

SINE2020 General Assembly

Bilbao, May 28th 2019

WP 8: INSTRUMENTATION - E-TOOLS

- E-tools for integrated simulation using neutronics and Monte Carlo ray-tracing
- Innovative Shielding Concepts and Materials
- Compact Instrumentation for Larmor Labelling applications at the ESS

DTU

Peter Willendrup,

29/5/19

This project is funded by the European Union (GA no. 654000)

1. Objectives

(and WP8 Structure)

- Task 8.1: E-tools for integrated simulation using neutronics and Monte Carlo ray-tracing

- Task 8.2: Innovative Shielding Concepts and Materials

! Task 8.3: Compact Instrumentation for Larmor Labelling applications at the ESS

1. Objectives

(and WP8 Structure)

Improve "cradle to grave" instrument-modeling capability beyond state of the art:

neutronics + ray-tracing — signal / simulation noise

! Task 8.1: E-tools for integrated using neutronics and Monte Carlo ray-tracing

! Task 8.2: Innovative Shielding

Concepts and Materials

! Task 8.3: Compact Instrumentation for Larmor Labelling applications at the ESS

(heavy concrete, laminar shielding)

Measure and understand (high-energy) background and utilise this to better shield our instruments using new shielding approaches

Investigate the effect of the ESS pancake / butterfly moderator on the design of NSE and Larmor labelling instruments at this facility

ISTSI 2019 - June 29th 2019
Holiday Inn Московские Ворота
St. Petersburg, Russia
Agenda:

9:30-9:40	**Welcome**	
9:40-10:00	*News from the RESTRAX/SIMRES project, including MCPL support and McStas bindings for SIMRES*	**Jan Šaroun, NPI**
10:00-10:20	*News from the Vitess project including MCPL support*	**Egor Vezhlev, FZJ**
10:20-10:40	*News from the McStas project, including interoperability solutions for SIMRES, Vitess and MCNP*	**Peter Willendrup, DTU/ESS**
10:40-11:00	*Developments in the MCPL software framework*	**Thomas Kittelmann, ESS**
11:00-11:20	**Coffee break**	
11:20-11:40	*An optimised neutron super mirror patch for MCNP*	**Miguel Magán, ESS-Bilbao**
11:40-12:00	*ESS-developed "duct source" for describing neutron guides in Geant4*	**Ken Andersen, ESS**
12:00-12:20	*CombLayer-driven MCNP-McStas simulations for simulating instrument signal to noise*	**Esben Klinkby, DTU/ESS**
12:20-12:40	*Applications of the neutron super mirror patch for MCNP*	**Octavio González, ESS-Bilbao**
12:40-14:00	*McStas and Scatter-logger driven calculations of prompt gamma shielding for neutron guides*	**Rodion Kolevatov, NPI**
14:00-14:20	**Lunch**	
14:20-14:40	*Studies of relevant design-parameters to enable compact Larmor devices in ESS designs*	**Katia Pappas, TUDelft**
14:40-15:00	*Magnetic field calculations for compact Larmor devices in ESS designs*	**Michel Thijs, TUDelft**
15:00-15:20	*Simulation benchmarks for experiments at the PSI BOA beamline*	**Erik Knudsen, DTU**
15:20-15:40	*Extensions to the Bonner Sphere Spectrometer at PSI, plus experiments and simulation benchmarking for newly developed concrete*	**Masako Yamada, PSI**
15:40-16:00	*Development and studies of Polyethylene-B4C concretes at ESS*	**Ken Andersen, ESS**
16:00-16:20	**Coffee break**	
16:20-16:40	*Studies of material composition and neutron activation*	**Eszter Dian, MTA-EK**
16:40-17:00	*Simulation studies of material irradiation*	**Esben Klinkby, DTU/ESS**
17:00-17:20	*Simulation studies of laminar shielding concepts*	**Miguel Magán, ESS-Bilbao**

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 654000.

Holiday Inn St. Petersburg, Russia, June 29th 2019

- Saturday before ECNS

Have held ~ 5 spots if anyone more from SINE wants to join!? Please let me know! (link)

25 participants, half are not from WP

- Fullfils WP8 MS5+MS6

ISTSI 2019 - June 29th 2019
Holiday Inn Московские Ворота
St. Petersburg, Russia
Agenda:

9:30-9:40	**Welcome**	
9:40-10:00	*News from the RESTRAX/SIMRES project, including MCPL support and McStas bindings for SIMRES*	Jan Šaroun, NPI
10:00-10:20	*News from the Vitess project including MCPL support*	Egor Vezhlev, FZJ
10:20-10:40	*News from the McStas project, including interoperability solutions for SIMRES, Vitess and MCNP*	Peter Willendrup, DTU/ESS
10:40-11:00	*Developments in the MCPL software framework*	Thomas Kittelmann, ESS
11:00-11:20	**Coffee break**	
11:20-11:40	*An optimised neutron super mirror patch for MCNP*	Miguel Magán, ESS-Bilbao
11:40-12:00	*ESS-developed "duct source" for describing neutron guides in Geant4*	Ken Andersen, ESS
12:00-12:20	*CombLayer-driven MCNP-McStas simulations for simulating instrument signal to noise*	Esben Klinkby, DTU/ESS
12:20-12:40	*Applications of the neutron super mirror patch for MCNP*	Octavio González, ESS-Bilbao
12:40-14:00	*McStas and Scatter-logger driven calculations of prompt gamma shielding for neutron guides*	Rodion Kolevatov, NPI
14:00-14:20	**Lunch**	
14:20-14:40	*Studies of relevant design-parameters to enable compact Larmor devices in ESS designs*	Katia Pappas, TUDelft
14:40-15:00	*Magnetic field calculations for compact Larmor devices in ESS designs*	Michel Thijs, TUDelft
15:00-15:20	*Simulation benchmarks for experiments at the PSI BOA beamline*	Erik Knudsen, DTU
15:20-15:40	*Extensions to the Bonner Sphere Spectrometer at PSI, plus experiments and simulation benchmarking for newly developed concrete*	Masako Yamada, PSI
15:40-16:00	*Development and studies of Polyethylene-B4C concretes at ESS*	Ken Andersen, ESS
16:00-16:20	**Coffee break**	
16:20-16:40	*Studies of material composition and neutron activation*	Eszter Dian, MTA-EK
16:40-17:00	*Simulati*[redacted]	
17:00-17:20	*Simulati*[redacted]	

***This pr*[redacted]**
***progran*[redacted]**

Holiday Inn St. Petersburg, Russia, June 29th 2019

- Saturday before ECNS

Have held ~ 5 spots if anyone more from SINE wants to join!? Please let me know! (link)

