FIRST STEPS FOR THE OPTIMIZATION OF EXPERIMENTAL FACILITIES AT FRM II DURING CONVERSION

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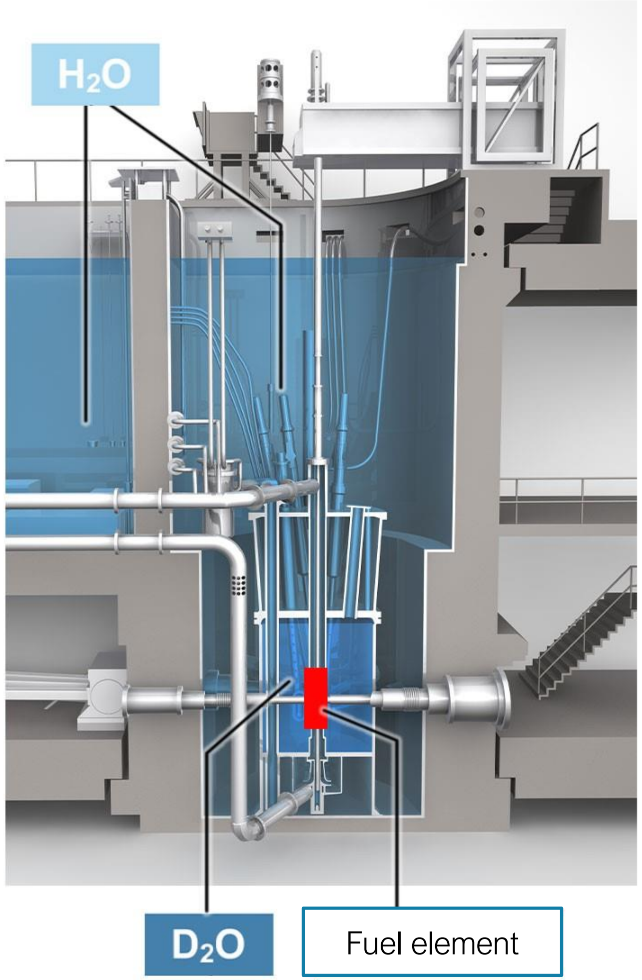
CONTEXT: FRM II AFTER CONVERSION

- Currently, FRM II is the reactor with the highest flux-to-power ratio worldwide
- However, conversion will affect the neutron flux arriving at the instruments.
- Instrument scientists want the best possible estimates for changes in neutron flux after conversion at their instrument. In this way, they can come up with improvements outside the core to minimize the losses of neutron flux.
- Ideally, scientists should be able to estimate the impact not only of conversion but also of any other future change in the moderator tank.

