ILL College 7 seminar

Grenoble, November 18th 2019

Progress in simulation software, shielding methods and compact Larmor devices:

- A report from SINE2020 WP8

DTU
Peter Willendrup,
Technical University of Denmark

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

Agenda

- 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

- McStas heading for the GPU… (short teaser, 1-2 slides)

This project was 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

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

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

- Task 8.2: Innovative Shielding Concepts and Materials

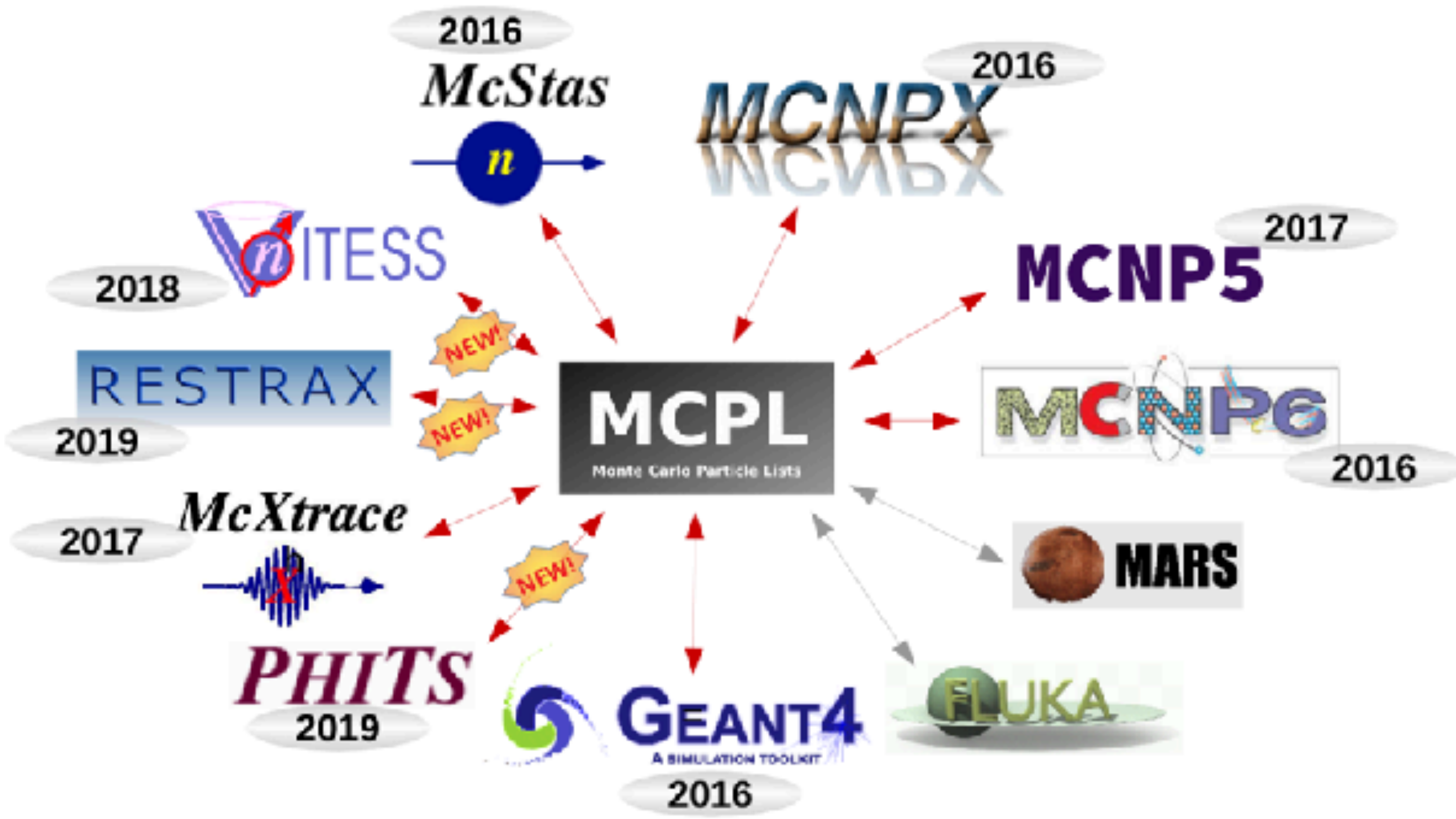
Measure
and understand (high-energy) background and utilise this to better shield our instruments using new shielding approaches (heavy concrete, laminar shielding)

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

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

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

Task 1 achievements 1: MCPL interchange format



T. Kittelmann, et al., Monte Carlo Particle Lists: MCPL, *Computer Physics Communications*, Volume 218, September 2017, Pages 17-42, ISSN 0010-4655, https://doi.org/10.1016/j.cpc.2017.04.012

Task 1 achievements 1: MCPL interchange format

4_McStas — -bash — 127×37

```
pkwi-mbp2018:4_McStas pkwi$ mcpltool W3.mcpl.gz
Opened MCPL file W3.mcpl.gz:

Basic info
  Format               : MCPL-2
  No. of particles     : 174450495
  Header storage       : 171 bytes
  Data storage         : 6280217820 bytes

Custom meta data
  Source               : "MCNPX-2.7.0"
  Number of comments   : 2
        -> comment 0 : "MCNP(X) SSW file converted to MCPL with ssw2mcpl"
        -> comment 1 : "Title/description encoded in SSW file: 'Input File:'"
  Number of blobs      : 0

Particle data format
  User flags           : no
  Polarisation info    : no
  Fixed part. type     : no
  Fixed part. weight   : no
  FP precision         : single
  Endianness           : little
  Storage              : 36 bytes/particle
```

File properties & stats

Simulation metadata

Particle storage properties

index	pdgcode	ekin[MeV]	x[cm]	y[cm]	z[cm]	ux	uy	uz	time[ms]	weight
0	2112	0.018837	131.29	150.88	19.66	0.61947	0.77528	0.1233	0.0013887	7.7394e-27
1	2112	0.021846	139.8	163.02	14	0.66303	0.73946	0.11659	0.0012184	1.4012e-28
2	2112	0.34503	135.14	167.44	18.926	0.6868	0.7196	0.10242	0.0003827	3.361e-17
3	2112	0.39514	129.99	152	11.639	0.67837	0.73181	0.065348	0.00034582	2.1271e-28
4	2112	0.39995	134.82	147.73	11.244	0.69895	0.71234	0.063561	0.00034449	4.8273e-26
5	2112	0.43034	134.34	148.16	13.595	0.70471	0.706	0.070283	0.00032745	2.436e-23
6	2112	0.023844	137.39	165.34	18.262	0.74022	0.33843	-0.58098	0.00033134	1.1614e-20
7	2112	0.44336	130.45	151.6	12.905	0.67163	0.73335	0.10538	0.000306	4.6873e-26
8	2112	0.44692	136.01	146.63	15.649	0.69704	0.70795	0.11372	0.00030363	4.9599e-25
9	2112	0.46274	129.51	152.4	9.4062	0.68973	0.7206	0.070773	0.0002787	1.0161e-21

```
pkwi-mbp2018:4_McStas pkwi$
```

Includes excellent command line tools for filtering, merging etc.

* MCPL is included with McStas since v.2.4

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

Task 1 achievements 1: MCPL interchange format

McCode — pkwi@pkwi-mbp2018: ~/Projects — bash — 98×35

```
pkwi@pkwi-mbp2018:~/Projects$ pymcpltool --stats /Users/pkwi/Projects/SINE2020BIFROST/W3.mcpl.gz

------------------------------------------------------------------------------
nparticles     : 174450495
sum(weights)   : 18527.8
------------------------------------------------------------------------------
               :            mean            rms             min             max
------------------------------------------------------------------------------
ekin     [MeV] :         1.38306        9.65091     2.07568e-15         1990.84
x         [cm] :          169.62        28.6837         97.6746             200
y         [cm] :         3.42827        101.954        -174.527         174.527
z         [cm] :         14.2431        3.27836          8.5598         19.9434
ux             :        0.815141       0.194949       -0.844703               1
uy             :      0.00809299       0.534939       -0.999928               1
uz             :      0.00137547       0.106366       -0.999943        0.999988
time      [ms] :        0.485192       0.782116     2.36574e-05         993.475
weight         :     0.000106207     0.00949162               0         3.40407
polx           :               0              0               0               0
poly           :               0              0               0               0
polz           :               0              0               0               0
------------------------------------------------------------------------------
pdgcode        :         2112 (n)               11856.2 [63.99%]
                           22 (gamma)           6667.51 [35.99%]
                         2212 (p)               3.04239 [ 0.02%]
                   1000010020 (D)               1.00065 [ 0.01%]
                         -211 (pi-)         7.77578e-06 [ 0.00%]
                          211 (pi+)         2.22455e-06 [ 0.00%]
                   1000010030 (T)           3.87931e-10 [ 0.00%]
                   1000020040 (alpha)       5.22881e-11 [ 0.00%]
                     [ values ]            [ weighted counts ]
------------------------------------------------------------------------------
userflags      :            0 (0x00000000)      18527.8 [100.00%]
                     [ values ]            [ weighted counts ]
------------------------------------------------------------------------------
pkwi@pkwi-mbp2018:~/Projects$ 
```

Gaussian stats on particle Properties

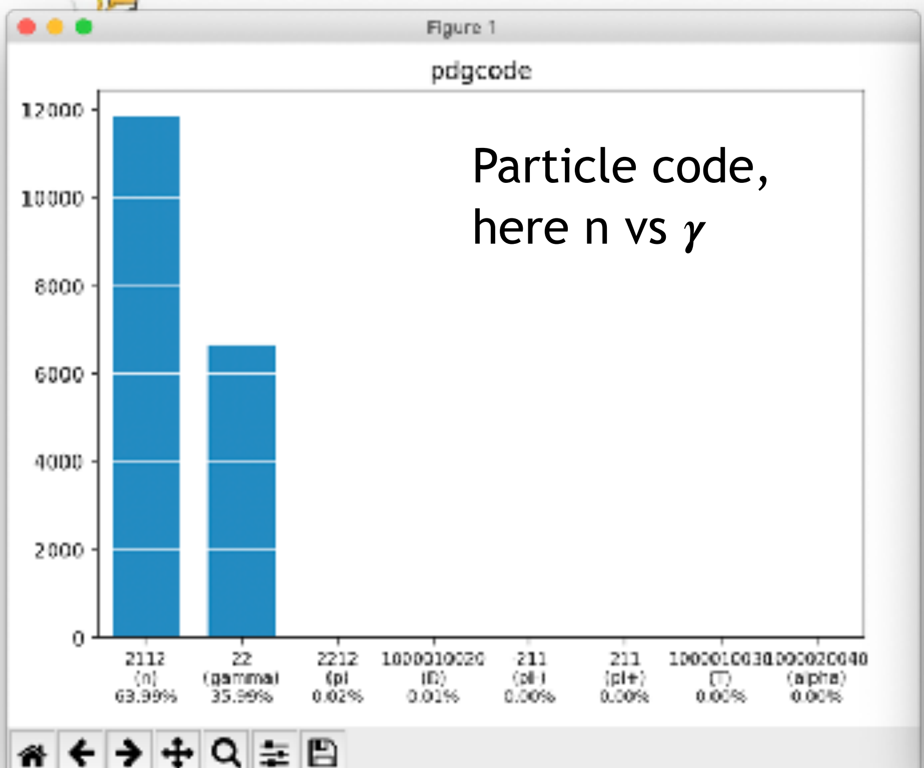
Particle type stats

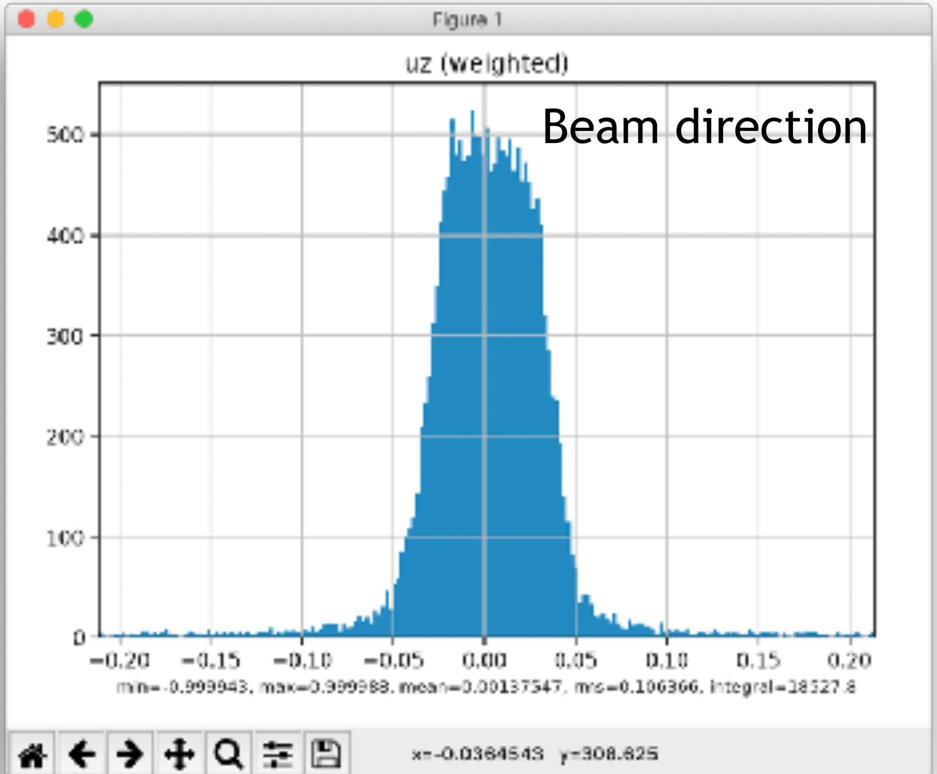
Includes command line tools for stats…

* pymcpltool is included with McStas from next release

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

Task 1 achievements 1: MCPL interchange format





... plus gui tools for stats...