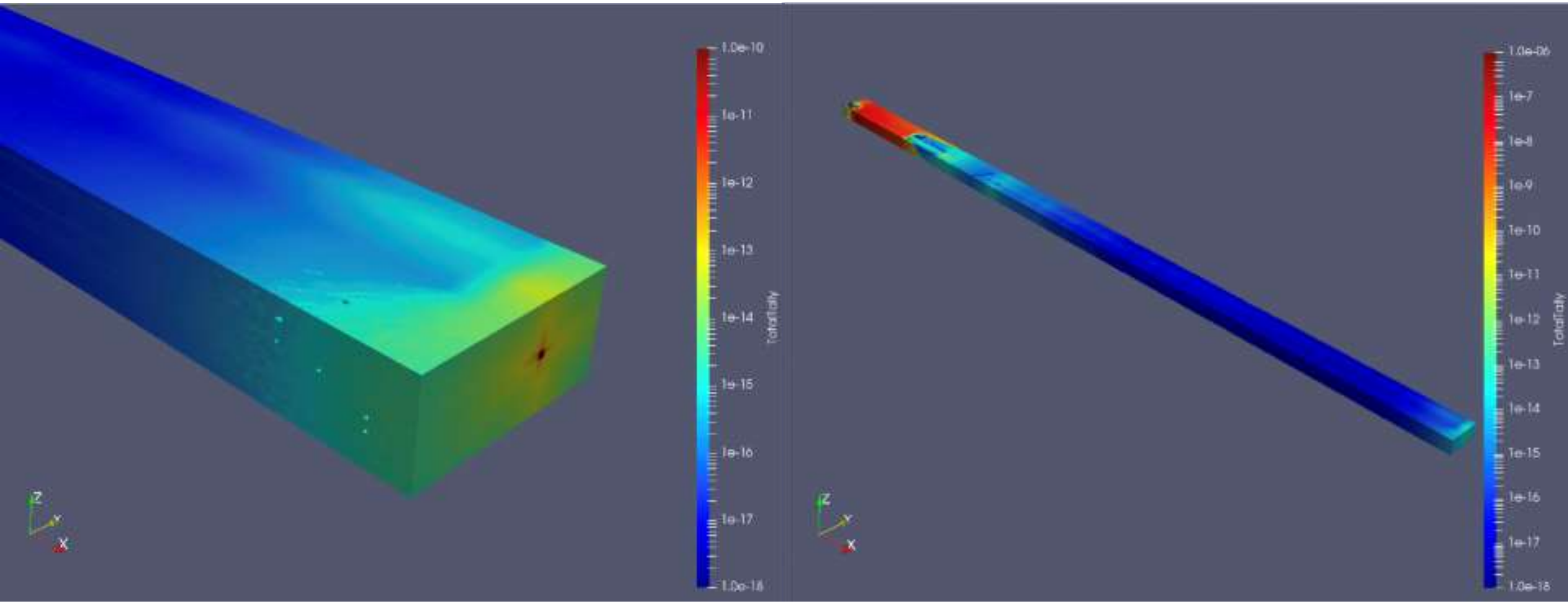
25 participants, half are not from WP

- Fullfils WP8 MS5+MS6

2. Work carried out: D8.3 Computational tests, multiple platforms

This project is funded by the European Union (GA no. 654000)

Optimisation of super-mirror patch to MCNP(X)[1], now allows both MPI[2] and use of DxTran[3] sphere variance reduction, allowing “deterministic transport” of both reflected and non-reflected intensity



This project is funded by the European Union (GA no. 654000)

[1]F. Gallmeier ORNL, U. Filges PSI - original patch to MCNPX 2.5, Esben Klinkby MCNPX 2.7,

[2]Ryan Bergmann, Emmanouela Rantsiou PSI, stable use of Message Passing Interface parallelisation for MCNPX

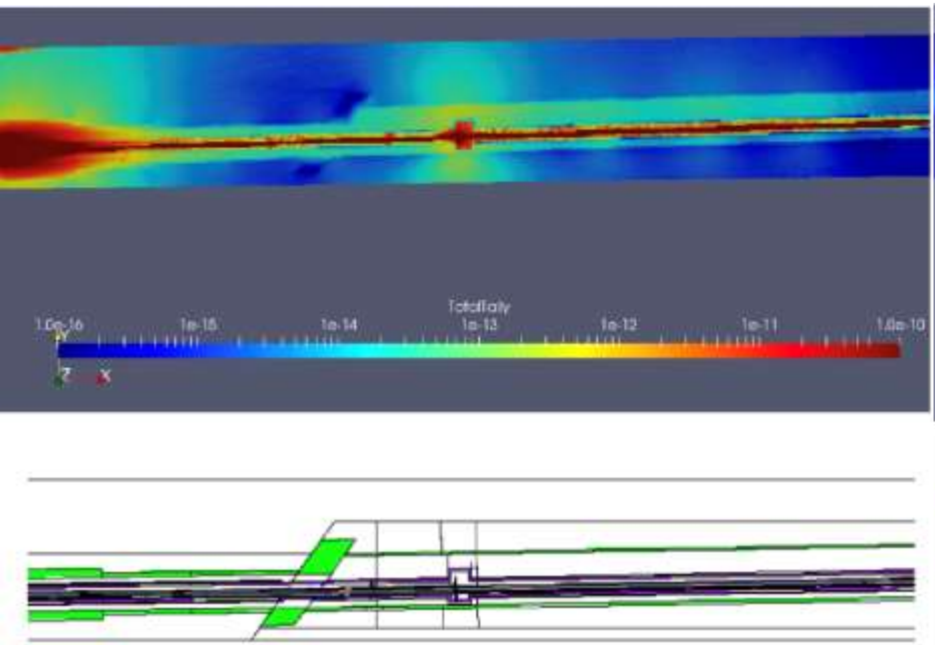
[3]Ryan Bergmann, Mguel Magán ESS-Bilbao, improved patch allowing use of variance reduction, i.e. definition of geometrical “area of interest” along / at end of guide for MCNP 6/6.1/6.2

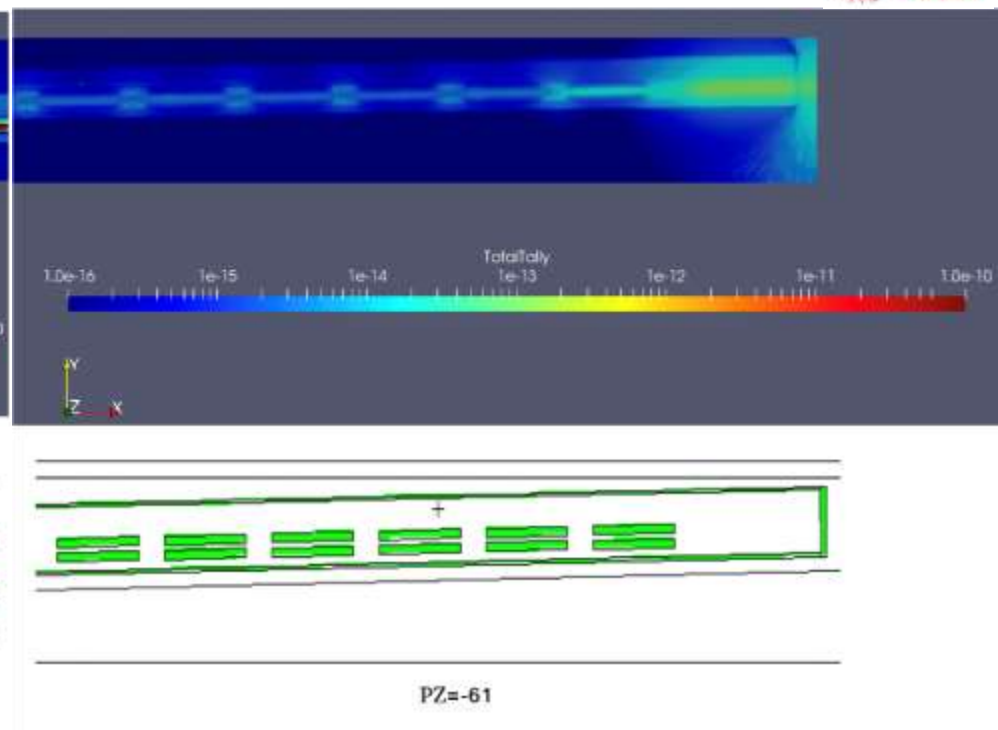
This project is funded by the European Union (GA no. 654000)

2. Work carried out: D8.3 Computational tests, multiple platforms

This project is funded by the European Union (GA no. 654000)

Optimisation of super-mirror patch to MCNP, now allows both MPI and use of DxTran sphere variance reduction, allowing "deterministic transport" of both reflected and non-reflected intensity





This project is funded by the European Union (GA no. 654000)

- Developed solution agrees very well with legacy implementation in MCNPX
- Initial assessment shows 80% speedup of shielding calculations near end of MIRACLES guide
- We have contacted the MCNP team at LANL to enquire about the legal / license terms under which the patch could be distributed

2. Work carried out: D8.8 Port of selected scattering kernels from McStas to SIMRES

DTU

By use of MCPL input / output (see D8.2), we have implemented wrapper-instruments of the McStas components

- PowderN (Debye-Scherrer cones)
- Single_crystal (bragg spots, multiple scattering, secondary extinction…) • Isotropic_Sqw (Inelastic scattering from isotropic materials) - further components e.g. for SANS are in the pipe.