Best way to obtain these fluxes: Monte Carlo simulations

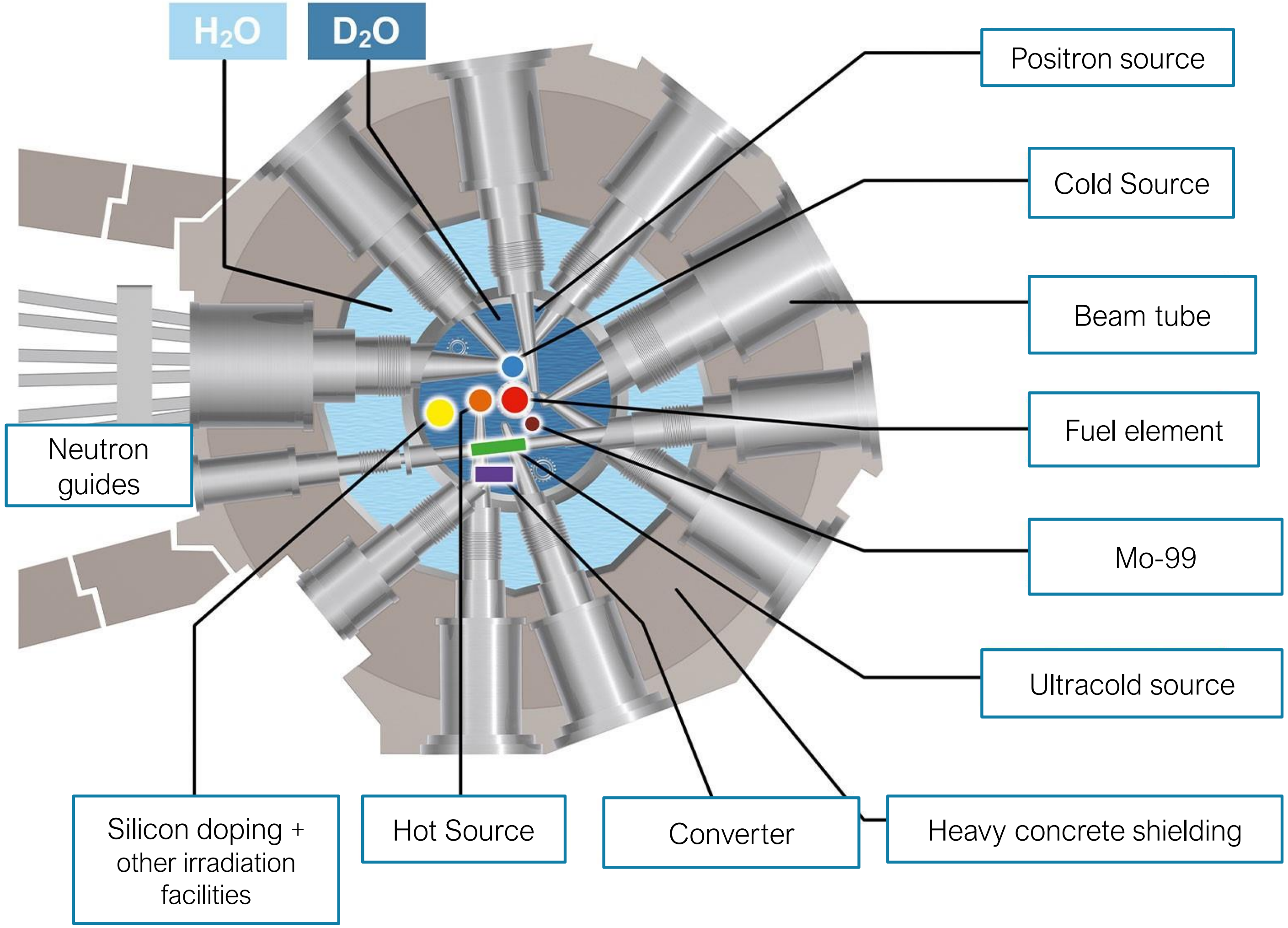
FRM II: CORE AND BEAM TUBES



H_2O

D_2O

Fuel element



H_2O

D_2O

Neutron guides

Positron source

Cold Source

Beam tube

Fuel element

Mo-99

Ultracold source

Silicon doping + other irradiation facilities

Hot Source

Converter

Heavy concrete shielding

FRM2/TUM ©

FRM II: INSTRUMENTS

- More than 30 instruments, using neutrons in all spectral regions from cold to fast.
- Some of them are a few meters away from the source, others more than 30 m.
- Space can be scarce, placing and size of elements is important.

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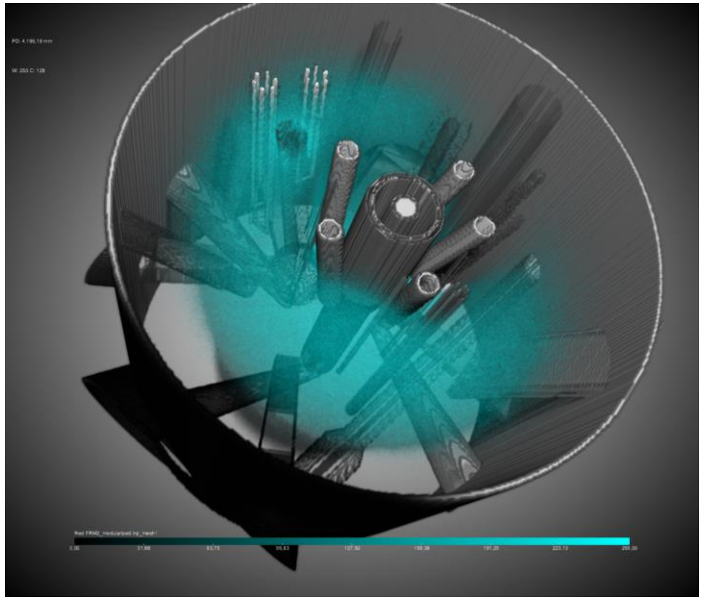
CONTEXT: MONTE CARLO CODES AT FRM II

