MOTIVATION FOR A MCSTAS-SERPENT COUPLING

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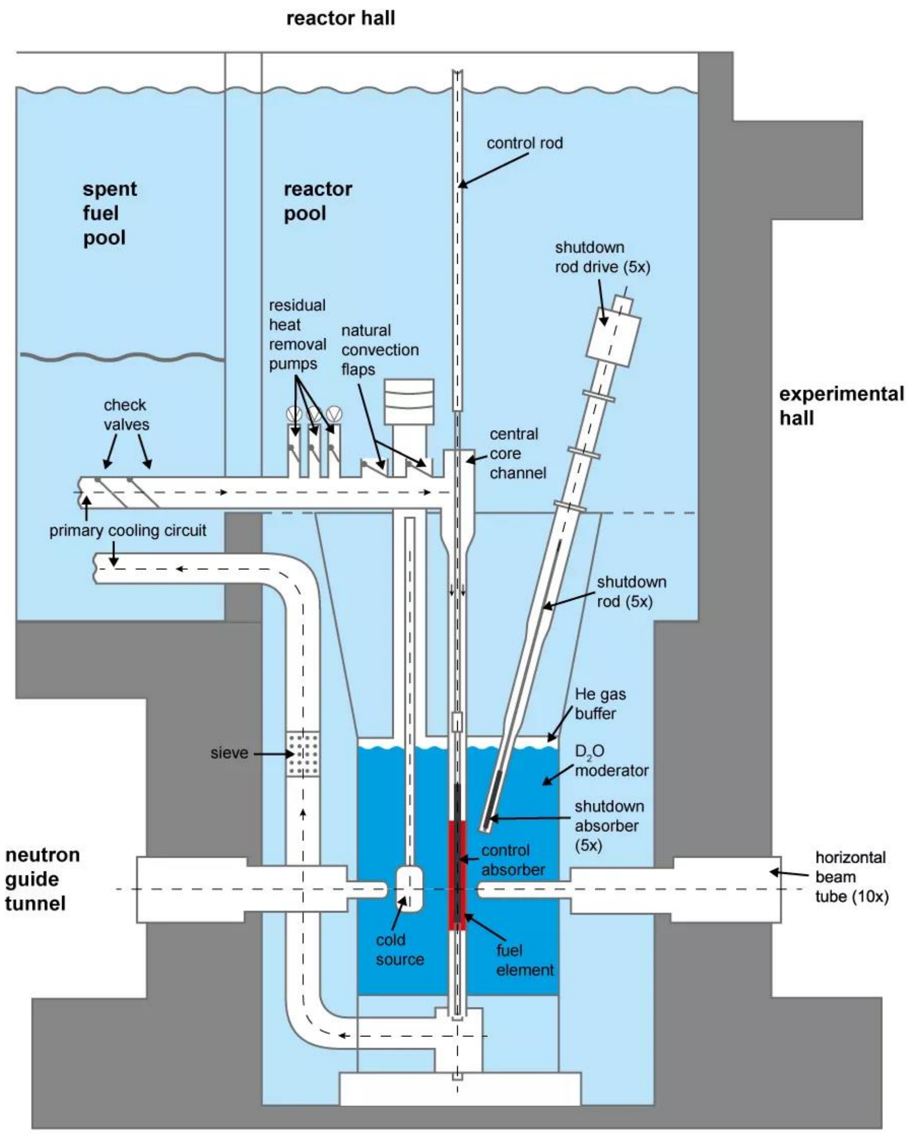
Serpent User Group Meeting

CONTEXT (I)

- Currently, FRM II is the reactor with the higher flux-to-power ratio worldwide
- However, conversion to LEU will affect the neutron flux arriving at the instruments (~ -9%).
- Instrument scientists want to know exactly how their instruments will be affected, if possible **before** the new reactor starts operations
- Additionally, the operation history of FRM II has shown that “things can happen” in the reactor tank, possibly affecting the neutron spectra at the instruments. Up to now, this had to be done manually