This project is funded by the European Union (GA no. 654000)

All
parameters and
inputs
are retained and
as
standard in McStas

Example

2. Work carried out: D8.8 Port of selected scattering kernels from McStas to SIMRES

By use of MCPL input / output (see D8.2), we have implemented wrapper-instruments of the McStas components

- PowderN (Debye-Scherrer cones)

This project is funded by the European Union (GA no. 654000)

- Single_crystal (bragg spots, multiple scattering, secondary extinction…) • Isotropic_Sqw (Inelastic scattering from isotropic materials) - further components e.g. for SANS are in the pipe.

All parameters and inputs are retained and as standard in McStas

The resulting executables can be used transparently from within SIMRES, and next official SIMRES release will include MCPL support, plus these McStas plugins.

Example

This project is funded by the European Union (GA no. 654000)

2. Work carried out: D8.12 Software documentation and report on combined RESTRAX + McStas simulations

Why combine RESTRAX + McStas?

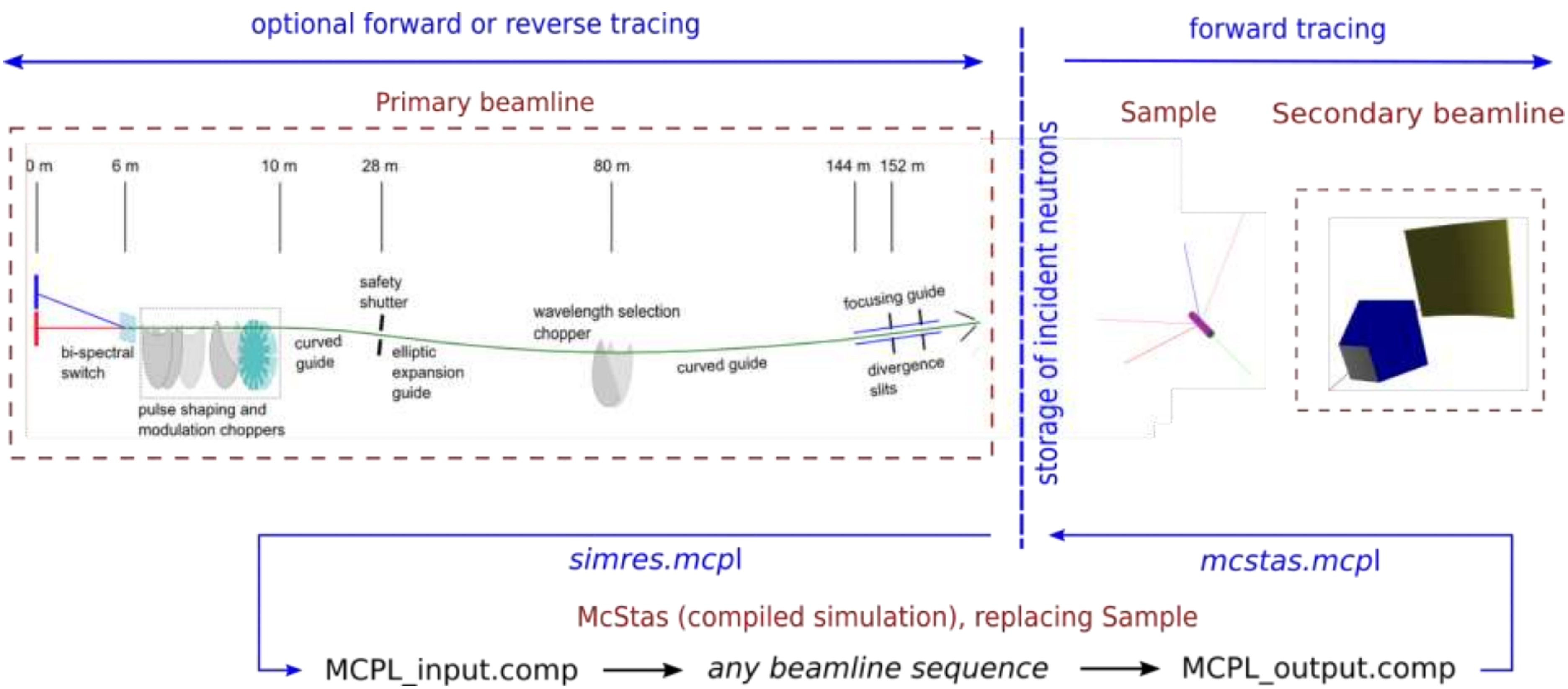
- Independent code validation by performing inter-comparison tests
- Complementarity: Each package includes unique features and models not available in the other two.
- Performance options: For example, efficient sampling strategy allowing fast simulations at a single CPU in SIMRES, versus highly configurable programming environment which is paid off by slower simulations in McStas.

This project is funded by the European Union (GA no. 654000)

2. Work carried out: D8.12 Software documentation and report on combined RESTRAX + McStas simulations

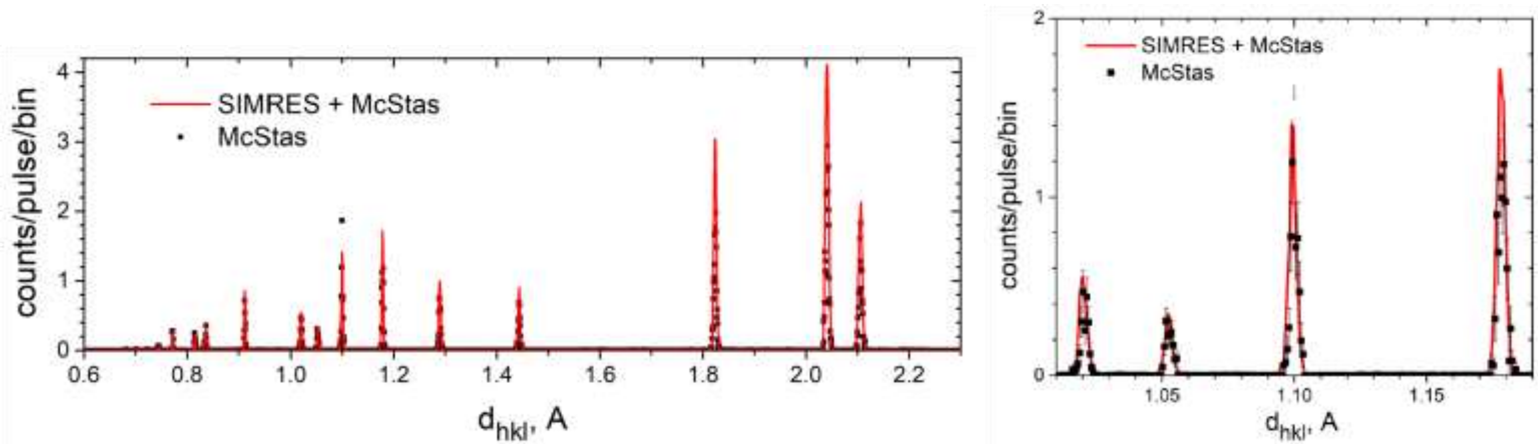
This project is funded by the European Union (GA no. 654000)

Case study: BEER@ESS



This project is funded by the European Union (GA no. 654000)

2. Work carried out: D8.12 Software documentation and report on combined RESTRAX + McStas simulations



Case study: BEER@ESS

This project is funded by the European Union (GA no. 654000)

2. Work carried out: D8.12 Software documentation and report combined RESTRAX + McStas simulations

Figure 2. Diffractograms simulated by the combined SIMRES+McStas ray-tracing (red line) and by McStas only (black points).The detail on the right permits to assess differences, which are within the statistical errors.

Table 1. Comparison of computing times and statistical errors for the primary beam intensity.