- Serpent is the main tool at FRM II for full reactor simulations.
- Serpent:
  - Monte Carlo *continuous particle transport code* being developed by VTT (Finland) since 2004. Similar to MCNP, more convenient for our reactor.
  - Used for mainly for criticality and burnup simulations. Occasionally for dosimetry and photon transport.
- However, instruments are far away from the neutron source and most beam tubes include neutron reflectors, lenses, collimators, etc.
- Problems:
  - 1) Codes like Serpent are not well suited for interactions with these elements. They cannot handle coherent scattering (cold-thermal neutrons).
  - 2) One simulation for each part of the neutron path would be needed to achieve reasonable statistics.

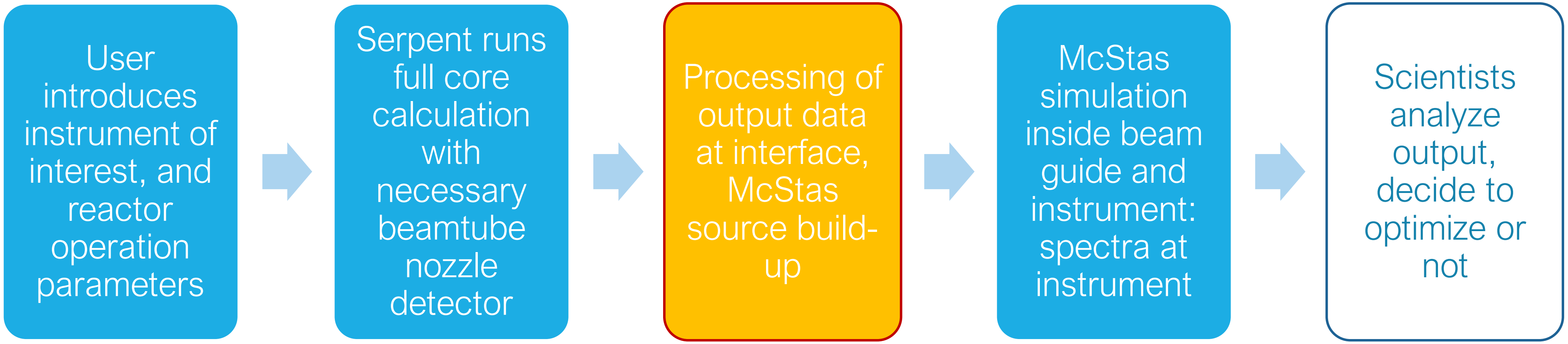


MCSTAS

- To solve Serpent’s limitations, MC *ray-tracing* software is used: 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.

SOLUTION: SERPENT-MCSTAS COUPLING

- 2 problems (recall):
  1) Codes like Serpent are not well suited for interactions with these elements. They cannot handle coherent scattering (cold-thermal neutrons).
  2) One simulation for each part of the neutron path would be needed to achieve reasonable statistics.
- Solution: One-way, script-based, coupling of Serpent and McStas to have everything in one run for a given core (reactor) design:



User introduces instrument of interest, and reactor operation parameters

Serpent runs full core calculation with necessary beamtube nozzle detector

Processing of output data at interface, McStas source build-up

McStas simulation inside beam guide and instrument: spectra at instrument

Scientists analyze output, decide to optimize or not

PRECEDENT: MCNPX-MCSTAS COUPLING

- Described in “Interfacing MCNPX and McStas for simulation of neutron transport”, E. Klinkby et al., 2012. Work from DTU and ILL. 3 approaches:

1. *Tally:* Analytical fit to flux spectral density tally at interface with several Maxwellians, which are then used by McStas to sample the source:
   - 🟩 Allows for repetition of McStas simulation without repeating the MCNPX part.
   - 🟥 Information on individual particle position and momentum is lost.
2. *Ptrac*: Surface neutron collection, i.e. writing position, momentum and statistical weight of each particle into a *Ptrac* file. McStas has built-in feature to read these files.
   - Limitations (MCNPX): only one interface allowed and not MPI-friendly.

