Developing an interface between MCNPX and McStas for simulation of neutron moderators

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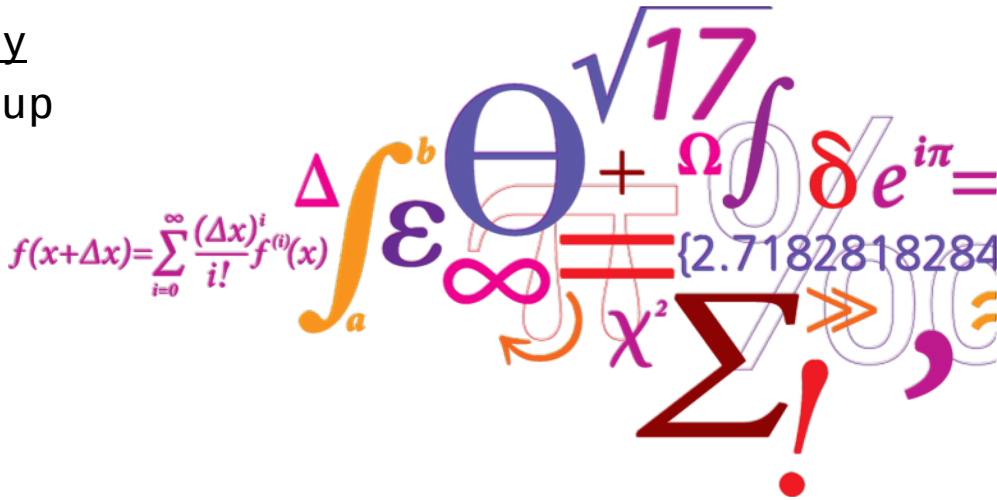


DTU Nutech
Center for Nuclear Technologies

Motivation

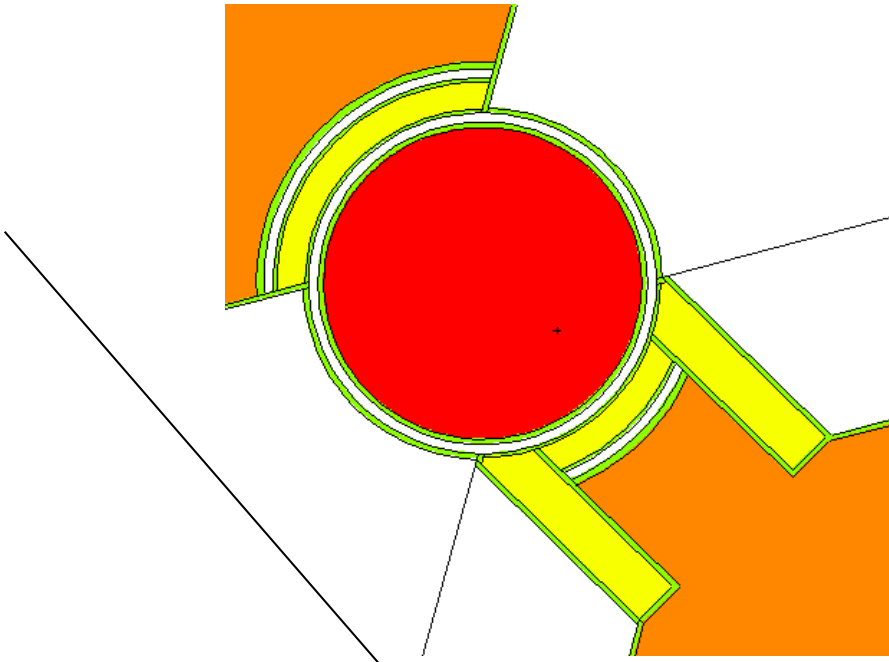
- Traditionally two decoupled Monte Carlo codes covers different needs in Neutron Scattering simulations:
  - MCNP/X used for TMS calculations
  - Neutron ray tracing code, e.g. McStas (talk by P.Willendrup) used for instrument design + data analysis

- 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.

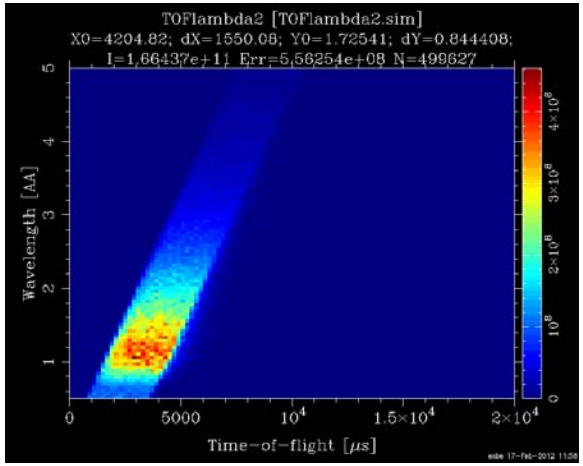
- **Prospects**: usage of direct MCNP/X McStas coupling:
  - Optimization of complex moderator design
  - Shielding along neutron guide
  - Crosstalk between neutron guides
- Test case: ESS TMS and guide systems.