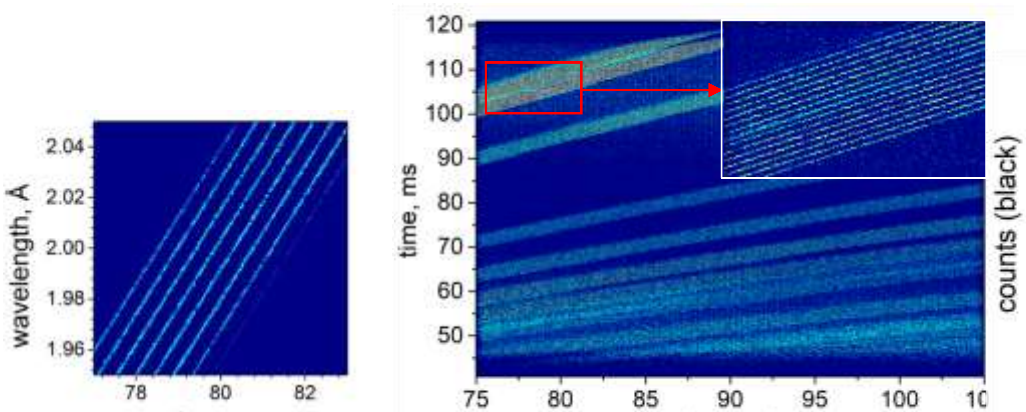
	Rel. error (primary beam)	Computing time
SIMRES + McStas 1.1 % 56 s		

McStas 1.8 % 1110 s

Substantial speed gain!

This project is funded by the European Union (GA no. 654000)

Case study: BEER@ESS



b)

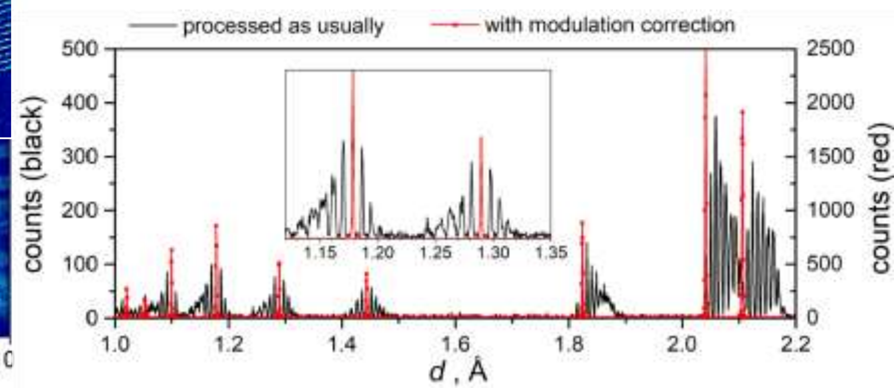


Figure 3. (a) Modulated beam structure at the primary slit – SIMRES MCPL output passed to McStas. (b) ToF – 2q map of events registered by the detector component (`NPI_tof_theta_monitor.comp`) in McStas; multiplexed diffraction lines from the duplex steel sample (`PowderN.comp`).

a)

This project is funded by the European Union (GA no. 654000)

Figure 4. Diffractogram produced by the McStas component `NPI_tof_dhkl_detector` with the [redacted]ed off (black, left scale) and on (red, right scale).

This project is funded by the European Union (GA no. 654000)

2. Work carried out: D8.12 Software documentation and report on combined RESTRAX + McStas simulations

Case study: BEER@ESS

Takes advantage of
- Flexibility in McStas-based samples, newly developed combined PowderN-SANS sample

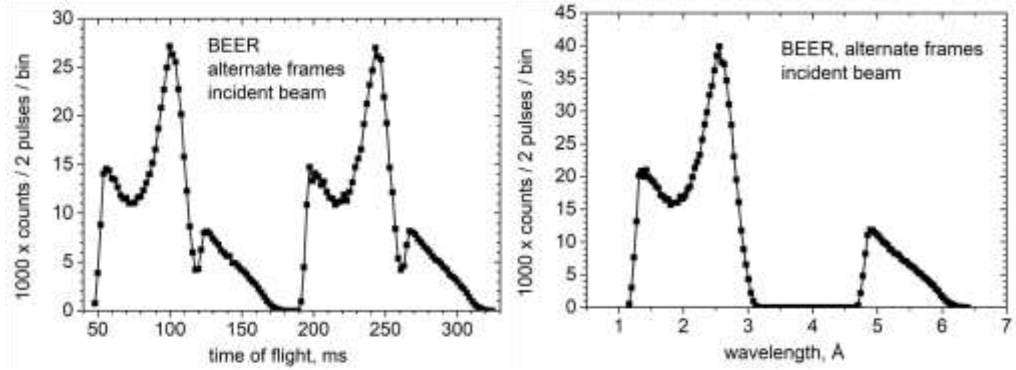


Figure 7. Time structure (left) and spectrum (right) of the primary beam simulated by SIMRES for BEER in the alternating frame mode. It was used as MCPL input to the subsequent McStas simulation of the sample and secondary beamline (see Figure 8).

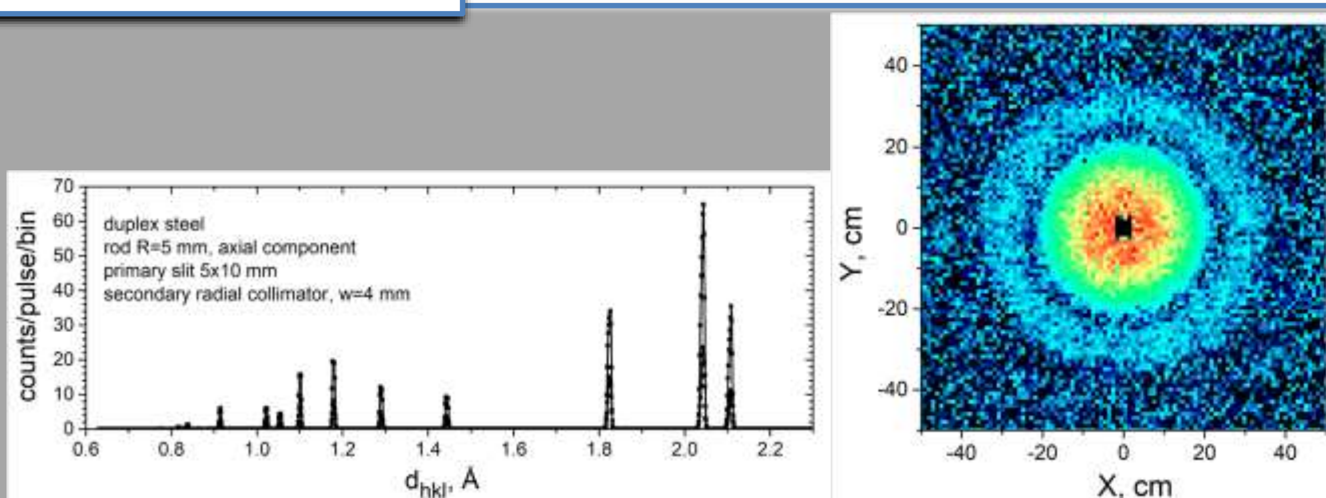


Figure 8. Diffractogram and SANS pattern “measured’ simultaneously on the same sample- output of the McStas simulation of the secondary beam.

