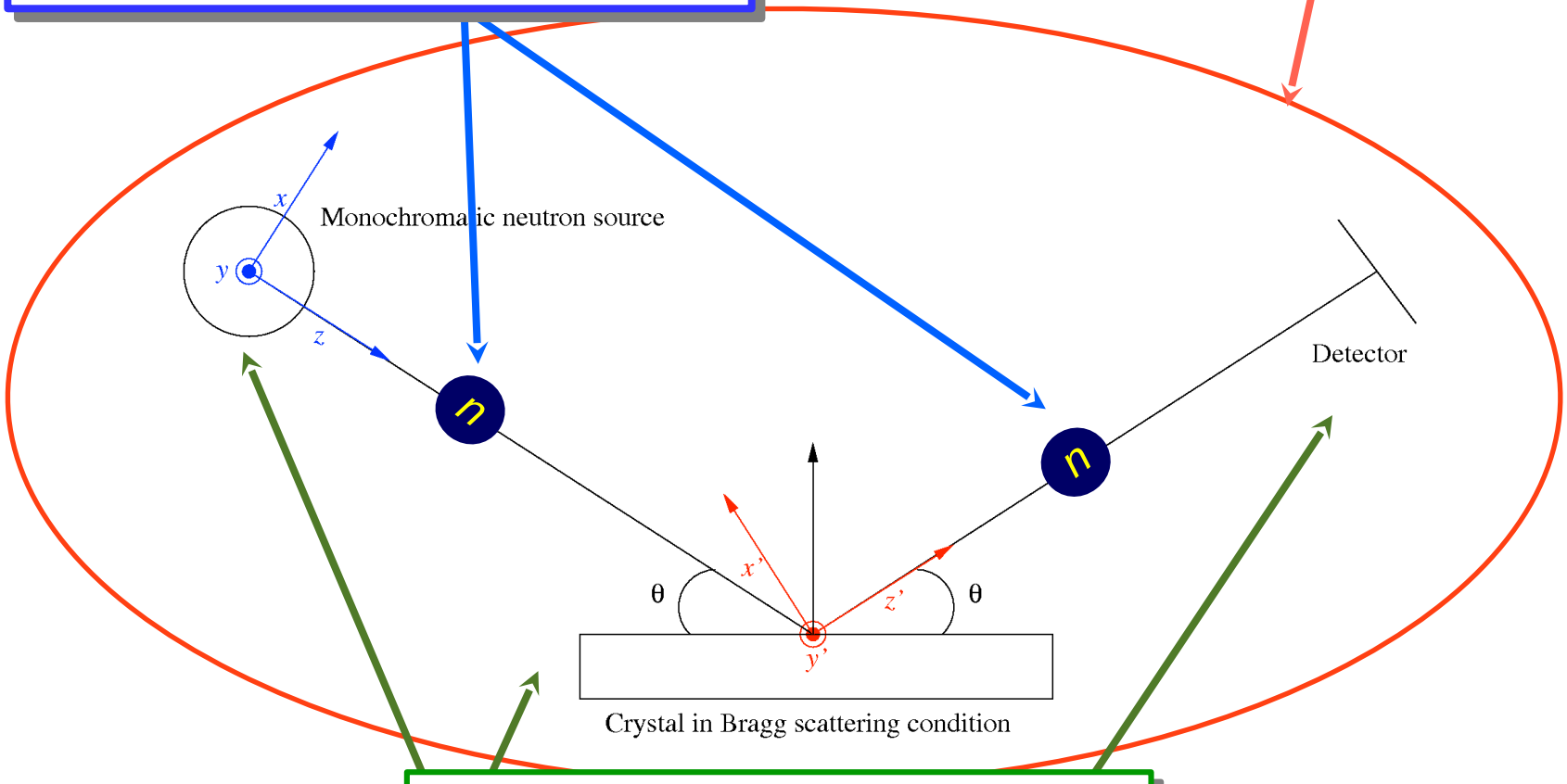
Project mailing list at
mcstas-users@mcxtrace.org

- 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.

McStas particle model and validity

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

MCNP overview

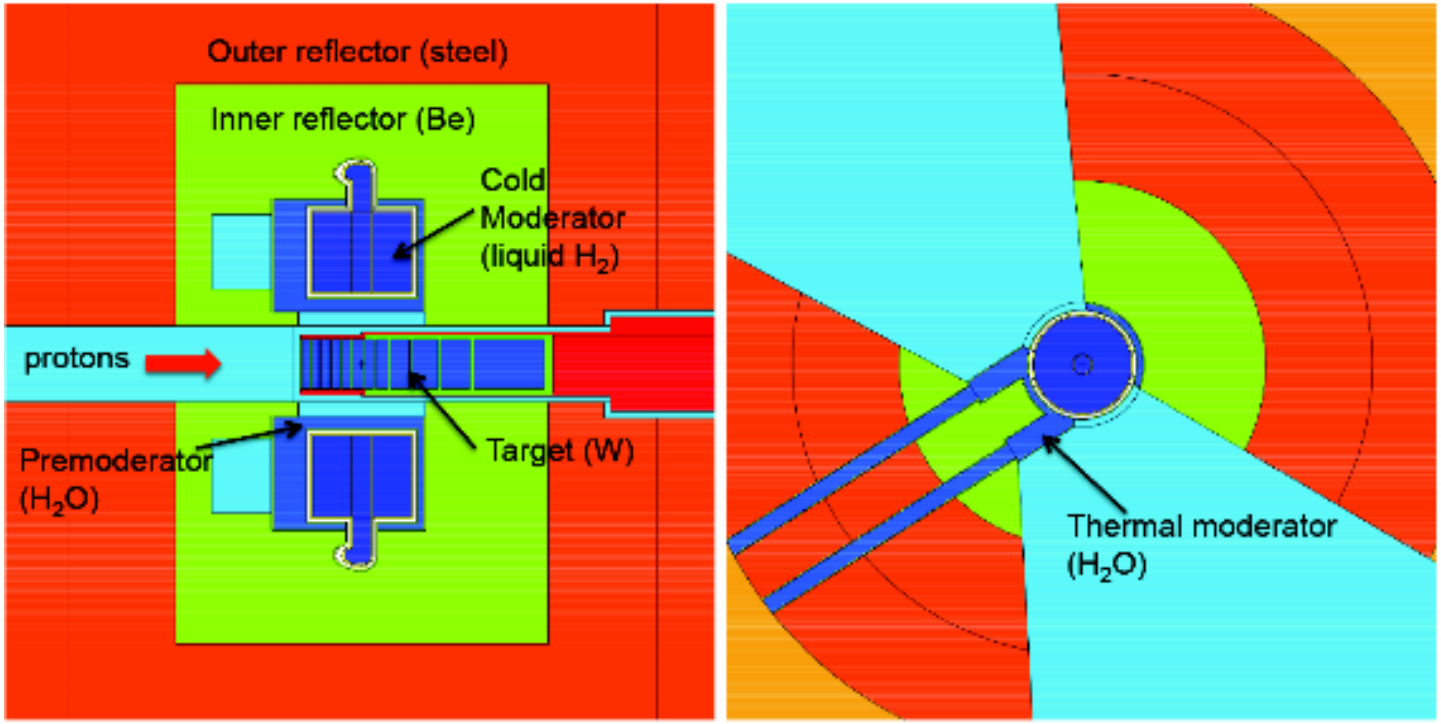
- Distributed “Freely” by RSICC.
- Source code available.
- Restrictive licensing-terms.
- Parallelism through MPI: MCNP6/MCNPx (most functionality)