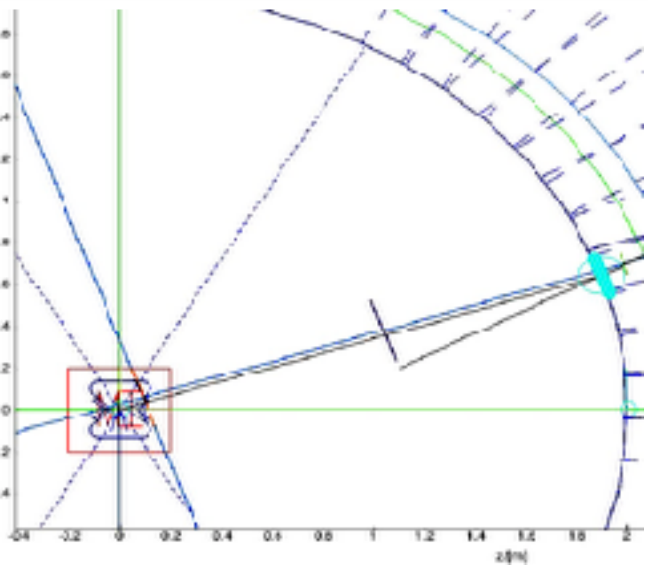
MCPL
Monte Carlo Particle Lists

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

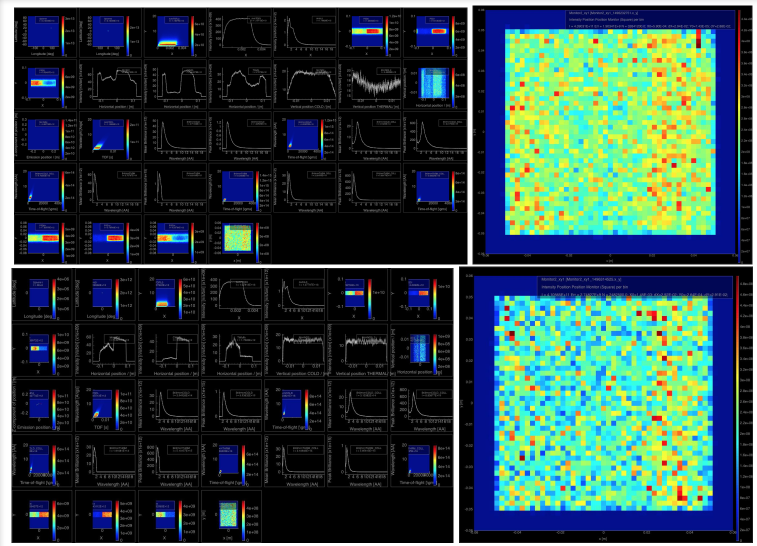
* pymcpltool is included with McStas from next release

Task 1 achievements 1: MCPL interchange format

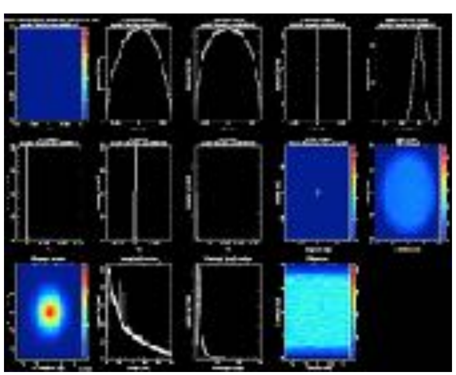
Used for bringing MCNP-based source-terms to McStas at multiple facilities: ESS, HIFR



Visualisation of events in the file W8.mcpl.gz within the ESS_butterfly_MCPL instrument. The coordinate system of choice is the TARGET coordinate system.



Output from MCPL-based and analytical ESS sources:
- overview plot and "end of curved guide" PSD for W8.



MCNP output from the ORNL HIFR source available for transport in McStas.

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

Task 1 achievements 2: (improved) Supermirror patch to MCNP-6

1. Initial implementation 2009 for MCNPX:

F. X. Gallmeier et. al. (**2009**) Implementation of Neutron Mirror Modeling Capability into MCNPX and Its Demonstration in First Applications, *Nuclear Technology*, 168:3, 768-772, DOI: 10.13182/NT09-A9304

2. Improved implementation 2013, MCNPX and enabling MPI support:

E. B. Klinkby, et. al. (2013) Interfacing MCNPX and McStas for simulation of neutron transport, *Nuclear Instruments and Methods A*, 700, 106-110 DOI: 10.1016/j.nima.2012.10.052

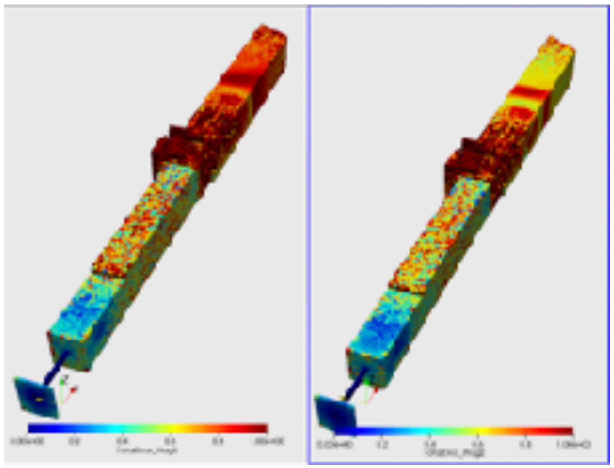
3. Current, MCNP6, MPI and standard variance reduction schemes:
Much improved implementation, allows standard variance reduction schemes and allows “deterministic propagation” in neutron guide volumes
M. Magan & R. Bergmann, Supermirror physics with event biasing in MCNP6, NIMA-D-19-00551, submitted in October 2019.

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

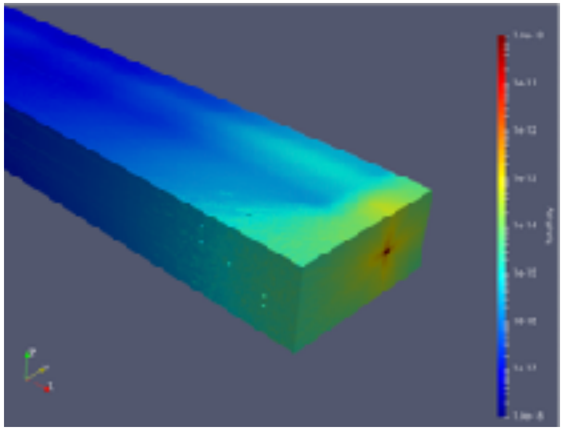
* Patch licensing still(!) under evaluation by MCNP team @ LANL

Task 1 achievements 2: (improved) Supermirror patch to MCNP-6

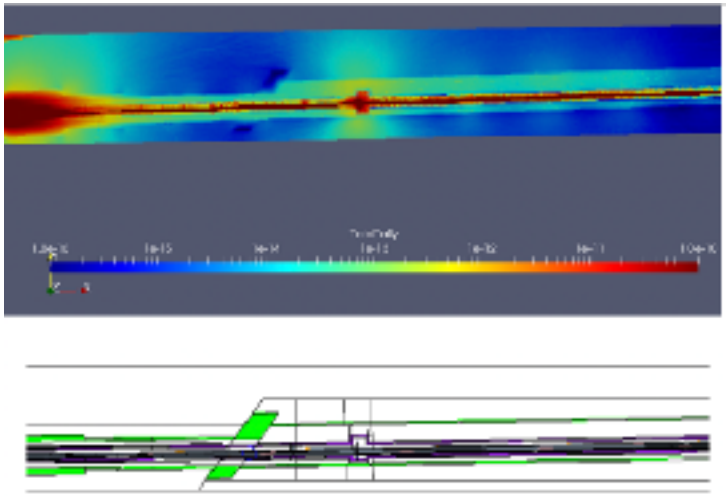
Prior to D8.3 work, the standard MCNP variance reduction tool of DXTRAN spheres was not possible together with the super mirror patch!



Comparison of stochastic (left) Vs deterministic guide reflection. Relative errors.



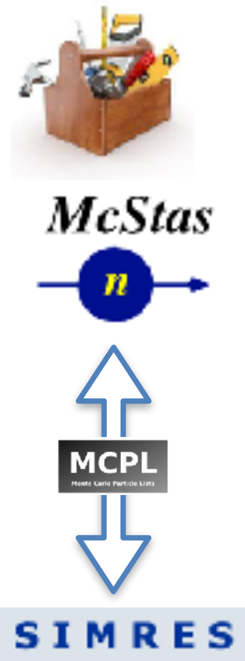
Neutron flux (per source particle) in the MIRACLES Geometry: detail at the end of the guide.



Radiation creation at features like neutron choppers is clearly visible and solved.

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

Task 1 achievements 3: McStas <-> SIMRES interchange



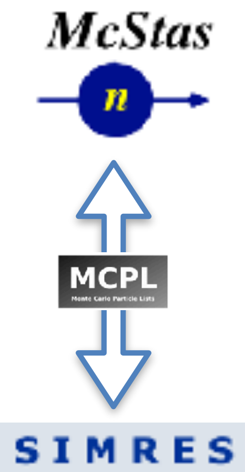
Why combine SIMRES + McStas?

- 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)

Task 1 achievements 3: McStas <-> SIMRES interchange

D8.11: Transport of sample models from McStas to SIMRES:
- Uses MCPL to "sandwich" e.g. the McStas Single_crystal in a SIMRES simulation workflow.
- Mechanism not limited to samples, but can expose any McStas component in SIMRES



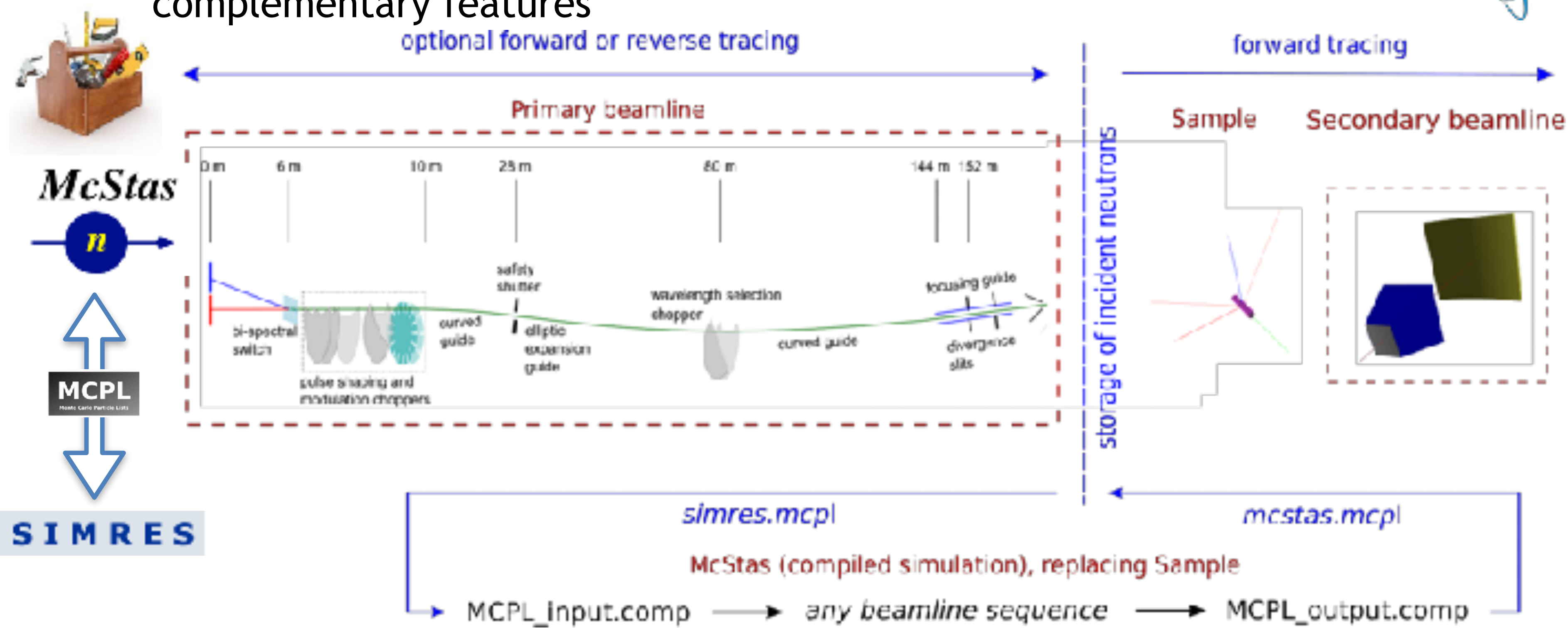

```
COMPONENT in = MCPL_input(repeat=1, filename="vin.mcpl")
AT(0,0,0) RELATIVE Origin

COMPONENT single_crystal = Single_crystal(
      reflections="Al2O3_sapphire.lau",
      yheight=0.05, radius=0.01, mosaic=1, delta_d_d=1e-4,
      ax=4.757, ay=0, az=0, bx=2.3785, by=0, bz=-3.364,
      cx=0, cy=12.9877, cz=0,
      p_transmit=0.1)
AT (0, 0, 0) RELATIVE PREVIOUS

COMPONENT out = MCPL_output(filename="vout.mcpl")
AT(0,0,0) RELATIVE PREVIOUS
```

Multiple examples of this were released with McStas 2.5

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

Task 1 achievements 3: McStas <-> SIMRES interchange

D8.12: Full ESS BEER beam line simulation combining McStas and SIMRES complementary features

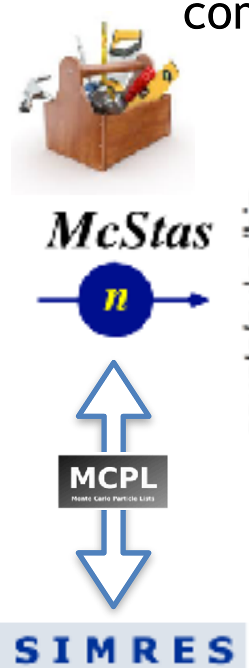


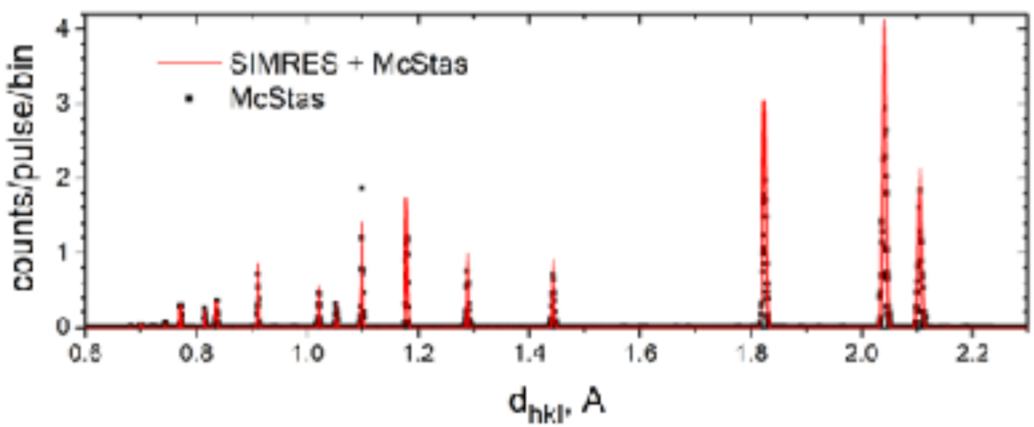
A schematics showing the flow of neutrons in a simulation combining SIMRES and McStas. The sample component of SIMRES is replaced by a compiled McStas simulation executable. It uses primary beam neutrons from SIMRES monitor and returns back the result by using the MCPL input/output components. The 3rd step (secondary beam simulation by SIMRES) is optional, simulations can be finished already by the McStas part.