- Other approaches: *Source Surface Write/Read (SSW/R)*, compile together, supermirror.

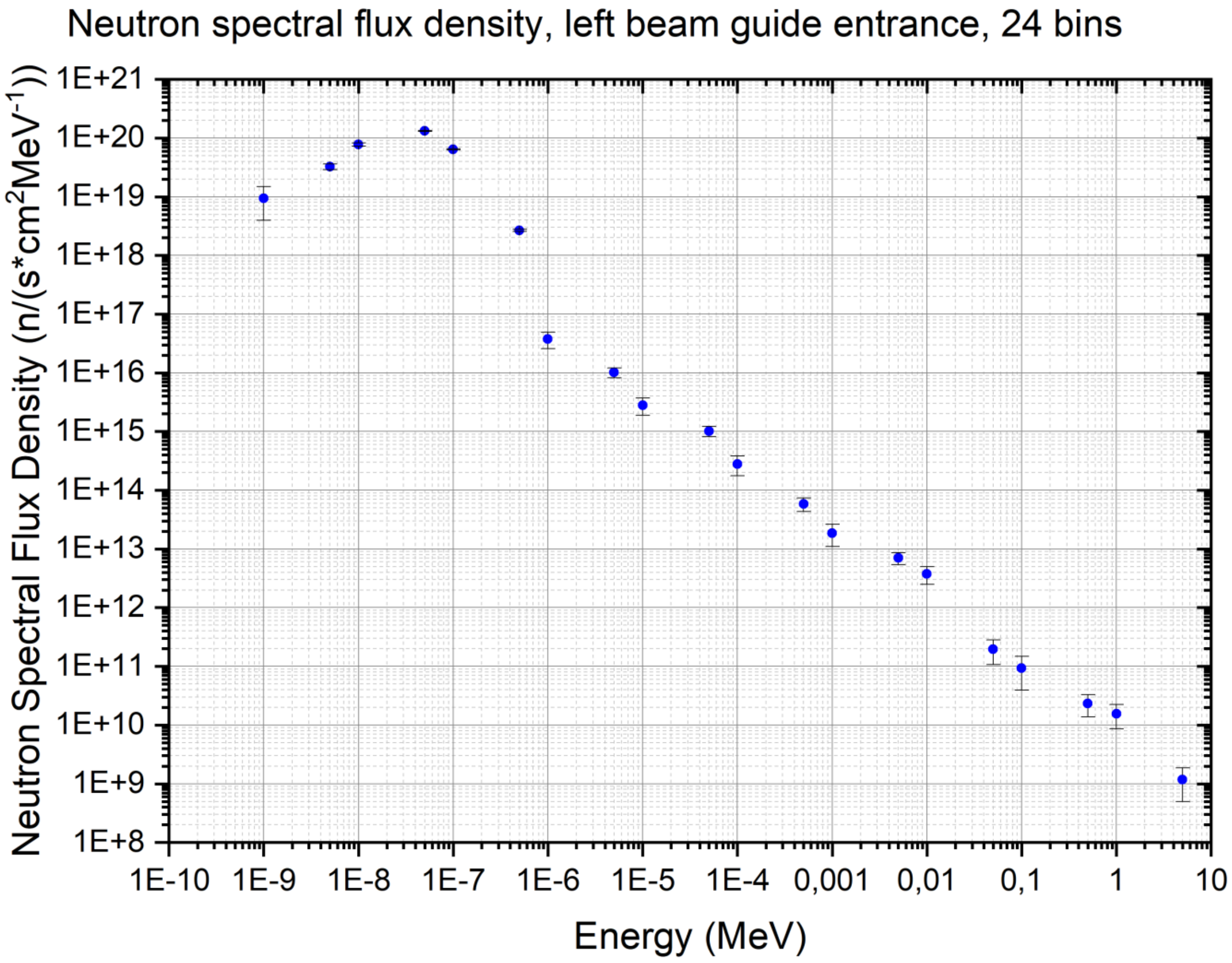
ADAPTATION FOR SERPENT-MCSTAS COUPLING

- *SSW/R* option does not exist as such in Serpent. *Compiling* and *Supermirror* are disadvantageous when compared to *tally* and *Ptrac.*

1. *Tally* (=flux detector) option is straight forward but requires someone or something to do the Maxwellian fitting.
2. *Ptrac* (~ surface current detector) is much less limited in Serpent, since two-way coupling would be possible, but some file formatting must take place to adapt to the McStas Ptrac-reading virtual component.