- Not restricted to neutrons (MCNPx / MCNP6)

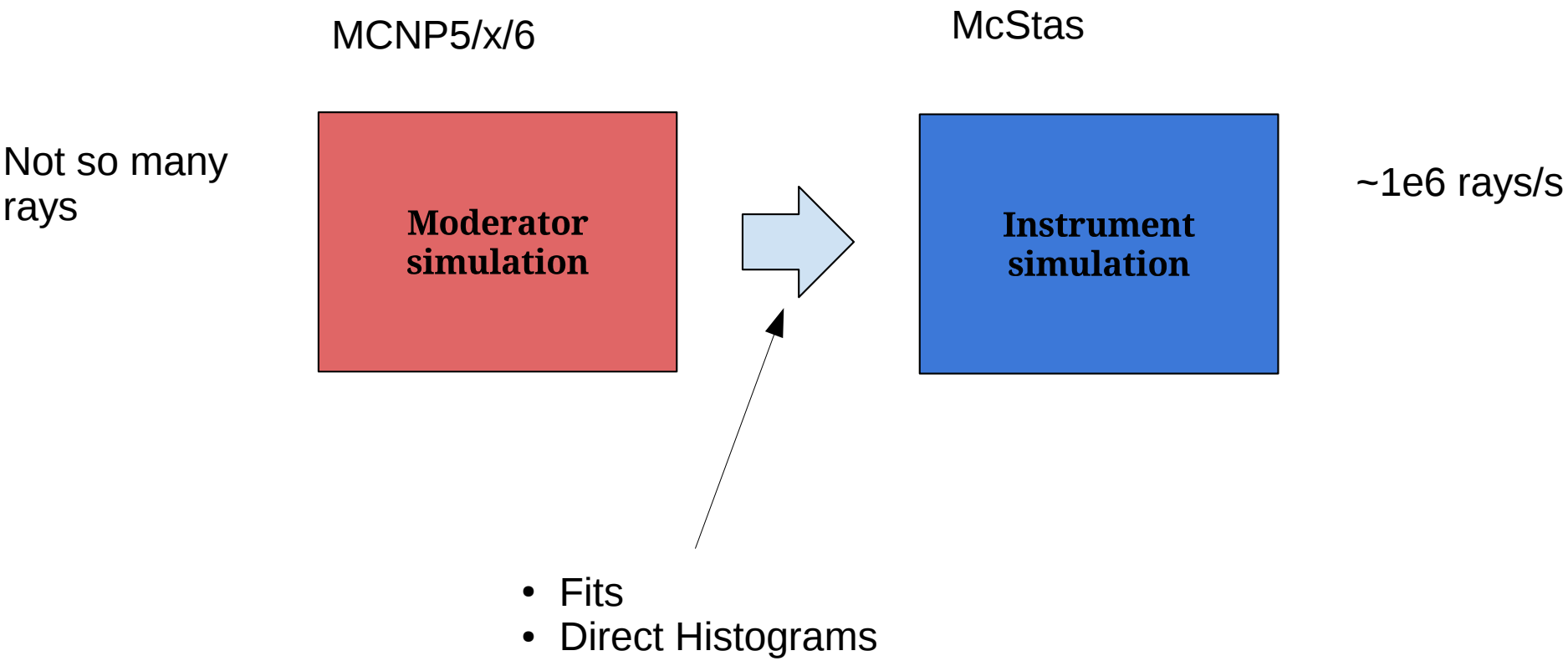
MCNP particle models and validity

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

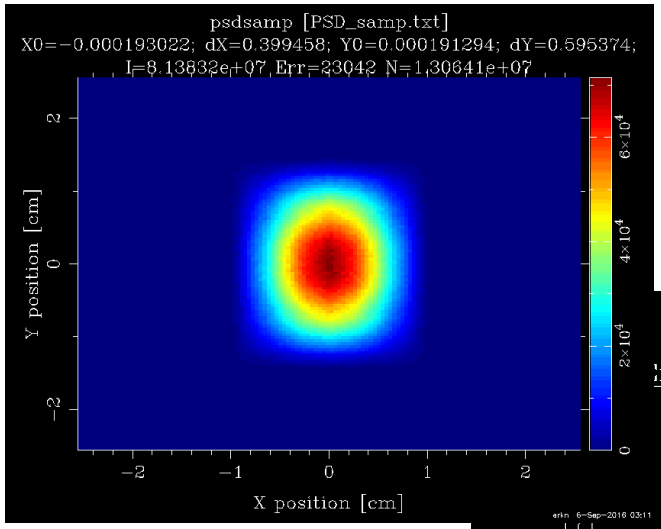

Outer reflector (steel)
Inner reflector (Be)
Cold
Moderator
(liquid H_2)
protons
Premoderator
(H_2O)
Target (W)
Thermal moderator
(H_2O)