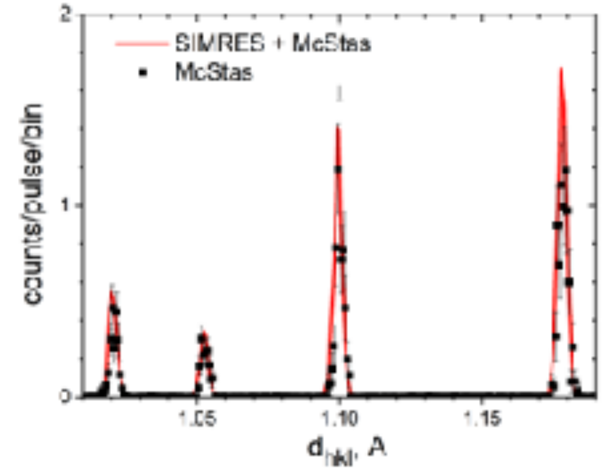
This project was funded by the European Union (GA no. 654000)

Task 1 achievements 3: McStas <-> SIMRES interchange

D8.12: Full ESS BEER beam line simulation combining McStas and SIMRES complementary features







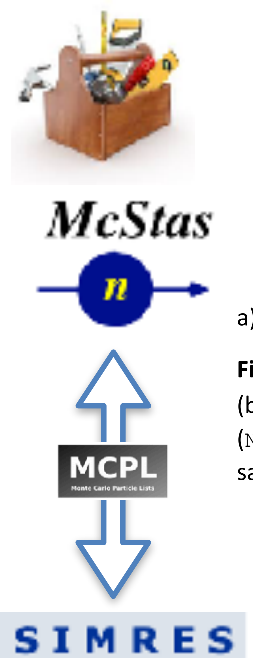
Diffractograms simulated by the combined SIMRES+McStas ray-tracing (red line) and by McStas only (black points).The detail on the right permits to assess differences, which are within the statistical errors.

	Rel. error (primary beam)	Computing time
SIMRES + McStas	1.1 %	56 s
McStas	1.8 %	1110 s

!

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

Task 1 achievements 3: McStas <-> SIMRES interchange



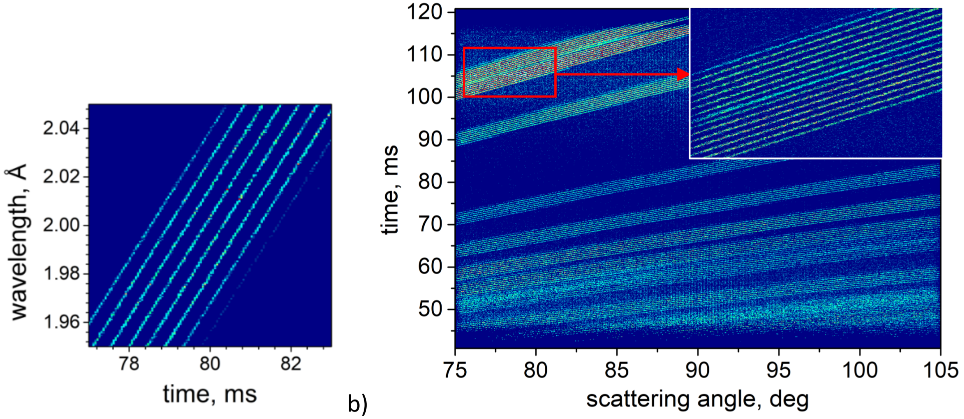


Figure 3. (a) Modulated beam structure at the primary slit – SIMRES MCPL output passed to McStas. (b) ToF – 2θ map of events registered by the detector component (`NPI_tof_theta_monitor.comp`) in McStas; multiplexed diffraction lines from the duplex steel sample (`PowderN.comp`).

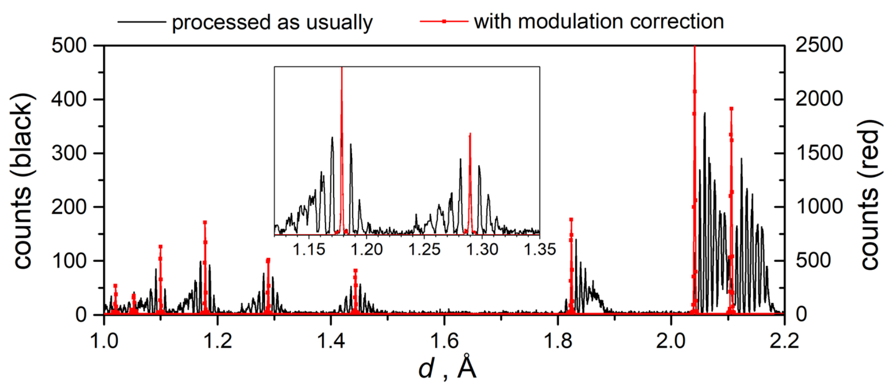


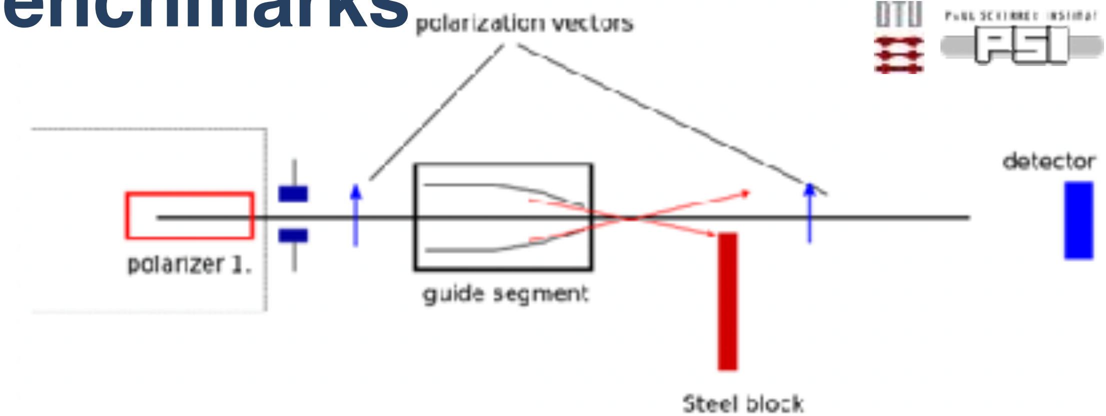
Figure 4. Diffractogram produced by the McStas component `NPI_tof_dhkl_detector` with the modulation analysis switched off (black, left scale) and on (red, right scale).

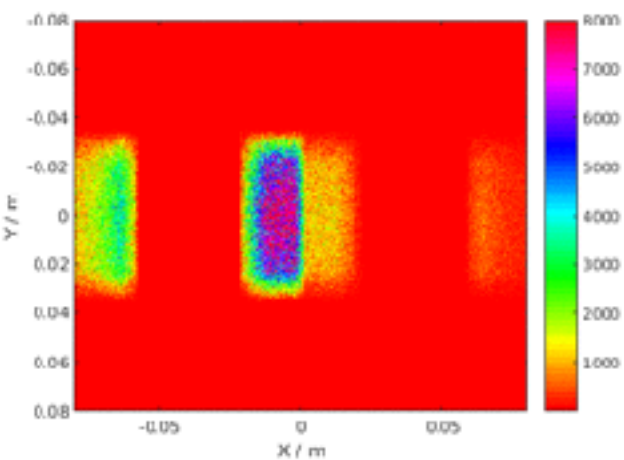
Takes advantage of
- SIMRES for small gauge-volume in strain measurements
- Flexibility in McStas-based data-evaluation -> reconstructed peaks from modulation signals

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

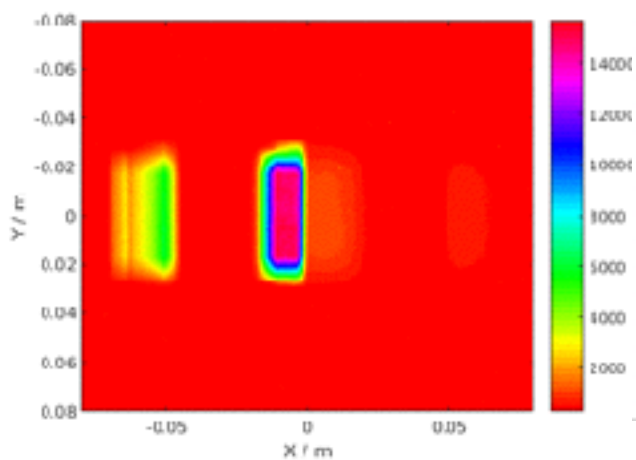
Task 1 achievements 4: experiments and benchmarks

D8.4 experiments, McStas and MCNP calculations at the PSI BOA beam line

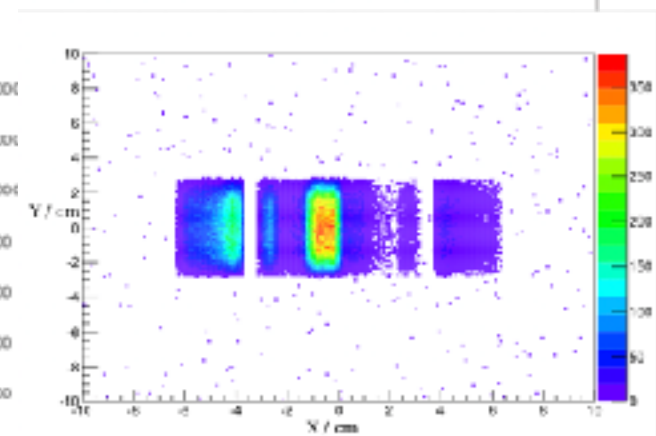




McStas



Experimental data

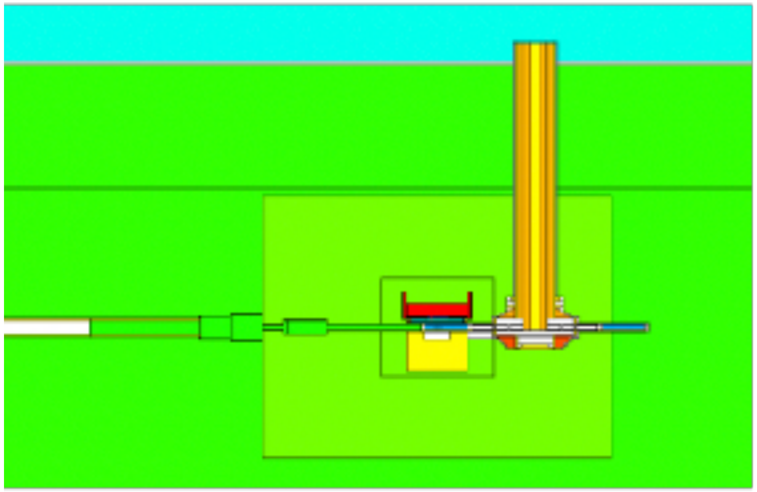


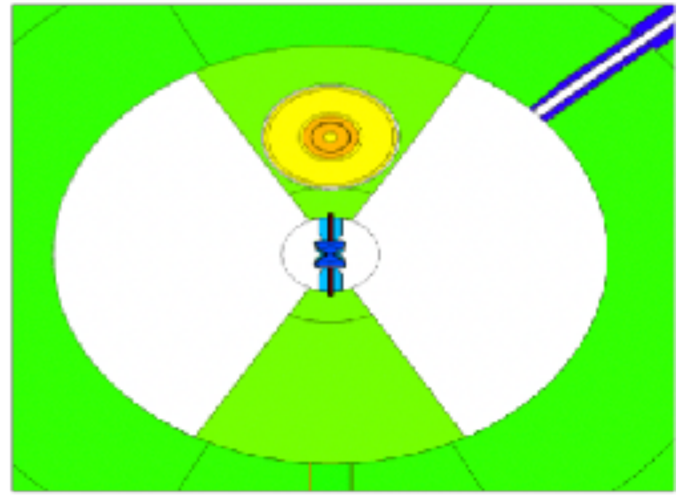
MCNP6

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

Task 1 achievements 5: illustrated example cases w/ code

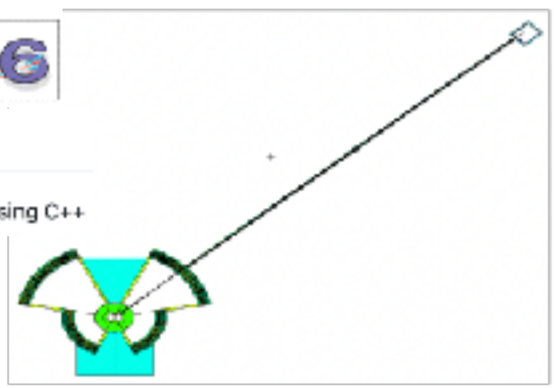
D8.13 Simulation tool-suite applied to BIFROST at ESS

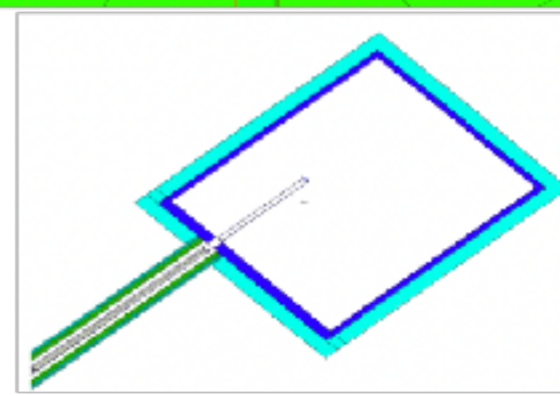




CombLayer

MCNP(X) project builder using C++





CombLayer-driven MCNP6 model of ESS source and the BIFROST instrument up to sample pos

