MCNPX-McStas interface for cold/thermal neutron moderator and guide simulation

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Publication date:
2012

Citation (APA):
Klinkby, E. B., Lauritzen, B., Nonbøl, E., Willendrup, P. K., Filges, U., & Panzner, T. (2012). MCNPX-McStas interface for cold/thermal neutron moderator and guide simulation [Sound/Visual production (digital)]. International Workshop on Neutron Delivery Systems, Grenoble, France, 09/07/2012, http://www.ill.eu/news-events/past-events/2012/nds-2012/

MCNPX-McStas interface for cold/thermal neutron moderator and guide simulation

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Motivation

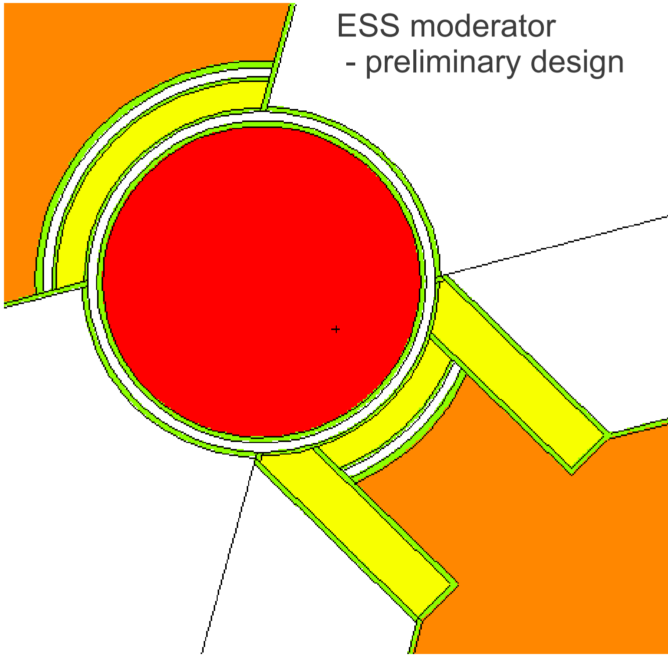
- Traditionally two decoupled Monte Carlo codes cover different needs in Neutron Scattering simulations:
  - MCNP/X used for TMS calculations
  - Neutron ray tracing code, e.g. McStas (talks by P.Willendrup & E. Farhi) used for instrument design + data analysis

- Even more precise simulations may be possible by combining the best of the two worlds: The detailed description of incoherent scattering from MCNP/X with the coherent scattering of McStas.

- **Prospects**: usage of direct MCNP/X McStas coupling:
  - Optimization of complex moderator design
  - Shielding calcutions along neutron guide
  - Crosstalk between neutron guides
  - Background at instruments

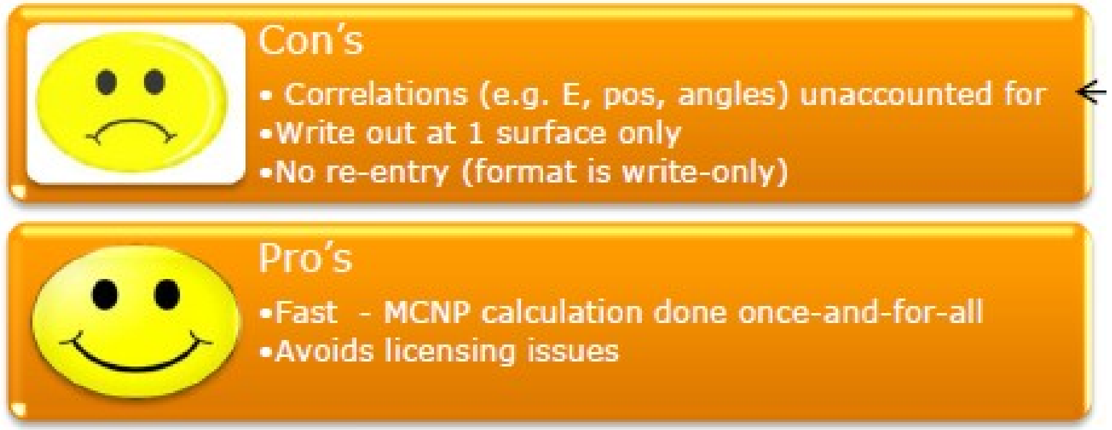
Outline

- **Explored interfaces:**
  - Tally fit
  - Ptrac
  - SSW/SSR
  - Compile
  - Supermirror
- **Validation**
  - First results
- **Summarizing experiences**
  - Cross comparisons
- **First usage**
  - Guide measurements and simulation (BOA, PSI)
  - Toward γ background estimates



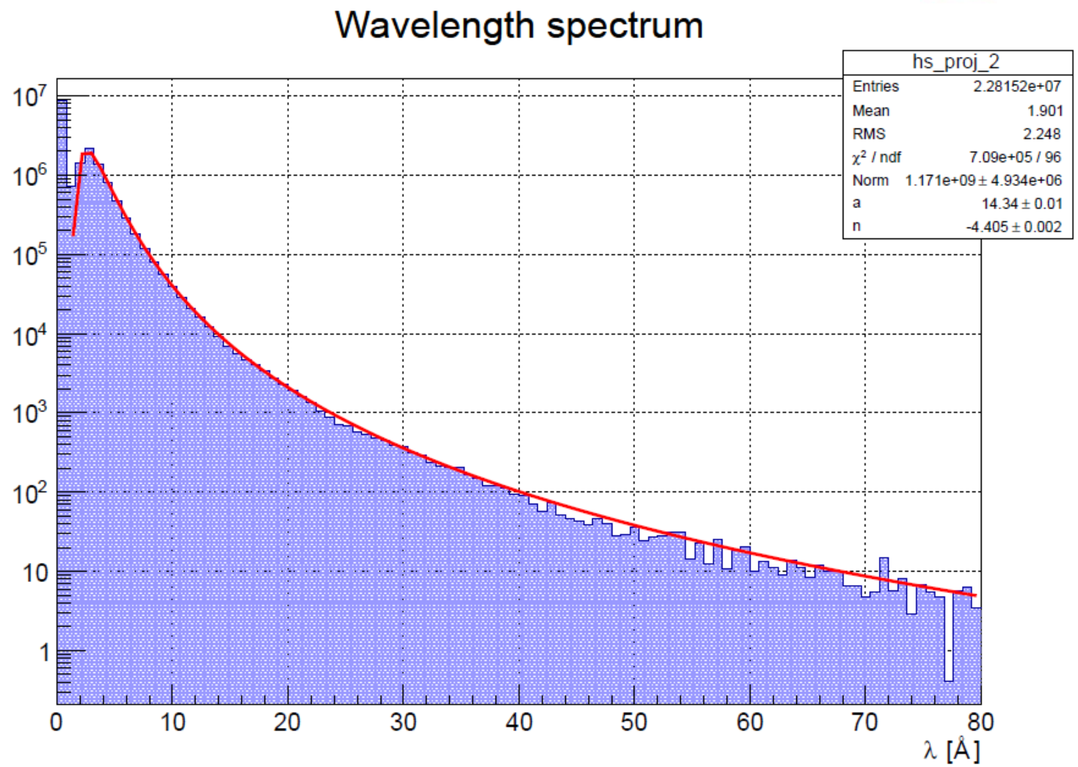
Tally fitting (present default approach)

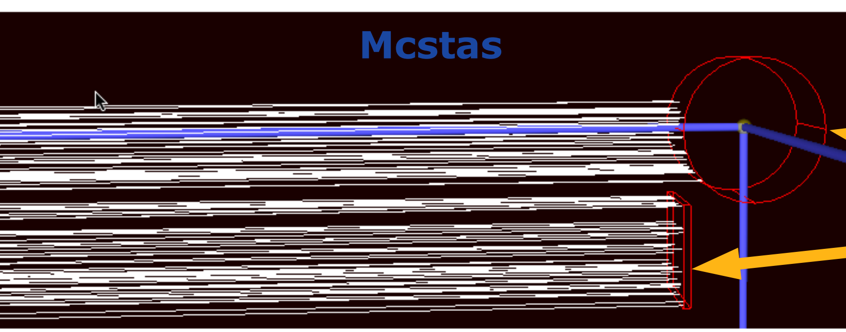
1. Neutron spectrum calculated with MCNP/X at the moderator surface
2. Spectrum is approximated by Maxwellian fits which serves as input to McStas.