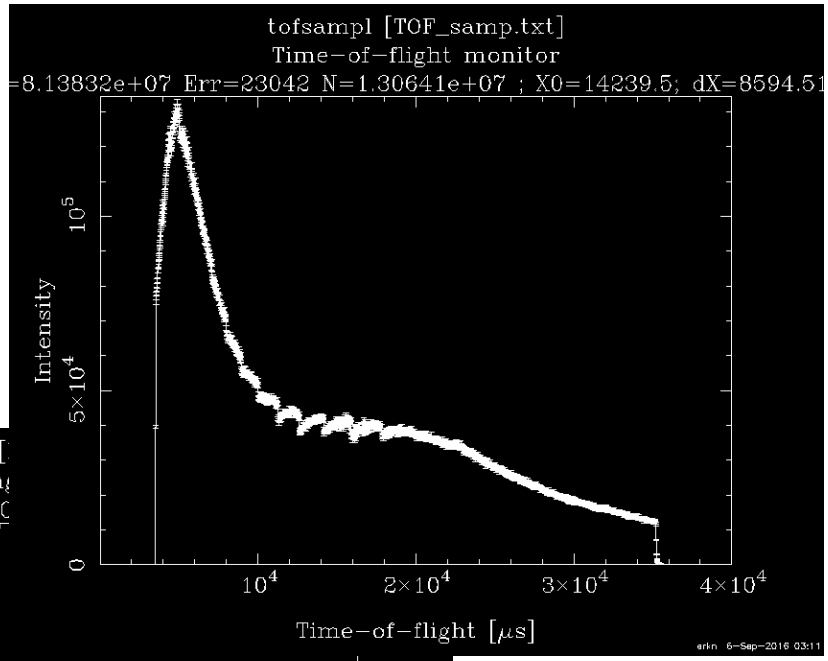
Present day normal

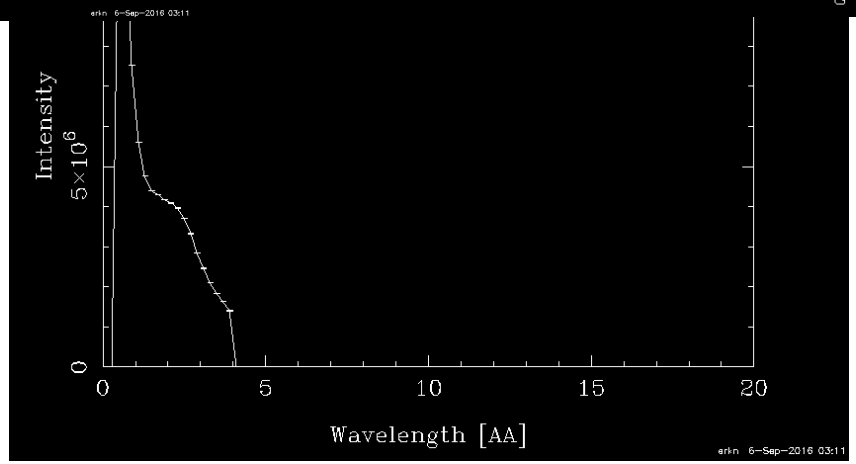


Examples

- ISIS_moderator
- SNS_source
- ESS_moderator/butterfly





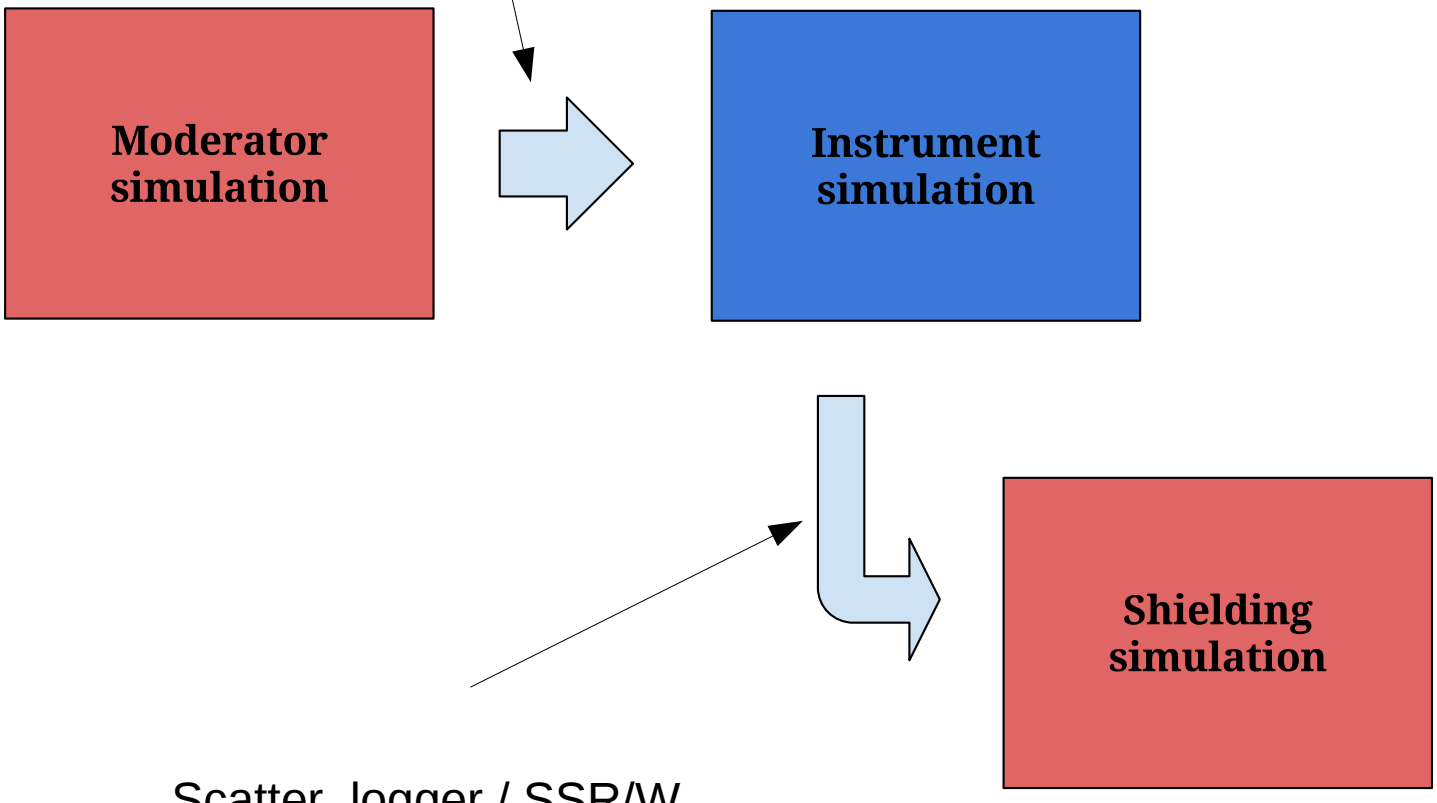


Present day

- Fits
- Direct Histograms

MCNP5/x/6

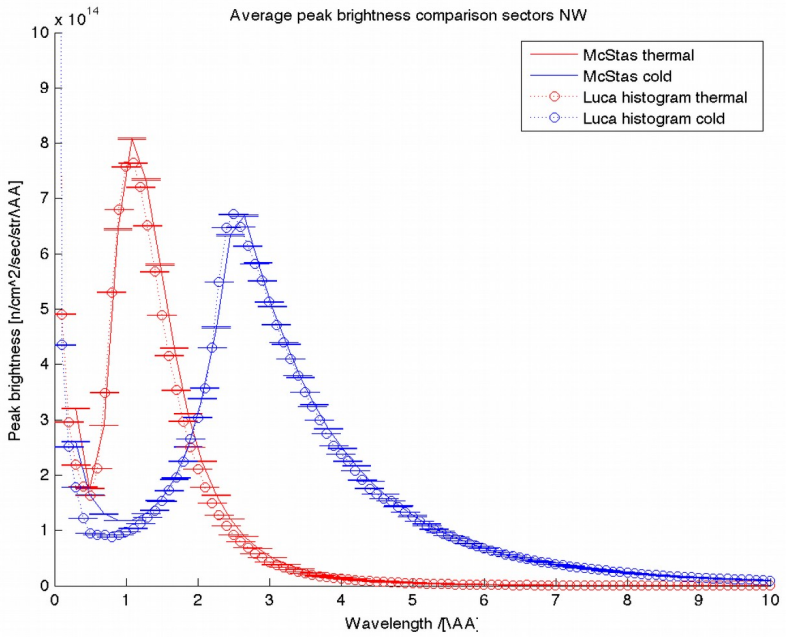
McStas

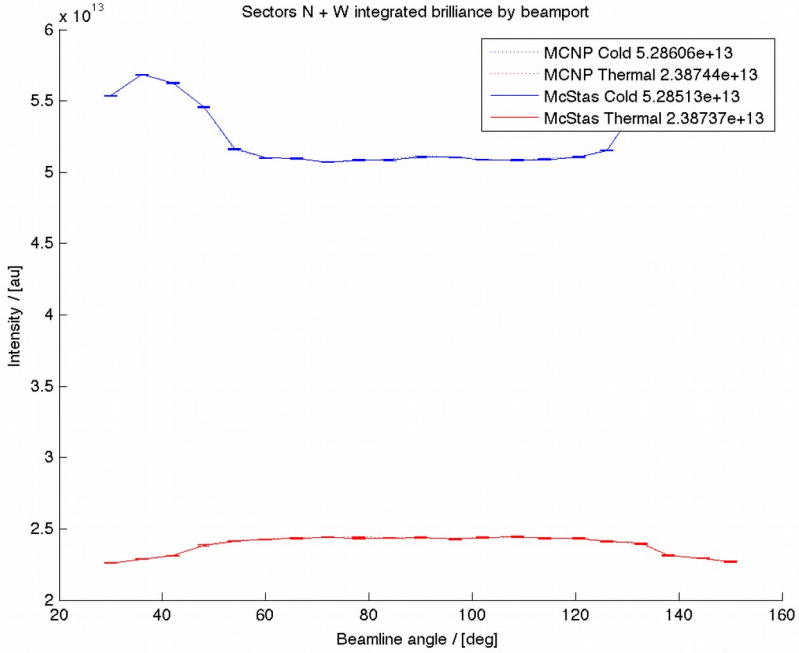


History: possible routes

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