Ansell, Stuart (2016). CombLayer - A fast parametric MCNP(X) model constructor (JAEA-Conf--2015-002). Arai, MasatoshiYonemura, Masao, Yonemura, Masao, & Suzuki, Jun-ichi (Eds.). Japan

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

Task 1 achievements 5: illustrated example cases w/ code

D8.13 Simulation tool-suite applied to BIFROST at ESS

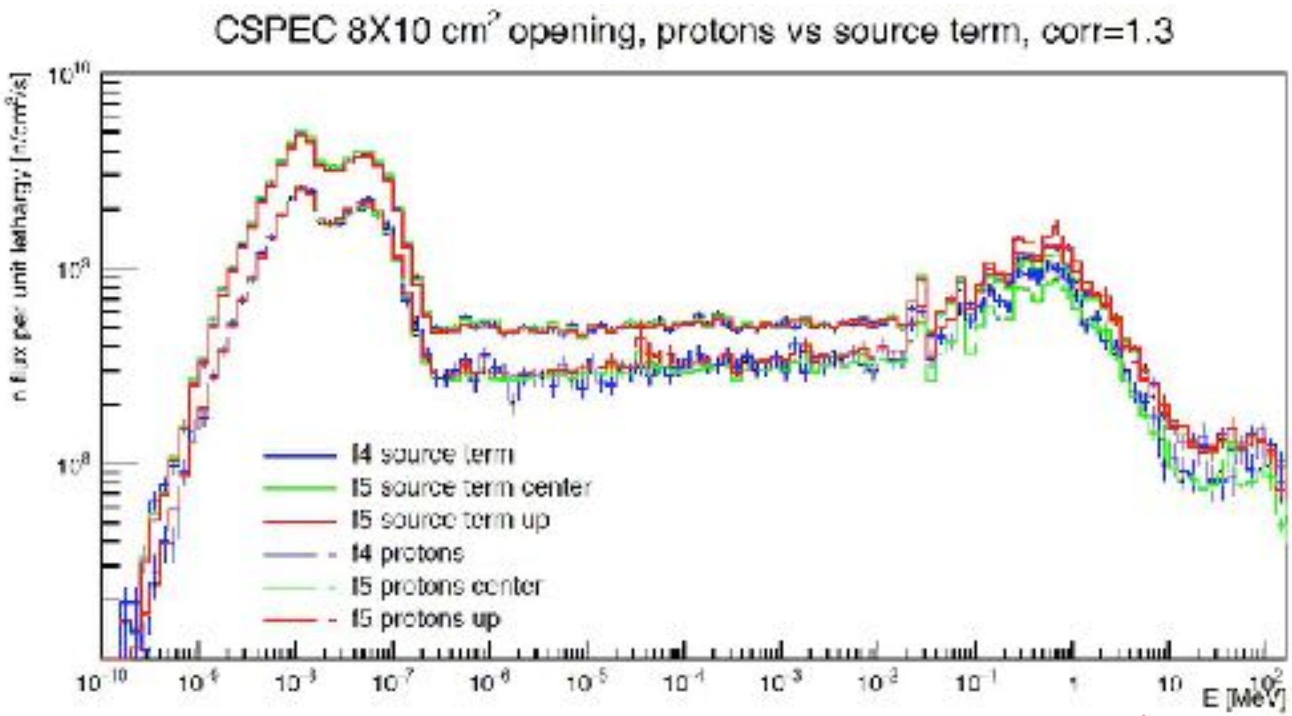
Supermirror patch applied to MCNP6

```
REFLE53 953 1 -4359
REFF1 0.99 2.19E-2 4 6.07 3E-3 $supermirror
RFLAG1 2
```

MCNP6

CombLayer

MCNP(X) project builder using C++

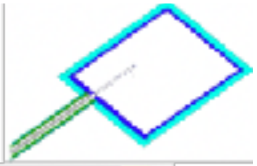


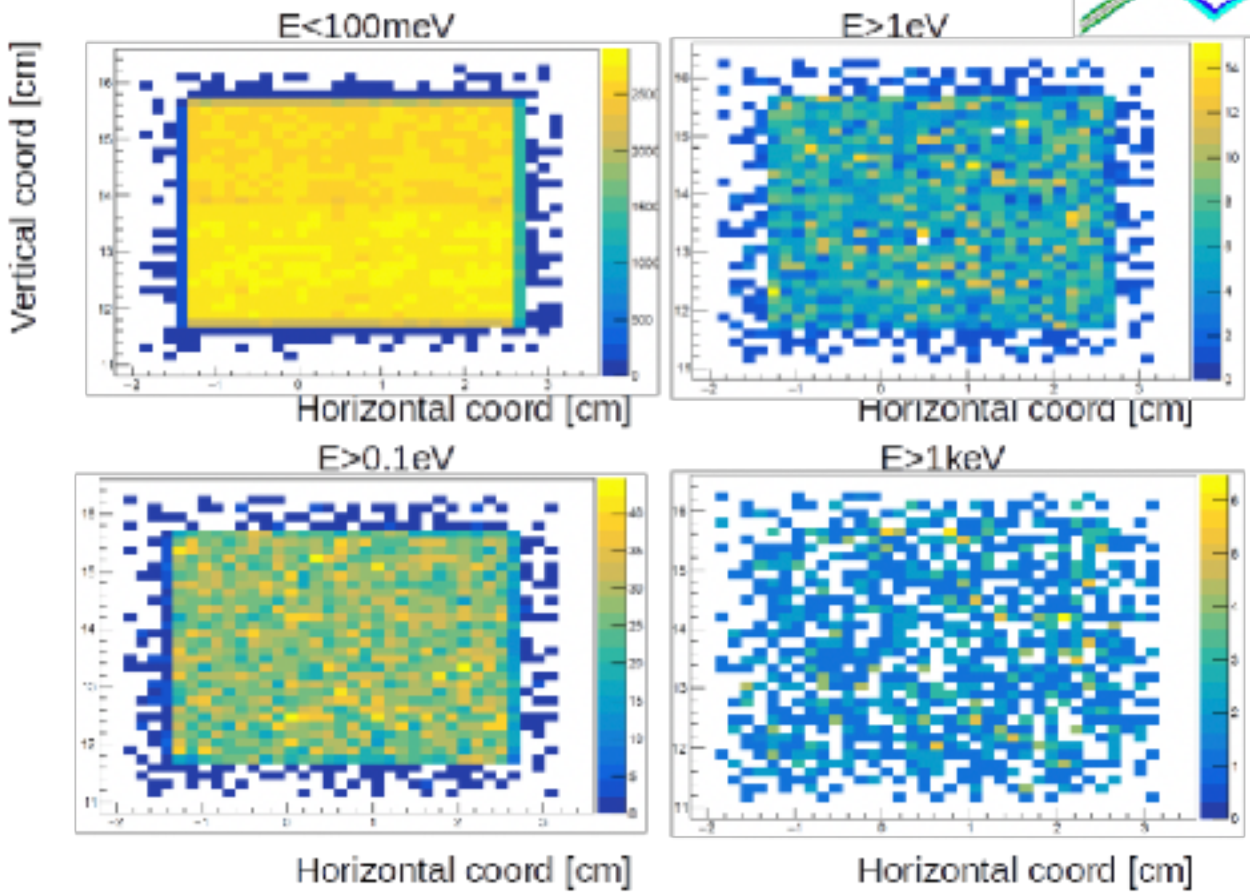
Synthesising neutron-source from proton source in MCNP6

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

Task 1 achievements 5: illustrated example cases w/ code

D8.13 Simulation tool-suite applied to BIFROST at ESS



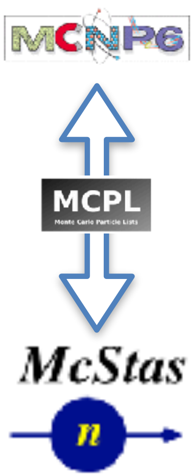


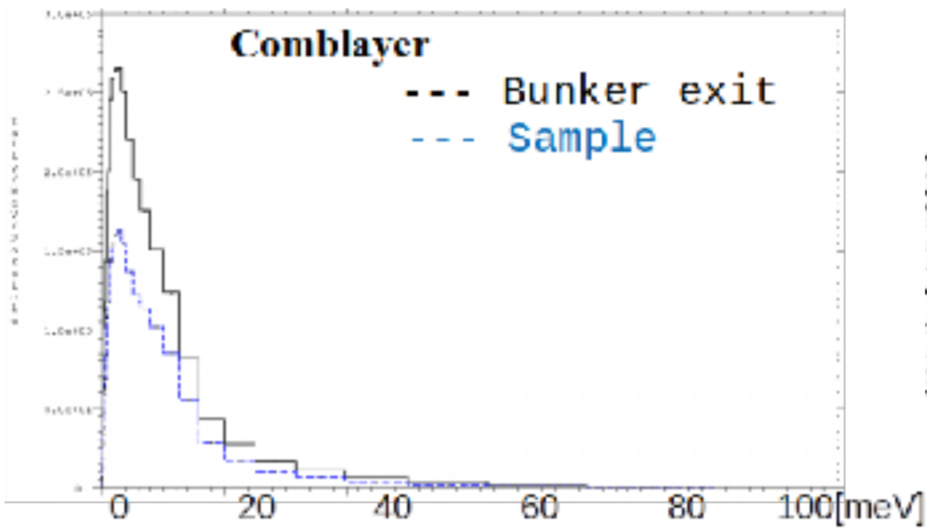
Beam cross section at sample position, all transported by

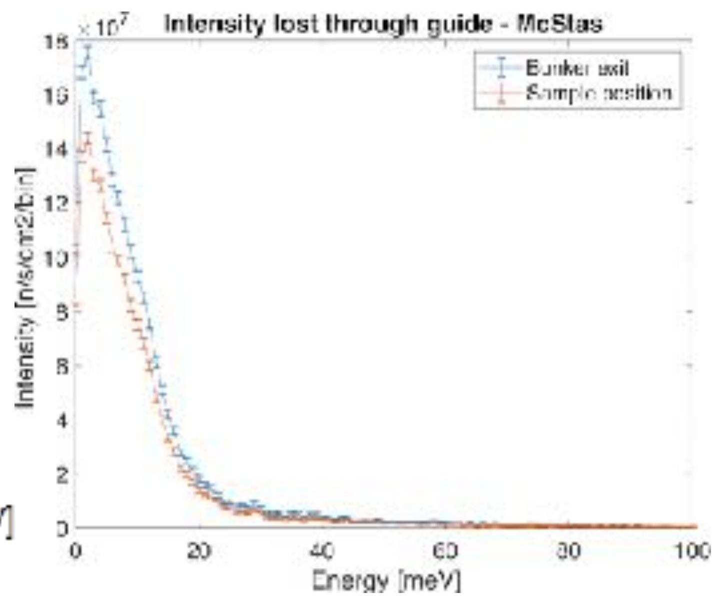
Task 1 achievements 5: illustrated example cases w/ code

D8.13 Simulation tool-suite applied to BIFROST at ESS

Beam losses along beamline, MCNP6 +SM vs McStas







The intensity loss in the McStas simulation is **22%**, whereas the corresponding loss found in the SM MCNP simulations where **37%**. These differences are thought to be due to small differences in the guide geometry - in the SM MCNP case the geometry is inherited from its CombLayer implementation, whereas the McStas geometry originate from the instrument team directly.

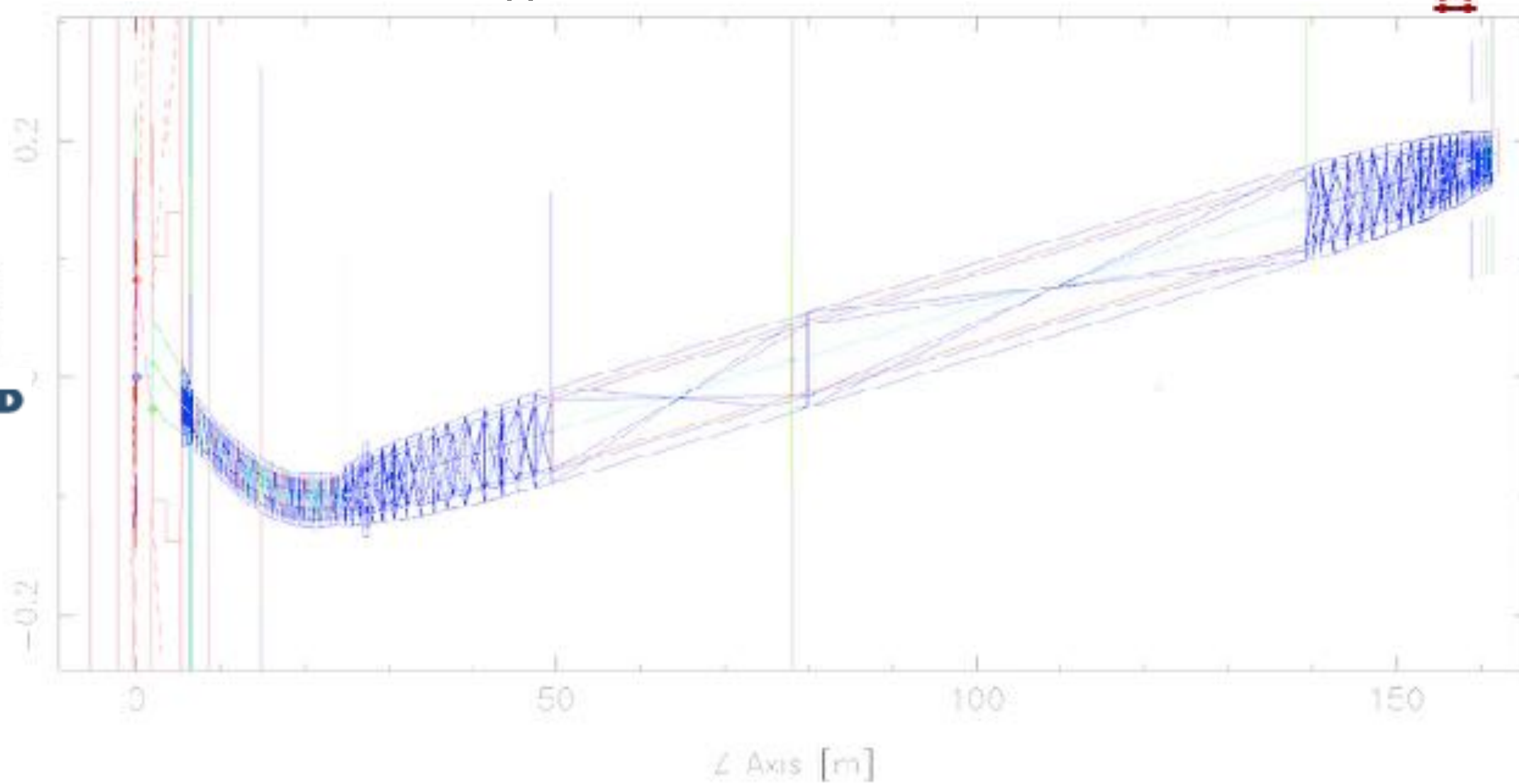
This project was funded by the European Union (GA no. 654000)

