SINE2020 GA

Parma, June 6th 2018

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,
Technical University of Denmark

Explanations of the work carried out

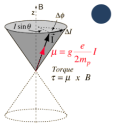
1. WP structure and objectives
2. Overview of work carried out so far
3. Highlights from the WP
4. KPI status and delays

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 WP

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

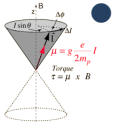
Improve
"cradle to grave" instrument-modeling capability beyond state of the art:

neutronics + ray-tracing → signal / noise

Science & Technology Facilities Council

- Task 8.2: Innovative Shielding Concepts and Materials

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



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

Conceptualise
and "develop" how Larmor labelling approaches can be used as "plug-in" technology at the ESS instruments, taking the above knowledge & methods into account

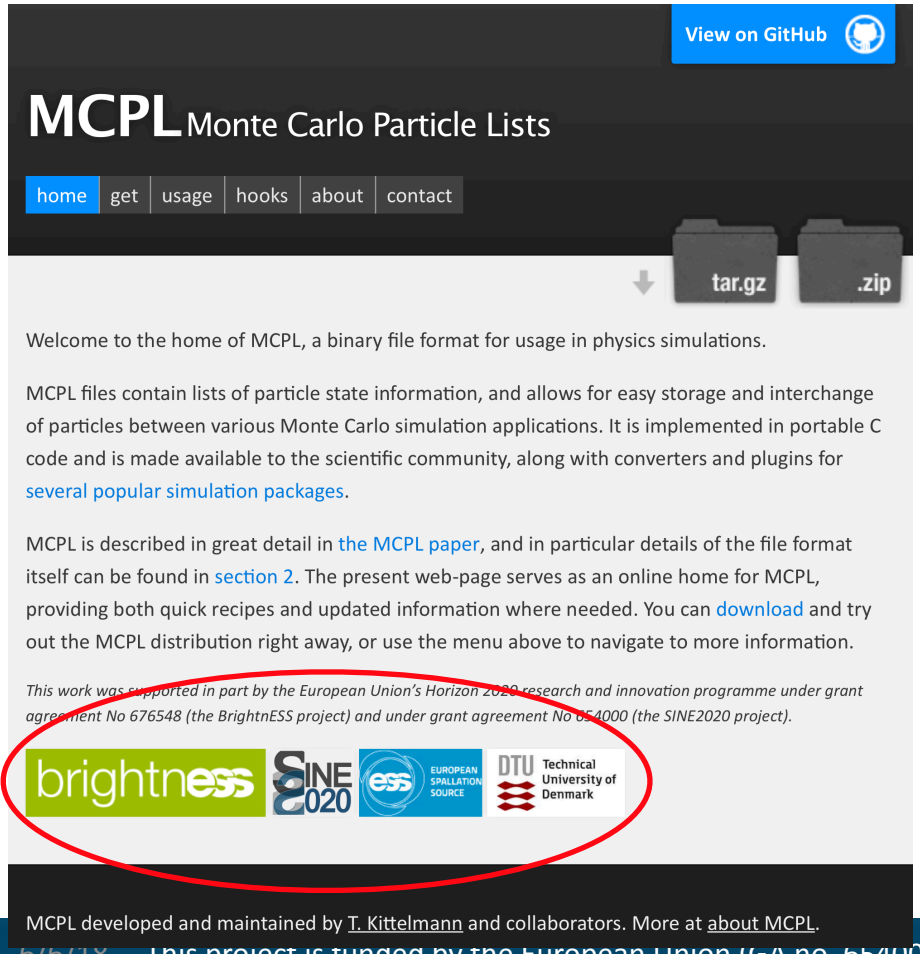
2. Work carried out - Task 8.1

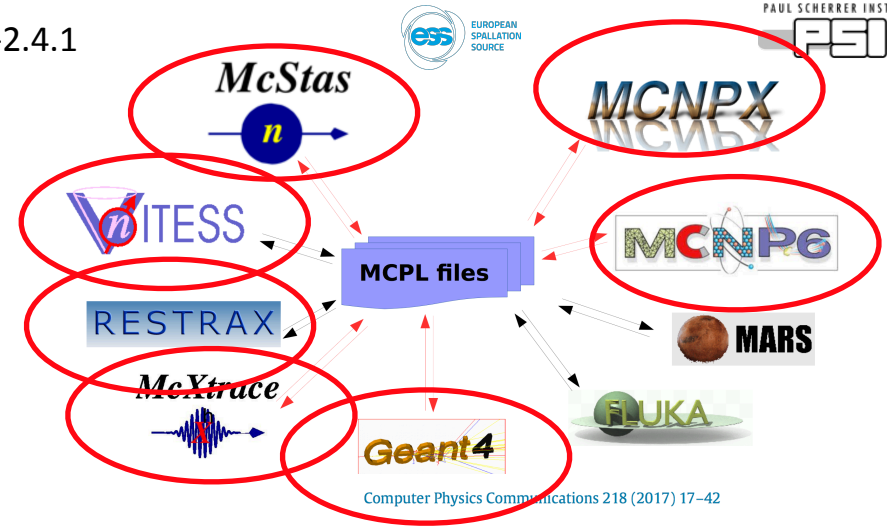
- Task 8.1: *E-tools for integrated simulation using neutronics and Monte Carlo ray-tracing*
  - *D8.2: Improved code interface, pre-release*
  - *MS2: Workshop: "Requirements/Development for a reverse Monte Carlo variance reduction method applied to neutron beamline transport systems".*
  - *D8.3: Computational tests*
  - *D8.4: Experimental test A - "BOA@PSI"& Experimental test B - "ChipIR@ISIS"*
  - *D8.8:Port of selected scattering kernel code from McStas to RESTRAX*
  - *D8.9: Improved description of materials for high-energy neutron transport*