- Plan:
    1. Try approaches 1 and 2 with manual fitting, file formatting, etc. for a given beam tube (BT-8).
    2. Discuss results with instrument scientists, possibly compare with available experimental data.
    3. Write script for preferred approach

SERPENT SPECTRUM AT BEAM TUBE 8



POTENTIAL FUTURE WORK

- Two way coupling. McStas-MCNPX coupling work has been used for secondary gamma production calculations along the neutron guides at ESS. Could be useful for FRM II too.
- Validation with experimental data at several instruments (still with HEU core)

SUMMARY

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

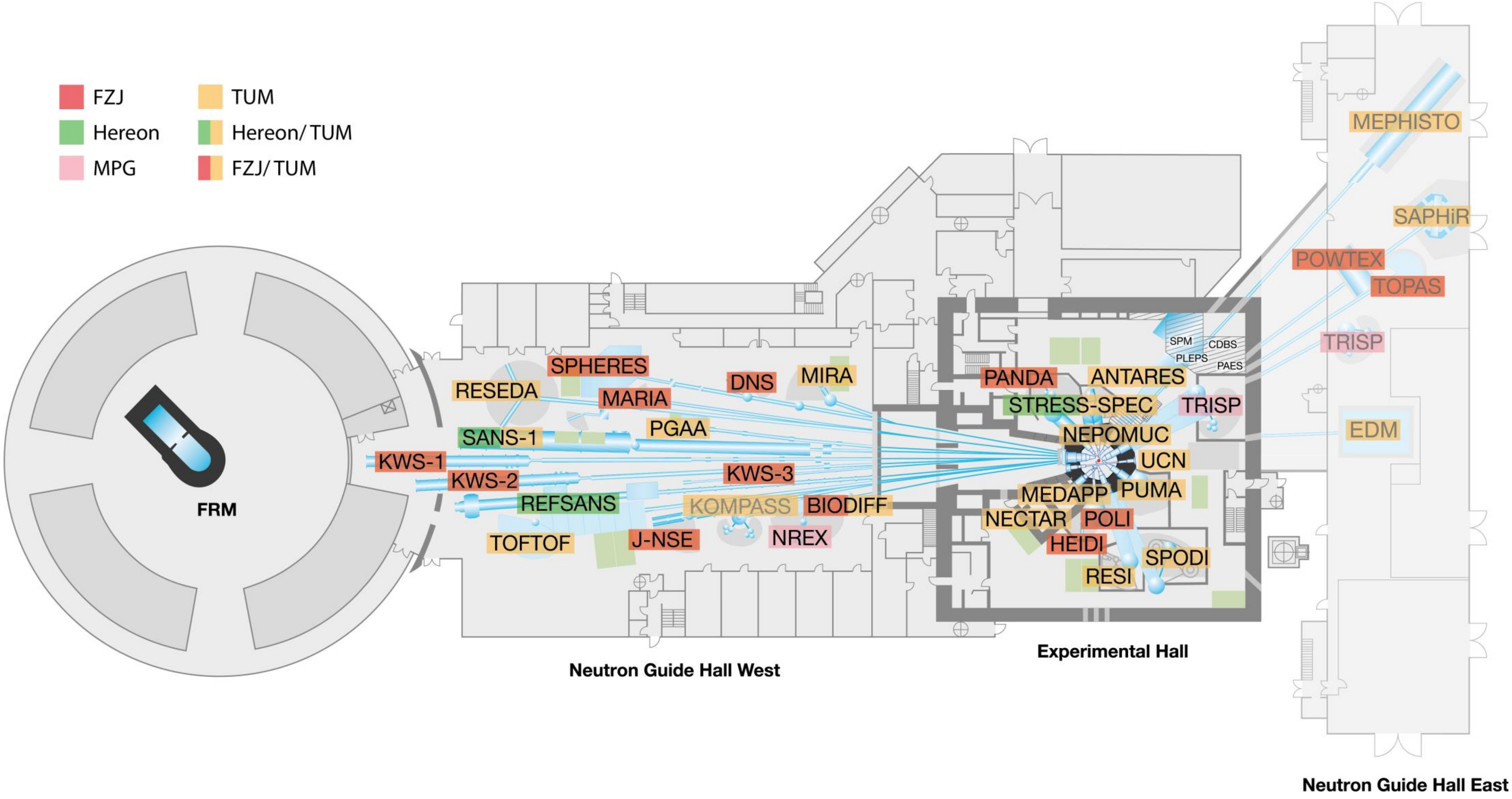
Problem: spectra available to instrument scientists today are very rough estimations, and they lack knowledge to accurately calculate them themselves now & in the future