Task 1 achievements 5: illustrated example cases w/ code

D8.13 Simulation tool-suite applied to BIFROST at ESS

.stl

.off

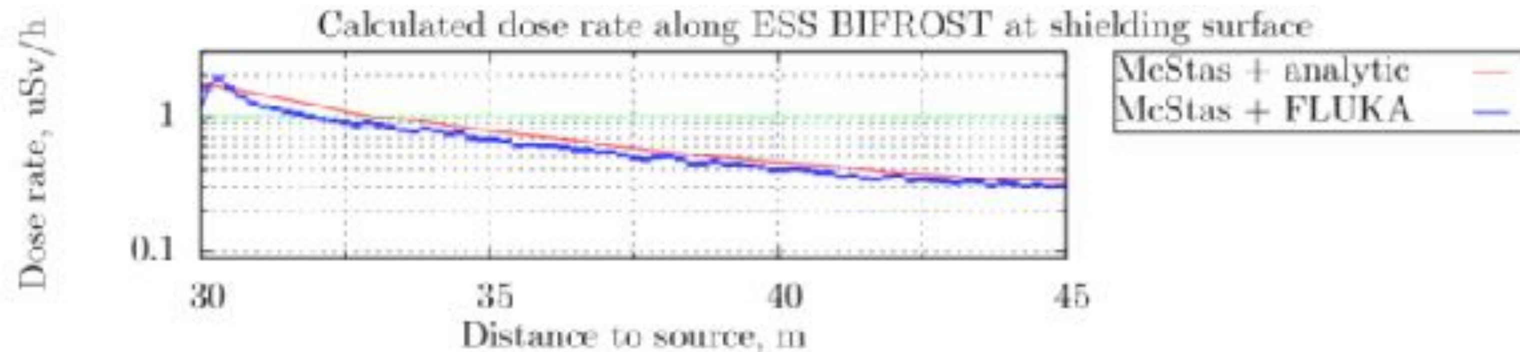


*CAD model (blue) overlayed with McStas instrument geometry. The precision in placement of the sample position is **of the order cm** over the 150 m instrument length.*

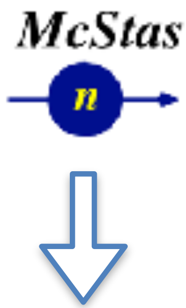
This project was funded by the European Union (GA no. 654000)

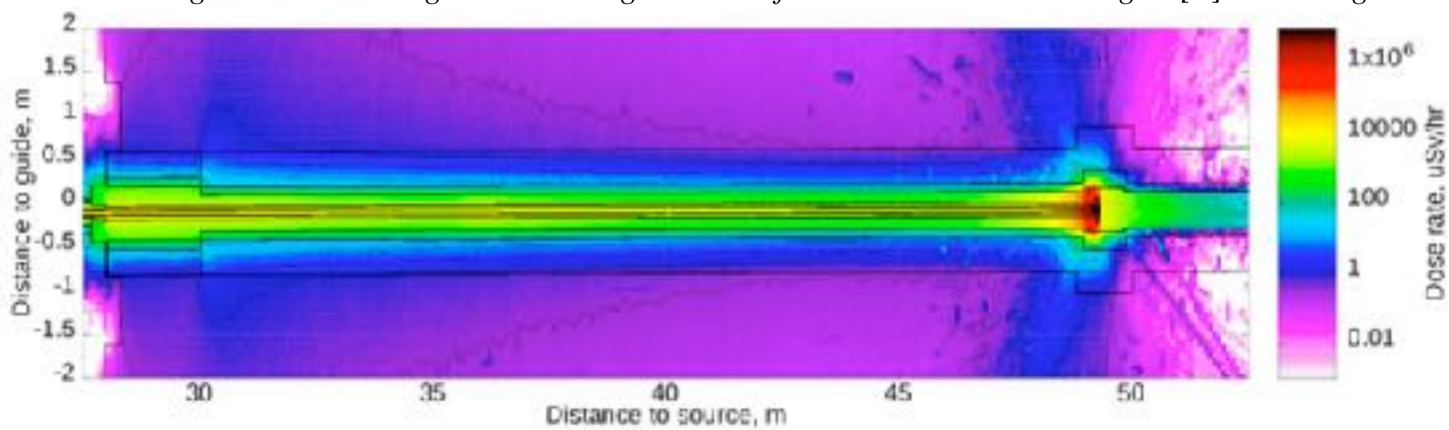
Task 1 achievements 5: illustrated example cases w/ code

D8.13 Simulation tool-suite applied to BIFROST at ESS



Dose rate along ESS BIFROST guide shielding at the surface calculated according to [3] and using FLUKA





γ-dose rate Estimates

Dose rate distribution in the shielding around BIFROST guide, cut by horizontal plane at guide height.

[3] **R. Kolevatov** et.al. Neutron absorption in supermirror coatings: Effects on shielding NIM. A 2019, **922**, pp. 98-107 https://doi.org/10.1016/j.nima.2018.12.069

[6] **R. Kolevatov,** McStas and Scatter Logger driven calculations of prompt gamma shielding for the neutron guides**, submitted to JNR ISTSI proceedings**

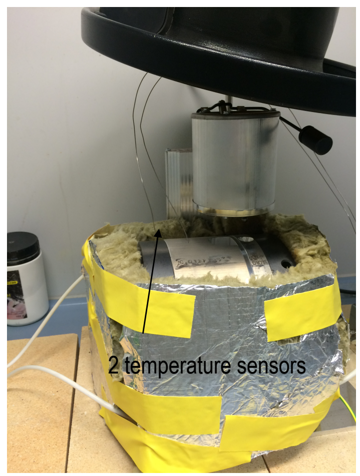
Related Vitess-deliverable was D8.18 from Wigner

* Experimental validation at PSI 2020 spring

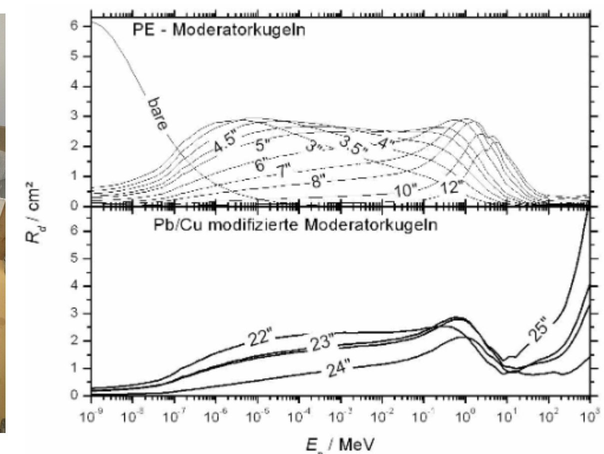
This project was funded by the Eu

Task 2 achievements 1: Improved Bonner Sphere Spectrometer

SINE2020 WP8-developed BSS-system with PE moderators, Cu and Pb shells



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



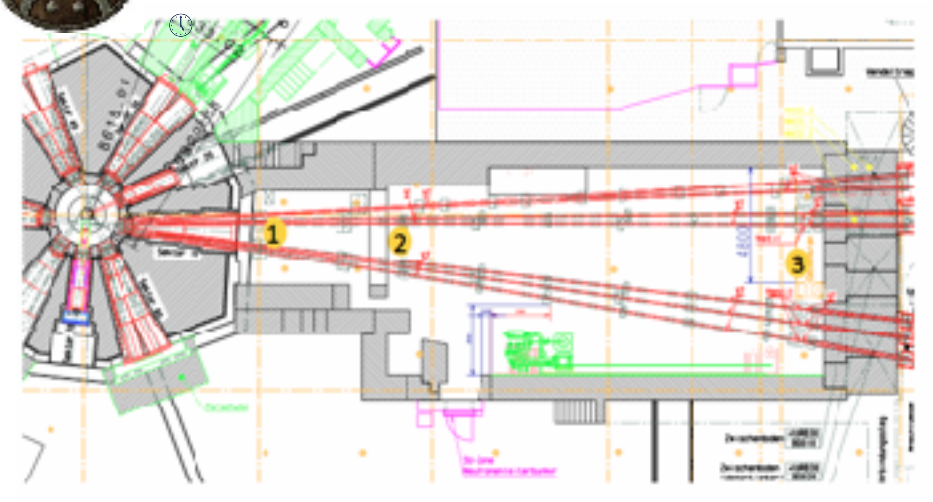
Range extension:

~20 MeV-> ~5 GeV!

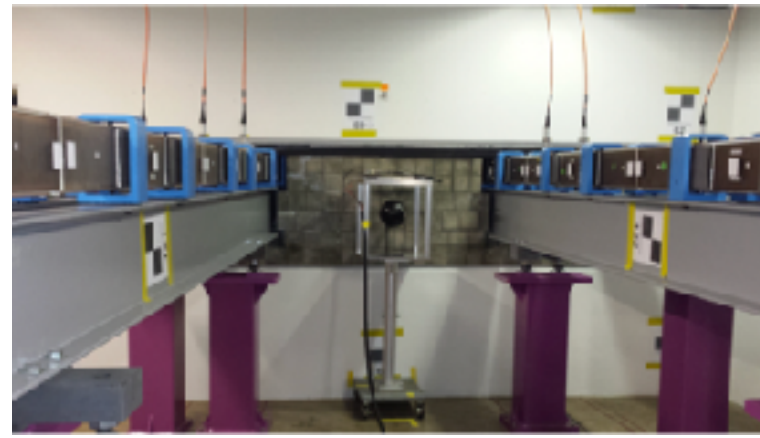
This project was funded by the European Union (GA no. 654000)

Task 2 achievements 2: Understanding facility backgrounds - PSI

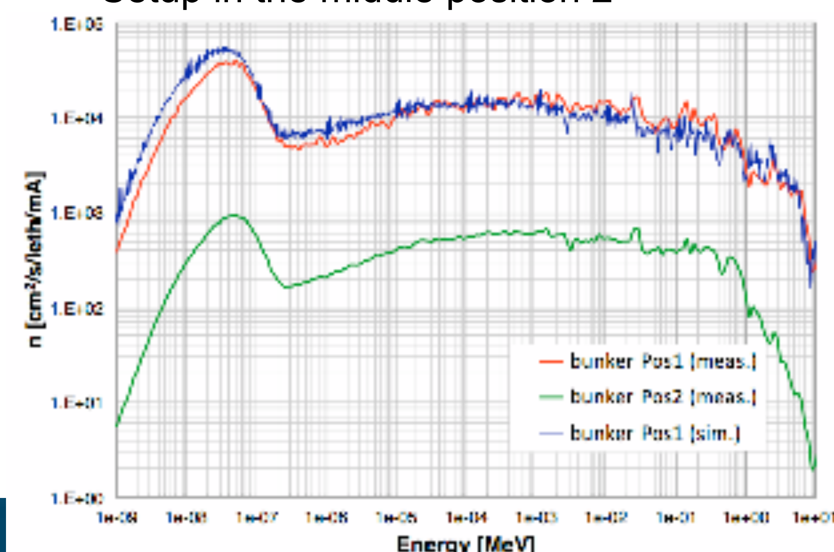
PSI measurements & simulations



SINQ neutron guide bunker with the three measurement position



Setup in the middle position 2

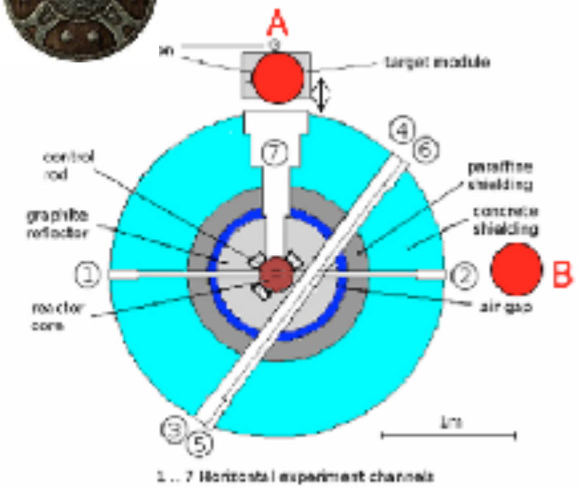


The agreement between simulations and measurement is very good. The small differences in the thermal region could be scattering effects which are not fully implemented in the MCNPX model.