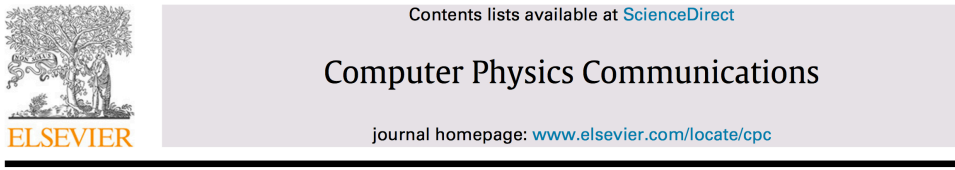
2. Work carried out - Task 8.1

- *D8.2: Improved code interface, pre-release*

https://mctools.github.io/mcpl and in McStas 2.3-2.4.1







Monte Carlo Particle Lists: MCPL☆

T. Kittelmann [a,*], E. Klinkby [b], E.B. Knudsen [c], P. Willendrup [c,a], X.X. Cai [a,b], K. Kanaki [a]
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[b] DTU Nutech, Technical University of Denmark, Denmark
[c] DTU Physics, Technical University of Denmark, Denmark

KPI #2

https://doi.org/10.1016/j.cpc.2017.04.012

D8.3 under way: (delayed from M18 - staff availability + scope change)

- Reformulated to include benchmarking of the WP8-developed tools against
  - Pure Geant4-based solution from D. DiJulio @ ESS
  - PHITS-based solution from J-PARC

Model Used

Previous studies used a very schematic neutron guide with basic shielding and no choppers. Also, we used a watts fission spectrum that provided a wide spectrum of neutrons, but did not have the cold/thermal part that is of interest in ESS and othe spallation sources. Therefore, we have switched to a more detailed model, that was used for preliminary MIRACLES calculations. This model includes the source kindly provided by D. DiJulio.

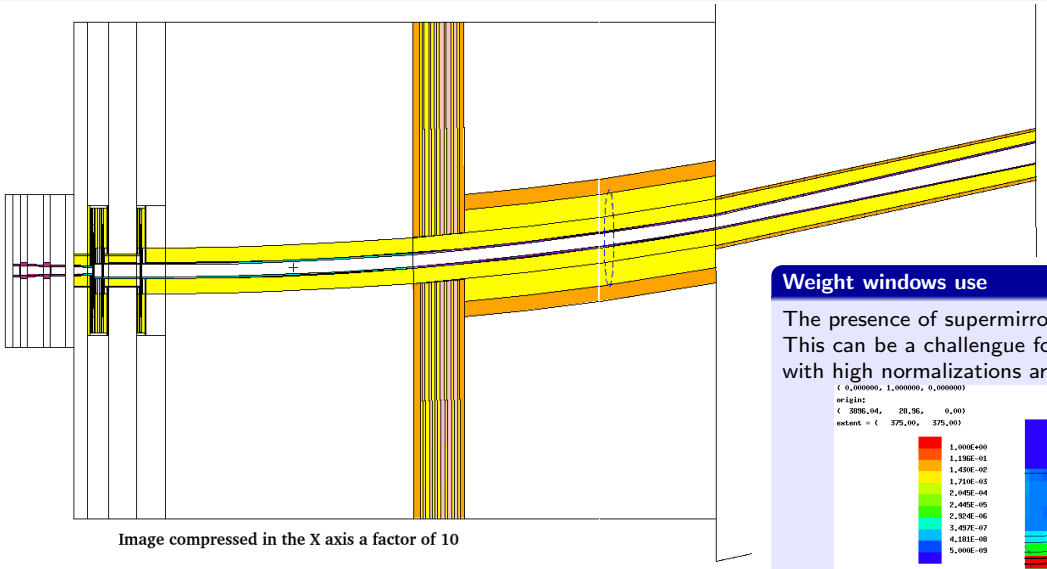
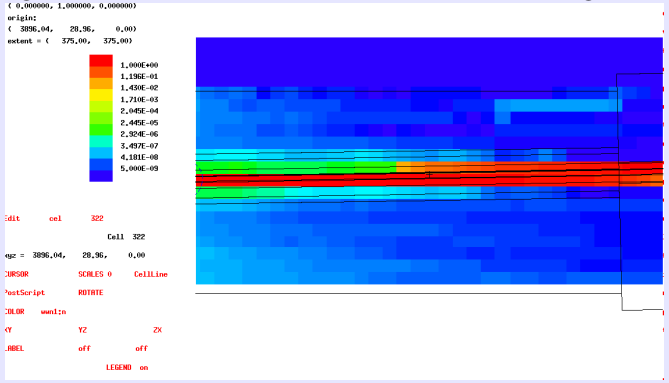