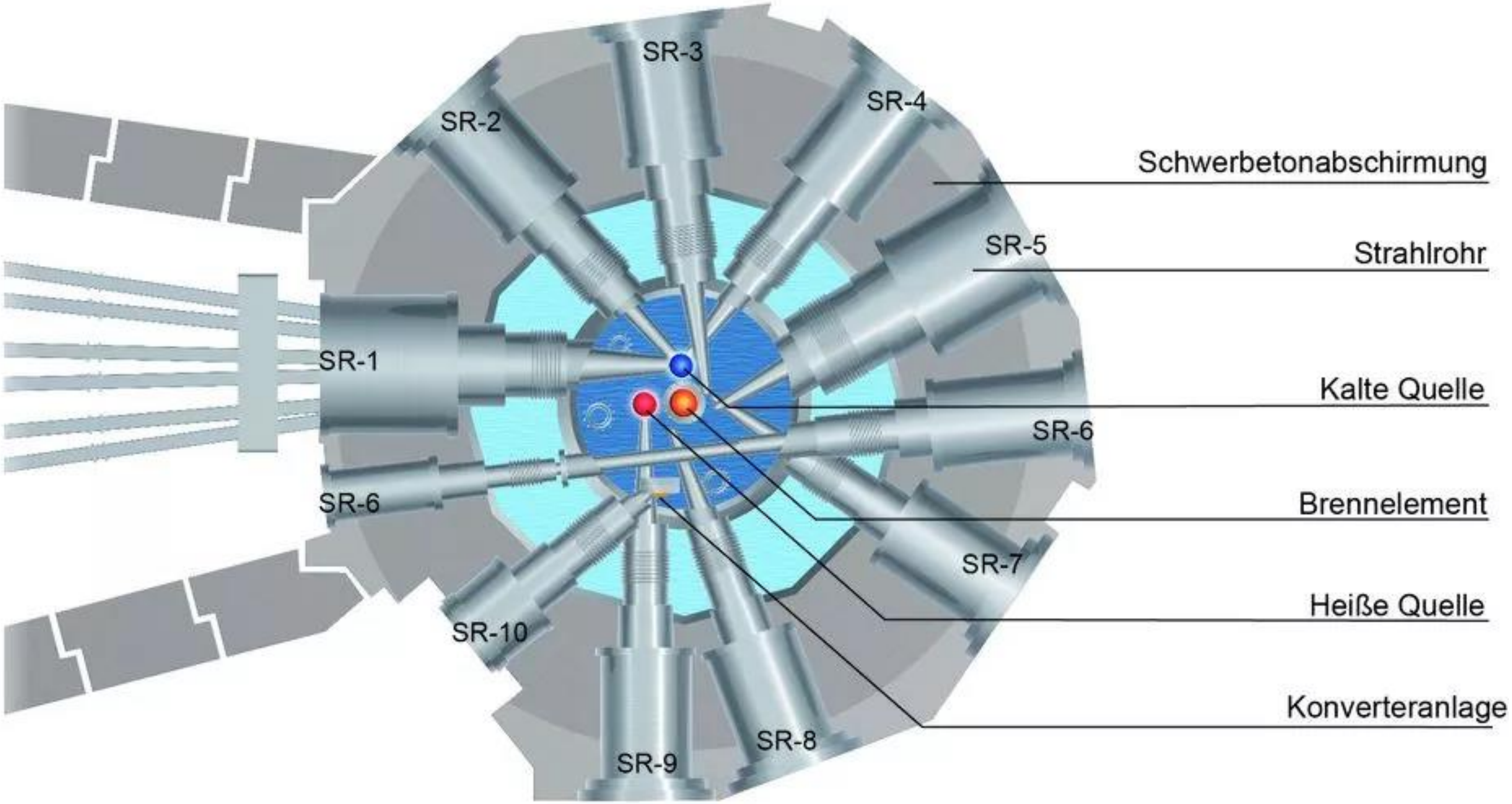
Source: FRM2 website

CONTEXT (II)