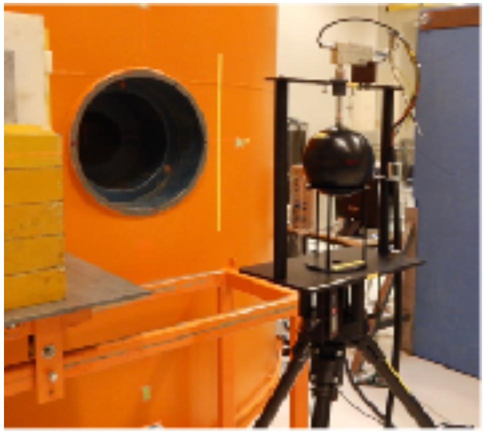
This project was funded by the European Union (GA no. 654000)

Task 2 achievements 2: Understanding facility backgrounds - PSI

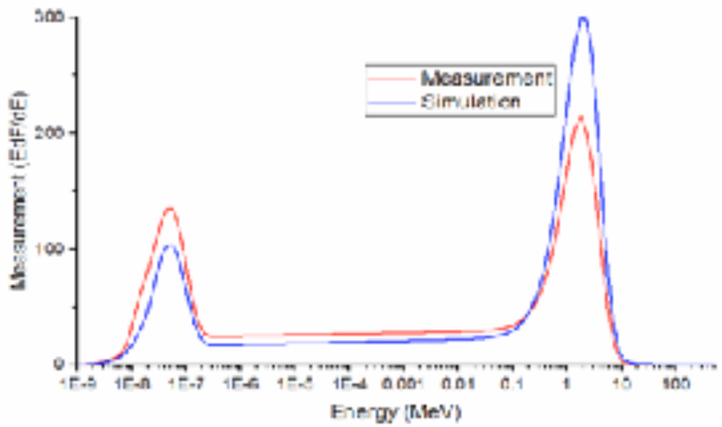
AKR-2 Dresden measurements & simulations



Cross section of the reactor setup and the two measurement positions

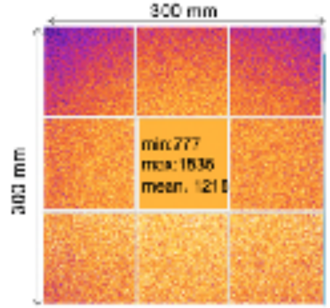


Measurement setup at position A



Measurements and Simulations for Position A

Data evaluation / modelling done for position A, as the spheres are not fully illuminated in position B which thus requires more complex data interpretation



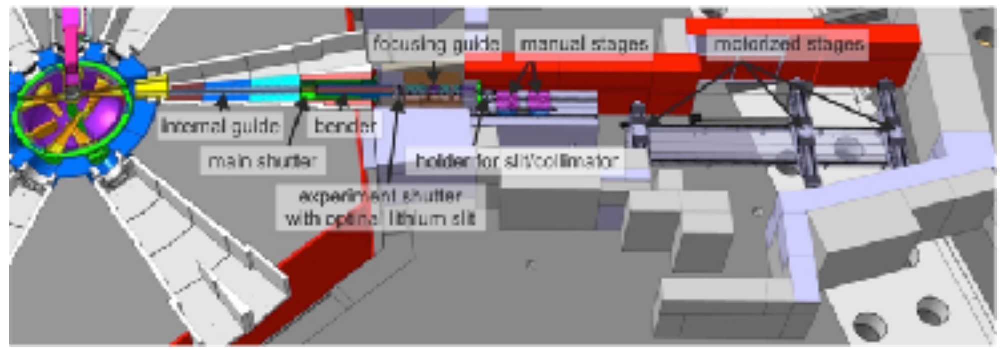
Thermal Neutron flux distribution of position A

This project was funded by the European Union (GA 654000)

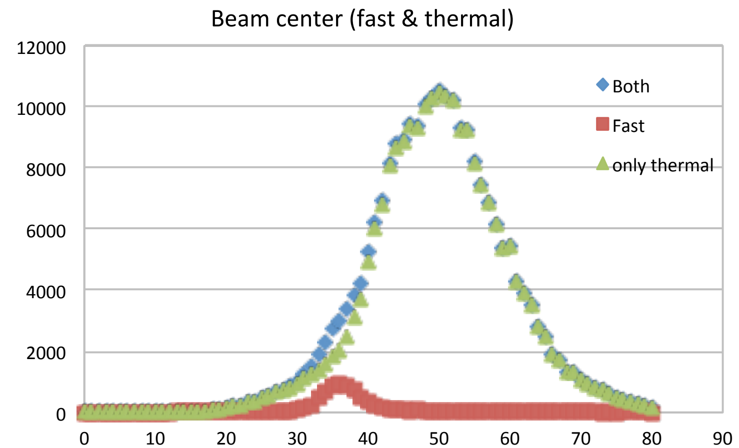
Task 2 achievements 2: Understanding facility backgrounds - PSI

Use of the BSS spectrometer with BOA@PSI

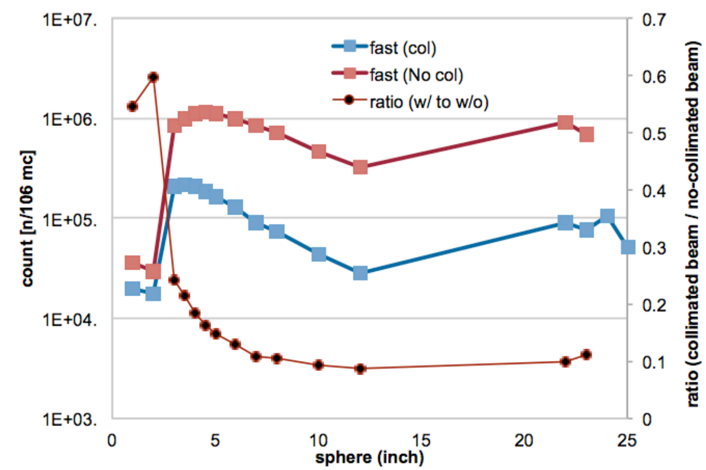
BSS-system with PE moderators and Cu shells



BOA beamline



Fast and thermal neutron flux distribution at the BOA beamline

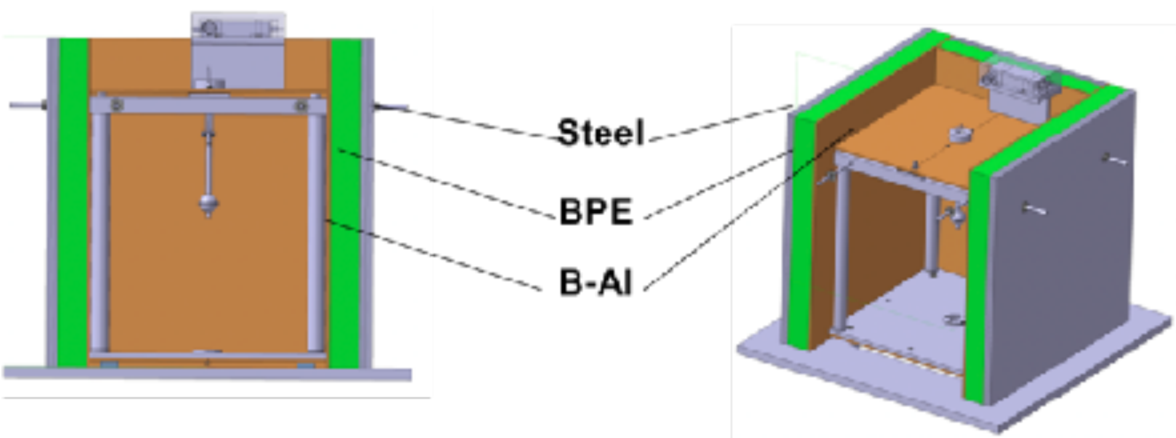


BOA – Fast neutron spectrum measured by the BSS system

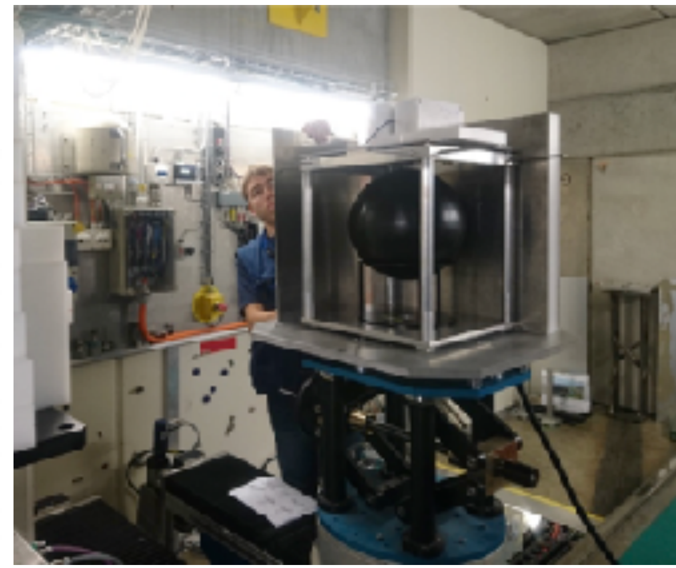
This project was funded by the European Union (GA no. 654000)

Task 2 achievements 2: Understanding facility backgrounds - PSI

Shielding-box setup



Shielding box for material investigations



Measurement setup at BOA beamline

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

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

Task 2 achievements 2: Understanding facility backgrounds - PSI

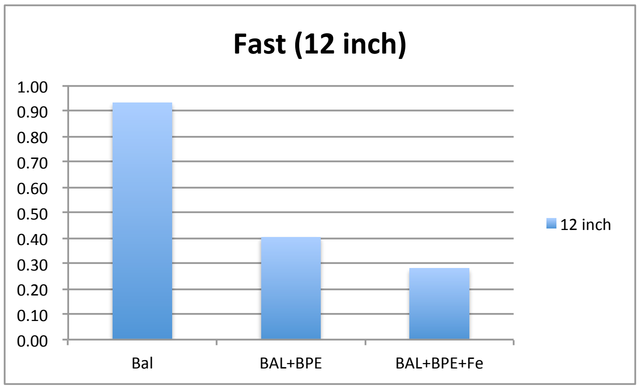


Figure 8a: Fast neutron transmission

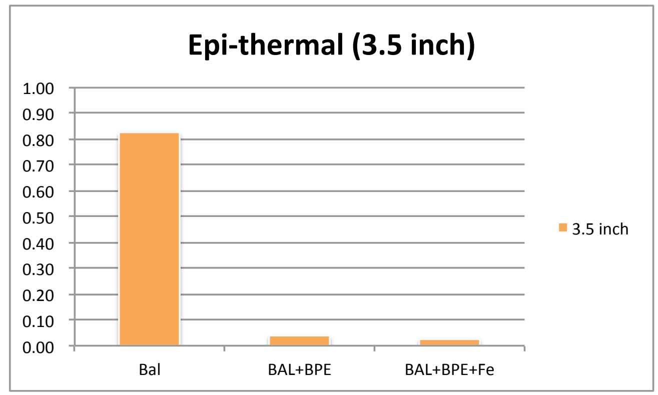


Figure 8b: Epi-thermal neutron transmission

Created for

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

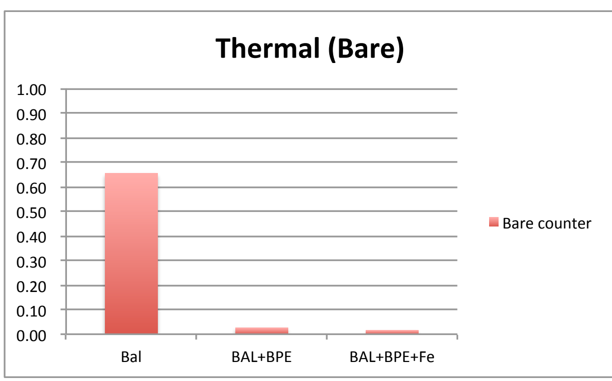
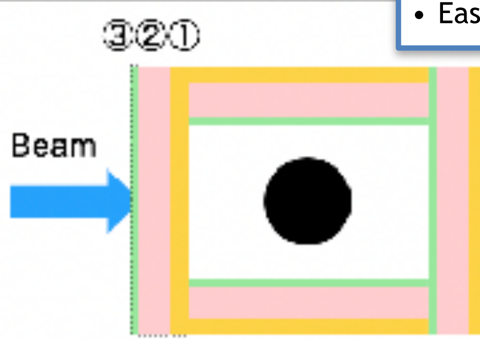


Figure 8c: Thermal neutron transmission

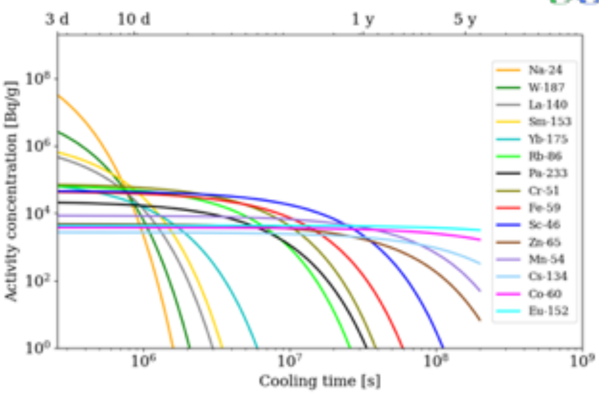


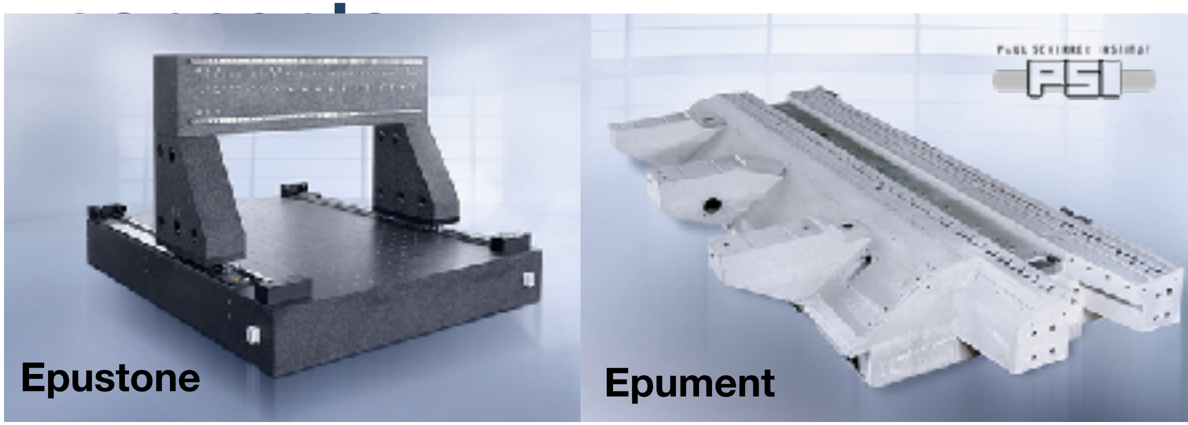
1 Yellow is steel

2 Pink layer is B-PE

3 Green layer is BAl

Task 2 achievements 3: New shielding



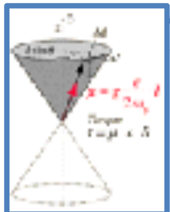


- 14 different mineral cast samples were investigated.
- Epument 130 and Epument 145 are comparible to concrete
- Epustone 161 is specially made as a replacement for granite
- Epument is usually without Boron (test samples have 1 and 3 % B4C)