This project is funded by the European Union (GA no. 654000)

2. Work carried out: D8.10 Several background measurement series at different facilities in Europe

Background measurements at spallation source SINQ@PSI and small research reactor AKR-2@TU Dresden

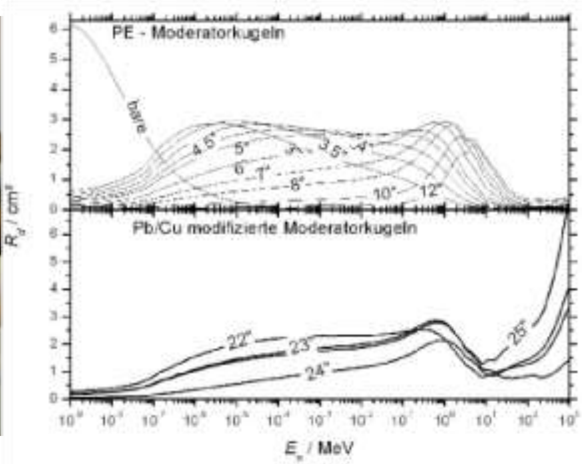
Two very different types of facilities

This project is funded by the European Union (GA no. 654000)

Systematic use of the enhanced Bonner Sphere Spectrometer (BSS)

SINE2020-developed BSS-system with PE moderators, Cu and Pb shells

Temperature controlled heading and cooling
(at least 3-4 times per sphere)



This project is funded by the European Union (GA no. 654000)

Range -> ~5 GeV!

2. Work carried out: D8.10 Several background measurement series at different facilities in Europe

PSI measurements & simulations

Setup in the middle position 2

SINQ neutron guide bunker with the three measurement position

This project is funded by the European Union (GA no. 654000)

The agreement between simulations and measurement is very good. The small differences in the thermal region could be scattering effects which are not fully implemented in the MCNPX model.

2. Work carried out: D8.10 Several background measurement series at different facilities in Europe

AKR-2 measurements & simulations

This project is funded by the European Union (GA no. 654000)

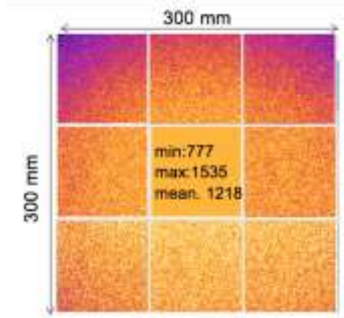
Cross section of the reactor setup and the two measurement positions

Measurement setup at position A

Measurements and Simulations for Position A

[redacted]ion A, as the

[redacted]al Neutron



flux distribution requires more

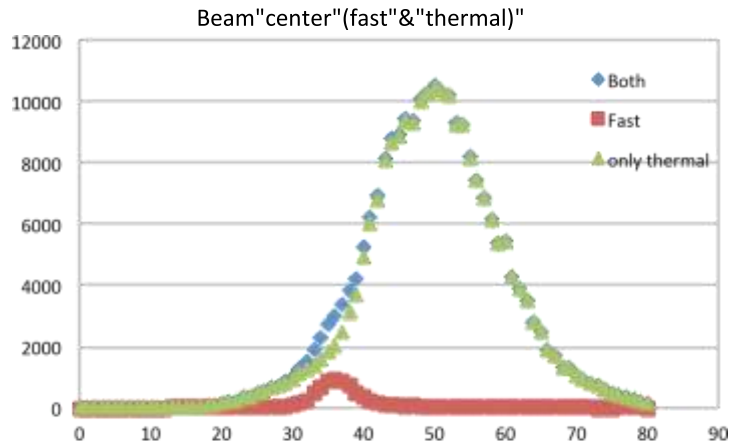
2. Work carried out: D8.14 Investigation of effective shielding concepts for high energy particles

Use of the BSS spectrometer with BOA@PSI

BSS-system with PE moderators and Cu shells

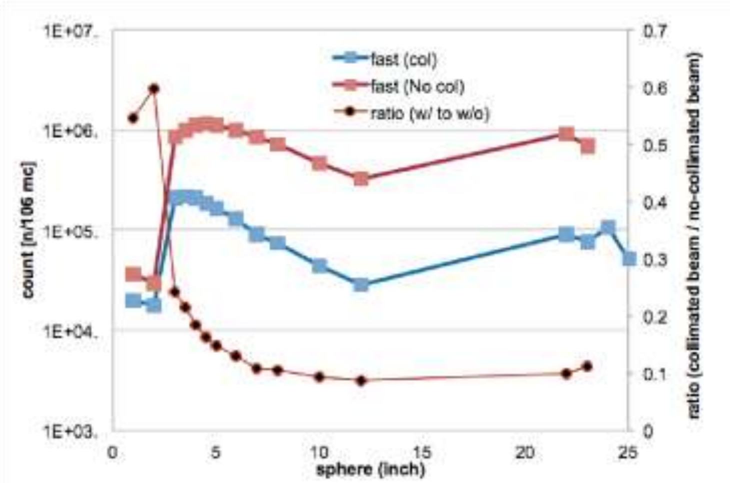
BOA beamline

This project is funded by the European Union (GA no. 654000)



Fast and thermal neutron flux distribution at the BOA beamline

This project is funded by the European Union (GA no. 654000)

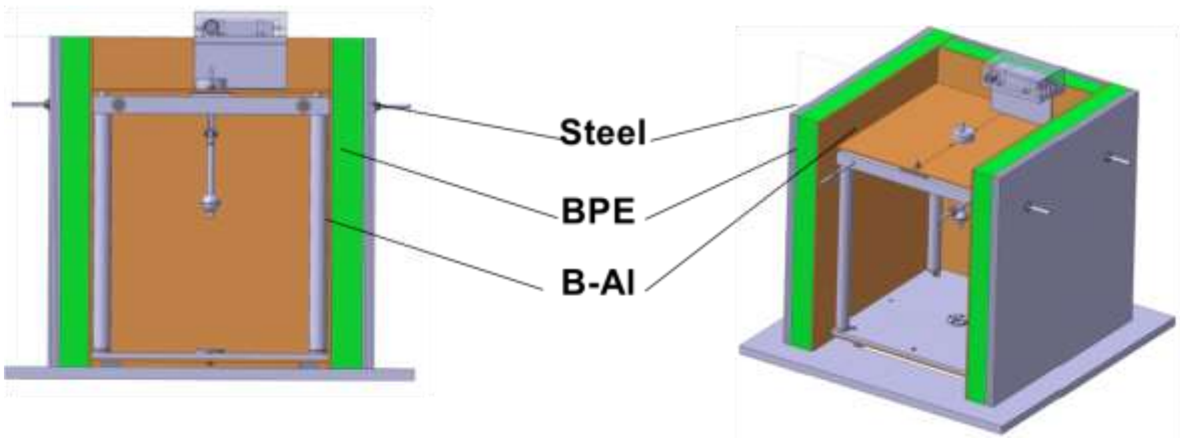


BOA – Fast neutron spectrum measured by the BSS system

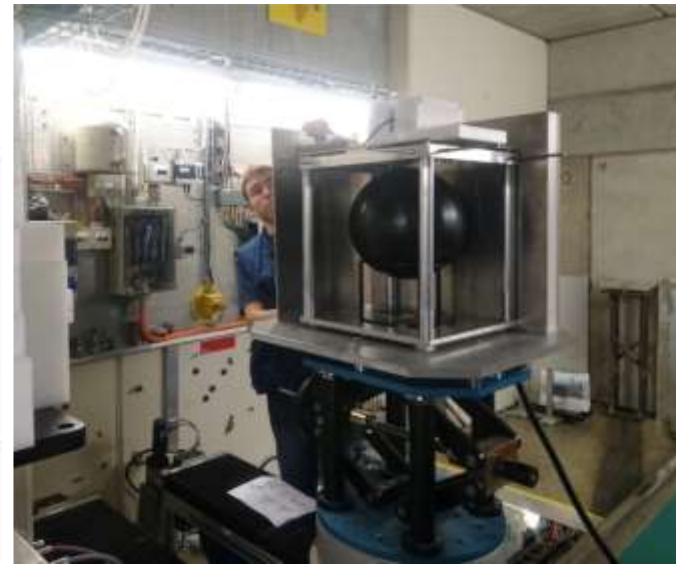
This project is funded by the European Union (GA no. 654000)

2. Work carried out: D8.14 Investigation of effective shielding concepts for high energy particles

Shielding-box setup



Shielding box for material investigations



Measurement setup at BOA beamline

[redacted]ifferent directions, e.g. sky-shine vs.