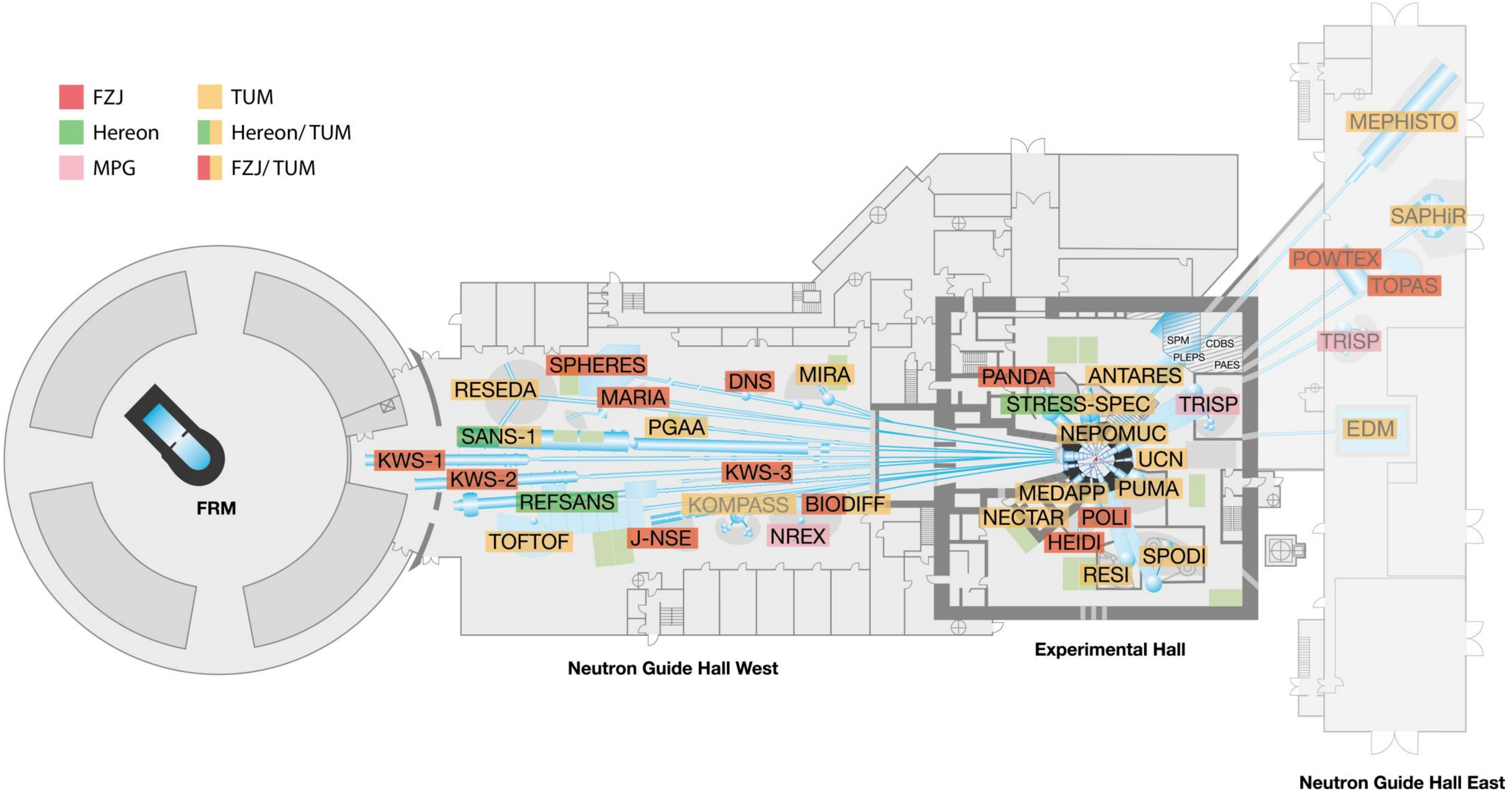
- We already use Serpent for full reactor calculations & to obtain spectra at beam tube nozzles.
- However, instruments are far away from the neutron source and most beam tubes include neutron reflectors, lenses, collimators, etc.*
- Monte Carlo *continuous particle transport codes* like Serpent are not well suited for interactions with these elements. Instead, MC *ray-tracing* software is used: McStas.
- Solution to make things easier: couple Serpent and McStas to have everything in one run for a given core (reactor) design.
- With the results, instrument scientists can decide whether and how to adapt or optimize the neutron optics.