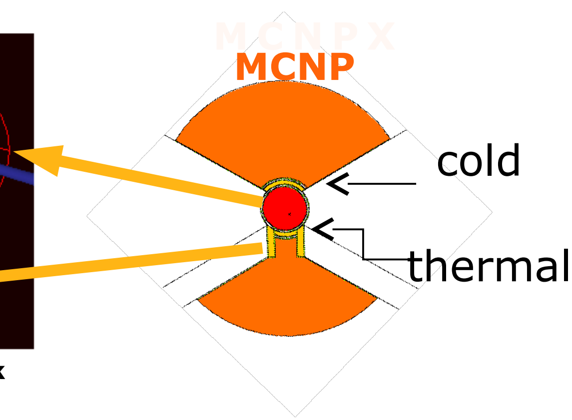


Tally fitting (ESS update)

- Major neutron sources has their own McStas source component
- Based on the latest MCNPX ESS target station (bi-spectral) geometry, we are updating the McStas ESS source mimicking both geometry, spectra and correlations between neutron parameters







Ptrac

- MCNP/X can output an ascii file containing individual neutron states: pos, angles, energy, time & weight
- The McStas component: *MCNP_Virtual_Input* (written by E.Farhi) converts the neutron state into McStas readable and works as a source

Con's

- ascii file enormous: ~0.2kB/evt
- Write out at 1 surface only
- No re-entry (format is write-only)
- Cannot run MPI