Image compressed in the X axis a factor of 10

Weight windows use

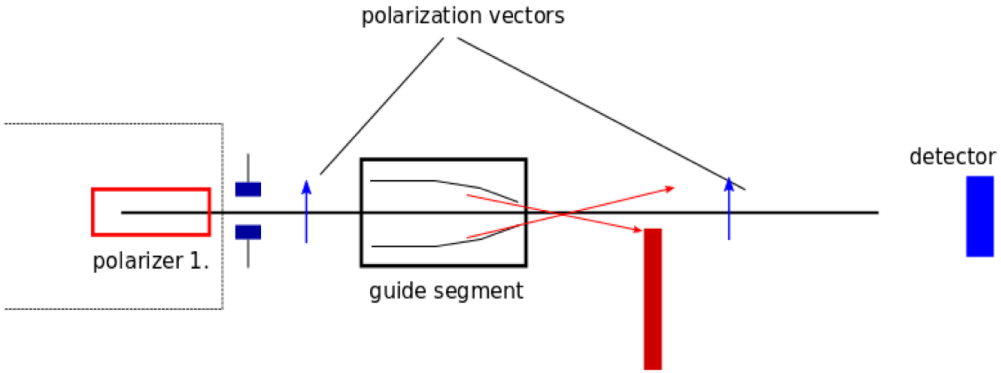
The presence of supermirrors causes, by design, very abrupt gradients at the edge of the guide. This can be a challengue for MAGIC-like methods. To mitigate this, agressive weight window with high normalizations are used to reduce the difference in weight between the guide and the rest.

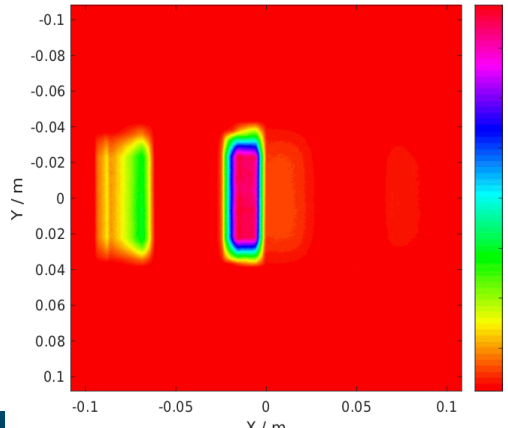


 This project is funded by the European Union (GA no. 6540

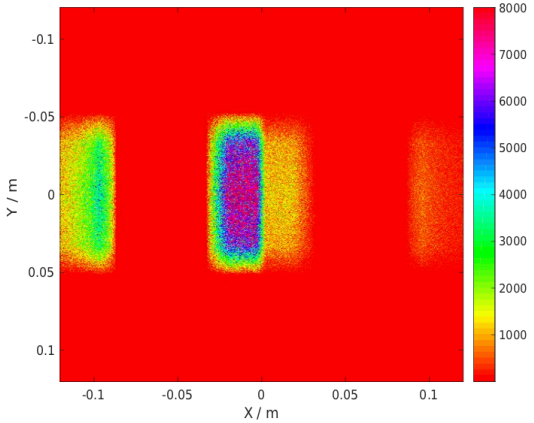
D8.4 report incoming: 2 benchmarking experiments @ BOA, PSI (delayed from M18, facility availability)

- Overall goal: take well curated data for simulation benchmarking
- BOA chosen since good models exist in McStas & MCNP
- Artificial background created by separating the beam and letting a part impinge on a steel rod.