Fits and functions





- Fast
- Robust

- No reentry
- Highly dependent on quality of documentaion

Ptracs

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

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
```

- Fast

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

SSW/SSR files

Source **S**urface **W**rite/**R**ead in MCNP stops/starts simulations at a given logical point.

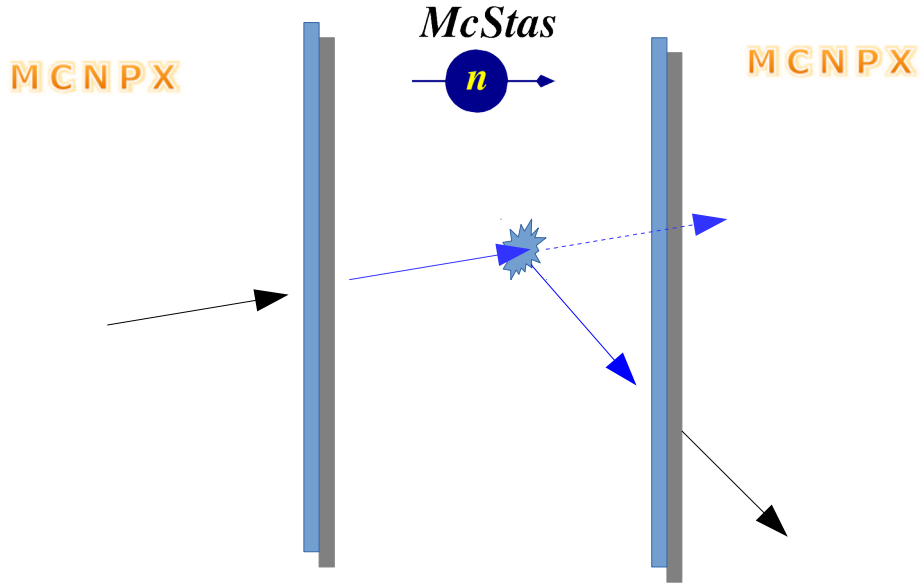
Neutron state is written to a binary file