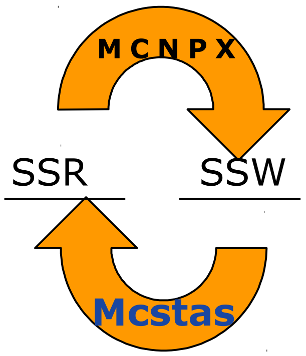
Pro's

- Correlations conserved (e.g. E,pos)
- Fast

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
………………………………..
```

SSW/SSR



- **S**ource **S**urface **R**ead/**W**rite in MCNPX starts/stops simulations at a given (set of) surface(s)
- Neutron state written to binary file.
- New McStas (v2.0) components :

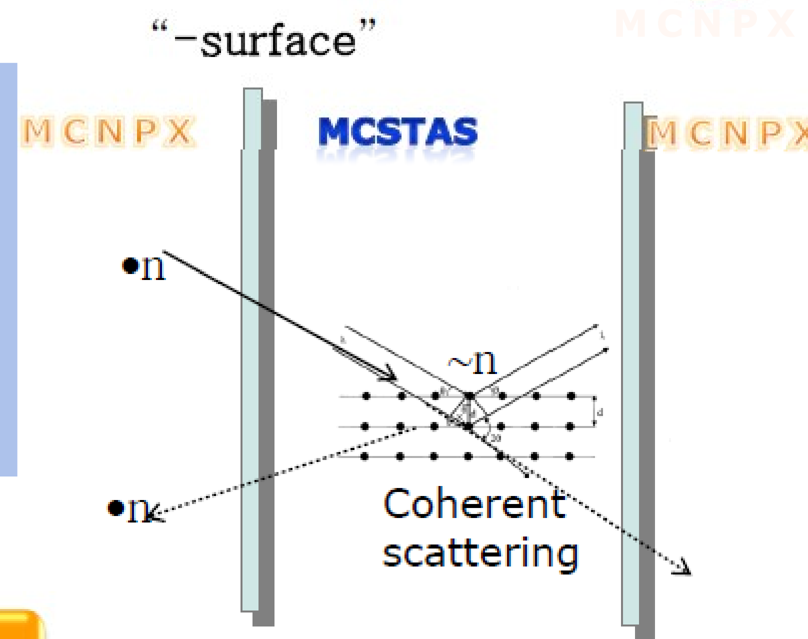
MCNP_Virtual_ss_Input & *MCNP_Virtual_ss_Output* read MCNPX output and write MCNPX input

- Neutron propagation started in MCNPX, continued in McStas and finalizing in MCNPX

ascii file sizable: ~0.1kB/evt
- Write out at selected surfaces only
- Has not (yet) been tested with MPI

All McStas functionality usable
- Re-entry supported
- Correlations conserved (e.g. E,pos)

Combined compilation



Method

- McStas surface *flag* introduced in MCNPX
- Neutron crossing McStas surface causes initiation of McStas simulation, based on neutron state.
- Updated neutron state returned to MCNPX

Technically difficult to make general

- Licensing issue
- Slow: MCNPX called for each neutron

Potentially very flexible (but not yet fully developed)

- All McStas functionality usable
- Re-entry supported
- Correlations conserved (e.g. E,pos)

<u>in MCNPX input file:</u>

.....

-110 PX -0.2

-120 PX -0.4

Supermirror

- Existing implementation, introducing McStas inspired supermirrors as a surface card in MCNPX (Gallmeier et all, Nuc.Tech. 168(3))

- Reflectivity $R=R_0$ if $Q<Q_c$
- $R=R_0/2\{1-\tanh[(Q-mQ_c)/W]\}\{1-a(Q-Q_c)\}$ if $Q>Q_c$

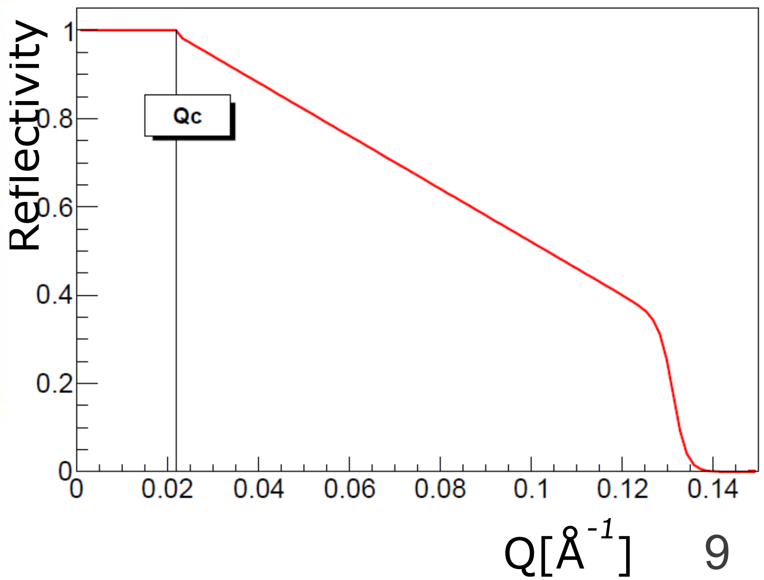
- Ported to MCNPX 2.7

Doesn't scale: workload per functionality significant. Only McStas mirrors ported

- Licensing issue

Re-entry supported