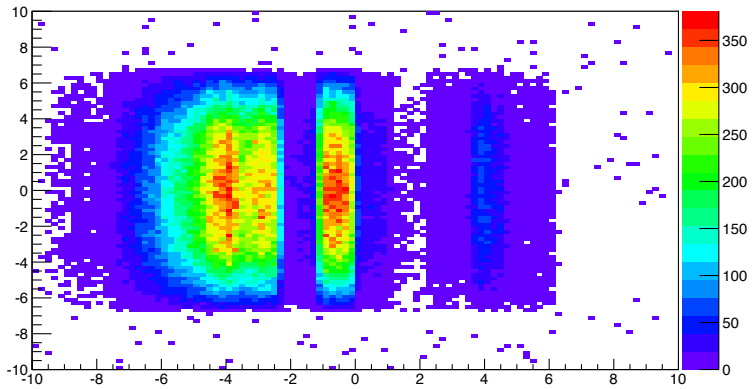




Experiment

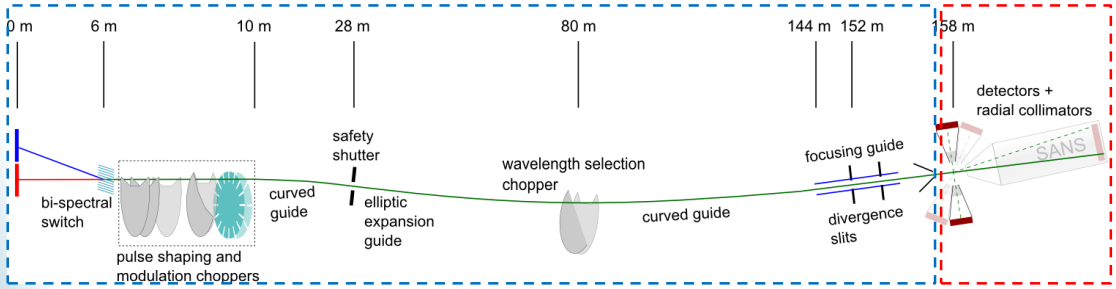


Simulation McStas



Simulation MCNP

Combined SIMRES + McStas simulations of BEER@ESS employing MCPL I/O

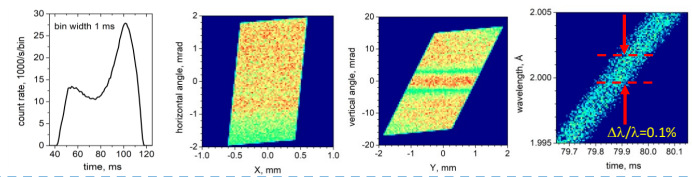


SIMRES

McStas

- Very high speed allowed by reverse tracing method and adaptive variance reduction.
- **Particularly useful for very small sampling volumes / high resolution**

Example: 1x2 mm^2 beam for *strain scanning*, single pulse, $\Delta\lambda/\lambda$ = 0.1%, bi-spectral source; computing time ~ 6 min/10^6 final events at 1 CPU



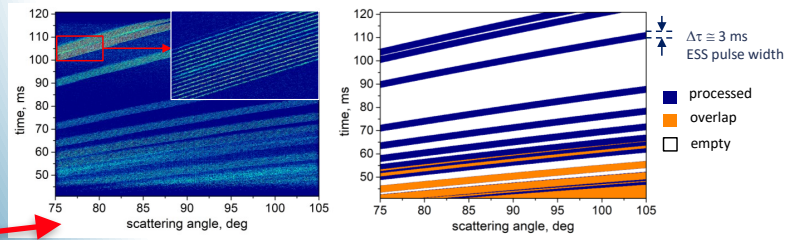
MCPL export

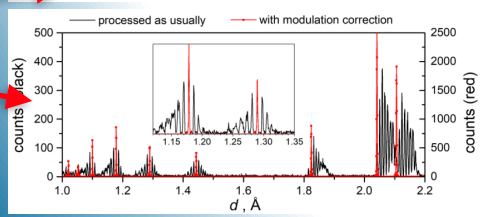
Combination-simulation based on reverse tracing in SIMRES and Powder sample from McStas allows efficient simulation of the BEER@ESS modulation mode

MCPL will be available in SIMRES v. 6.3.5

New component `tof_dhkl_detector.comp`
allows for **event based data reduction in modulation regime**

- Accounts for spatial and time resolution of the detector
- Performs conversion (x, y, time) -> (2θ, time) -> d_{hkl}
- Requires a list of expected peaks with d_{hkl} estimates:
  - Estimates the index of the nearest t_0 chopper window and corrects for its phase.
  - Excludes line overlaps and empty regions in (2θ, time) map





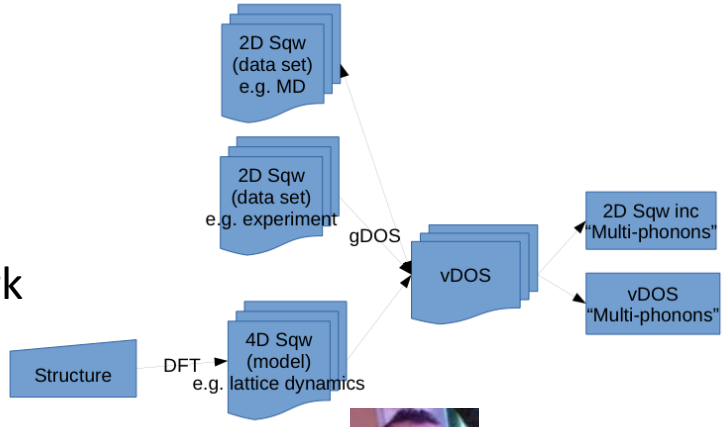
Accumulated diffractograms:

1. *assuming a single chopper window (blac*
2. *with account for the modulation (red)*

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

D8.9: *Improved description of materials for high-energy neutron transport*

- NDEF cross-section data well-known to be of limited reliability in the the meV range[1]
- Framework / algorithm devised to allow use of MD, DFT and experimental data for describing improved neutronic cross-sections (e.g. for MCNP 'scattering kernels')
- Limited 2D S(q,w) + structure -> full scattering kernel description
- To become available via the iFit code framework http://ifit.mccode.org
- For details see D8.9 report