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)

Combined compilation



Prototype exists for MCNPx

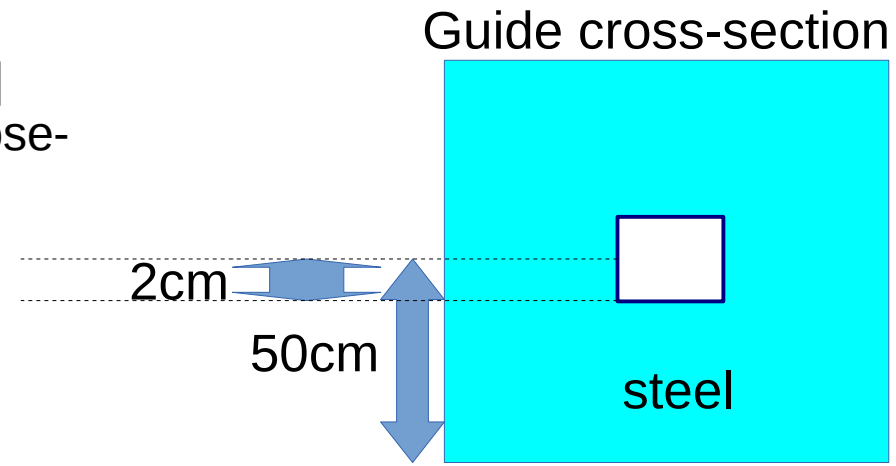
- McStas entry surface defined in MCNPx
- Neutrons crossing the surface trigger
- a McStas simulation.
- Upon reentry the neutron state is updated.
-

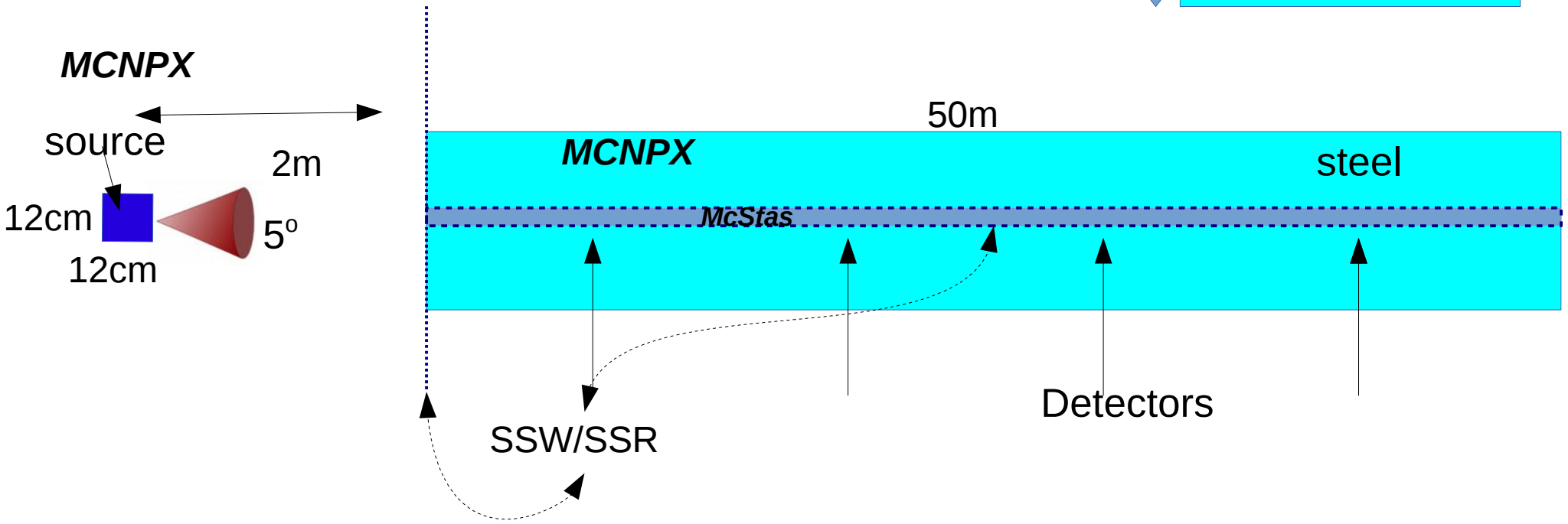
- Flexible
  - Access to full McStas functionality
  - Access to full MCNPx functionality