Outline

- **Explored interfaces:**
  - Tally fit
  - Ptrac
  - SSW/SSR
  - Compile
  - Supermirror



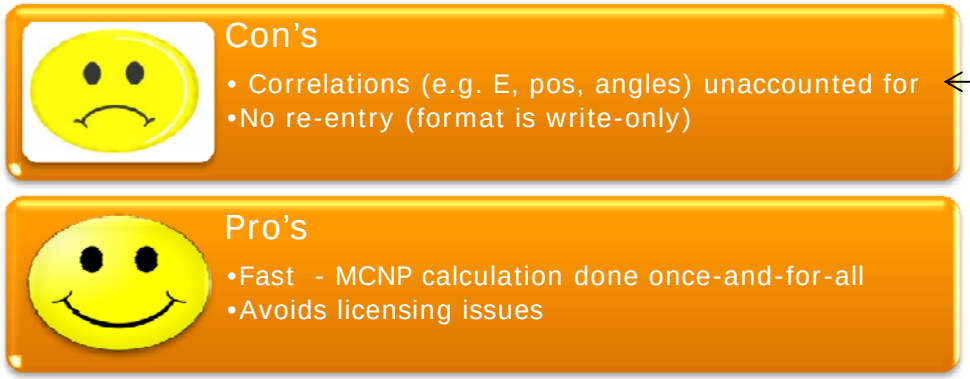
- **Validation**
  - First results
  - Upcomming



- **Summarizing experiences**
  - Cross comparisons

Tally fitting (present default approach)

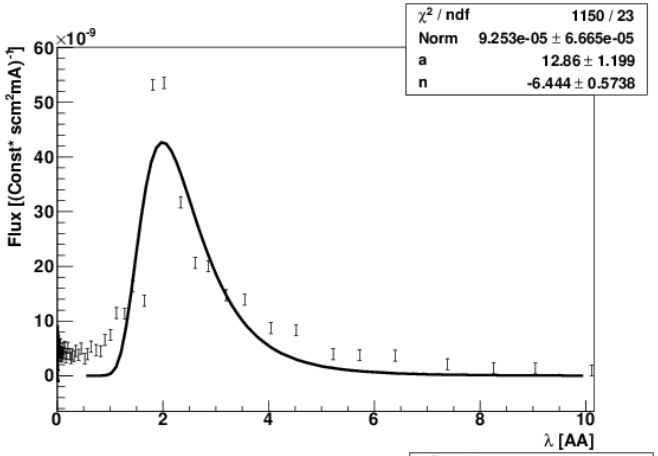
1. Neutron spectrum calculated with MCNP/X at the moderator surface
2. Spectrum is approximated by simple functions which serves as input to McStas.

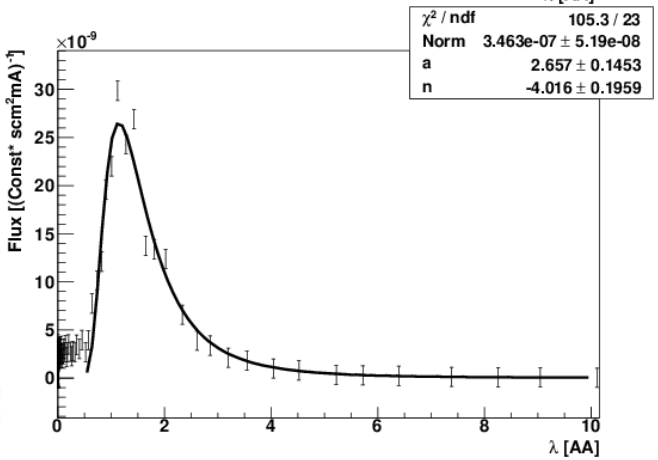


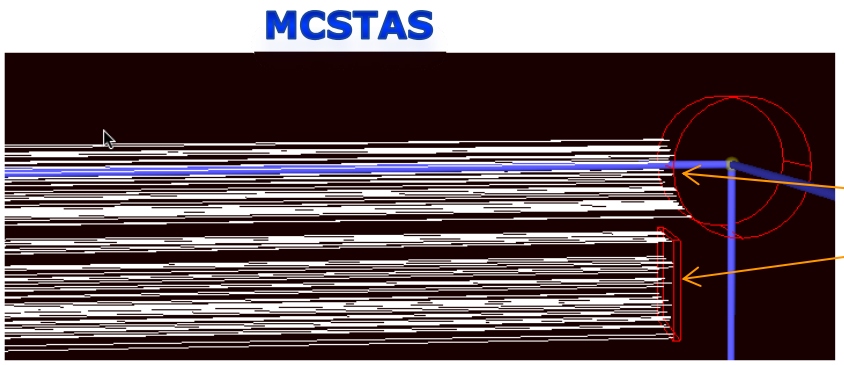
Discussed later

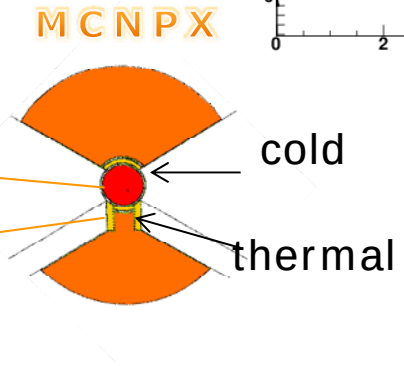
Tally fitting (update)

- Based on the latest MCNPX ESS target station (bi-spectral) geometry from ESS-Bilbao (see presentation by F.Sordo), we have developed a McStas component mimicking both geometry and spectra.
- The component is named: *ESS_Moderator_revised*, and is expected to be released shortly.