Solution: calculate spectra with a full-core Serpent simulation and feed them automatically to McStas, taking inspiration in the *tally*/flux detector and *Ptrac*/surface current detector approaches used in the MCNPX-McStas coupling literature.

THANK YOU FOR YOUR ATTENTION!

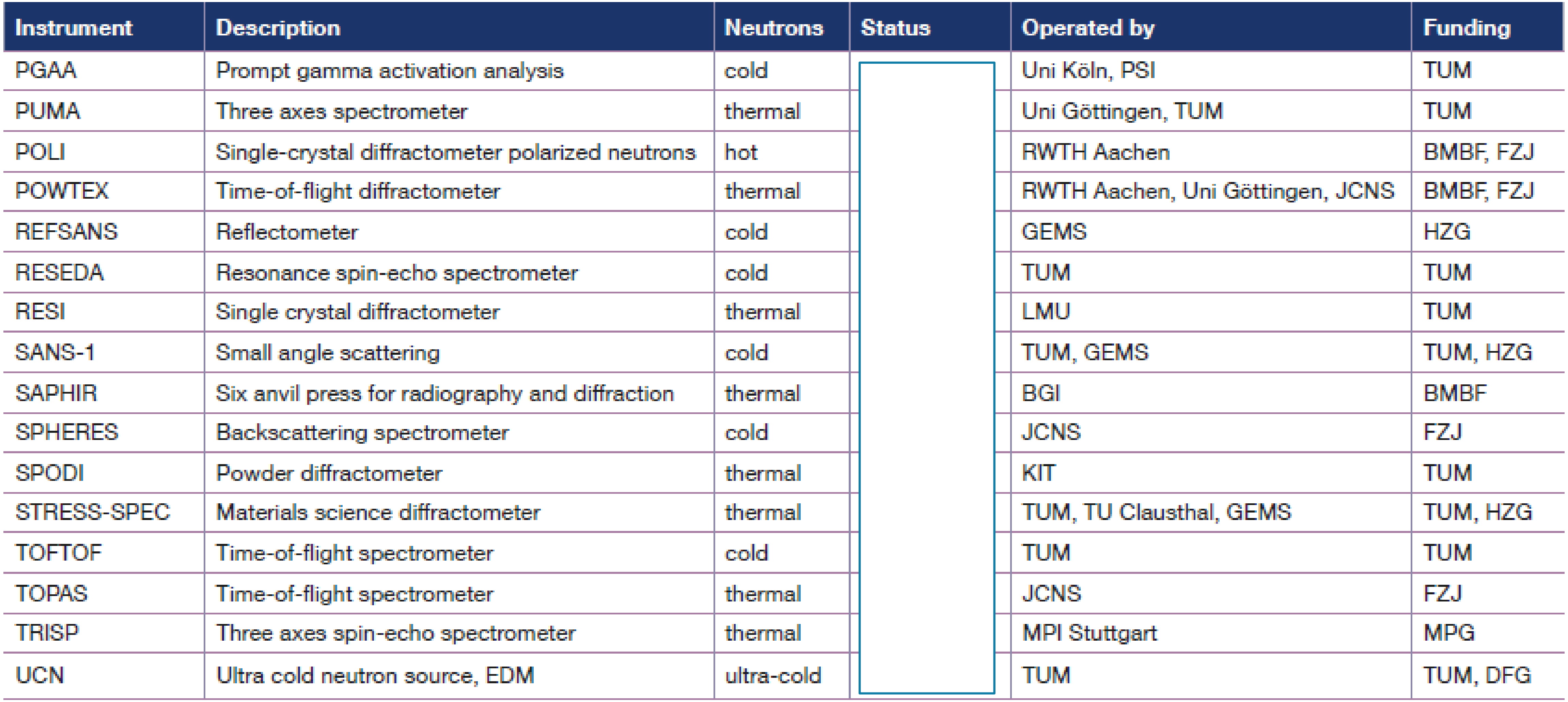
ANY QUESTIONS?