- *Some instruments like MEDAPP (BT-10) only have a collimator and can be simulated with Serpent as part of a 2-step calculation (talk at Serpent UGM 2020)

FRM II BEAMTUBES AND INSTRUMENTS



Source: FRM2 website



Source: MLZ website

Instrument	Description	Neutrons	Status	Operated by	Funding
ANTARES	Radiography and tomography	cold	operation	TUM	TUM
BIODIFF	Diffractometer for large unit cells	cold	operation	TUM, JCNS	TUM, FZJ
DNS	Diffuse scattering spectrometer	cold	operation	JCNS	FZJ
HEIDI	Single crystal diffractometer	hot	operation	RWTH Aachen	FZJ
J-NSE	Spin-echo spectrometer	cold	operation	JCNS	FZJ
KOMPASS	Three axes spectrometer	cold	construction	Uni Köln, TUM	BMBF
KWS-1	Small angle scattering	cold	operation	JCNS	FZJ
KWS-2	Small angle scattering	cold	operation	JCNS	FZJ
KWS-3	Very small angle scattering	cold	operation	JCNS	FZJ
MARIA	Magnetic reflectometer	cold	operation	JCNS	FZJ
MEPHISTO	Facility for particle physics, PERC	cold	reconstruction	TUM	TUM, DFG
MIRA	Multipurpose instrument	cold	operation	TUM	TUM
MEDAPP	Medical irradiation treatment	fast	operation	TUM	TUM
NECTAR	Radiography and tomography	fast	operation	TUM	TUM
NEPOMUC	Positron source, CDBS, PAES, PLEPS, SPM	-	operation	TUM, UniBw München	TUM, BMBF
NREX	Reflectometer with X-ray option	cold	operation	MPI Stuttgart	MPG
PANDA	Three axes spectrometer	cold	operation	TU Dresden, JCNS	FZJ

Instrument	Description	Neutrons	Status	Operated by	Funding
PGAA	Prompt gamma activation analysis	cold	operation	Uni Köln, PSI	TUM
PUMA	Three axes spectrometer	thermal	operation	Uni Göttingen, TUM	TUM
POLI	Single-crystal diffractometer polarized neutrons	hot	operation	RWTH Aachen	BMBF, FZJ
POWTEX	Time-of-flight diffractometer	thermal	construction	RWTH Aachen, Uni Göttingen, JCNS	BMBF, FZJ
REFSANS	Reflectometer	cold	operation	GEMS	HZG
RESEDA	Resonance spin-echo spectrometer	cold	operation	TUM	TUM
RESI	Single crystal diffractometer	thermal	operation	LMU	TUM
SANS-1	Small angle scattering	cold	operation	TUM, GEMS	TUM, HZG
SAPHIR	Six anvil press for radiography and diffraction	thermal	construction	BGI	BMBF
SPHERES	Backscattering spectrometer	cold	operation	JCNS	FZJ
SPODI	Powder diffractometer	thermal	operation	KIT	TUM
STRESS-SPEC	Materials science diffractometer	thermal	operation	TUM, TU Clausthal, GEMS	TUM, HZG
TOFTOF	Time-of-flight spectrometer	cold	operation	TUM	TUM
TOPAS	Time-of-flight spectrometer	thermal	construction	JCNS	FZJ
TRISP	Three axes spin-echo spectrometer	thermal	operation	MPI Stuttgart	MPG
UCN	Ultra cold neutron source, EDM	ultra-cold	construction	TUM	TUM, DFG