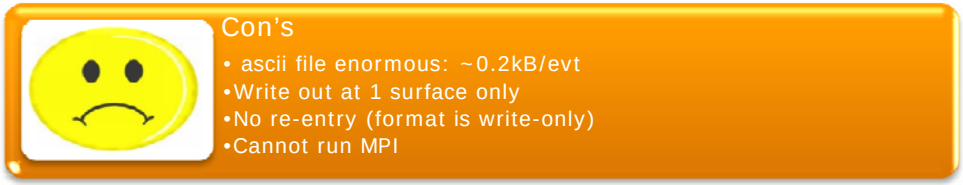






Ptrac

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

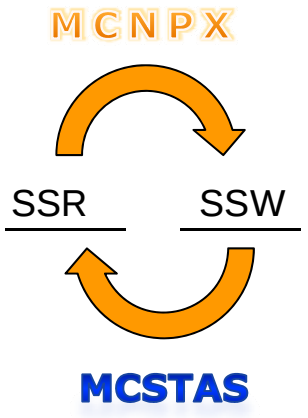


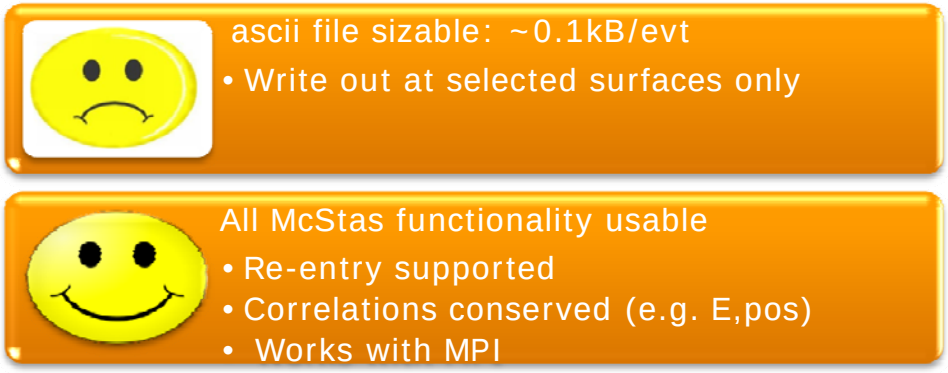
Ptrac format

```
.....
 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)
- The neutron state written to binary file.
- New McStas components:
  MCNP_Virtual_ss_Input & *MCNP_Virtual_ss_Output*
  reads MCNPX output and writes MCNPX input
- Neutron propagation started in MCNPX, continued in McStas and finalizing in MCNP

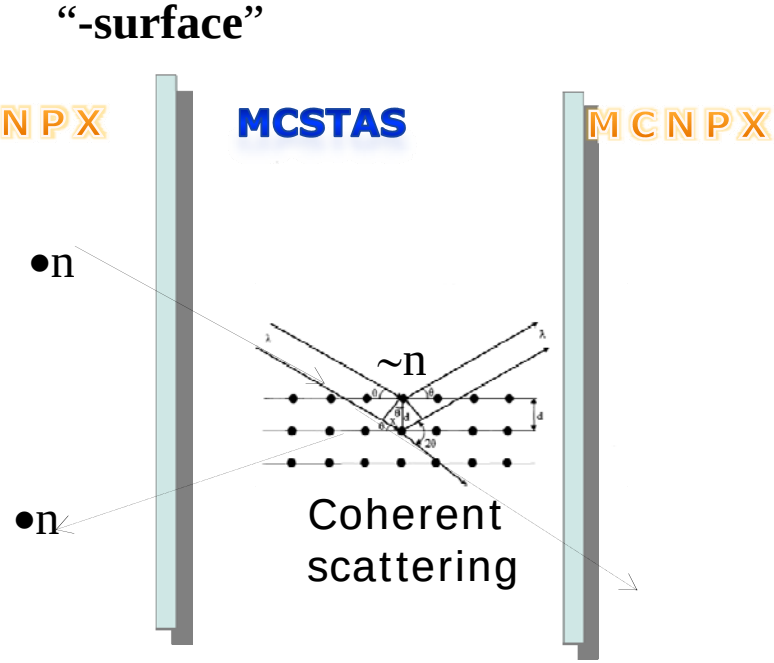




Combined compilation

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



- 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)

in MCNPX input file:

…..

-110 PX -0.2

-120 PX -0.4

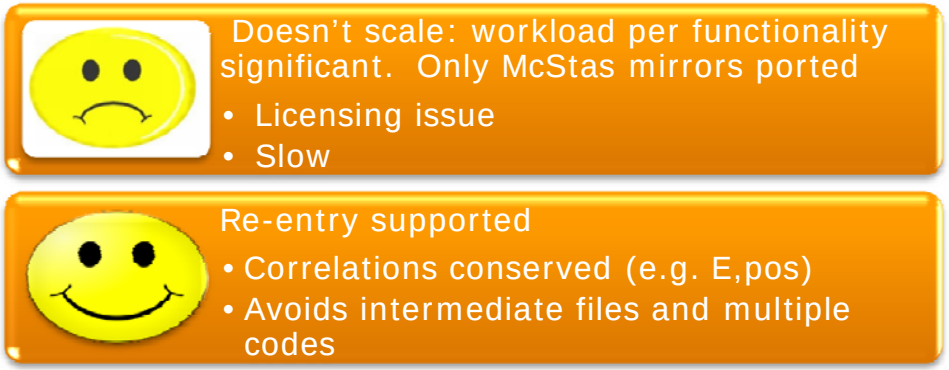