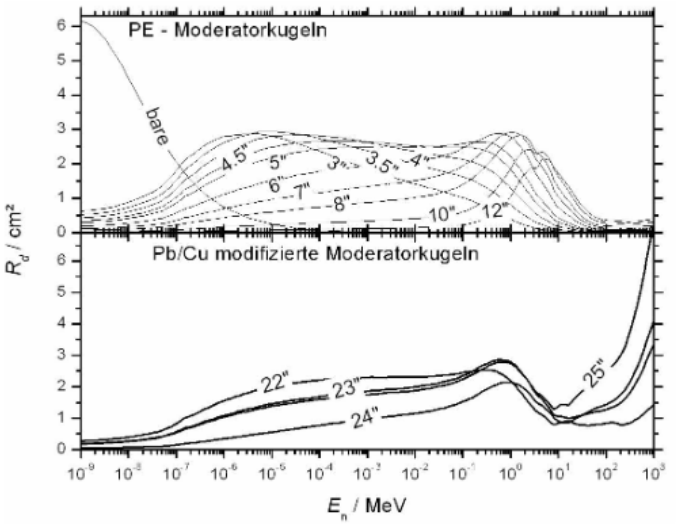
E Farhi, ILL (WP8 Observer)

[1] F. Cantargi, J. R. Granada, and R. E. Mayer. Annals of Nuclear Energy, 80. 43-46 (2015) ; see also subsequent papers at <http://www.cab.cnea.gov.ar/nyr/tsl_eng.html>.

2. Work carried out - Task 8.2

- Task 8.2: *Innovative Shielding Concepts and Materials*
  - *D8.1: Evaluation of detectors for fast neutron and gamma spectroscopy – mainly for background measurements*
  - *D8.5: Simulating laminate shielding concepts*
  - *D8.6:* Evaluation of material compositions & Developing special heavy concretes for fast neutron shielding
  - D8.10: Several background measurement series at different facilities in Europe (PSI, ISIS, TUM) scattering generic instrumentation
  - D8.16: Activation studies, radiation resistance

Measurements by Extended BSS System



Field Test with BSS system

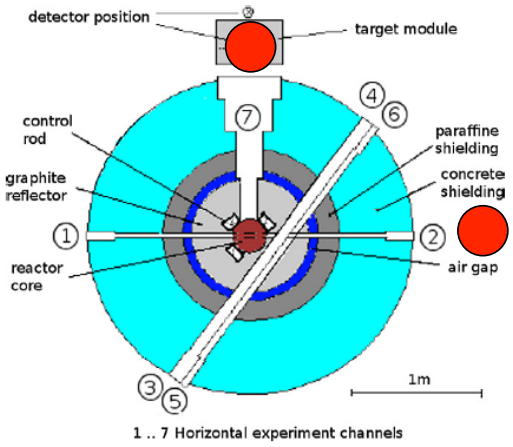
- detailed MCNP model exists
- at position A the fast neutron spectrum was measured by another group (proton recoil method)

Field test was in April 2018

(1) Verification of the known n-spectrum

(2) Measurement an un-known n-spectrum (Pos. B)

Data evaluation will be done in June 2018



Measurement range extended to 6 GeV

D8.6: Evaluation of material compositions & Developing special heavy concretes for fast neutron shielding

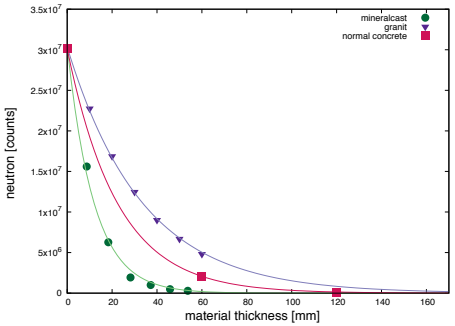
PAUL SCHERRER INSTITUT PSI

PSI - Development of New Shielding Materials

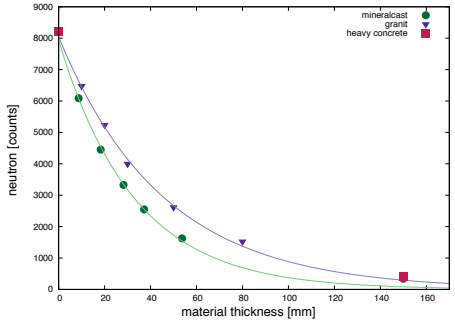
Investigate new shielding materials for use in AMOR/PSI and ESTIA/ESS (also for in house usage in upcoming SINQ upgrade).
Conditions apply: -- highly polish-able (replace granite in Estia) -- non-magnetic (poralized beamlines) – very compact (space limitations, shielding within vacuum housing)
New mineral cast materials tested: Epustone (to replace granite in Estia's design) and Epument (in place of heavy concrete where needed). Enriched with B4C and epoxy for better shielding on thermal and fast range.
Also new heavy concrete compositions tested
Transmission and activation tests performed for a range of various compositions for Epustone, Epument (14 different samples) and concrete (7 different samples).
Good candidates identified for all three types
In general: mineral casts perform better as normal concrete or granite and as good an heavy concrete