Probennummer	Bezeichnung	Basismineralguss	Modifizierung	Anzahl Prismen
1	17:013_1	EPUMENT 130/3 A1	Standard	6
2	17:014_2	EPUMENT 140/3 A1	+ 1% Borcarbid auf Komp. C	6
3	17:013_3	EPUMENT 130/3 A1	+ 3% Borcarbid auf Komp. C	6
4	17:017_1	EPUMENT 130/3 A1	ohne EFA (Opalia)	6
5	17:017_2	EPUMENT 130/3 A1	ohne EFA (Opalia) + 1% Borcarbid auf Komp. C	6
6	17:017_3	EPUMENT 130/3 A1	ohne EFA (Opalia) + 3% Borcarbid auf Komp. C	6
7	17:023_1	EPUMENT 161. St2	Standard	6
8	17:023_2	EPUMENT 161. St2	+ 1% Borcarbid auf Komp. C	6
9	17:023_3	EPUMENT 161. St2	+ 3% Borcarbid auf Komp. C	6
10	17:023_4	EPUMENT 161. St2	+ 1% Borcarbid auf Komp. C (- 1% Komp. C)	6
11	17:024_1	EPUMENT 161. St2	+ 3% Borcarbid auf Komp. C (- 1% Komp. C)	6
12	17:025_1	EPUMENT 145 B1	ohne EFA (Opalia), ohne Basalt B-11	6
13	17:025_2	EPUMENT 145 B1	ohne EFA (Opalia), ohne Basalt B-11, + 1% Borcarbid auf Komp. C	6
14	17:025_3	EPUMENT 145 B1	ohne EFA (Opalia), ohne Basalt B-11, + 3% Borcarbid auf Komp. C	6
			Summe	84

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

Task 3 achievement: Feasibility of Larmor-tech at ESS instruments



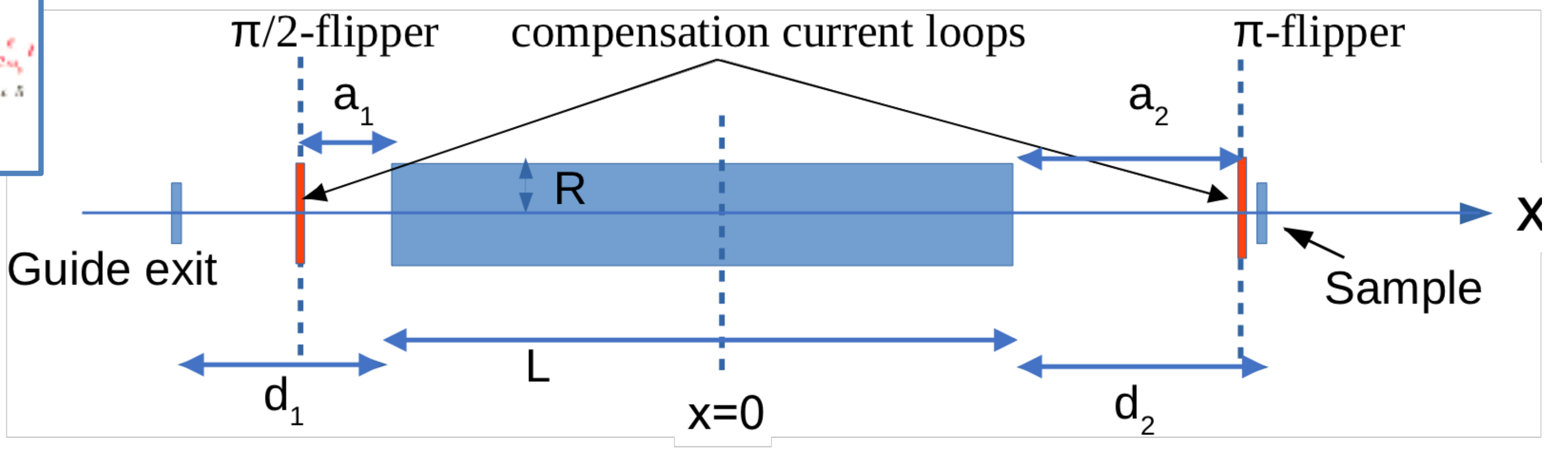
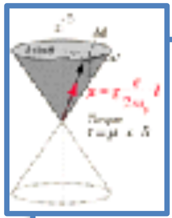


Fig. 1: Schematic representation of the configuration considered for the first arm of a NSE spectrometer. The layout is characterized by the lengths L, a_1, a_2 and R. The blue rectangular area represents the main precession coil.

Results show a clear gain with the "pancake moderator".
Rectangular beam cross-sections height / width ratio ~ 1:4,
ala ESS "pancake moderator" beams lead improved the homogeneity of the magnetic field integrals by at least 30 %.
Relative inhomogeneities become worse for shorter coils,
in order to reach high resolution, the length of the instruments cannot be reduced, i.e. not be more compact than e.g. at the ILL.

An IN15-like instrument will have gain in resolution at the ESS

Task 3 achievement: Feasibility of Larmor-tech at ESS instruments



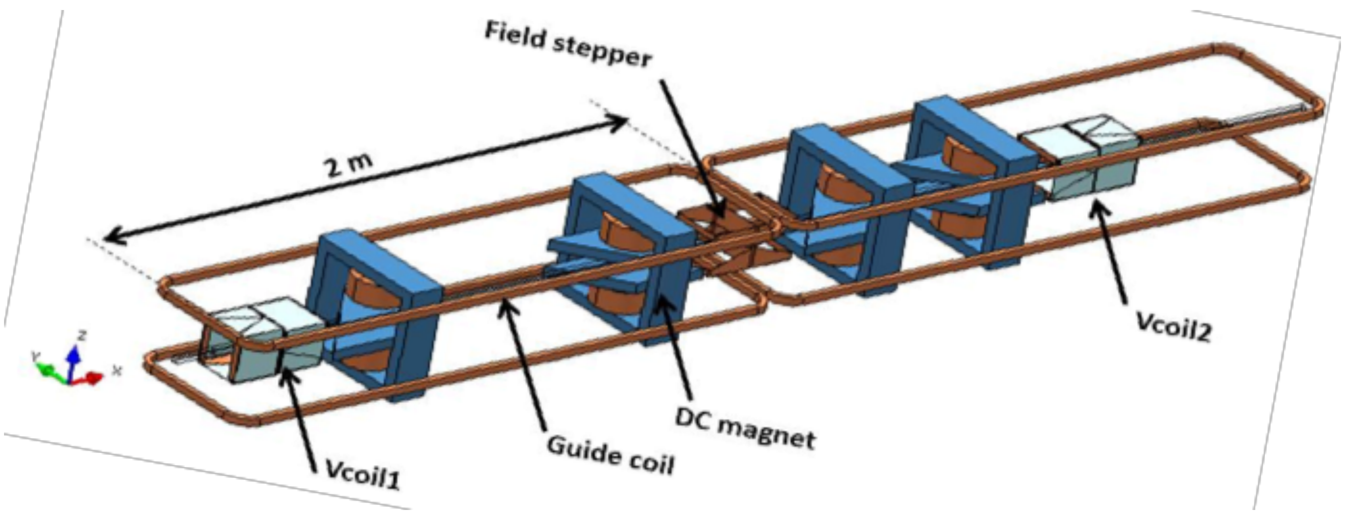


Figure 2: Schematic drawing of SEMSANS arrangement considered for the magnetic field calculations. The white boxes illustrate the Vcoils, which act as π/2 flippers, the blue components are DC magnets with parallelogram shaped pole shoes, the central coil is a field stepper. The long upper and lower create a homogenous magnetic field, which guides the beam polarisation.

Compact design could be easily implemented as an add-on. Could be installed and removed, according to the experimental requirements and would substantially extend the capabilities of the ESS. Instrument candidate SKADI, would allow simultanes SANS and SEMSANS. Another candidate is ODIN, add-on to be used for high resolution dark field imaging.

→

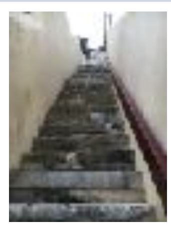
Only practically applicable dark-field method for ESS, by synchronising the fields with the source pulse

Workshop 1:

Neutrons: Cradle to Grave workshop, Coimbra, Portugal, September 6th 2016

- Requirements/Developments for a (bidirectional) Monte Carlo ***variance reduction*** *method applied to* ***neutron beamline transport systems.***

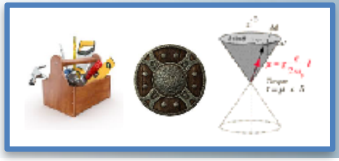
Speaker	Presentation topics	Video link
Peter Willendrup, DTU/ESS	Welcome, agenda, setup (No slides)	(no video)
Erik B Knudsen, DTU	McStas-MCNP interface solutions	Video #1 (partial)
Thomas Kittelmann, ESS	MCPL "Monte Carlo Particle List" interchange format	Video #1
Xiao Xiao Cai, DTU/ESS	NCrystal, coherent scattering library for Geant4	Video #1
Emmanouela Rantsiou, PSI	Code, simulations and experiments including guides at BOA, PSI	Video #2
Douglas Di Julio, ESS	Metaheuristics for Vitess, simulation of laminar shielding problems (**Talk cancelled**)	(no video)
Phil Bentley, ESS	Neutron acceptance diagram methods	Video #2
Steven Lilley, STFC	Initial experiences using Advantg in fusion and spallation	Video #2
Stuart Ansell, ESS	"MCNP model builder / CombLayer, "fast" beamline constructor, variance reduction. Instrument background calculations for long beamlines at the ESS."	Video #3
Jan Saroun, NPI	RESTRAX/SIMRES reverse tracing, optimisation, McStas *reverse tracing* prototype	Video #3



Website with talks and videos available at http://coimbra2016.essworkshop.org

(Videos also on McStas YouTube channel)

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



Workshop 2:

Innovative Simulation Tools, Shielding and Instrumentation 2019 (ISTSI2019) ECNS satellite

Talk title	Speaker
Welcome and SINE2020 / WP8 introduction	Peter Willendrup, DTU/ESS
News from the RESTRAX/SIMRES project, including MCPL support and McStas bindings for SIMRES	Jan Šaroun, NPI
News from the Vitess project including MCPL support	Egor Vezhlev, FZJ
News from the McStas project, including interoperability solutions for SIMRES, Vitess and MCNP	Peter Willendrup, DTU/ESS
Developments in the MCPL software framework	Thomas Kittelmann, ESS
An optimised neutron super mirror patch for MCNP, with applications (ESS-Bilbao)	Esben Klinkby, DTU/ESS
CombLayer-driven MCNP-McStas simulations for simulating instrument signal to noise	Esben Klinkby, DTU/ESS
McStas and Scatter-logger driven calculations of prompt gamma shielding for neutron guides	Rodion Kolevatov, IFE
Studies of relevant design-parameters to enable compact Larmor devices in ESS designs	Katia Pappas, TUDelft
Magnetic field calculations for compact Larmor devices in ESS designs	Michel Thijs, TUDelft
Simulation benchmarks for experiments at the PSI BOA beamline	Erik Knudsen, DTU
Extensions to the Bonner Sphere Spectrometer at PSI, plus experiments and simulation benchmarking for newly developed concrete	Masako Yamada, PSI
Studies of material composition and neutron activation, plus related simulations	Eszter Dian, MTA-EK and Esben Klinkby, DTU/ESS

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

- a SINE2020 WP8 "e-tools" satellite event of ECNS2019.

The workshop is held as a dissemination activity of the WP8 workpackage in the EU SINE2020 Project and is open to all ECNS2019 participants

Website with talks available at http://istsi2019.essworkshop.org

Access to the code, reports, results and examples

https://github.com/McStasMcXtrace/SINE2020WP8

README.md

SINE2020WP8

Repository for software and methods 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

Unless explicitly noted, all software and examples in this repository is licensed under GPL v2.0.

Other files and documentation are licensed under Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License

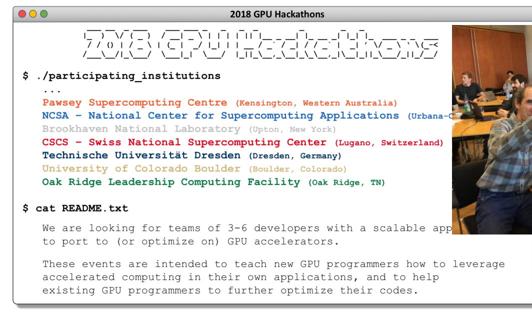
McStas heading for the GPU… March 2018

McCode on GPU?

McStas McXtrace NVIDIA

1st prototype, “null”-instrument with only one component.

Based on NVIDIA compiler technology, PGCC and OpenACC pragmas



More to come in 2019!