…..

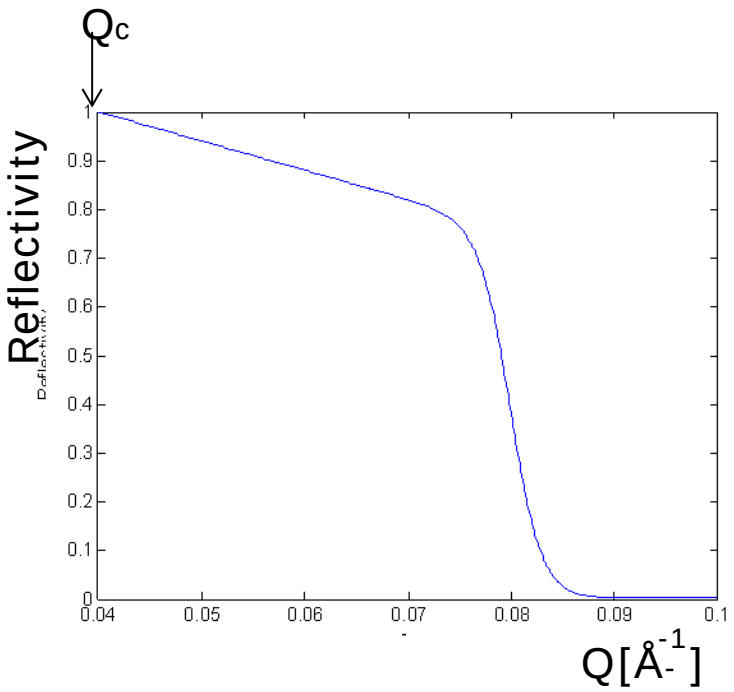
Supermirror

- 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* $Q \geq Q_c$

- Ported to MCNPX 2.7, but not yet validated





Validation:
Fitting distributions vs. importing neutron states

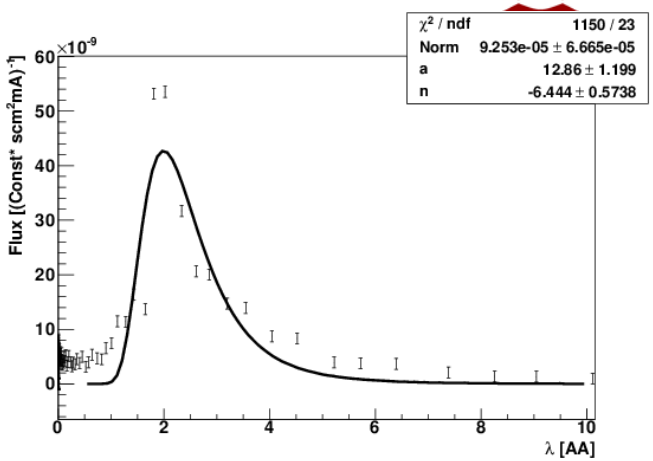
- Present approach used for instrument design & physics analysis relies on a once-and-for-all fit to a spectrum.
- Clear advantages over porting individual neutrons:
  - Preliminary ESS geometry (from ESS-Bilbao), simulation 1M protons with MCNPX takes ~1K CPU hours
  - McStas CPU cost for 1M neutrons: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

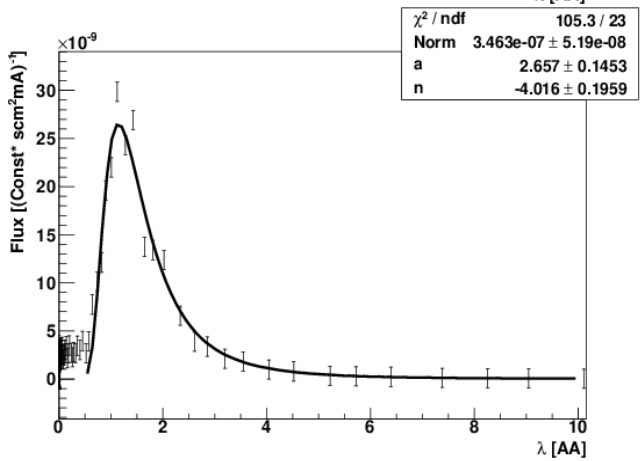
- Implicitly McStas assumes:
  - Spectrum fit is perfect