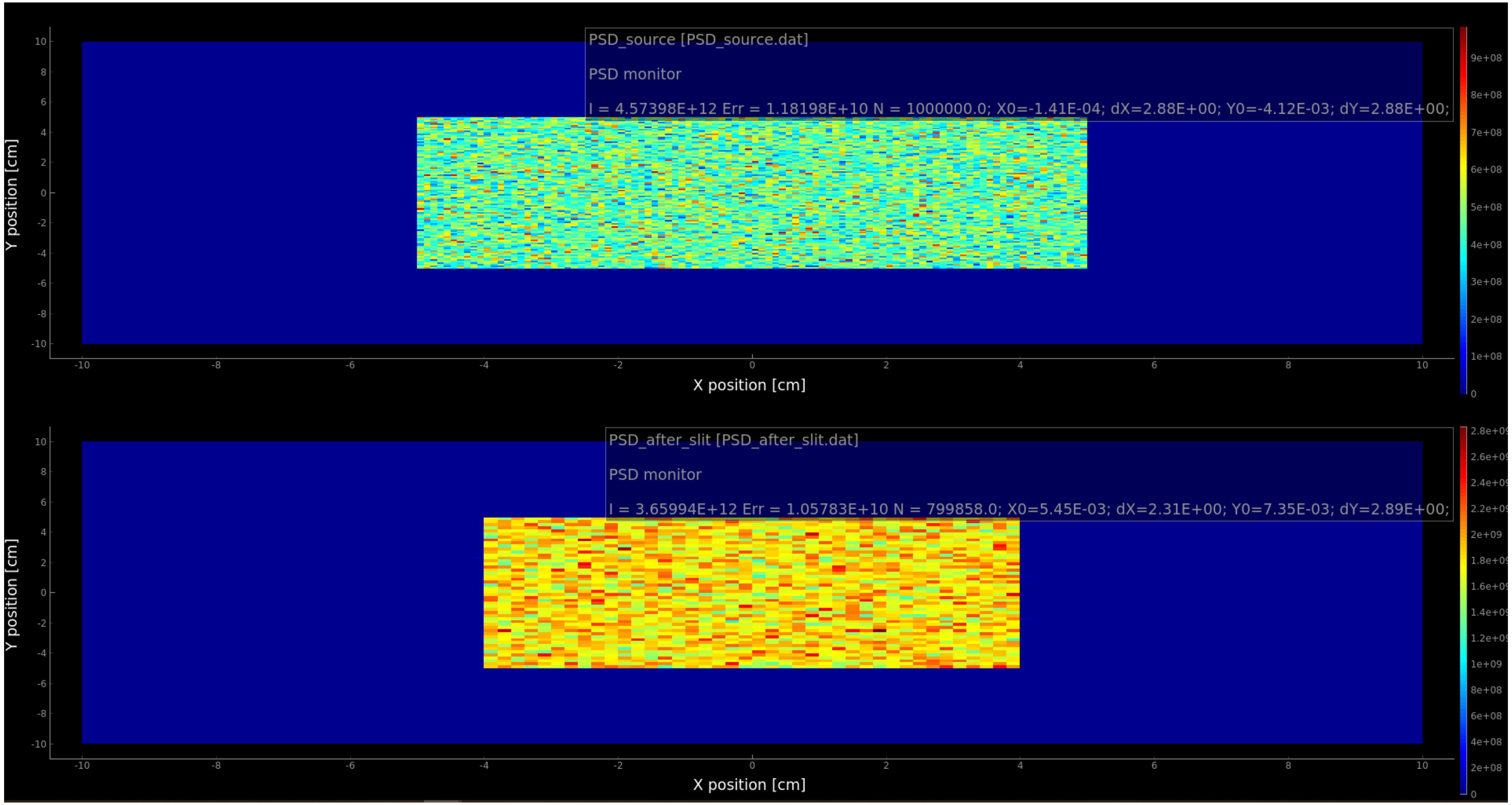
MCSTAS

- Tool for "carrying out Monte Carlo ray-tracing simulations of neutron scattering instruments with high complexity and precision" using both continuous and pulsing sources.
- Main developers from DTU; collaborations from ILL, U of Cologne and U of Copenhaguen. Initial release in 1998.
- Geometry are instruments consisting of neutron optics components along the neutron path at given positions.
- Elements added from libray, where users can add their instrument to
- Like in Serpent and other MC codes, particle weights, importance sampling, russian roulette etc are also used.
- Various ways of defining neutron sources are possible