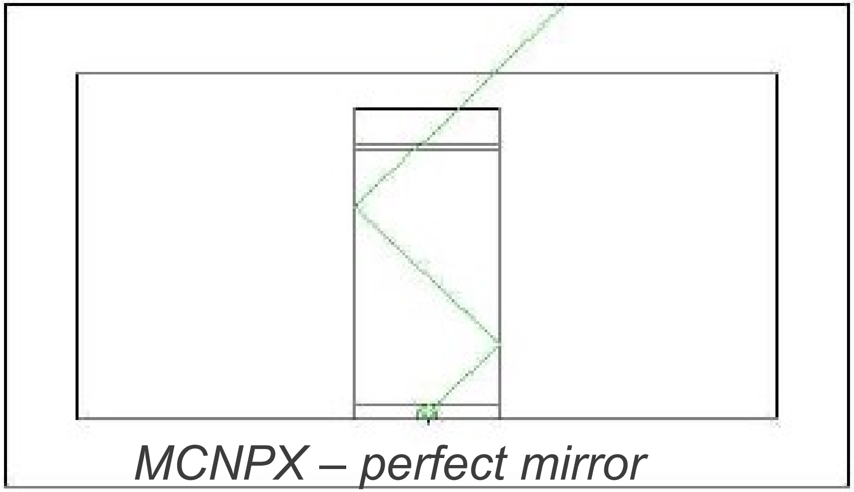
- Correlations conserved (e.g. E,pos)
- Avoids intermediate files and multiple codes



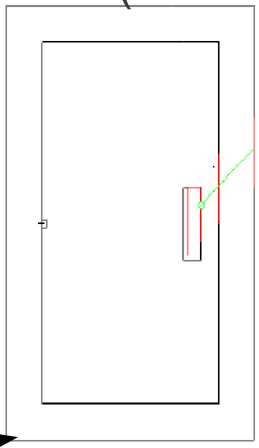
Validation setup

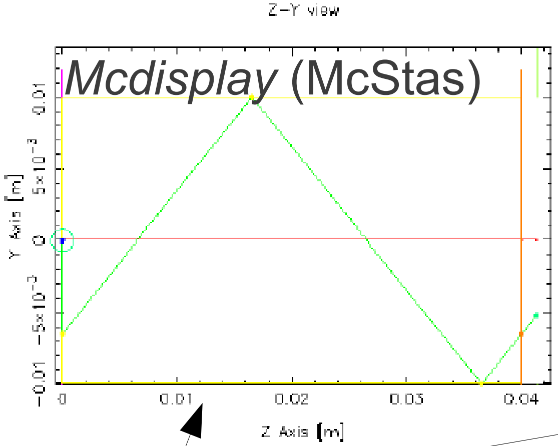
Strategy: consider dummy geometry, where the correct result is obvious:

- 20meV neutrons generated at disk and aimed 45 degree toward a perfectly reflecting 'guide wall' 1 cm away (in y)
- At z=4cm: check what comes through
- Assume vacuum in guide so that transport in McStas MCNPX should be identical

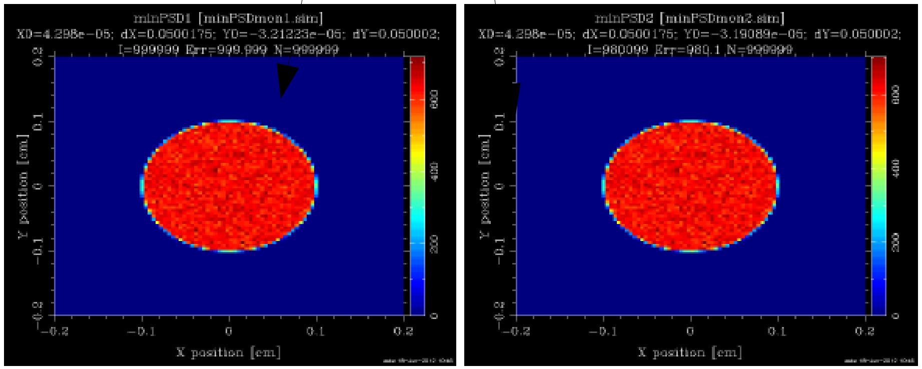


Vised (MCNPX)



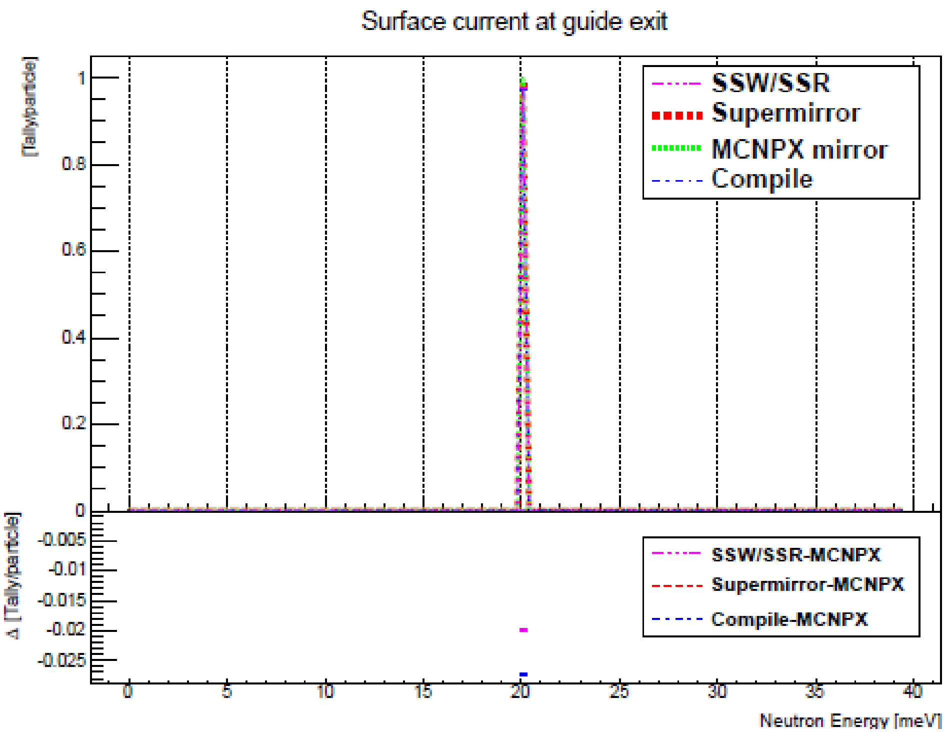


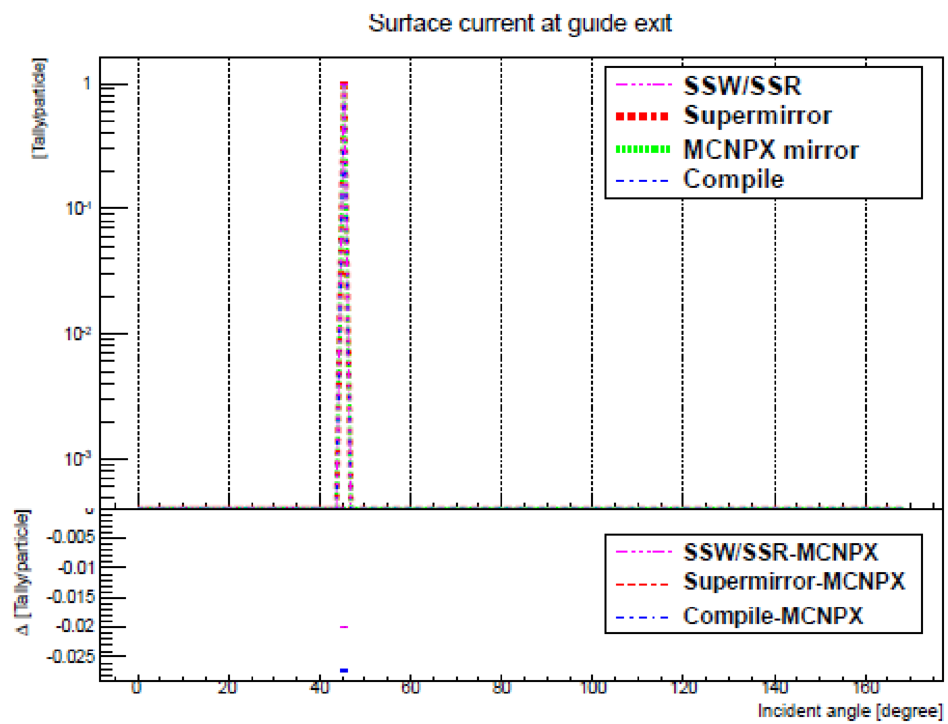
Flux $_{in}$ = Flux $_{out}$



SSR/SSW

Validation results



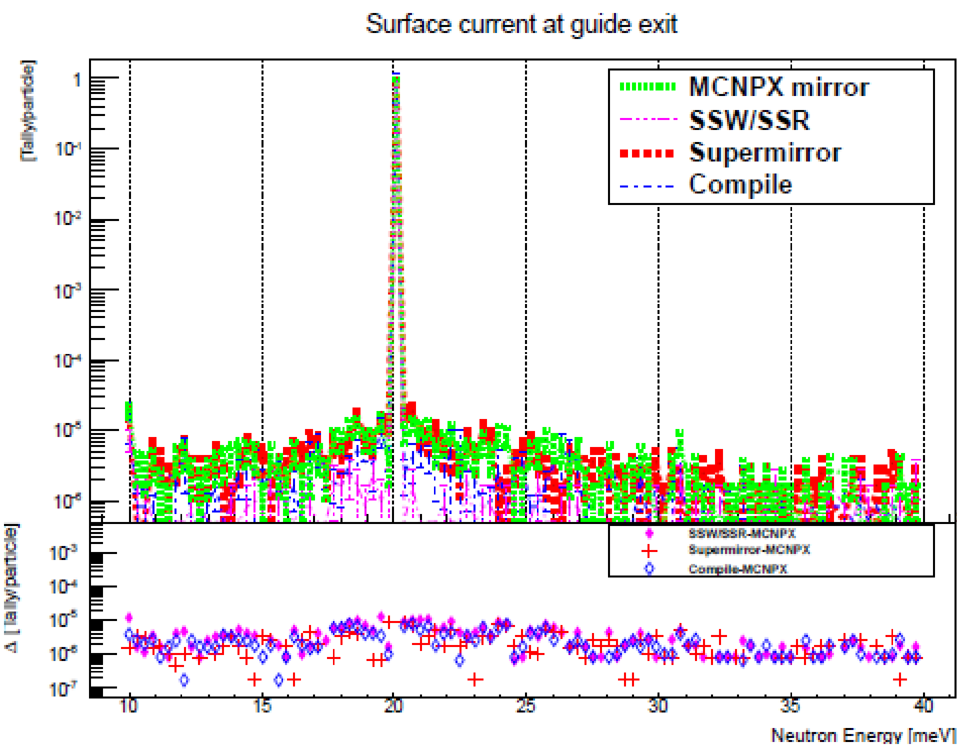


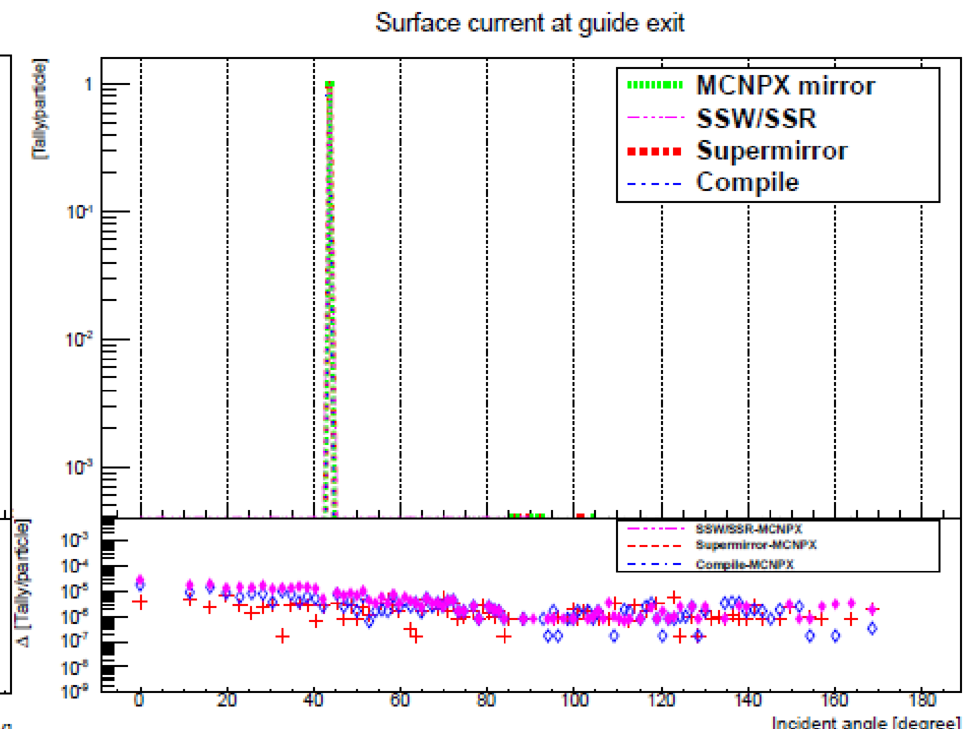
For all interfaces:

→ Neutron energy and angle conserved (45degree, scattered twice) √

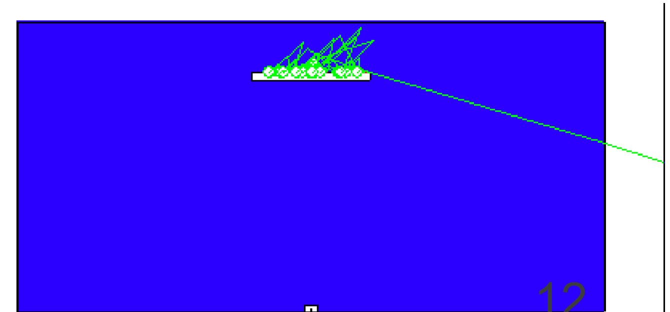
Validation results

For fun: repeat after filling the guide with air





At first glance, the tails in SSW/SSR histograms surprised me. However, the tails are due to backscattering in the air outside the “McStas world”



Cross comparison - *reminder*

	Re-entry neutrons	Speed	Single neutron trace	Require License	Comments
Tally	No	Fast*	No	No	Should try to determine validity at least once
Ptrac	No	Fast*	Yes	Yes	Somewhat outdated by SSW/SSR
SSW/SSR	Yes	Fast*	Yes	Yes	Works well
Compile	Yes	Very slow	Yes	Yes	Require (minor) changes to MCNPX source code
Supermirror	Yes	Slow	yes	yes	Generalizes poorly (but who cares?)

*) The computational heavy MCNP/X calculation can be performed once-and-for-all

Ongoing validation / example of usage: Comparison to real data