Comparison 1 – Standard mineral cast

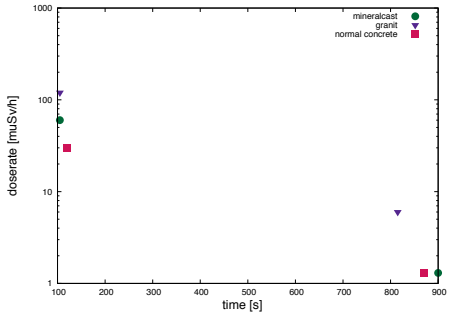
Thermal neutron transmission



Fast neutron transmission



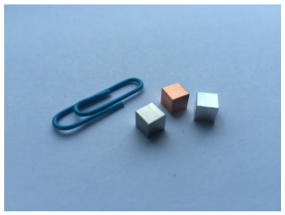
Activation decay (irradiation time 10 sec)

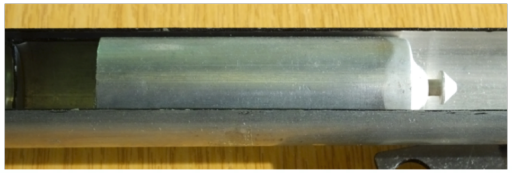


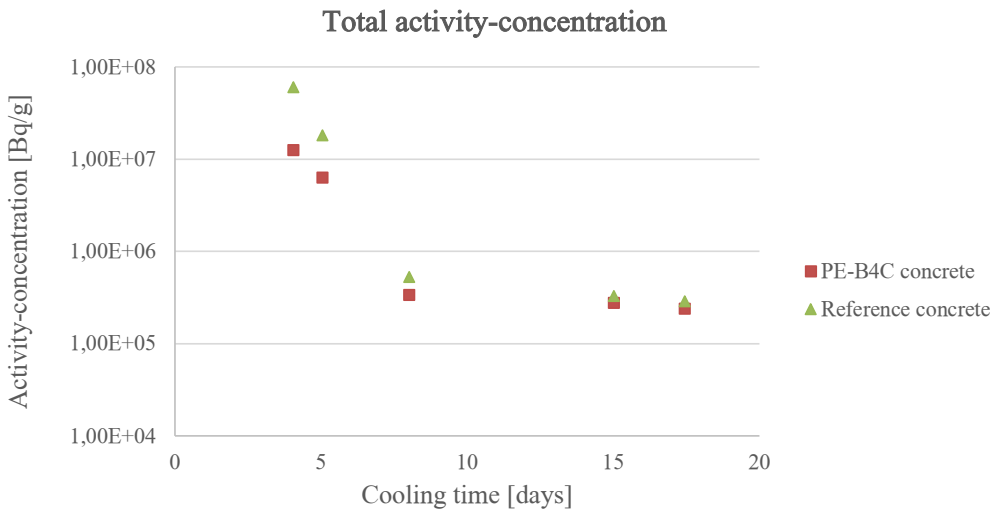
 This project is funded by the European Union (GA no. 654000)

Irradiation of concrete and metal samples at BRR

- Samples:
  - PE-B4C-concrete and a reference concrete
  - Metals: Al, Cu stainless steel
- Irradiation at Budapest Research Reactor
  - Vertical channels
- Activity measurement with HPGe detector
  - 1-3 day cooling
  - 2-3 week follow-up







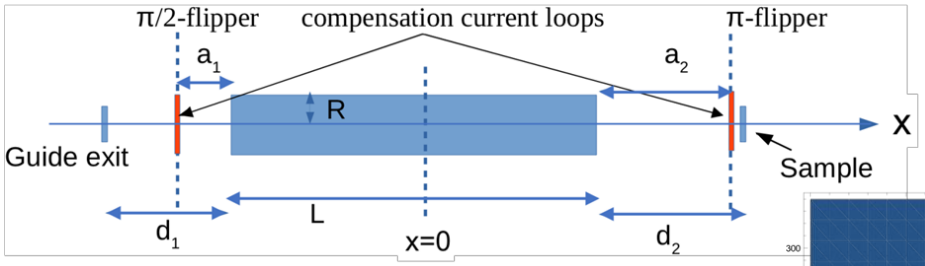
MAGYAR TUDOMÁNYOS AKADÉMIA
ENERGIATUDOMÁNYI KUTATÓKÖZPONT