  - No correlations between: Position at moderator surface, position at guide entrance, momentum
  - No scattering between moderator surface and guide entrance

- For TMS & instrument design these assumptions are worth questioning

Validation of Tally approach: Fits

- No fit is ever perfect – especially not mine

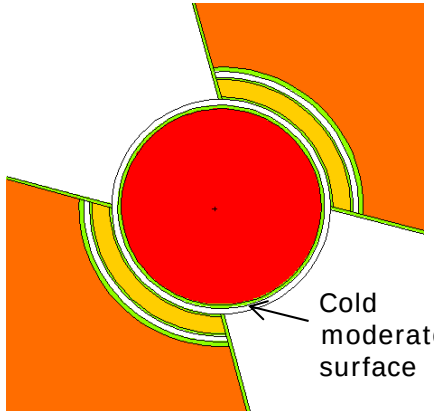


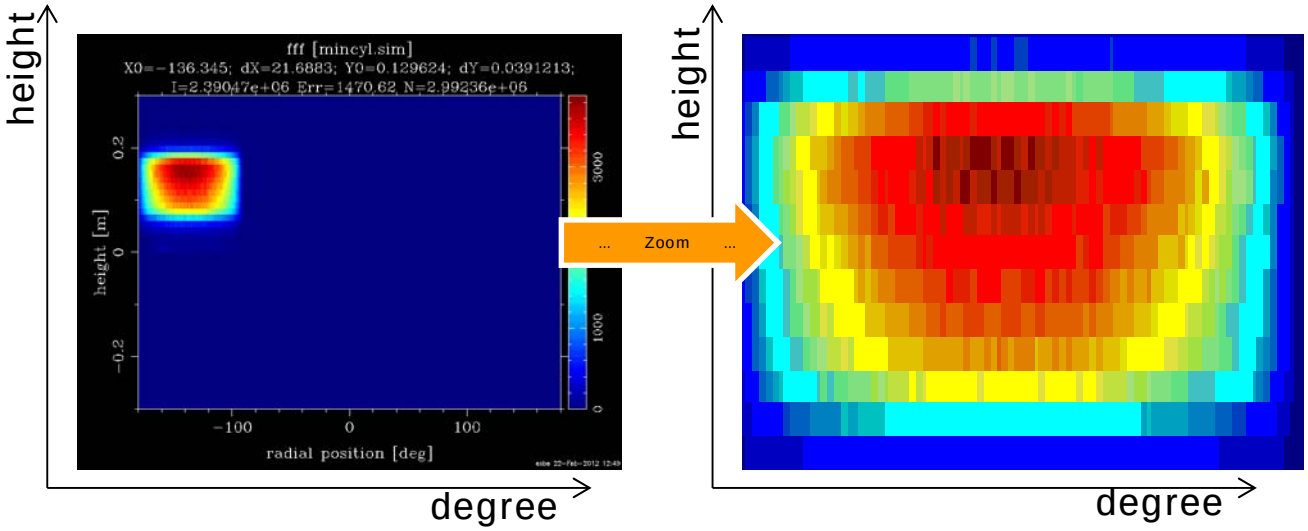


Validation of Tally approach: Correlations

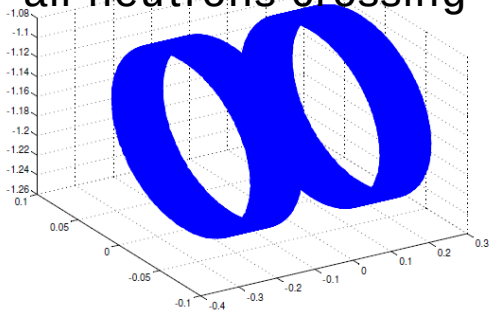
Stress test of the developed SSW/SSR approach:

- Simulate 1M 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 cold moderator surface gives:

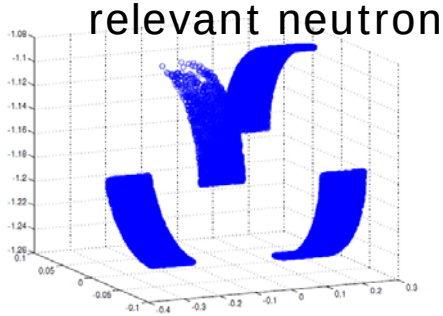




all neutrons crossing

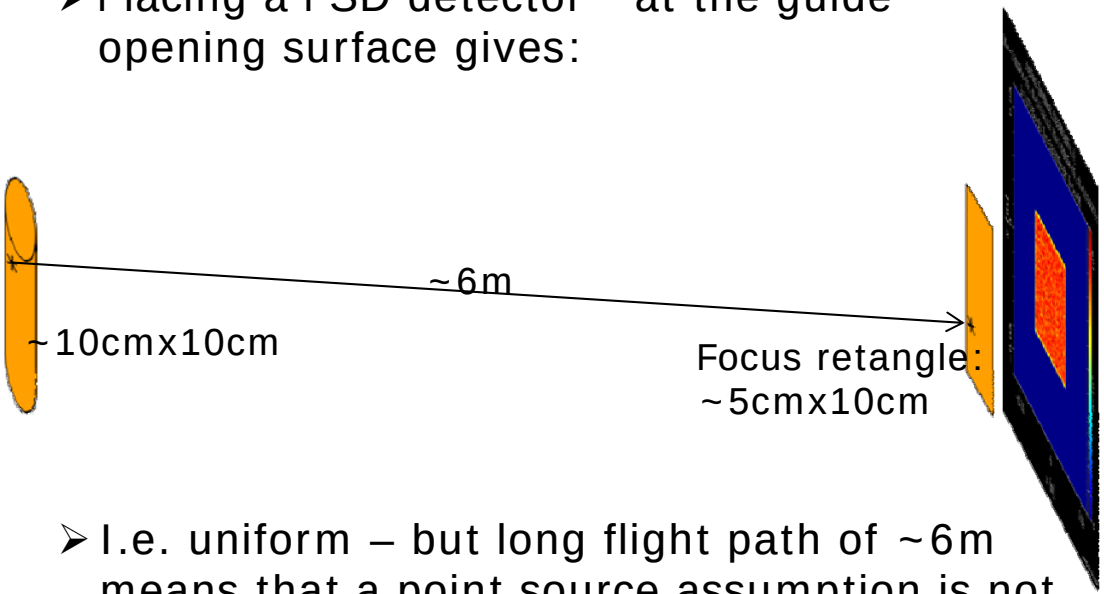


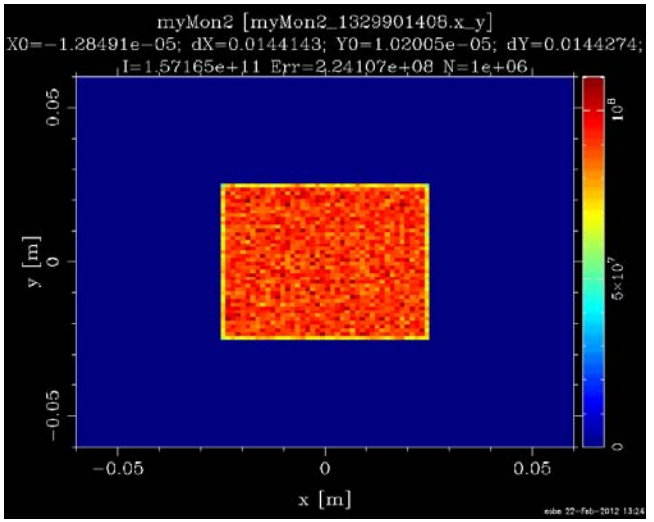
relevant neutrons