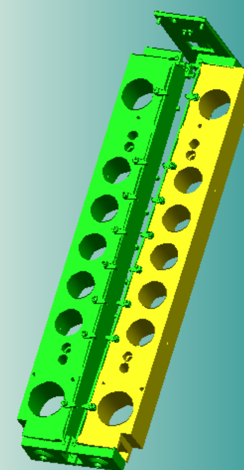
- In collaboration with U.Filges (et al) at PSI: a ESS prototype elliptical mirror was tested at the BOA beamline at SINQ.
- Allows cross validation of simulation approaches against real data
- <u>Basic idea:</u>

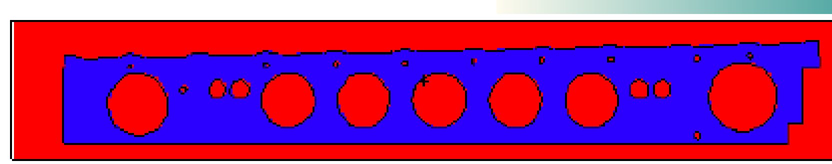
  → setup incl beam profile + spectrum known.

  → Intercept half beam by known material.

  → Use coupled MCNPX-McStas to describe the intensity loss.
- Status data looks promissing. Starting to work on the simulations.

CAD



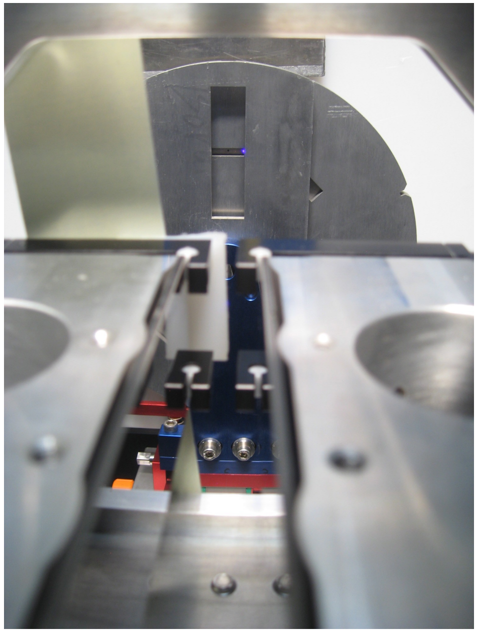


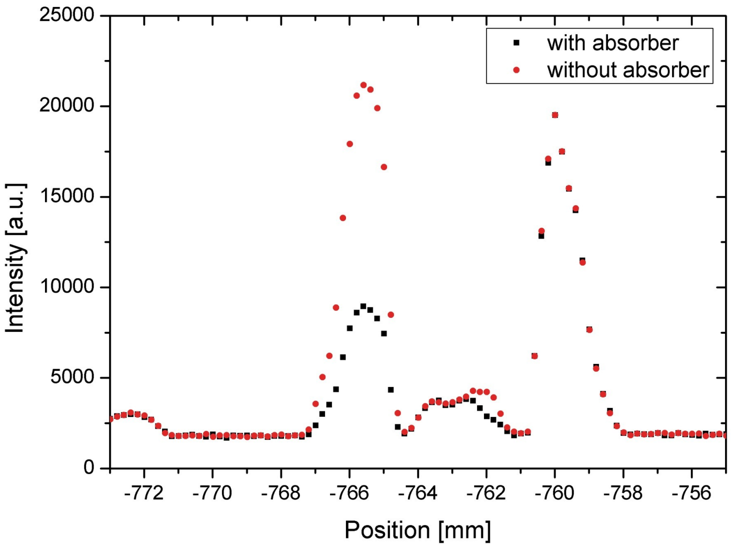
MCNPX

1)FDS Team, China. Y.Wu, FDS Team, CAD based interface programs for fusion neutron transport simulation, Fusion Engineering and Design 84 (2009) 1987-1992

Ongoing validation / example of usage: Comparison to real data

- Measurements were done at a defocus position (10 cm behind focus plane)





- Half of the guide segment was shielded (at the exit) by different materials (polyethylene: 1.4 mm, aluminium: 1 mm , vanadium: 0.3 mm).

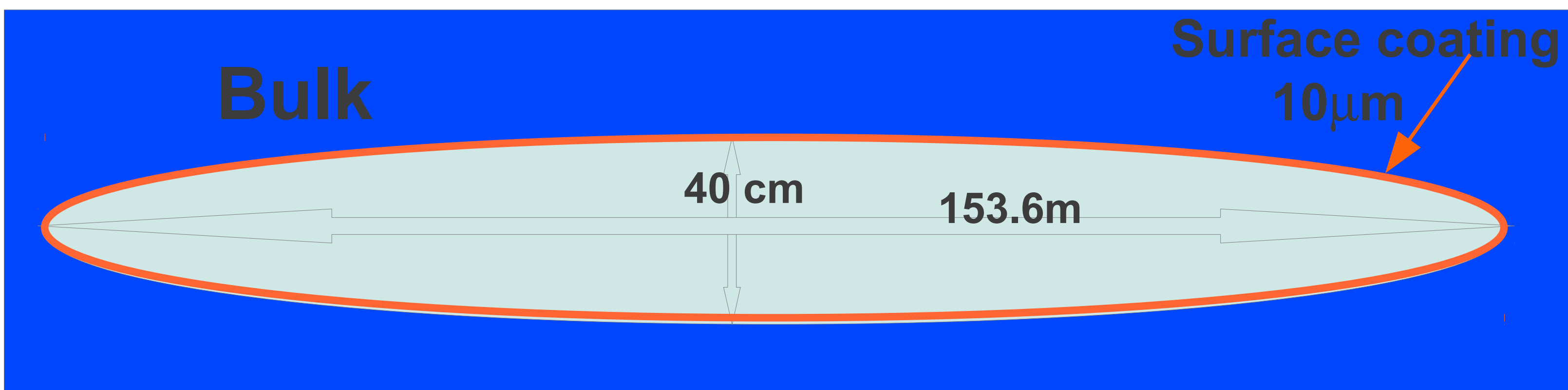
(slide from U.Filges)

Applications for shielding and γ/n background at sample

- Simulate ellitical (ESS-like) guide in MCNPX using introduced supermirrors
  - Fast neutron/γ background at sample
  - Shielding calculations
- Material composition inspired from: *http://en.wikipedia.org/wiki/Borosilicate_glass*
- *i.e.:*

Bulk				
SiO_2	B_2O_3	Na_2O	CaO	K_2O
70%	10%	8%	1%	8%

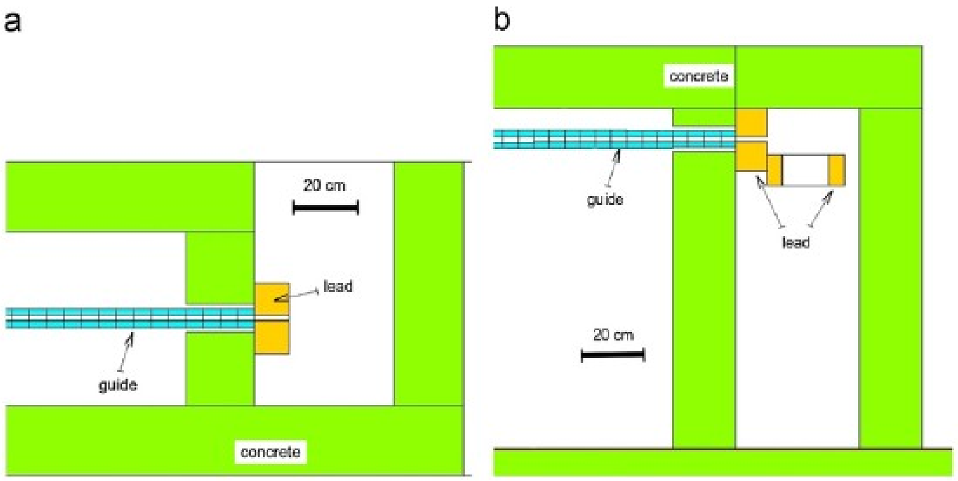
Surface coating	
Ni	Ti
50%	50%



- This study was only started recently, so no reliable results yet.

Applications for shielding and γ/n background at sample

- 1) γ background measurement at BOA is being planned now.