This project is funded by the European Union (GA no. 654000)

2. Work carried out: D8.14 Investigation of effective shielding concepts for high energy particles

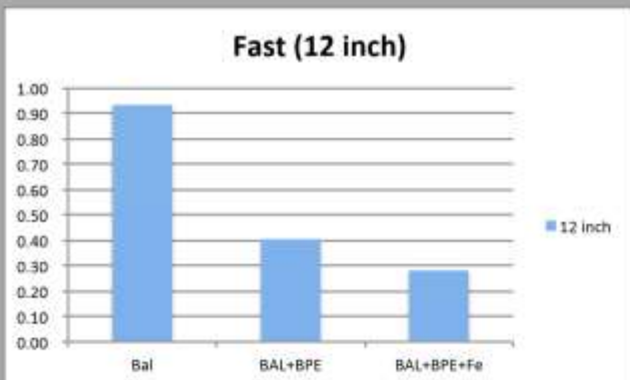


Figure 8a: Fast neutron transmission

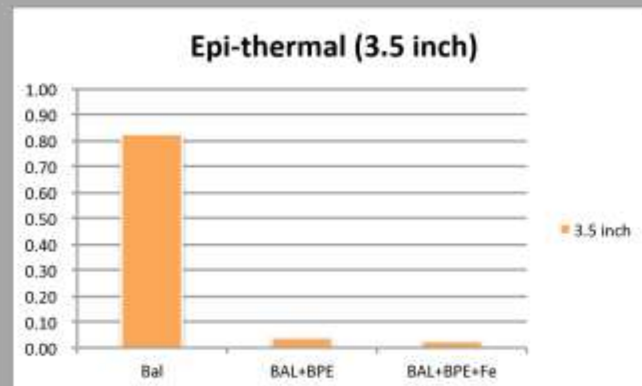
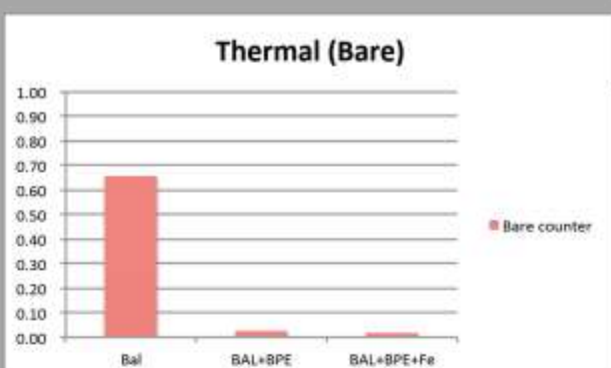
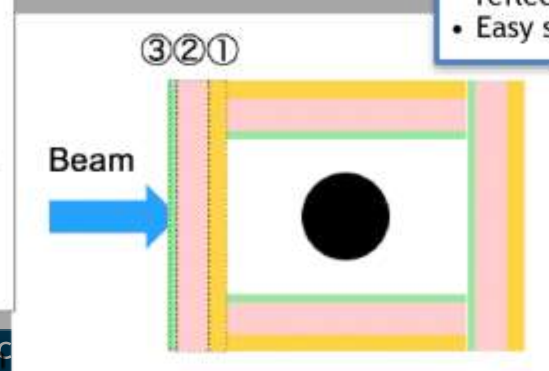


Figure 8b: Epi-thermal neutron transmission

Created for
- Easy decomposition of background from different directions, e.g. sky-shine vs. reflection from floor
- Easy setup/evaluation of laminar setups





1 Yellow is steel

2 Pink layer is B-PE

3 Green layer is BAl

Figure 8c: Thermal neutron transmission

This projec… no.

2. Work carried out: D8.15 Recommendations for ESS instruments

Owes much to the work of D8.7

- Compact Neutron Spin Echo Spectrometer
- Compact SEMSANS add-on for SANS and Imaging

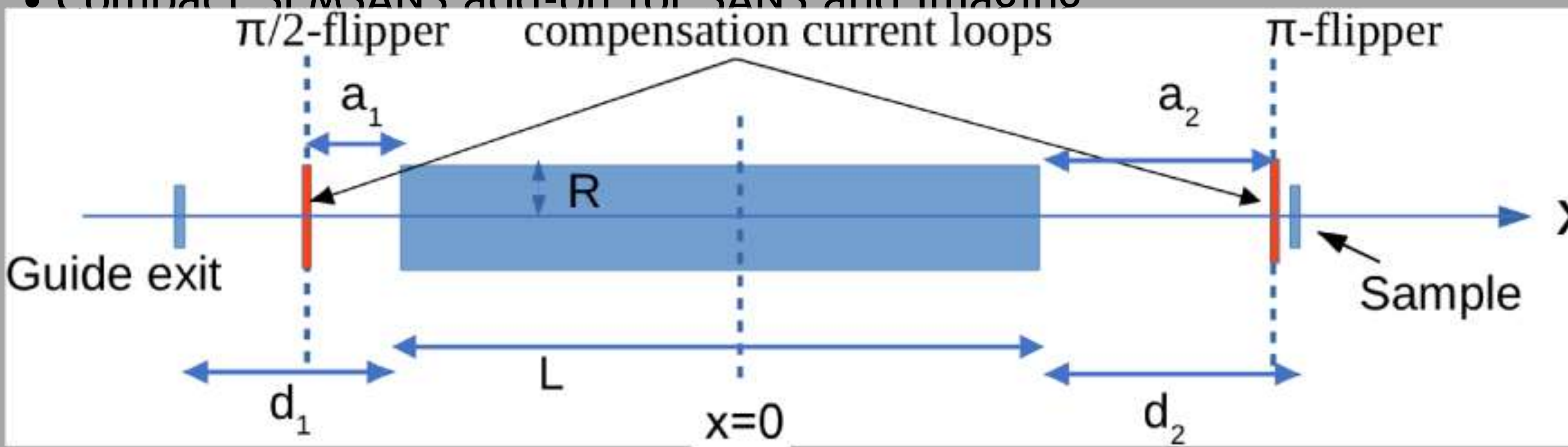


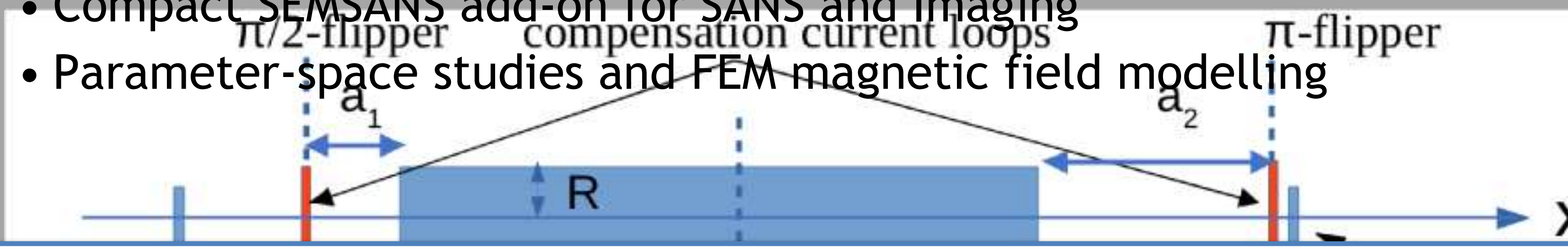
Fig. 1: Schematic representation of the configuration considered for the first arm of a NSE spectrometer. The layout is characterized by the lengths $0, 4_{/}, 4_2$ *and* 1*. The blue rectangular area represents the main precession coil.*

This project is funded by the European Union (GA no. 654000)

2. Work carried out: D8.15 Recommendations for ESS instruments

Owes much to the work of D8.7

- Compact Neutron Spin Echo Spectrometer
- Compact SEMSANS add-on for SANS and Imaging
- Parameter-space studies and FEM magnetic field modelling