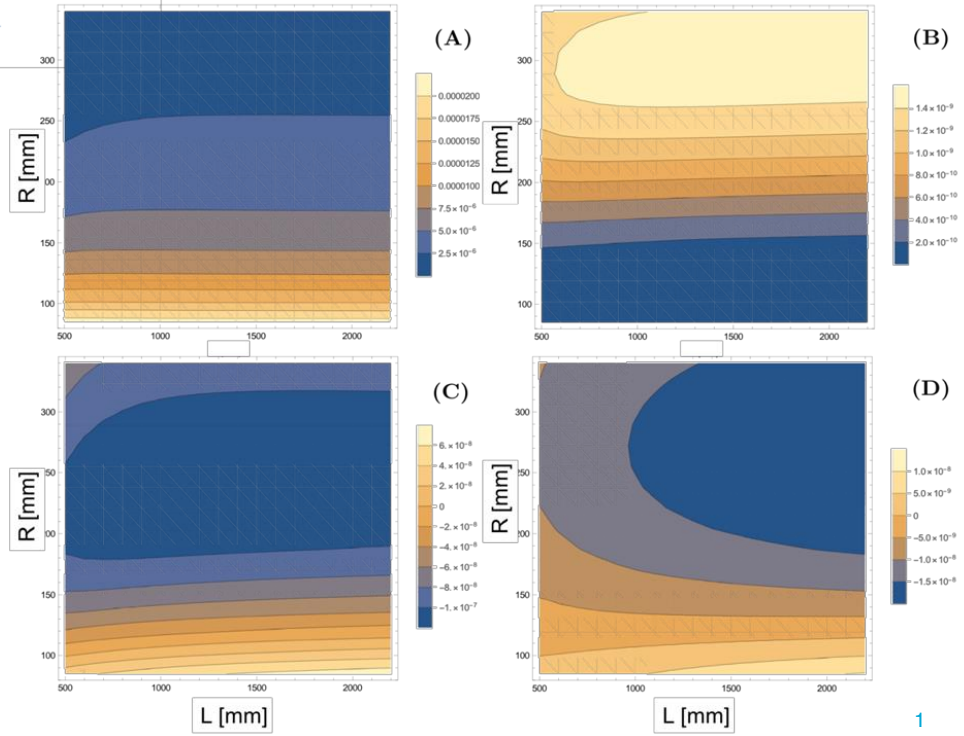
3. Work carried out - Task 8.3

- Task 8.3: Compact Instrumentation for Larmor Labelling applications at the ESS
  - D8.7: Analytical calculation of magnetic field configurations for compact Larmor schemes for ESS…

Inelastic spin-echo

- The case for inelastic spin-echo instruments
- Calculations through parameter space to investigate optima specific to ESS pancake moderator

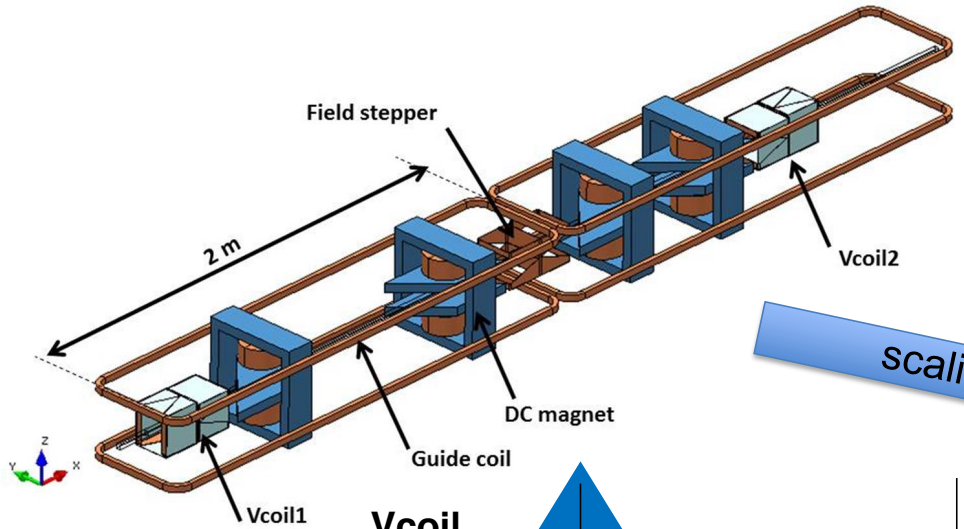


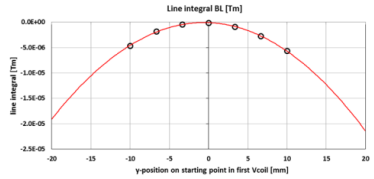


Calculated contributions the magnetic field inhomogeneity for an asymmetric magnetic layout of $a_1 = 0.3\ m$ and $a_2 = 0.5\ m$). The contour plots indicate the dependence of the different parameters influencing the magnetic field inhomogeneities on the radius R and length L of the main precession coil. (A) $F_0 = H^2$ (B) $F_{U2} = 4U^2/L_{tot}^2$, (C) $F_1 = 4HU/L_{tot}$ and (D) $F_3 = 4GU/L_{tot}^3$.