- 2) Comparison with previous results
  - **NIMA 634** (2011) S130–S133. A. Szaka et al
  - Measures #γ / #n with below setup (detector shielded by led → can't compare with presented results)



Name	gamma / ref. neutron	gamma / esc. neutron
Straight	1.15×10^{-6}	1.48×10^{-6}
Linearly conv.	8.99×10^{-7}	2.10×10^{-6}
Ellipt. foc.	1.74×10^{-6}	1.34×10^{-5}
Soller+Ellipt. foc.	2.81×10^{-6}	1.71×10^{-5}

- ***Plan:*** try to replica results using our developed framework →I.e. build corresponding MCNPX geometry, try to deduce source etc.

Conclusions

- Interfaces validated √
- Applications started....
  - Task decides which interface is more useful

Backup slides

Validation:
Fitting distributions vs. importing neutron states

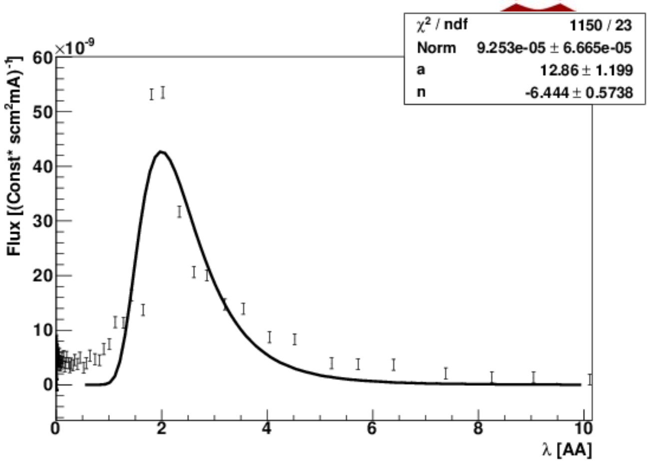
- Present approach used for instrument design & physics analysis relies on a once-and-for-all fit to a spectrum.
- Clear advantages over porting individual neutrons:
  - Preliminary ESS geometry (from ESS-Bilbao), simulation 1M protons with MCNPX takes ~1K CPU hours
  - McStas CPU cost for 1M neutrons: hardly measureable <1s

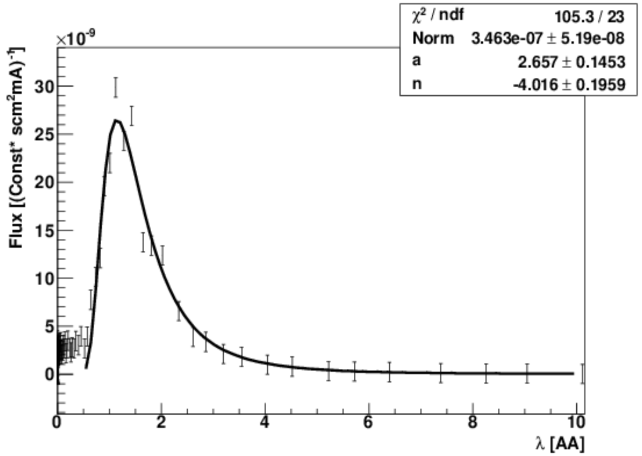
- Implicitly McStas assumes:
  - Spectrum fit is perfect
  - No correlations between: Position at moderator surface, position at guide entrance, momentum
  - No scattering between moderator surface and guide entrance

- For TMS & instrument design these assumptions are worth questioning

Validation of Tally approach: Fits

- No fit is ever perfect – especially not mine

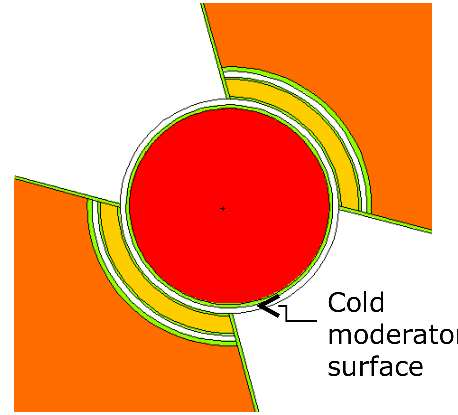


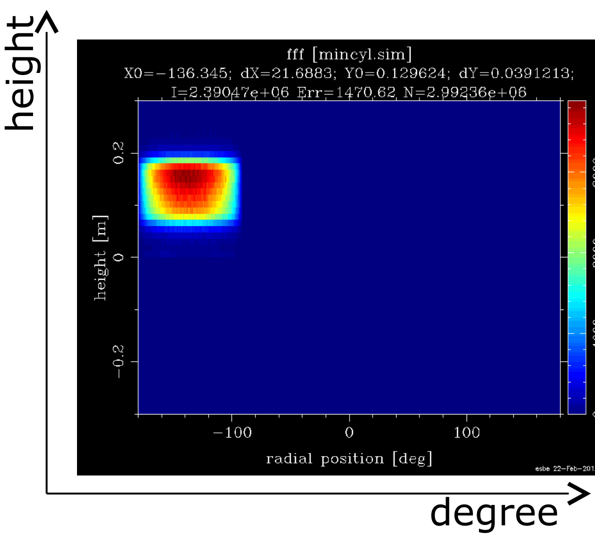


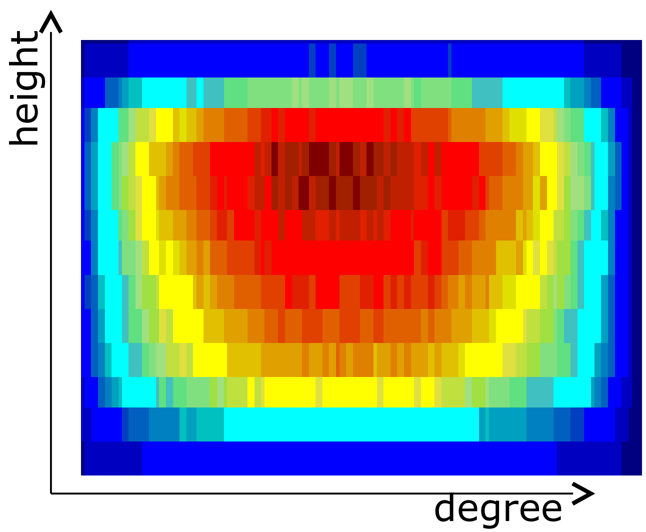
Validation of Tally approach: Correlations

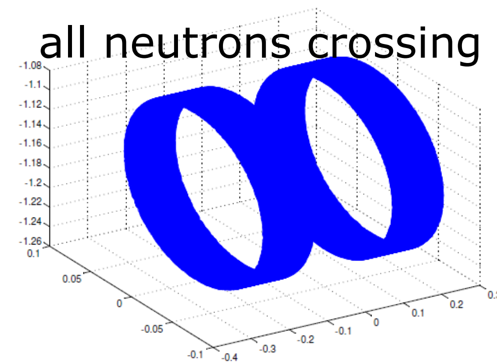