MCSTAS (II)

```
COMPONENT some_beamline = Arm()
  AT (0,0,0) RELATIVE a1
  ROTATED (0,0,0)  RELATIVE a1

/**************************************  source  ******************************************/
/* a typical McStas generic 3 Maxwell definition ******************************************/
COMPONENT MySource = Source_gen(
   yheight =  0.100, xwidth = 0.100,
   focus_xw = 0.100, focus_yh = 0.100, dist = 2.00,
   lambda0 = Lam, dlambda = dLam,
   T1=361.9,I1=7.22e12,
   T2=159.0,I2=6.74e12,
   T3=35.66,I3=6.435e12)
  AT (0,0,0)  RELATIVE some_beamline
  ROTATED (0,0,0) RELATIVE some_beamline

/* lets look what the source emmits */
COMPONENT PSD_source = PSD_monitor(xmin=-0.100, xmax=0.100, ymin=-0.100, ymax=0.100,
                                   nx=200, ny=200, filename="PSD_source.dat")
  AT (0,0,0.00001) RELATIVE PREVIOUS
  ROTATED (0,0,0)  RELATIVE PREVIOUS

/* somewhere the beamtube plug channel has an opening ... */

COMPONENT beamchannel_entry = Slit (xmin=-0.04, xmax=0.04, ymin=-0.05, ymax=0.05)
  AT (0,0,2.000)    RELATIVE some_beamline

/* lets look what passes the opening */
COMPONENT PSD_after_slit = PSD_monitor(xmin=-0.1, xmax=0.1, ymin=-0.10, ymax=0.10,
                                            nx=100, ny=100, filename="PSD_after_slit.dat")
  AT (0,0,0.00001) RELATIVE PREVIOUS
  ROTATED (0,0,0) RELATIVE PREVIOUS

/***********************************End of DEMO ***********************************/
```

MCSTAS (III)


PSD_source [PSD_source.dat]
PSD monitor
I = 4.57398E+12 Err = 1.18198E+10 N = 1000000.0; X0=-1.41E-04; dX=2.88E+00; Y0=-4.12E-03; dY=2.88E+00;
Y position [cm]
X position [cm]
PSD_after_slit [PSD_after_slit.dat]
PSD monitor
I = 3.65994E+12 Err = 1.05783E+10 N = 799858.0; X0=5.45E-03; dX=2.31E+00; Y0=7.35E-03; dY=2.89E+00;
Y position [cm]
X position [cm]

COUPLING

- First idea: One-way, script-based

User introduces instrument of interest, and reactor operation parameters → Serpent runs full core calculation with necessary beamtube nozzle detector → Spectra extraction from det file, data processing → McStas simulation: spectra at instrument

FUTURE POTENTIAL WORK

- Two way coupling. McStas and MCNP coupling work is ongoing allowing for e.g. dosimetry calculations for shielding purposes along the beamtube or instrument

SUMMARY

Context: instrument scientists might need/want to adapt their instruments after conversion

Problem: spectra available to instrument scientists today are very rough estimations, and they lack knowledge to accurately calculate them themselves now & in the future