- Reentrant

- Slow
- Requires MCNP source code
- Licensing Issues
- Not al 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





 [1] E. Klinkby et al. 'Interfacing MCNPX and McStas for simulation of neutron transport.' Nucl. Instr & Meth A , 700: p106, 2013.

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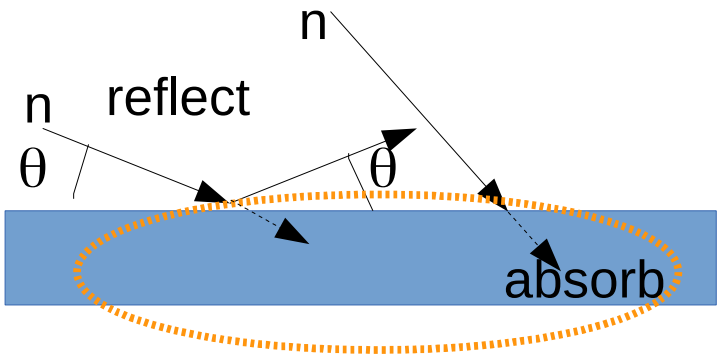


At each scattering:

⇒

Incomming state: $n_{in} = (\mathbf{x}, \mathbf{v}_{in}, t, w_{in})$

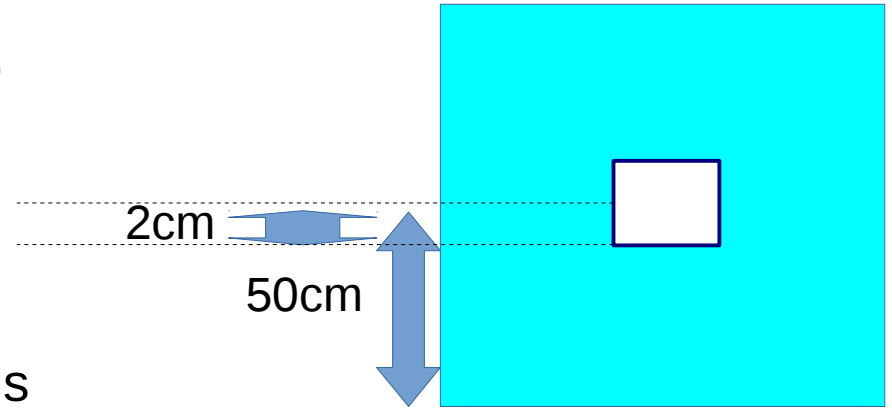
Transmitted state: $n_{trans} = (\mathbf{x}, \mathbf{v}_{in}, t, w_{trans})$

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

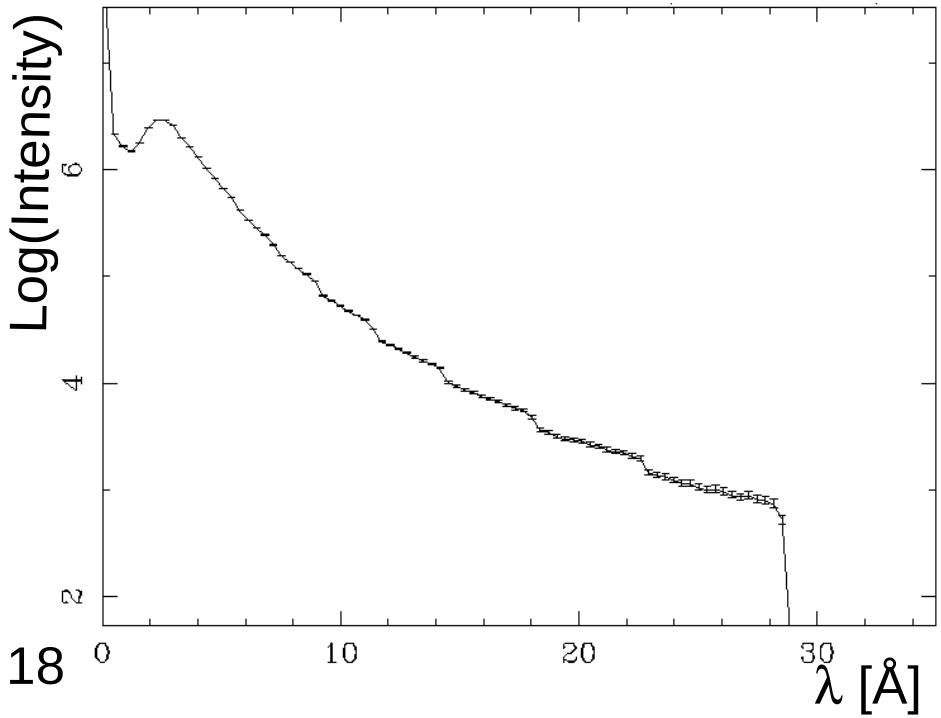
17

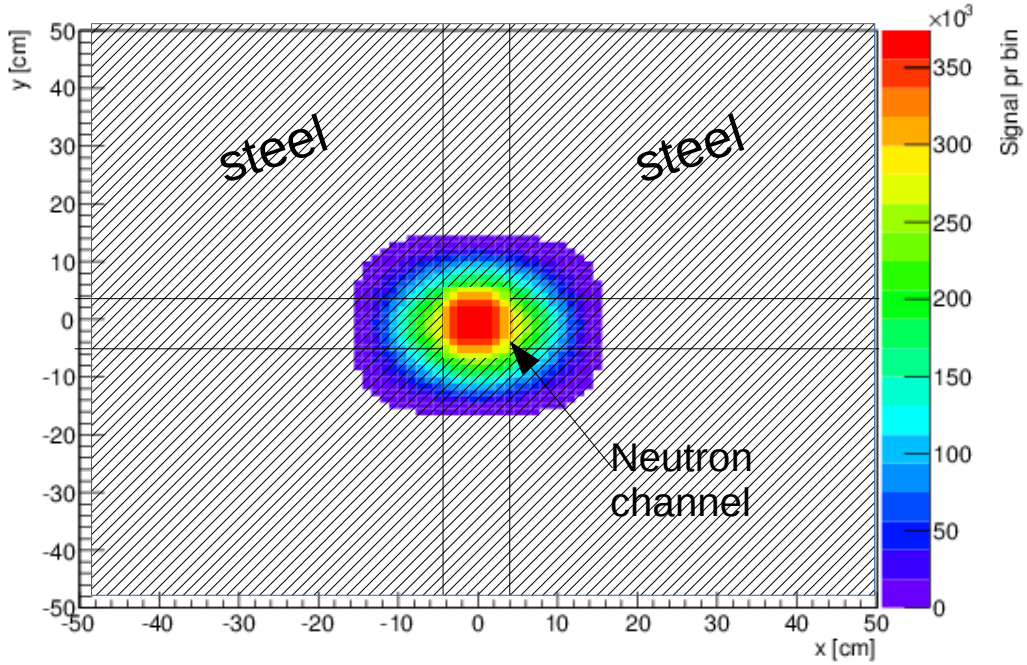
I. Neutrons generated with MCNPX
II. Handed to McStas through SSW interface [1]
→ **III. Unreflected neutrons returned to MCNPX for dose-rate calculation**

Guide cross-section