Stress test of the developed SSW/SSR approach:

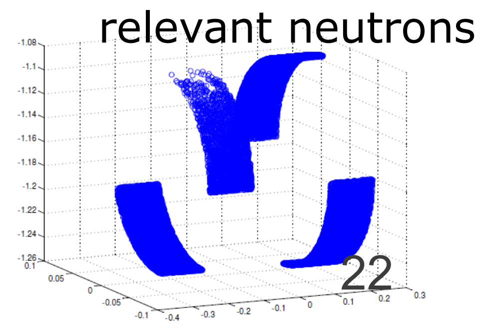
- Simulate1M protons hitting target wheel
- Dump all neutrons passing moderator surface to SSW output file (3.5Gb)
- In McStas, placing a **P**osition**S**ensitive**D**etector (PSD) ~at the surface gives:





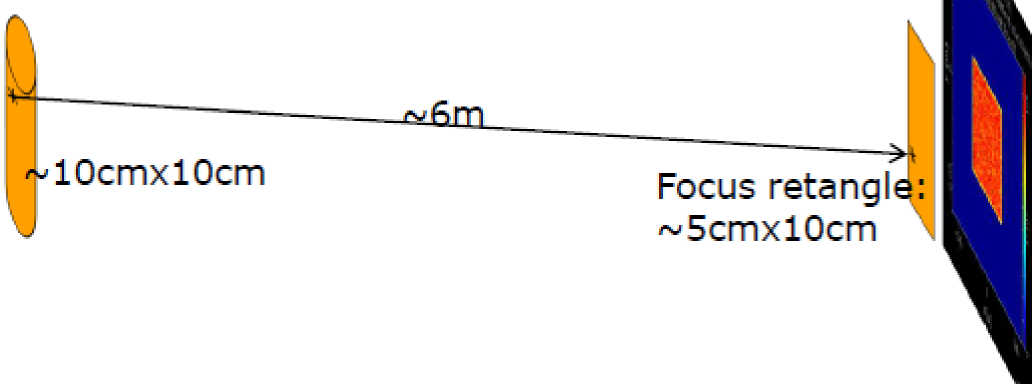


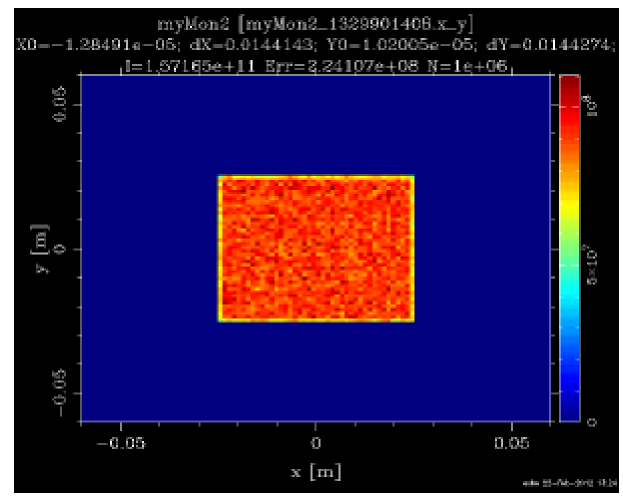




Validation of Tally approach: Correlations

- In McStas the procedure to provide neutron states is to connect randomly points at the moderator to points at the guide opening, and assign energy (based on a maxwellian function + modulation)
- Placing a PSD detector ~at the guide opening surface gives:

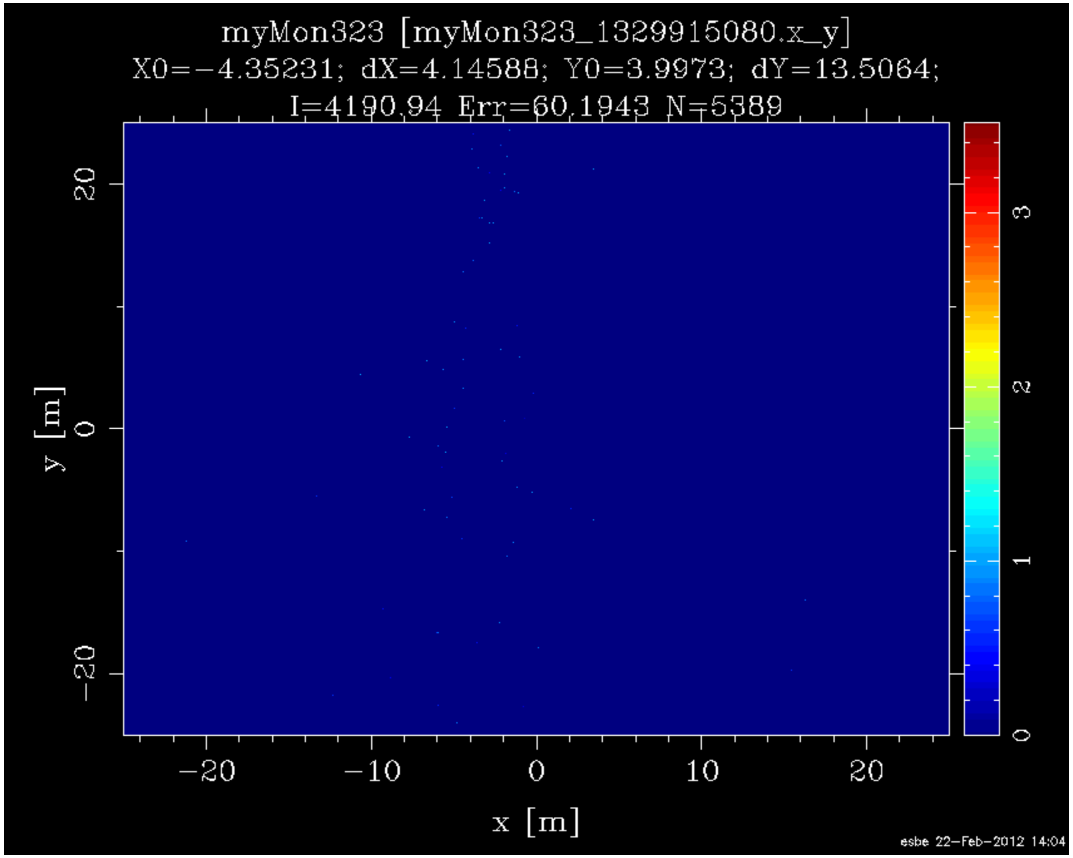




- I.e. uniform – but long flight path of ~6m means that a point source assumption is not too far off.
- **Q**: How would the distribution look in MCNP. I.e. SSW card at 6m?

Validation of Tally approach: Correlations

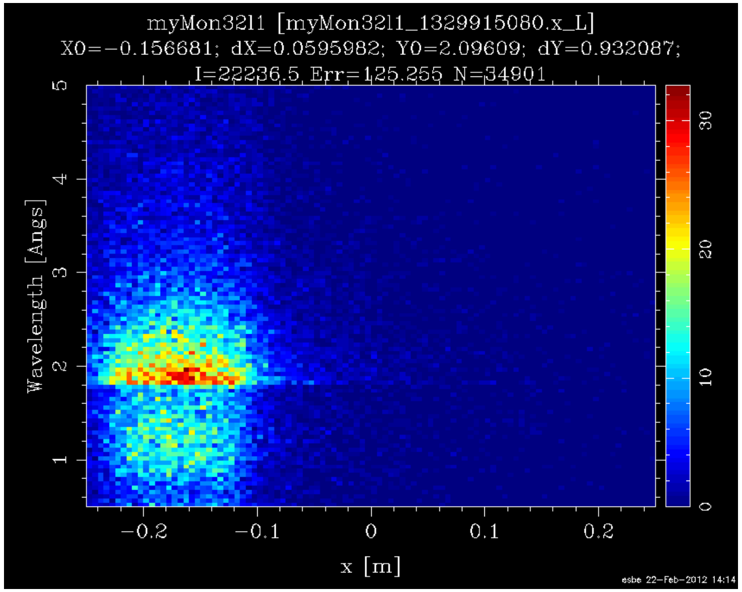
- **A**: Flat – in the empty sense of the word:

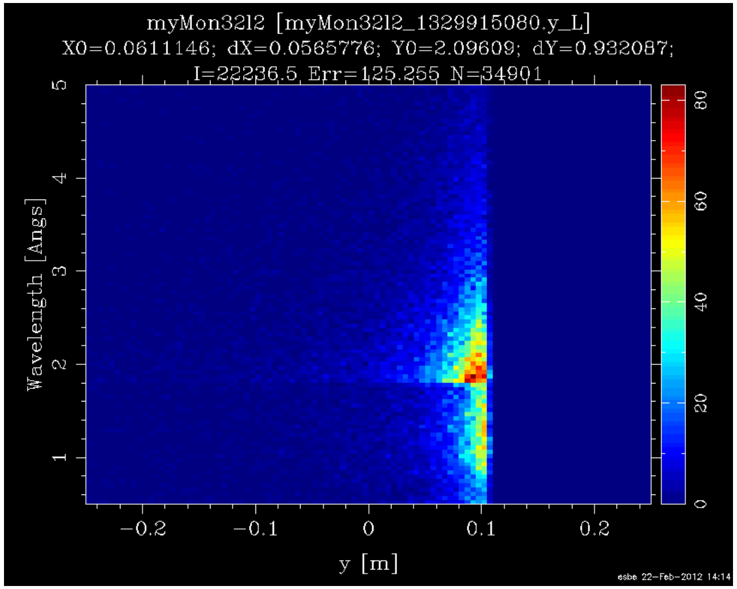


- No focus -> very few neutrons at guide

Validation of Tally approach: Correlations

- Lots of other comparisons to make:

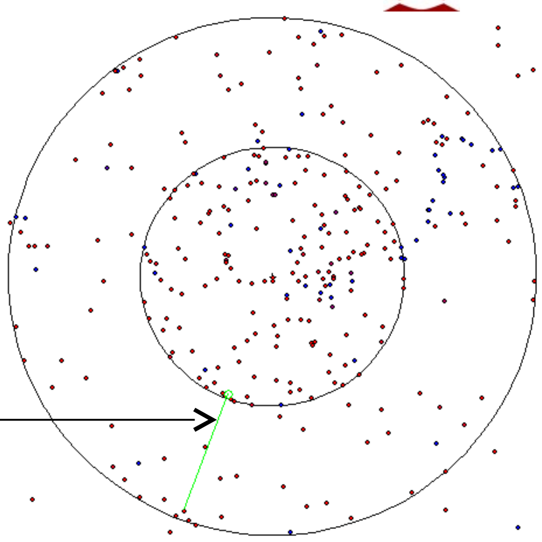


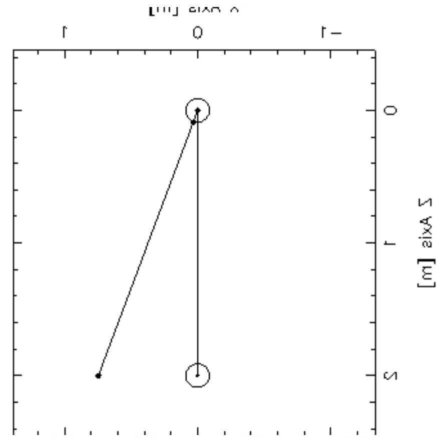


- I.e. correlations between position & energy exist. Important for moderator design etc, but perhaps not for instrument design (?). Being investigated.

Validation of SSW / SSR approach

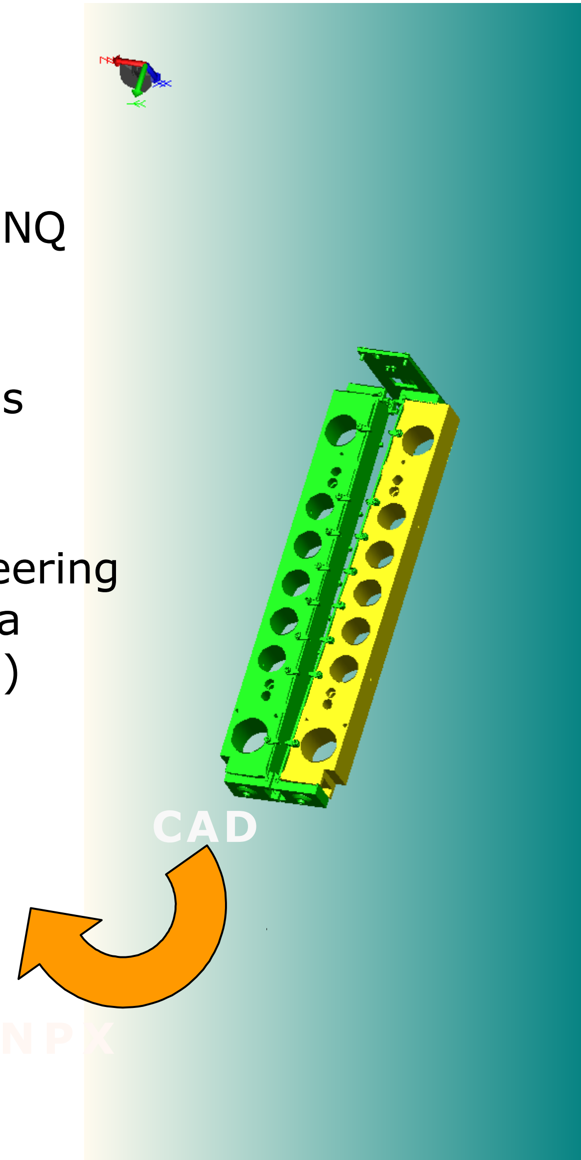
1. Define simplest possible geometry in MCNPX
2. Run test simulation
3. Visualize events and pick one
4. Import to McStas the neutron states as recorded by SSW card
5. Run simplest possible McStas simulation from SSW input: neutron transport