ADDITIONAL SLIDES

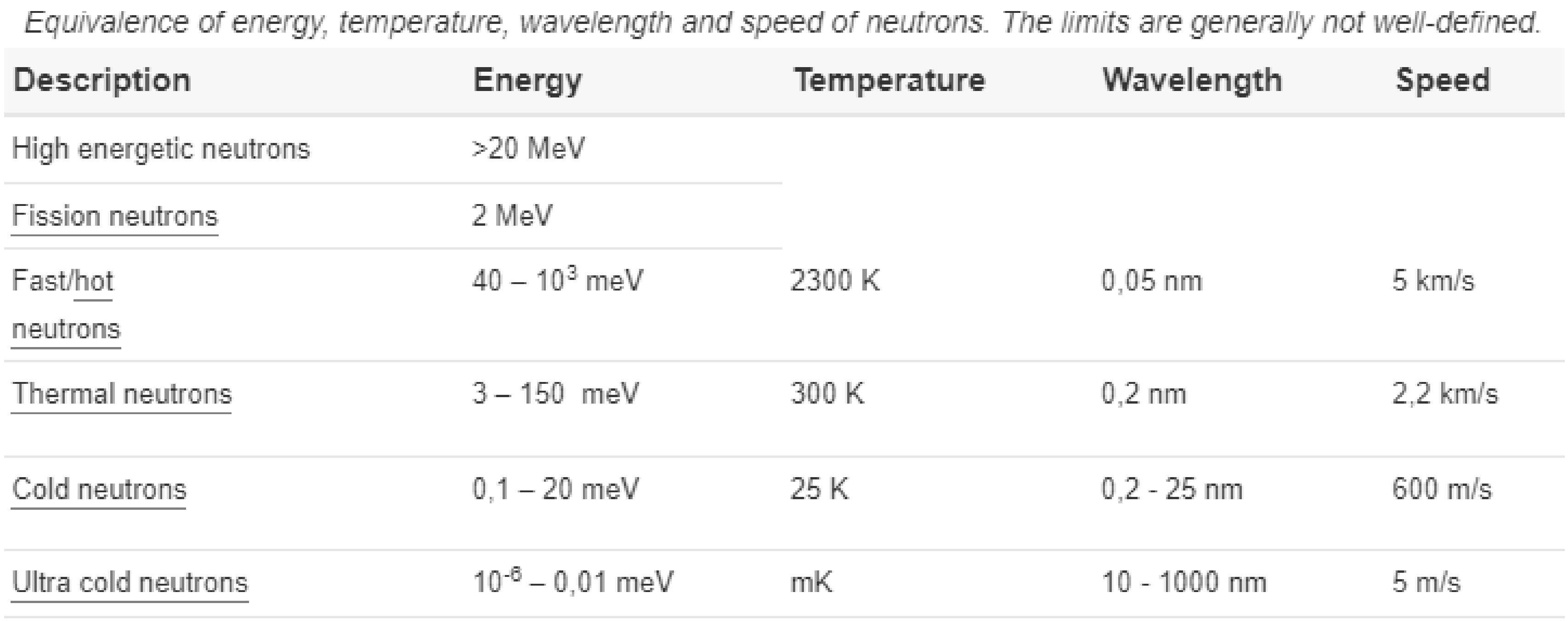


Source: MLZ website

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



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



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