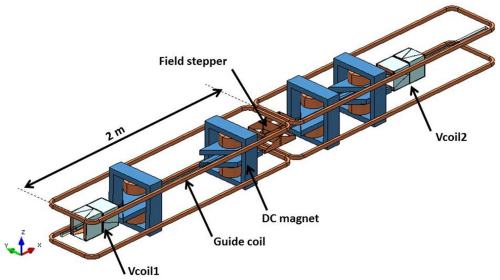
Elastic spin-echo

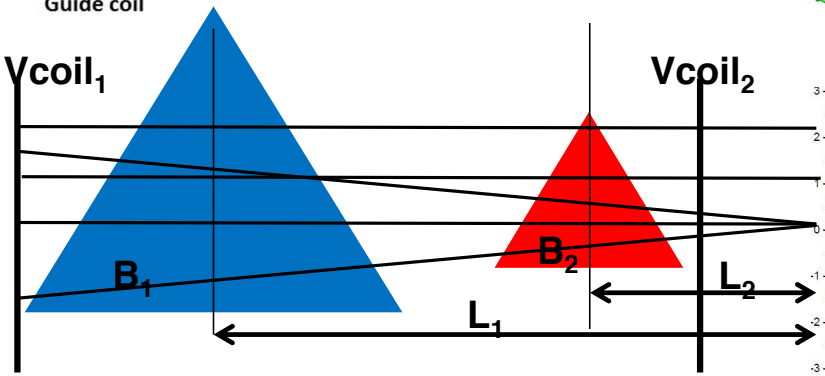
- Make optimal use of the pancake moderator at the ESS
- The case for elastic spin-echo instruments (SESANS type)
- Scaling to short and compact SEMSANS giving high intensity and tolerating high divergence

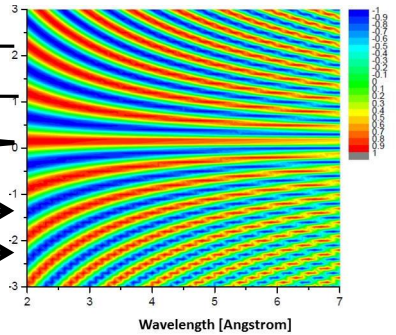




scaling







$B_1 L_1 = B_2 L_2$



Delays 1

Deliverable Number [14]	Deliverable Title	Lead beneficiary	Type [15]	Dissemination level [16]	Due Date (in months) [17]
D8.1	Evaluation of detectors for fast neutron and gamma spectroscopy	4 - PSI	Report	Public	9 ✓
D8.2	Improved code interface	13 - DTU	Other	Public	12 ✓
D8.3	Computational tests (multiple platforms)	15 - ESS-B	Report	Public	18
D8.4	Experimental test A - "BOA@PSI"& Experimental test B - "ChipIR@ISIS"	4 - PSI	Report	Public	18 ✓
D8.5	Simulating laminate shielding concepts	15 - ESS-B	Report	Public	18 ✓
D8.6	Evaluation of material compositions & Developing special heavy concretes for fast neutron shielding	4 - PSI	Report	Public	24

Delay to **M33**,
- availability of staff
- scope change
- WP meeting in Parma shows good progress
- Report **incoming**

!

Delay to M30,
- availability of facilities
- **Report received**, submission pending

Delay to **M33**,
- availability of facilities
- WP meeting in Parma shows excellent progress
- Report **incoming**

!

Delays 2

Deliverable Number [14]	Deliverable Title	Lead beneficiary	Type [15]	Dissemination level [16]	Due Date (in months) [17]
D8.7	Analytical calculation of magnetic field configurations for compact Larmor schemes for ESS instruments/ Evaluation of implications on the design of both inelastic and static neutron scattering generic instrumentation	8 - TU Delft	Report	Public	24 ✓
D8.8	Port of selected scattering kernel code from McStas to RESTRAX	13 - DTU	Other	Public	24
D8.9	Improved description of materials for high-energy neutron transport codes	1 - ILL	Websites, patents filling, etc.	Public	24 ✓
D8.10	Several background measurement series at different facilities in Europe	4 - PSI	Report	Public	24

Delay to M30,
- availability of staff
- **Report received**

Work **DONE**, report delay to **M33** !
- Part of work on D8.12 has come in early
- MCPL available in SIMRES
- Demonstration simulation BEER@ESS with McStas sample
- Report **incoming**

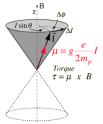
Delay to **M36**, !
- availability of facilities
- WP meeting in Parma shows good progress
- Report **incoming**

Impact

- General WP goals:

- Improving understanding signal-to-noise
  - **Increase instrument availability and utilisation**

- Background from high-energy neutrons, challenge for ESS
  - **Increase instrument availability and utilisation**



- Investigation of Larmor methods
  - **Increase method availability**

→ WP8 will pave the way for **optimised use of ESS**.

- Applications beyond neutron community:

- MCPL utilisation in other scientific disciplines, e.g. in cosmogenics (see mcpl paper) ✓

(cosmogenics == use of radionuclides produced in-situ by cosmic rays, earth surface science)

- Use of developed shielding methods beyond neutron community ?

KPI values - and current aims…

- KPI data overview

		Coimbra 2016	ICANS 2017	Other events	Current sum	… project aim
8 - Instrumentation E-tools	Number of presentations (poster, oral)	0+8	2+5	1+5	21	30
	Number of publications	1	2	3	6	8-10
	Number of workshop participants	15	10		25	all > 10

- … and a careful estimate of a ‘success’ definition
- We should
  - Get other current / incoming results written up
  - Arrange further workshops aiming at potential users!

Questions?