The results [1,2] show that there is a clear gain with the “pancake moderator” beams. Indeed, rectangular beam cross-sections with a height over width ratio, e.g. 1:4, that mimic the ESS “pancake moderator” beams lead to the best results, and improve the homogeneity of the magnetic field integrals by at least 30 %. On the other hand, because relative inhomogeneities become worse for shorter coils, in order to reach high resolution, i.e. long Fourier times, the length of the instruments *Fig. 1: Schematic representation of the configuration considered for the first arm of a NSE spectrometer. The* cannot be reduced. *layout is characterized by the lengths* Consequently, NSE

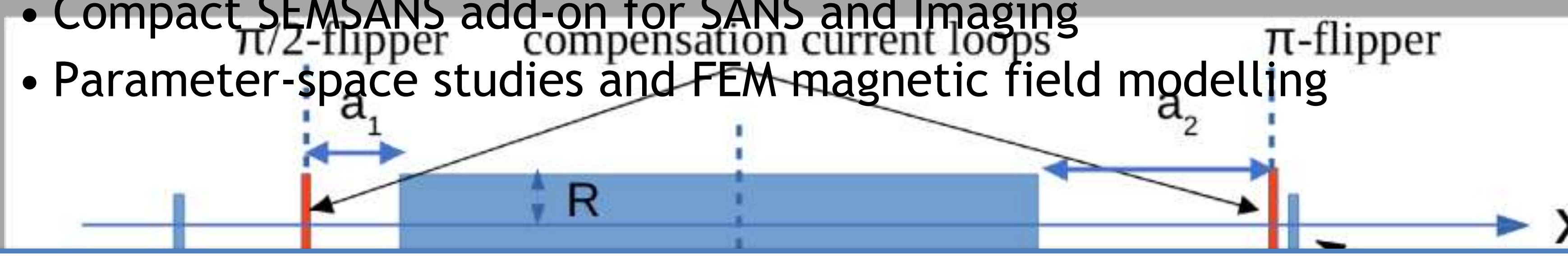
This project is funded by the European Union (GA no. 654000)

spectrometer0, 4/, 42 *and* 1. *The blue rectangular area represents the main* s will perform better at the ESS, as the required magnetic f*precession coil.*ield integral corrections (through Fresnel coils) will be weaker, but they will not be more compact than e.g. at the ILL or FRM2.

2. Work carried out: D8.15 Recommendations for ESS instruments

Owes much to the work of D8.7

- Compact Neutron Spin Echo Spectrometer
- Compact SEMSANS add-on for SANS and Imaging
- Parameter-space studies and FEM magnetic field modelling



The results [1,2] show that there is a clear gain with the "pancake moderator" beams. Indeed, rectangular beam cross-sections with a height over width ratio, e.g. 1:4, that mimic the ESS "pancake moderator" beams lead to the best results, and improve the homogeneity of the magnetic field integrals by at least 30 %. On the other hand, because relative inhomogeneities become worse for shorter coils, in order to reach high resolution, i.e. long Fourier times, the length of the instruments *Fig. 1: Schematic representation of the configuration considered for the first arm of a NSE spectrometer. The* cannot be reduced. *layout is characterized by the lengths* Consequently, NSE spectrometer$0, 4_/, 4_2$ *and* 1. *The blue rectangular area represents the main* s will perform better at the ESS, as the required magnetic f*precession coil.*ield integral corrections (through Fresnel coils) will be An IN15-like instrument will weaker, but they will not be more

compact than e.g. at the ILL or FRM2.

have gain in resolution at the ESS

This project is funded by the European Union (GA no. 654000)

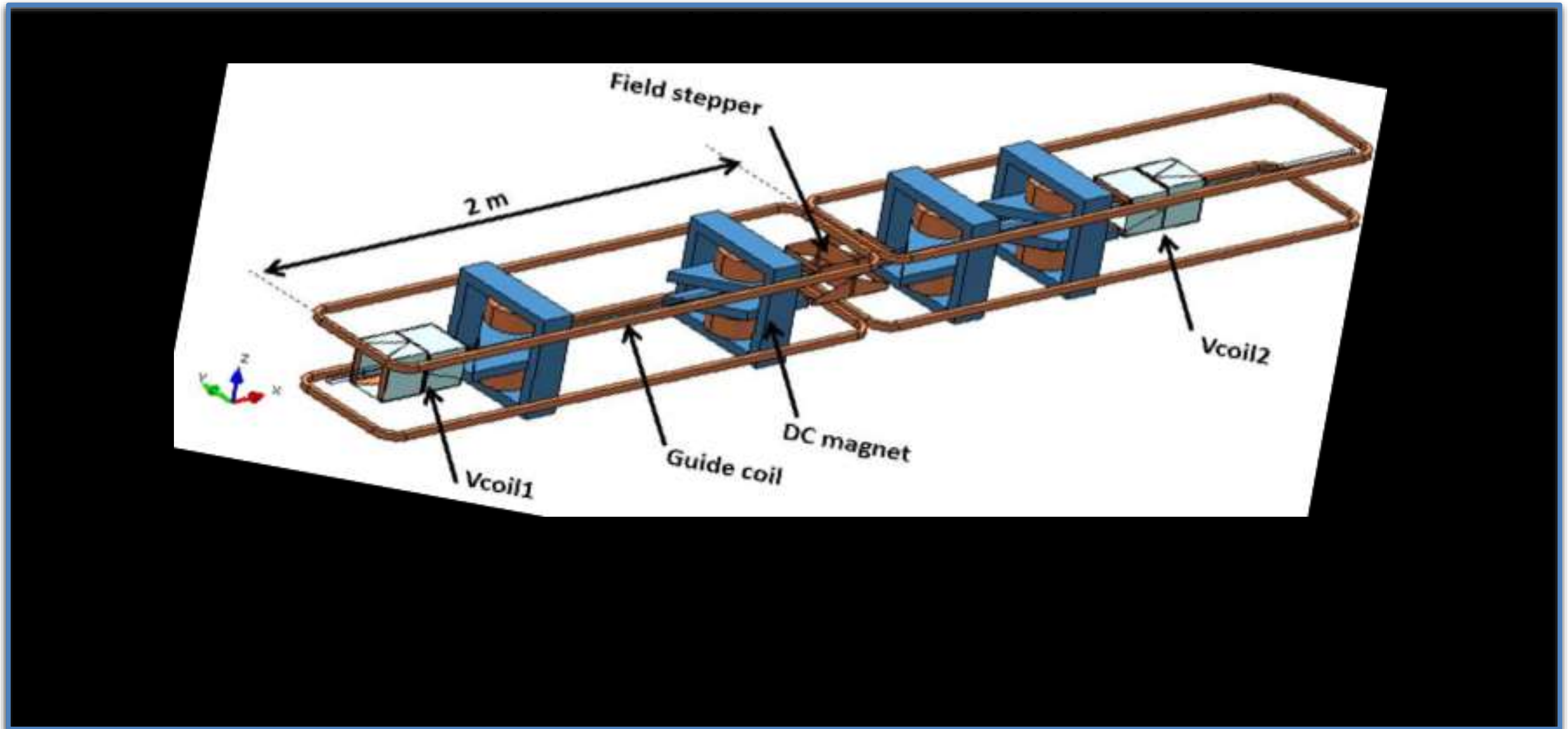
2. Work carried out: D8.15 Recommendations for ESS instruments

field, which guides the beam polarisation.