6. At z=2m, write SSW & visualize
7. Based on McStas SSW resume the MCNPX simulation, and visualize

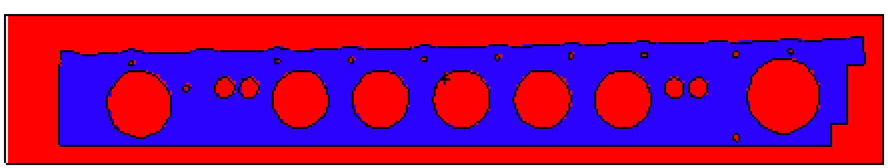




Validation: all approaches

- Test interfaces using ESS prototype guide at SINQ spallation source at PSI in summer 2012
- Allows cross validation of simulation approaches against real data
- Status (simulation-wise): Using MCAM[1)] engineering CAD model geometry has been translated into a MCNPX readable geometry (details missing still)

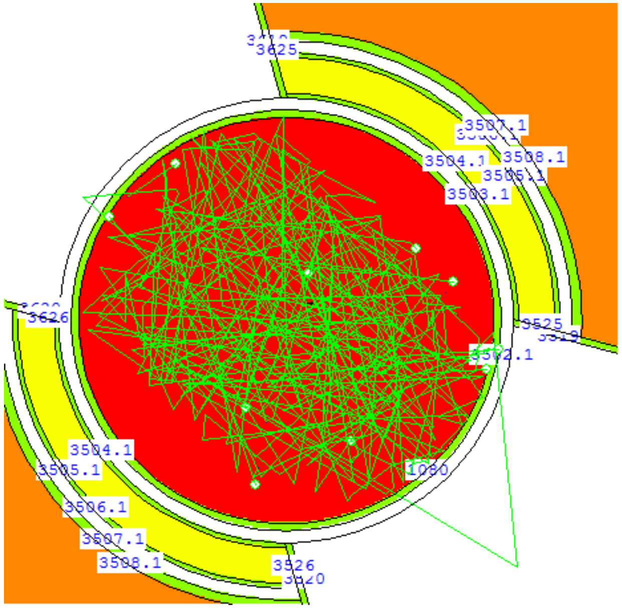




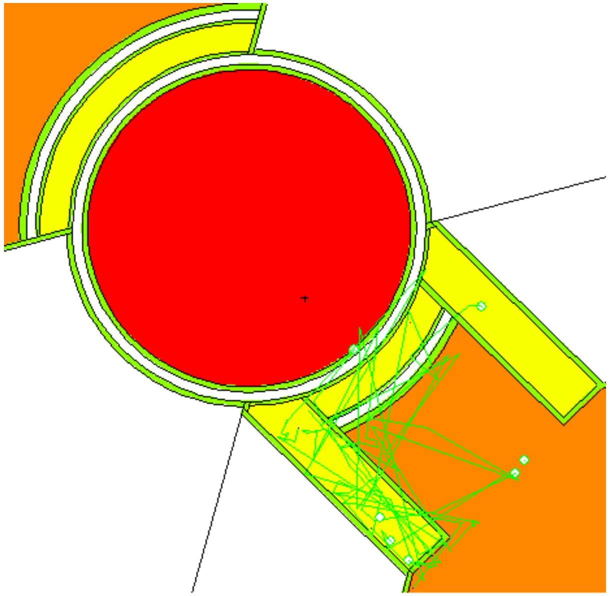
1)FDS Team, China. Y.Wu, FDS Team, CAD based interface programs for fusion neutron transport simulation, Fusion Engineering and Design 84 (2009) 1987-1992

Tally contributions

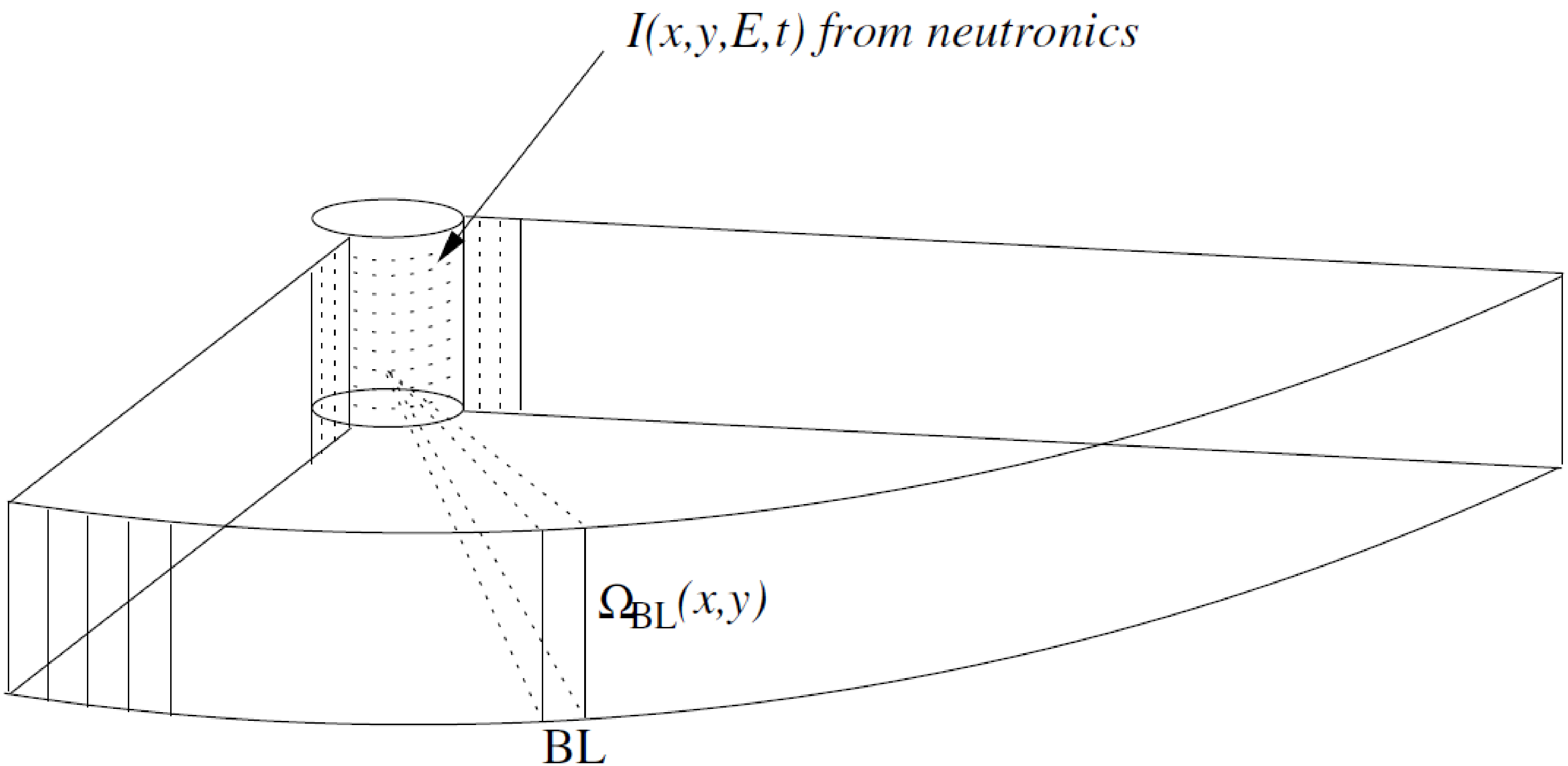
- Contributions to cold spectrum



- Contributions to thermal spectrum



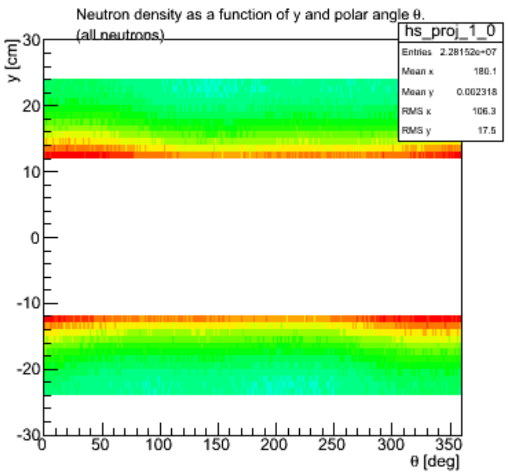
Revised tally approach

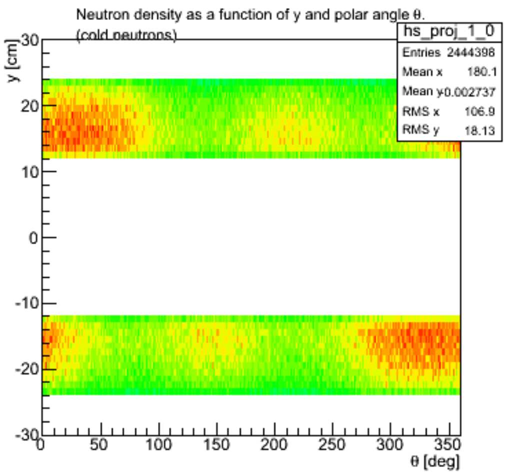


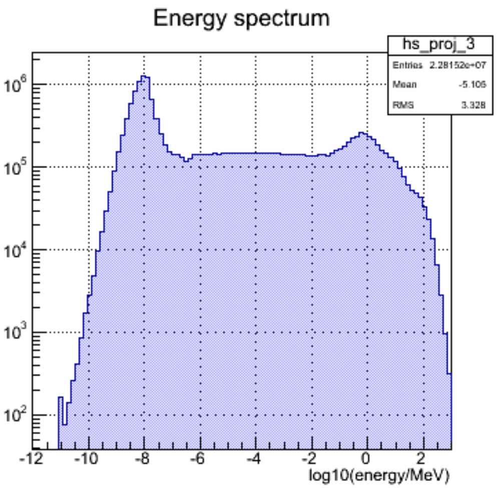
Per beamline:

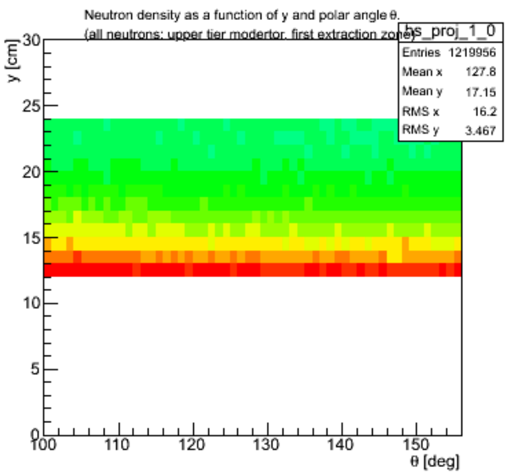
$$I_{BL}(x,y,E,t) = \frac{\Omega_{BL}(x,y)}{4\pi} I(x,y,E,t)$$

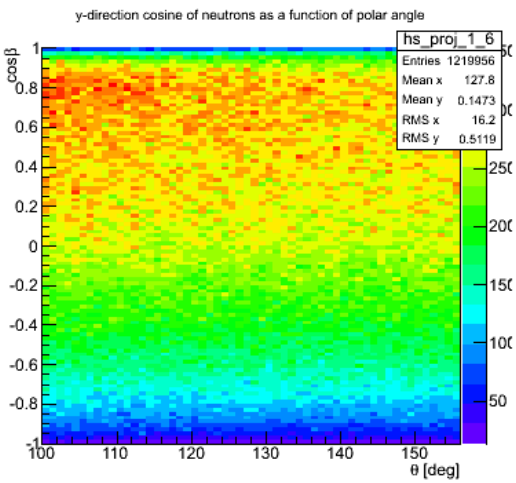
Revised tally approach

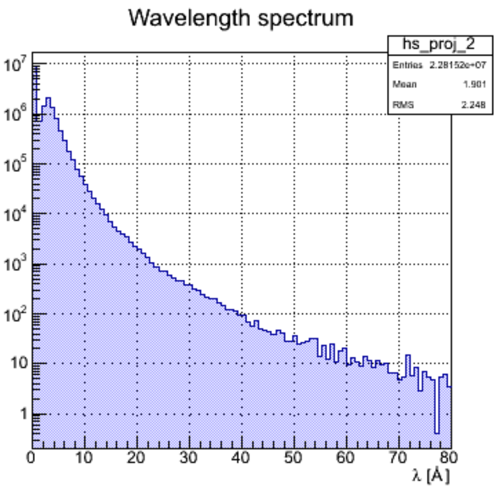




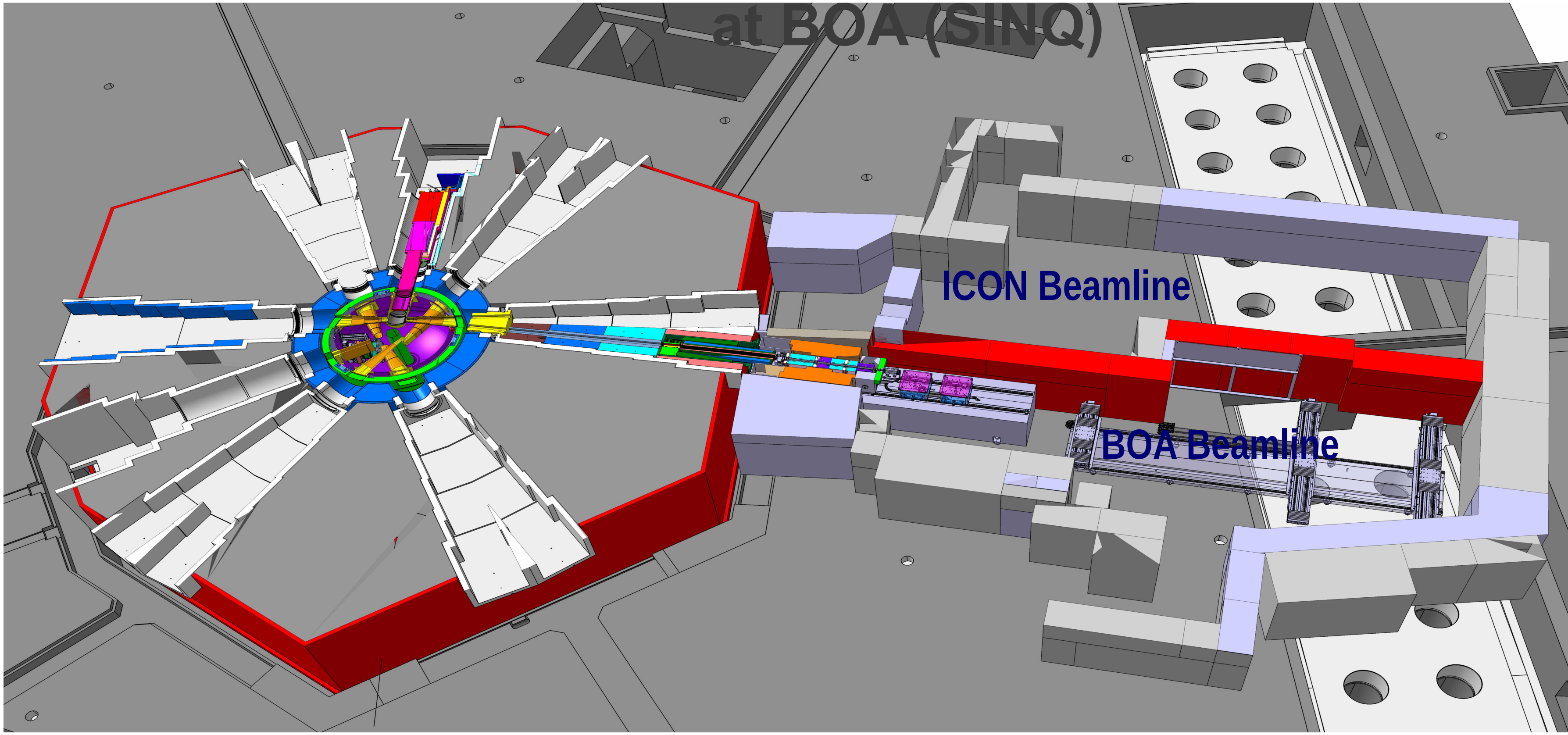








Validation of MCNPX/McStas model against measurements at BOA (SINQ)



Beamline description:

- polarized neutron beam 4x15 cm
- 9.7 m free neutron flight path (straight) behind second guide section
- 5 measurement positions with three turnable axis
- CCD detector / single He-3 detector / He-3 PSD detector with TOF
- chopper/selector at position 1 (double monochromator , analyzer system)

(slide from U.Filges)