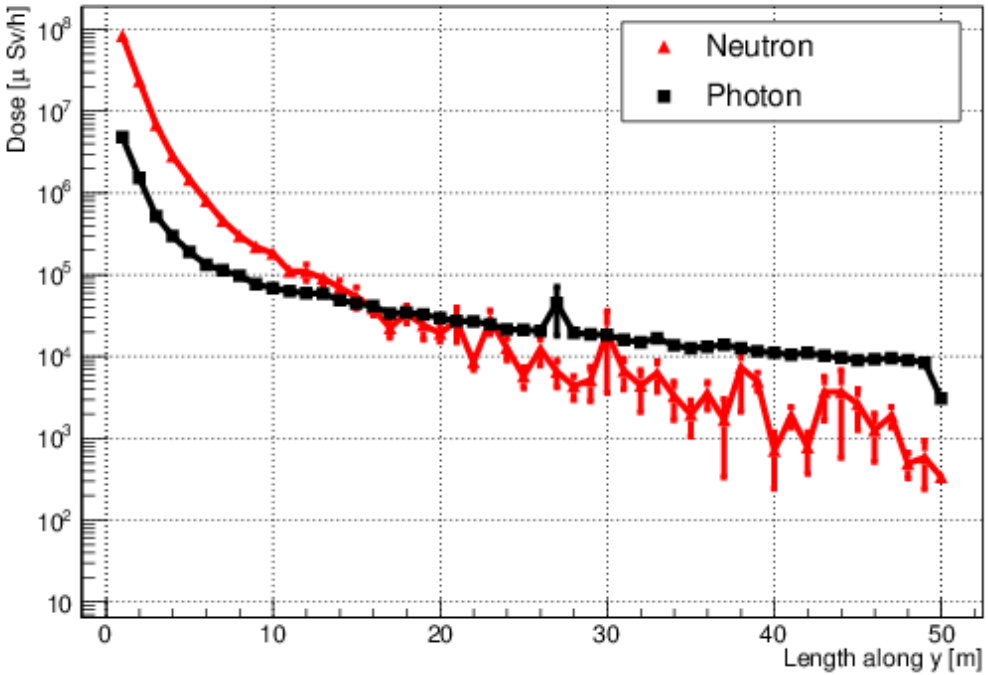


Guide end overilluminated by energetic neutrons

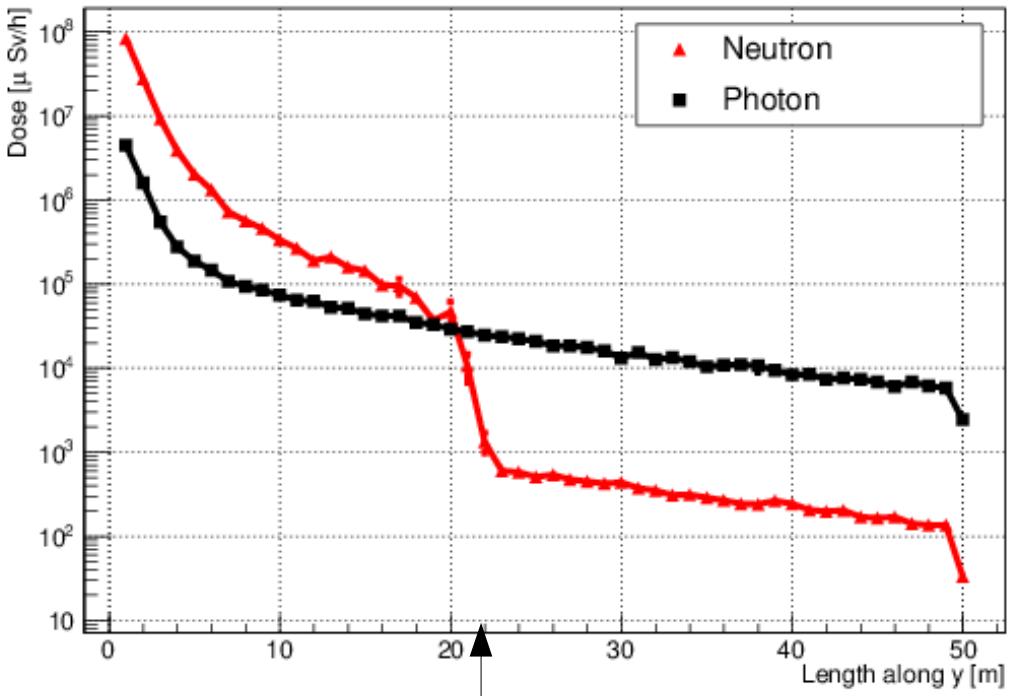




Straight guide



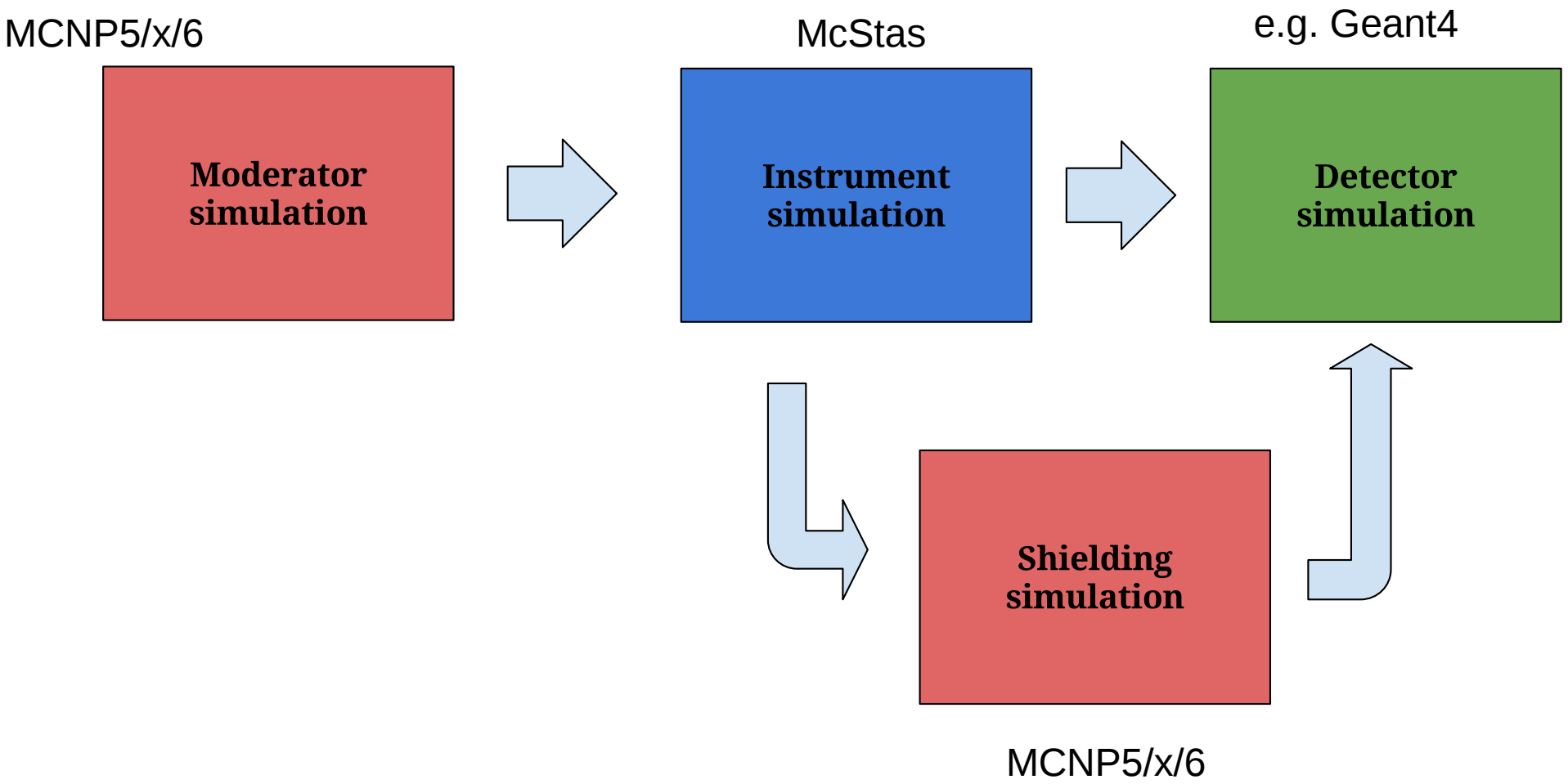
Curved guide ($r_{curvature}$=1500m)



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

19

Goal: Signal to Noise



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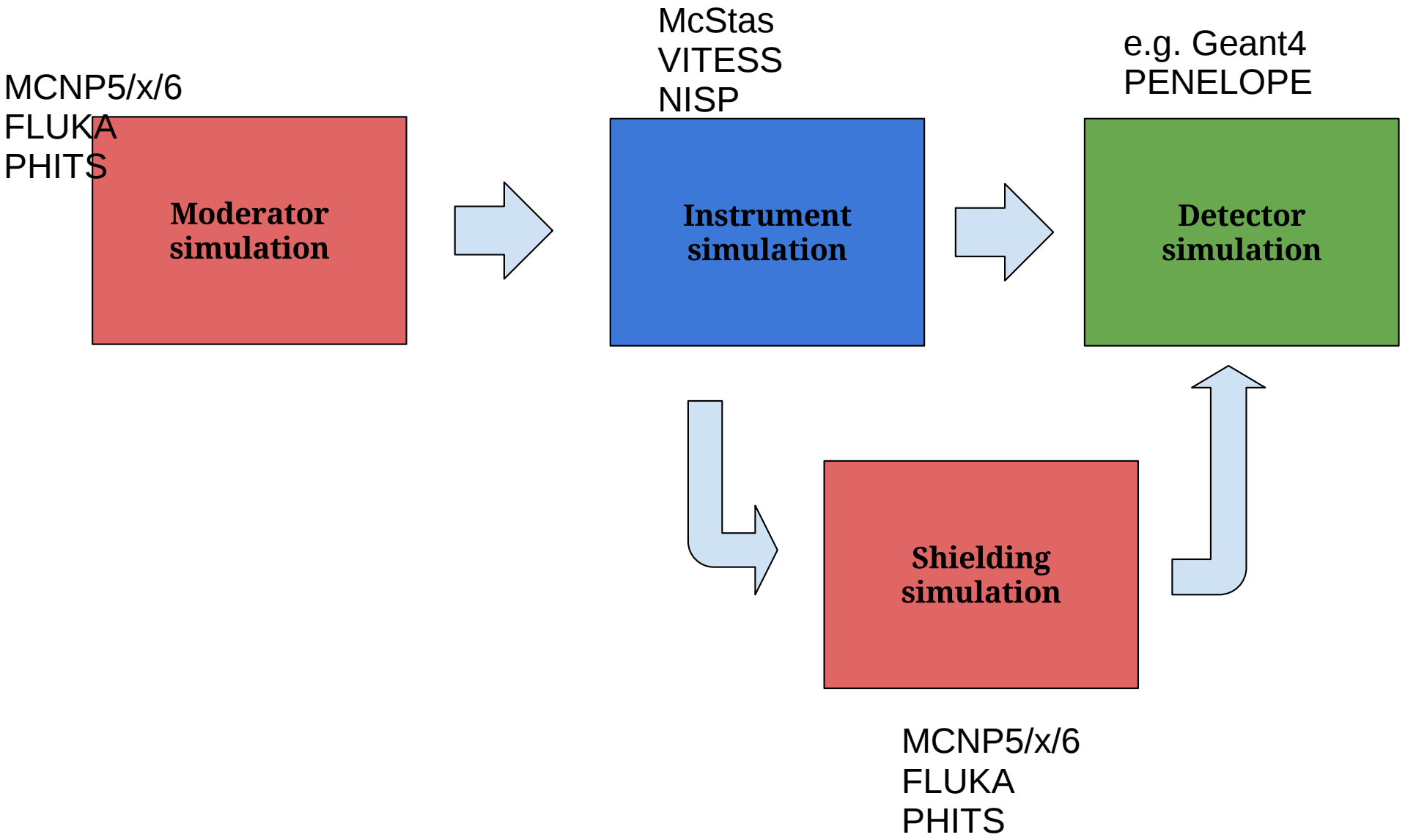

NONE OF THE ABOVE

Next talk by Thomas Kittelmann