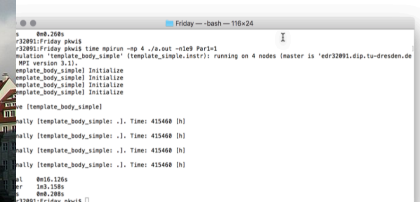
Port heavy part of component to GPU (Shows some potential)

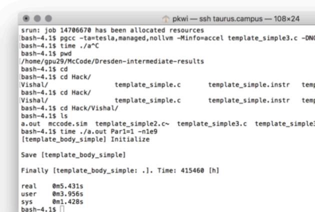
Port neutron loop to GPU
- Lots of code
- Code generation
- Compiles! Speed up today

McStas / McXtrace instrument

CPU MPI 4 cores (95 % usage)

GPU 5% usage





16.12 s (Single core 56.0 s)

5.43 s

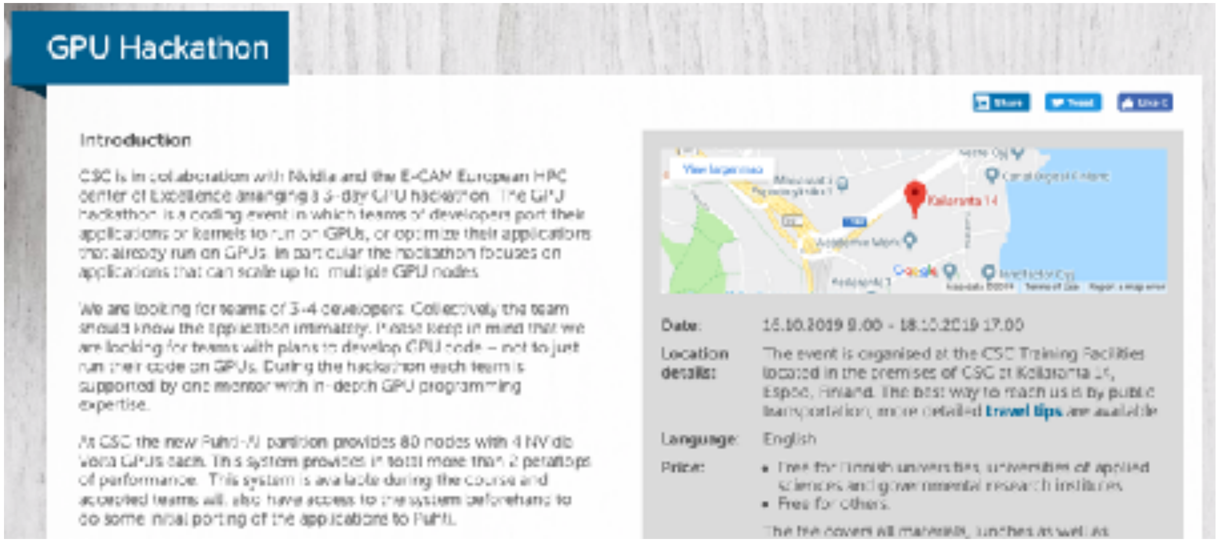
This project was funded by the European Union (GA no. 654000)

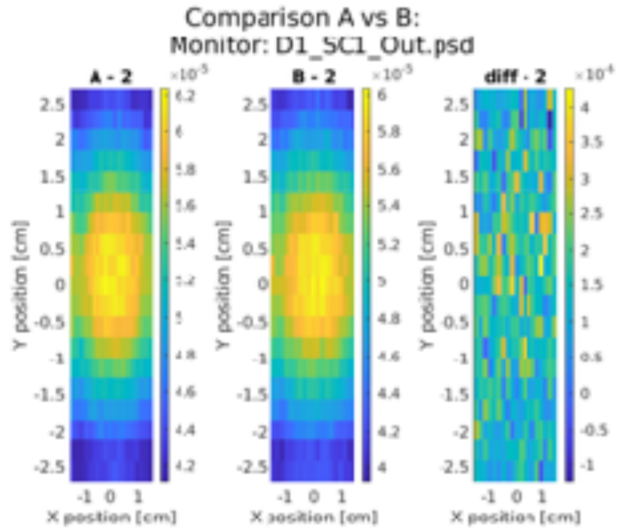
McStas heading for the GPU… October 2019

Rewritten code-generation with automated additions of OpenACC pragmas.

Quite transparent wrt. CPU vs. GPU

First simulations with meaningful output



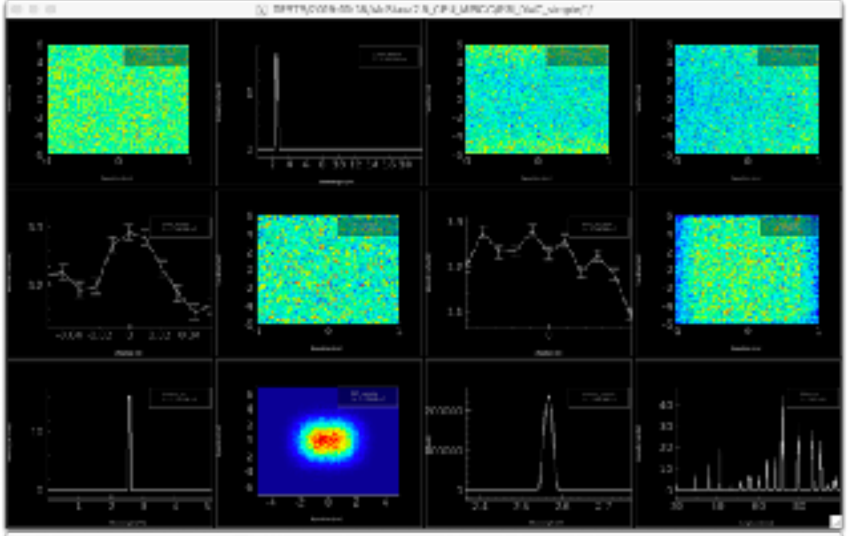


This project was funde
654000)

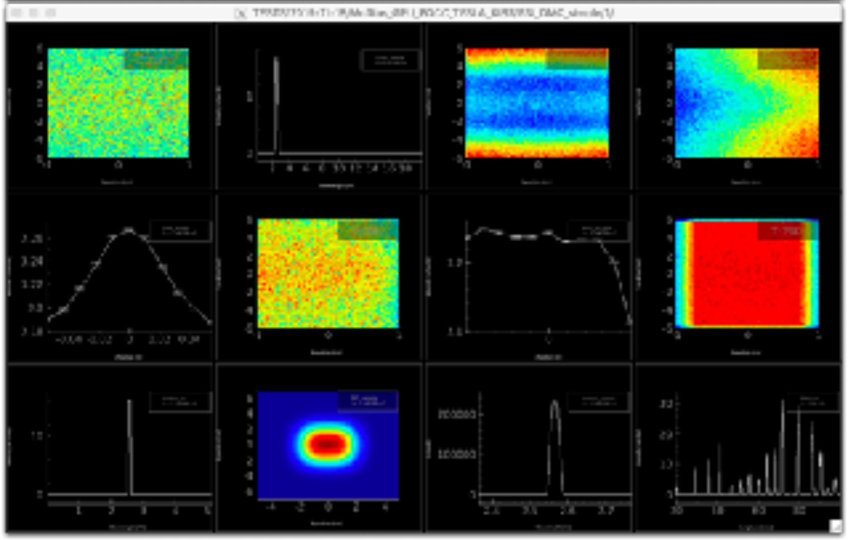
McStas heading for the GPU… Now

9 instruments fully ported, also realistic ones like PSI_DMC

10-core MPI run,
1e7 in 2 secs

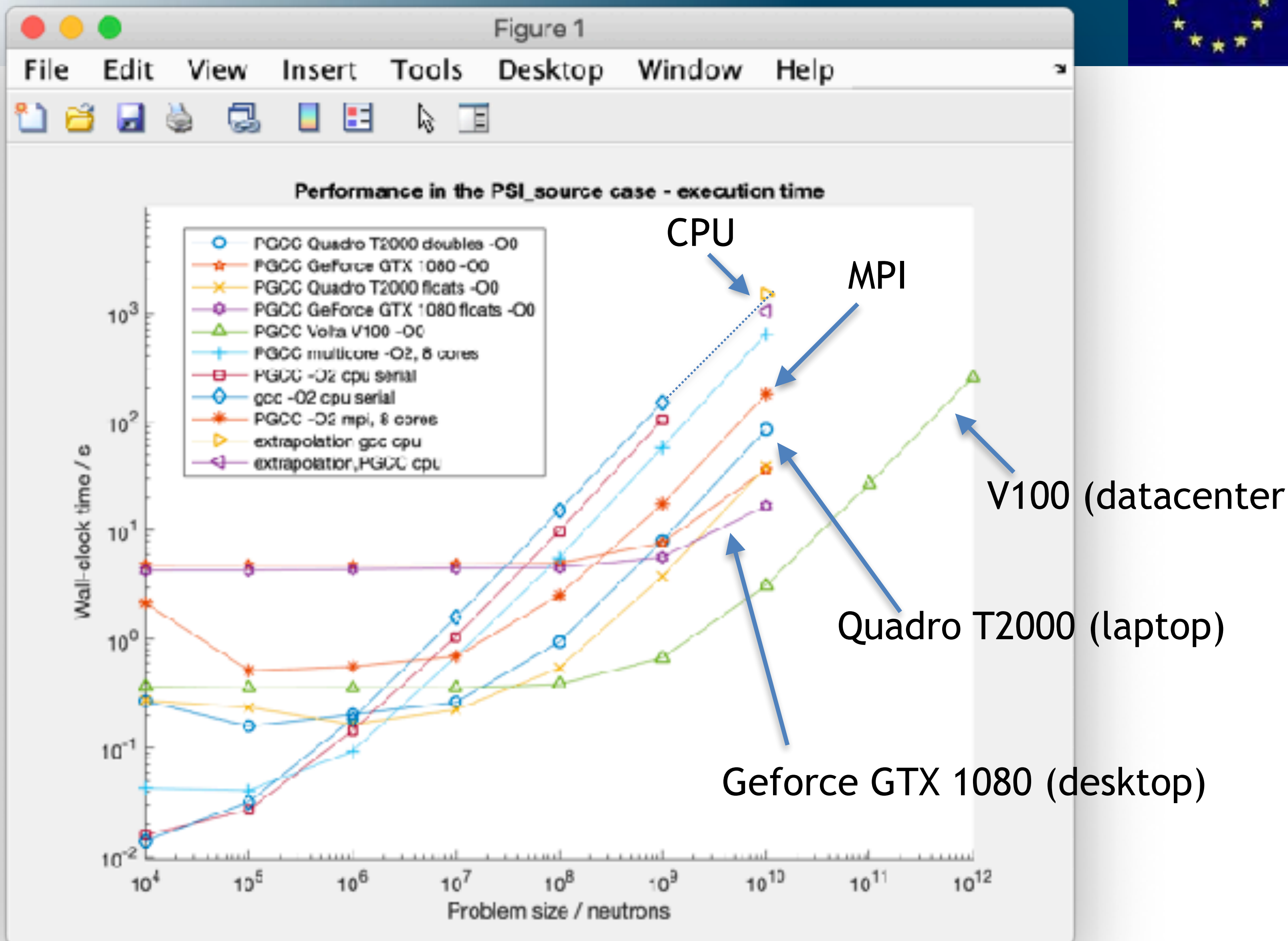


Tesla V100 run,
1e9 in 22 secs

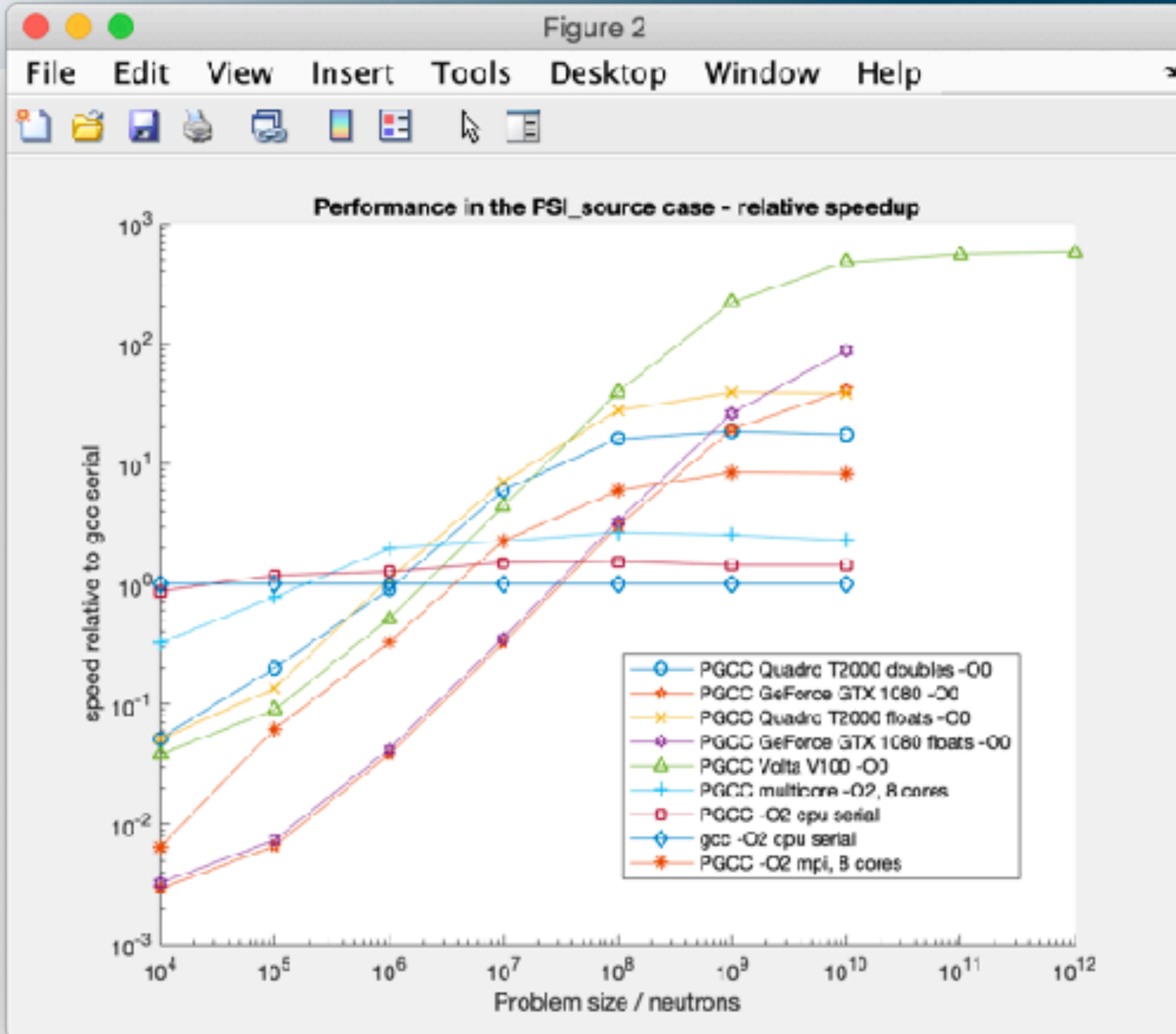


~ 2 orders of magnitude wrt. a
single, modern CPU core

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



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



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

McStas 3.0 - next generation code generator

- Limited-functionality “beta” release to be made public soon (jan-feb) after **2.6 (december)**
  - Expect bugs!
  - Only a subset of components / instruments
  - Event interchange with 2.6 possible via MCPL

- Main purpose: **get this working in ‘the wild’**
  - Your instruments will likely **require (limited) rewriting**
    - E.g. the declare section **cannot include assignments**
  - Your own components will **likely require rewriting**
    - E.g. the declare section **cannot include assignments**
    - Arrays must be declared/initialized using a new set of functions (i.e. not double PSD_I[nx][ny] with definition parms)

- Hence some backward compatibility is lost and we need **to increment major release #**

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

Questions?