This project is funded by the European Union (GA no. 654000)

Owes much to the work of D8.7

- Compact SEMSANS add-on for SANS and Imaging



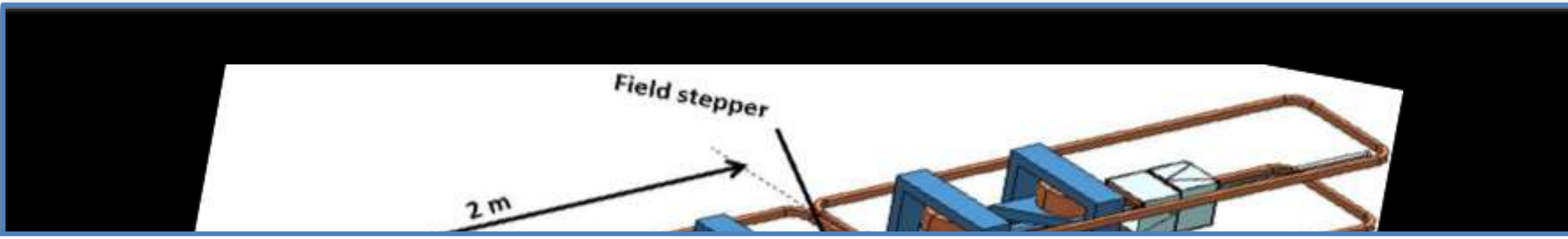
field, which guides the beam polarisation.

This project is funded by the European Union (GA no. 654000)

2. Work carried out: D8.15 Recommendations for ESS instruments

Owes much to the work of D8.7

- Compact SEMSANS add-on for SANS and Imaging



The results show that one can change the dimensions while keeping the optimised [x,z,y] ratios for the components. For the setup investigated, this implies that when considering the beam geometry of the ESS pancake moderators, the overall length can be reduced from 3.1 m to 1.1 m, which can be considered as the minimal length for such an add-on setup. Such a compact design could be easily implemented as an add-on. It could be installed and removed, according to the experimental requirements and would substantially extend the capabilities of the ESS. A possible host instrume nt would be the polarised *Figure 2: Schematic drawing of* neutron *SEMSANS* SANS*a*,*rrangeme* SKADI, *nt* where *considered for the* the add-on*magnetic* would *field calculations*allow simultaneously SA*. The white* NS and SE*box*MSANS*es illustrate* measurements. Another host instrument candidate is the neutron imaging instrume *the Vcoils, which act as π/2 flippers, the blue components are DC magnets with parallelogram* nt ODIN, *shaped pole shoes, the central coil is a field ste*where the add-on could be used for*pper* high resolution dark field imaging*. The long upper and lower create a homog* [4]. *enous magnetic*

2. Work carried out: D8.15 Recommendations for ESS instruments

Owes much to the work of D8.7

- Compact SEMSANS add-on for SANS and Imaging
- Parameter-space studies and FEM magnetic field modelling

field, which guides the beam polarisation.

This project is funded by the European Union (GA no. 654000)

The results show that one can change the dimensions while keeping the optimised [x,z,y] ratios for the components. For the setup investigated, this implies that when considering the beam geometry of the ESS pancake moderators, the overall length can be reduced from 3.1 m to 1.1 m, which can be considered as the minimal length for such an add-on setup. Such a compact design could be easily implemented as an add-on. It could be installed and removed, according to the experimental requirements and would substantially extend the capabilities of the ESS. A possible host instrume nt would be the polarised *Figure 2: Schematic drawing of* neutron *SEMSANS* SANS*a,rrangeme* SKADI, *nt* where *considered for the* the add-on*magnetic* would *field calculations*allow simultaneously SA*. The white* NS and SE*box*MSANS*es illustrate* measurements. Another host instrument candidat *the Vcoils, which act as π/2*

[redacted] *with parallelogram* Only practically applicable nstrument

ODIN, *shaped pole shoes, the central coil is a field ste*where the add-on could be used for*pper* high resolution dark f*. The long upper and lower* ield imagingdark-field me*create a homo* [4].*genous*thod for ESS, b *magnetic* y

synchronising the fields with the source pulse

field, which guides the beam polarisation.

This project is funded by the European Union (GA no. 654000)

Delays 1

- Delays: Have now caught up with those from last GA…

*+@	&# " /!	*48 ;%		
*+@	/$! !! & 242GR F !"" !"	2 &		
*+@	;&D! " /!" " "(,9! ! F !"F,G	*48 2 &		
*+@	# "(!/ // # "% (&"/%(% (&! "	2 &		
*+@	2 !"			

	/ " "	+4	[redacted]	8 neeting			Reason: Essentially other project obligations.

show good progress!

WP8 Instrumenta ls – P

Both expected around ISTSI workshop

Delays 2

- Delays: Have now caught up with those from last GA…

Status summary

D8.16	Activation studies, radiation resistance	16 - MTA EK	Report	Public	36
D8.17	Investigation of different test samples	3 - STFC	Report	Public	42
D8.18	Comparative Vitess+MCNP simulations	16 - MTA EK	Report	Public	46
D8.19	Validation of the measurements by Monte Carlo Simulations	15 - ESS-B	Report	Public	48
D8.20	Final release of all software	13 - DTU	Other	Public	48

Reason:

Essentially other project obligations, focus on scientific paper vs. deliverable report.

Expected around ISTSI workshop

= incoming / being written up

[redacted]

Remaining 1

D8.16	Activation studies, radiation resistance	16 - MTA EK	Report	Public	36
D8.17	Investigation of different test samples	3 - STFC	Report	Public	42
D8.18	Comparative Vitess+MCNP simulations	16 - MTA EK	Report	Public	46
D8.19	Validation of the measurements by Monte Carlo Simulations	15 - ESS-B	Report	Public	48
D8.20	Final release of all software	13 - DTU	Other	Public	48

Experiment scheduled for mid-June at ISIS. PSI and ESS-Bilbao in close contact on data-evaluation and simulation

Remaining 2

D8.16	Activation studies, radiation resistance	16 - MTA EK	Report	Public	36
D8.17	Investigation of different test samples	3 - STFC	Report	Public	42
D8.18	Comparative Vitess+MCNP simulations	16 - MTA EK	Report	Public	46
D8.19	Validation of the measurements by Monte Carlo Simulations	15 - ESS-B	Report	Public	48
D8.20	Final release of all software	13 - DTU	Other	Public	48

Wigner staff on track but not at this WP meeting. Will try to get them to **contribute talk and paper** in connection with **ISTSI**

Remaining 3

README.md

SINE2020WP8

Repository for software and methods and publications developed in WP8 under the EU SINE2020 project

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 654000

For more information, please visit the SINE2020 website at https://www.sine2020.eu

D8.1					
D8.1					
D8.1					
D8.1					
D8.20	Final release of all software	13 - DTU	Other	Public	48

Population of GitHub repository in progress:
https://github.com/McStasMcXtrace/SINE2020WP8

Impact

- General WP goals:

  - Improving understanding signal-to-noise
  - **Availability of well-documented software tools and methods**

  - Background from high-energy neutrons, challenge for ESS
  - **Bonner sphere spectrometer**
    - **New material solutions: B-PE, Epument cast, laminar shielding**

  - Investigation of Larmor methods at ESS
  - **Well-investigated parameter space**
    - **SE and SEMSANS concepts devised for use at ESS, promising “IN15 type”, compact SEMSANS add-on for SKADI and dark-field imaging at ODIN** WP8 will pave the way for **optimised use of ESS**.

Applications **beyond** neutron community: ✓

- MCPL utilisation in other scientific disciplines, e.g. in *cosmogenics and †plasma physics
- Bonner-sphere spectrometer in use in accelerator physics and nuclear waste storage

*cosmogenics == use of radionuclides produced in-situ by cosmic rays, earth surface science †A. S. Richardson, et al. Phys. Rev. Accel. Beams 22, 050401

KPI values - and current aims…

- KPI data overview

		Coimbra 2016	ICANS 2017	Other events*	Current sum	ISTSI 2019	… project aim
8 - Instrumentation E-tools	Number of presentations (poster, oral)	0+8	2+5	3+7	25	17	30
	Number of publications	1	2	3	6	16-17?	8-10
	Number of workshop participants	15	10	100	125	28	all > 10

- We should
  - Get current / incoming results written up

*McStas schools at ISIS, ORNL, CSNS, MDANSE2018, …

Questions?