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
- Placing a PSD detector ~at the guide opening surface gives:

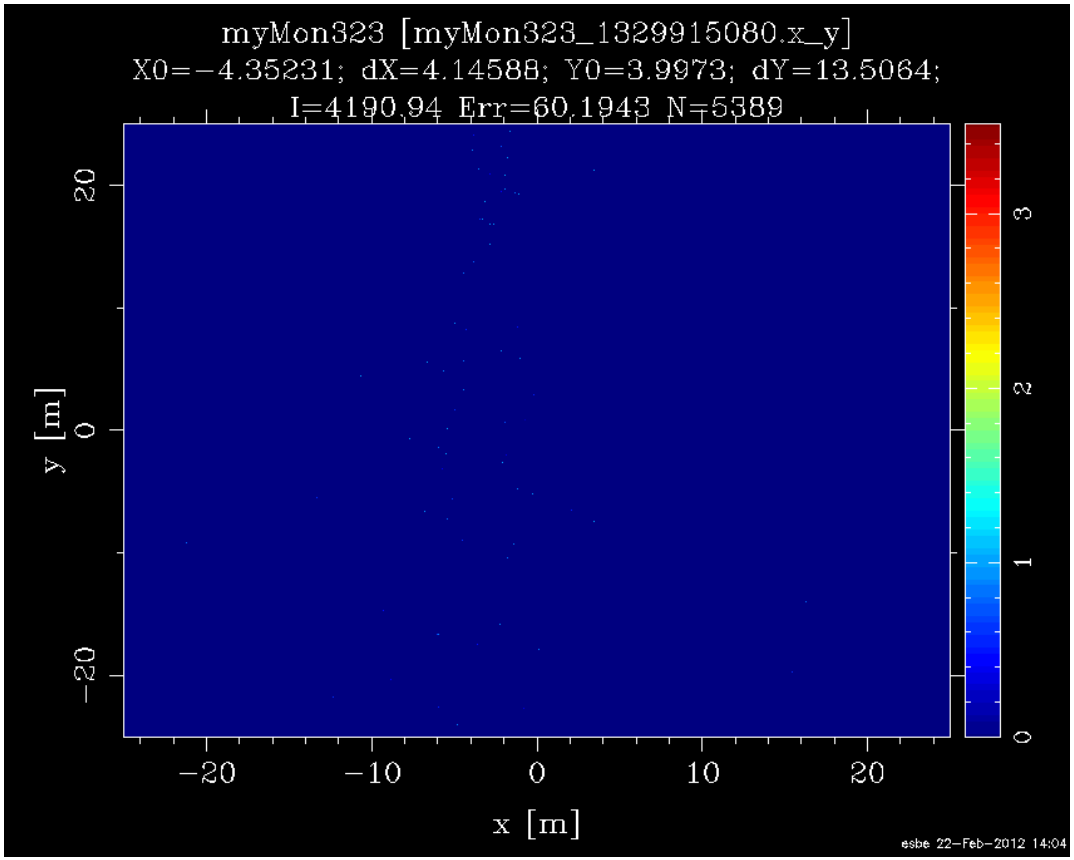




- I.e. uniform – but long flight path of ~6m means that a point source assumption is not too far off.
- **Q**: How would the distribution look in MCNP. I.e. SSW card at 6m?

Validation of Tally approach: Correlations

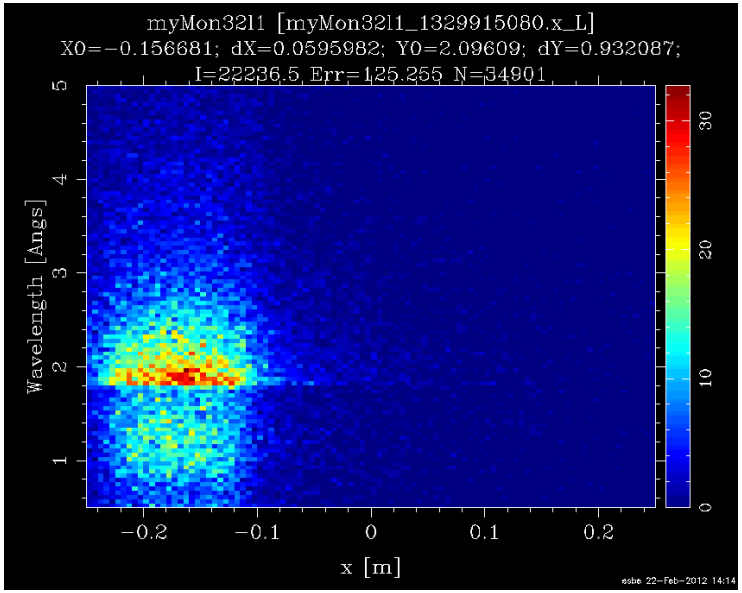
- **A**: Flat – in the empty sense of the word:

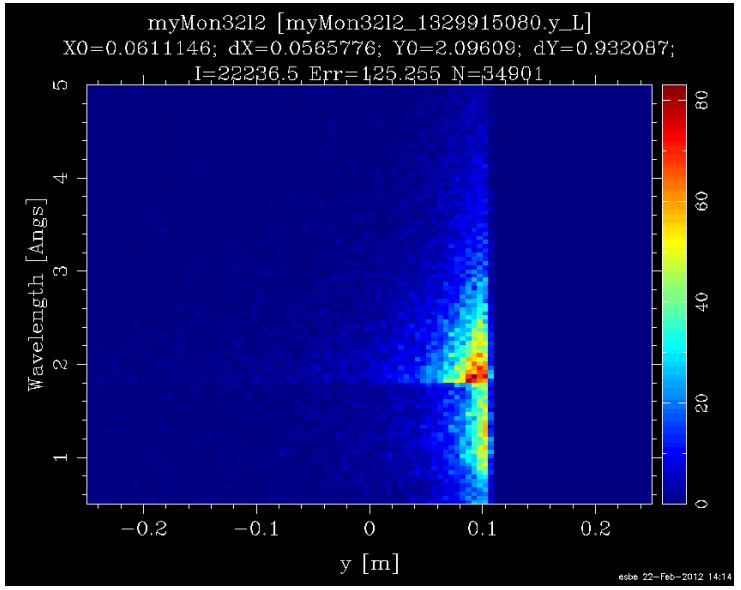


- No focus -> very few neutrons at guide

Validation of Tally approach: Correlations

- Lots of other comparisons to make:

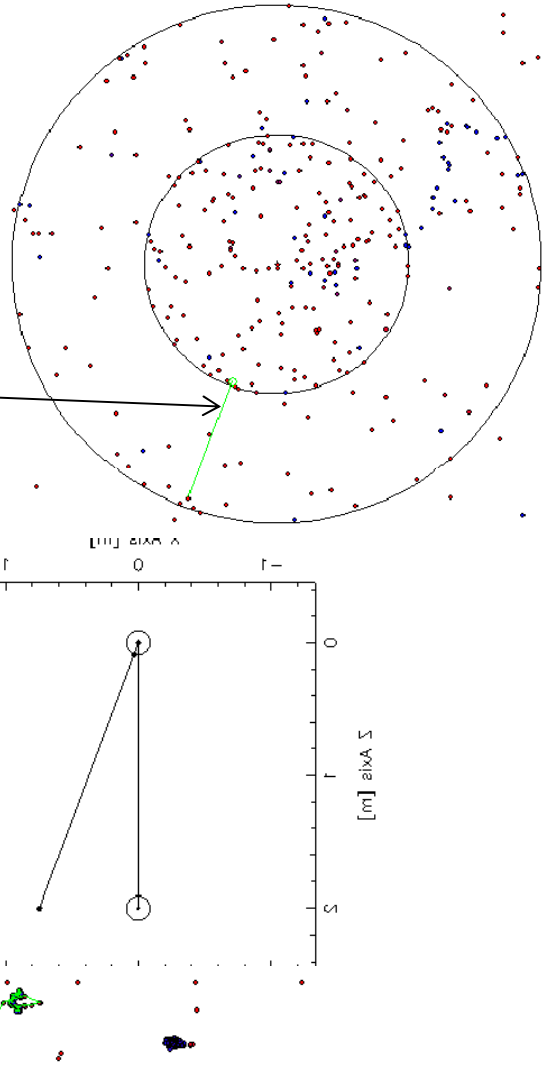




- I.e. correlations between position & energy exist. Important for moderator design etc, but perhaps not for instrument design (?). Being investigated.