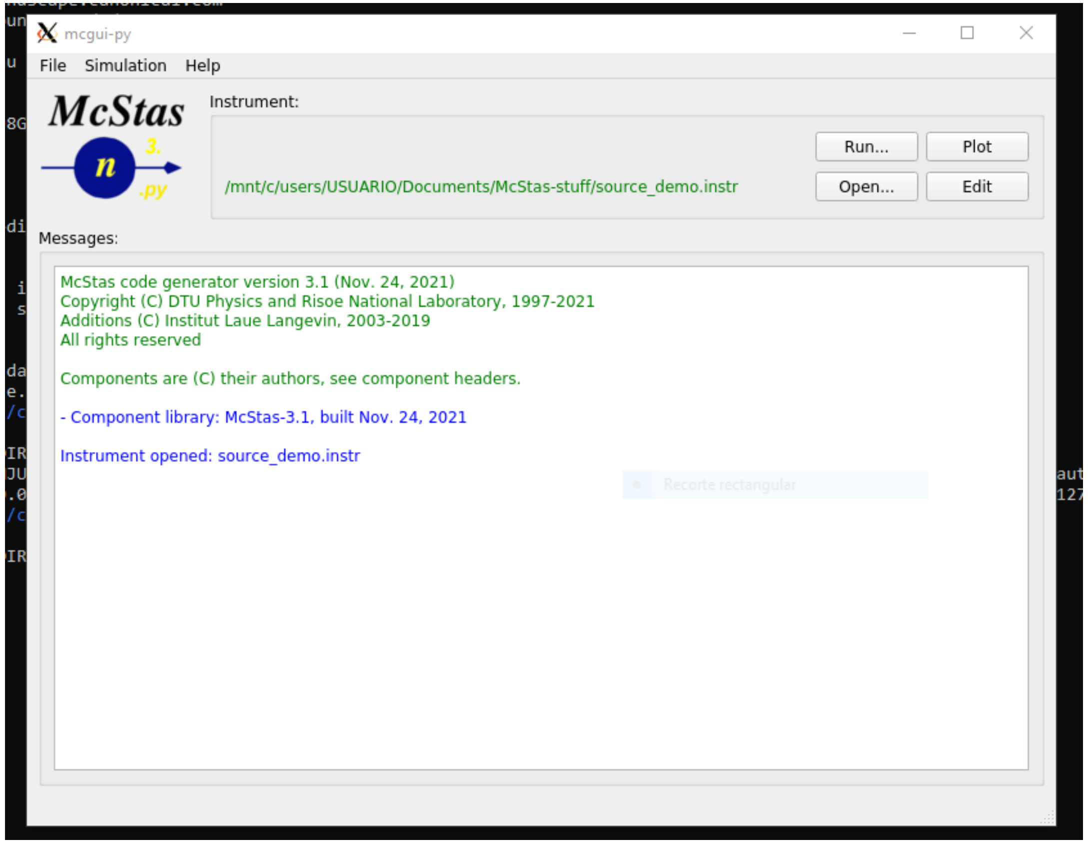
Solution: calculate spectra with a full-core Serpent simulation and feed them automatically to McStas.

THANK YOU FOR YOUR ATTENTION!

ANY QUESTIONS?

ANNEX

```
COMPONENT guide13 = Guide(w1=0.04507,
                         h1=0.04507,
                         w2=0.04347,
                         h2=0.04347,
                         l=1.0-0.0000001, R0=0.99, Qc=0.0217,  alpha=3,m=3.2,W=0.001)
                         AT (0, 0, 26.6) RELATIVE a1 ROTATED (0,0,0) RELATIVE a1
```



Equivalence of energy, temperature, wavelength and speed of neutrons. The limits are generally not well-defined.

Description	Energy	Temperature	Wavelength	Speed
High energetic neutrons	>20 MeV			
Fission neutrons	2 MeV			
Fast/hot neutrons	40 – 10^3 meV	2300 K	0,05 nm	5 km/s
Thermal neutrons	3 – 150 meV	300 K	0,2 nm	2,2 km/s
Cold neutrons	0,1 – 20 meV	25 K	0,2 - 25 nm	600 m/s
Ultra cold neutrons	10^{-6} – 0,01 meV	mK	10 - 1000 nm	5 m/s