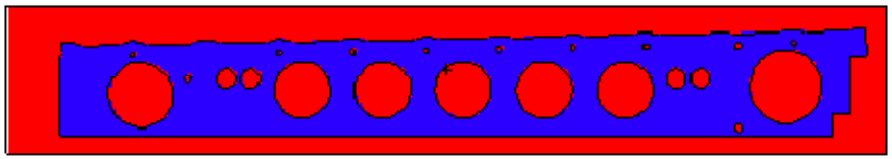
Validation of SSW / SSR approach

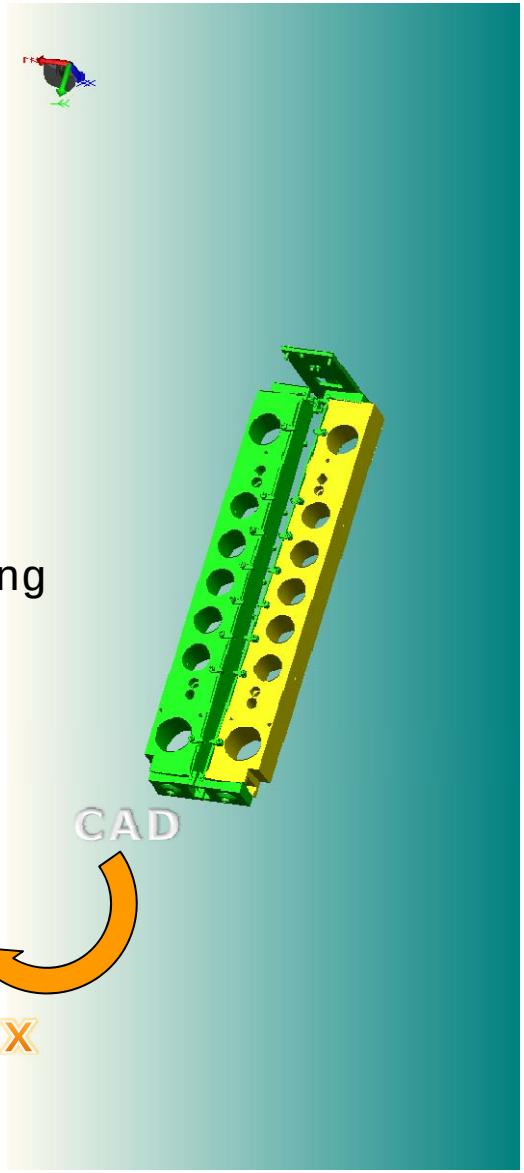
1. Define simplest possible geometry in MCNPX
2. Run test simulation
3. Visualize events and pick one
4. Import to McStas the neutron states as recorded by SSW card
5. Run simplest possible McStas simulation from SSW input: neutron transport
6. At z=2m, write SSW & visualize
7. Based on McStas SSW resume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



Validation: upcomming

- Test all 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

Cross comparison

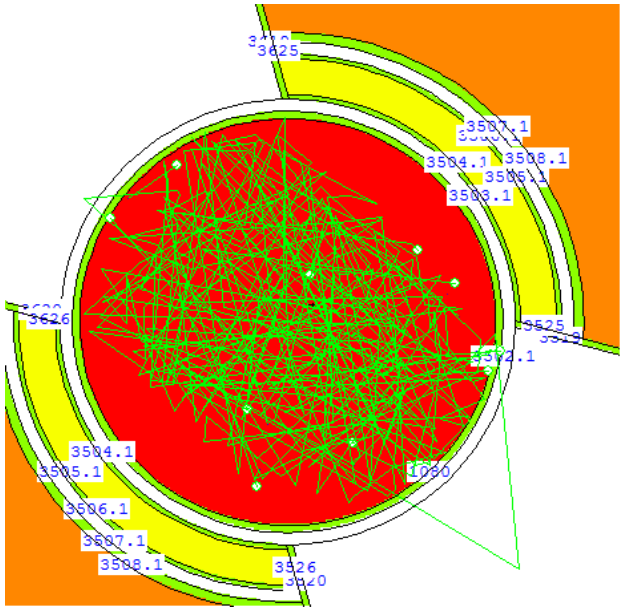
	Re-entry neutrons	Speed	Single neutron trace	Require License	Comments
Tally	No	Fast*	No	Yes/No	Should try to determine validity at least once
Ptrac	No	Fast*	Yes	Yes	Somewhat outdated by SSW/SSR
SSW/SSR	Yes	Fast*	Yes	Yes	Promising…
Compile	Yes	Slow	Yes	Yes	Generalizes poorly (auto gen c-code hacks)
Supermirror	Yes	Slow	yes	yes	Generalizes poorly (but who cares?)

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

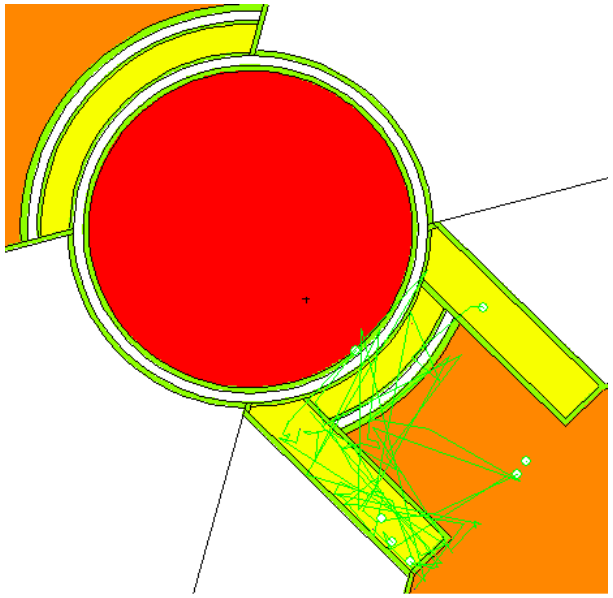
Backup slides

Tally contributions

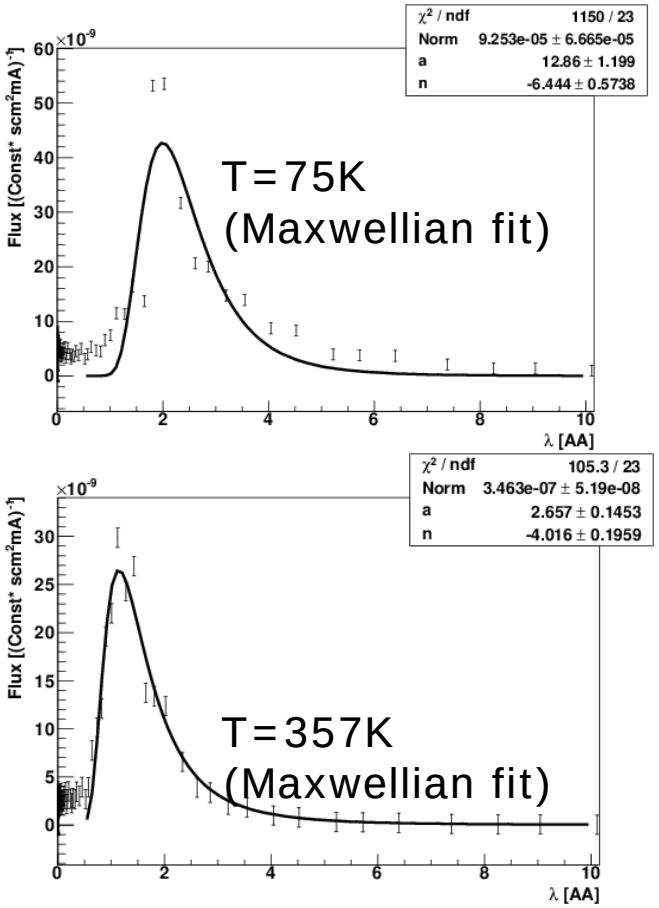
- Contributions to cold spectrum



- Contributions to thermal spectrum



Fits


χ² / ndf 1150 / 23
Norm 9.253e-05 ± 6.665e-05
a 12.86 ± 1.199
n -6.444 ± 0.5738
×10⁻⁹
Flux [(Const* scm²mA)⁻¹]
λ [AA]
T=75K
(Maxwellian fit)
χ² / ndf 105.3 / 23
Norm 3.463e-07 ± 5.19e-08
a 2.657 ± 0.1453
n -4.016 ± 0.1959
×10⁻⁹
Flux [(Const* scm²mA)⁻¹]
λ [AA]
T=357K
(Maxwellian fit)