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DTU contribution to the CRP

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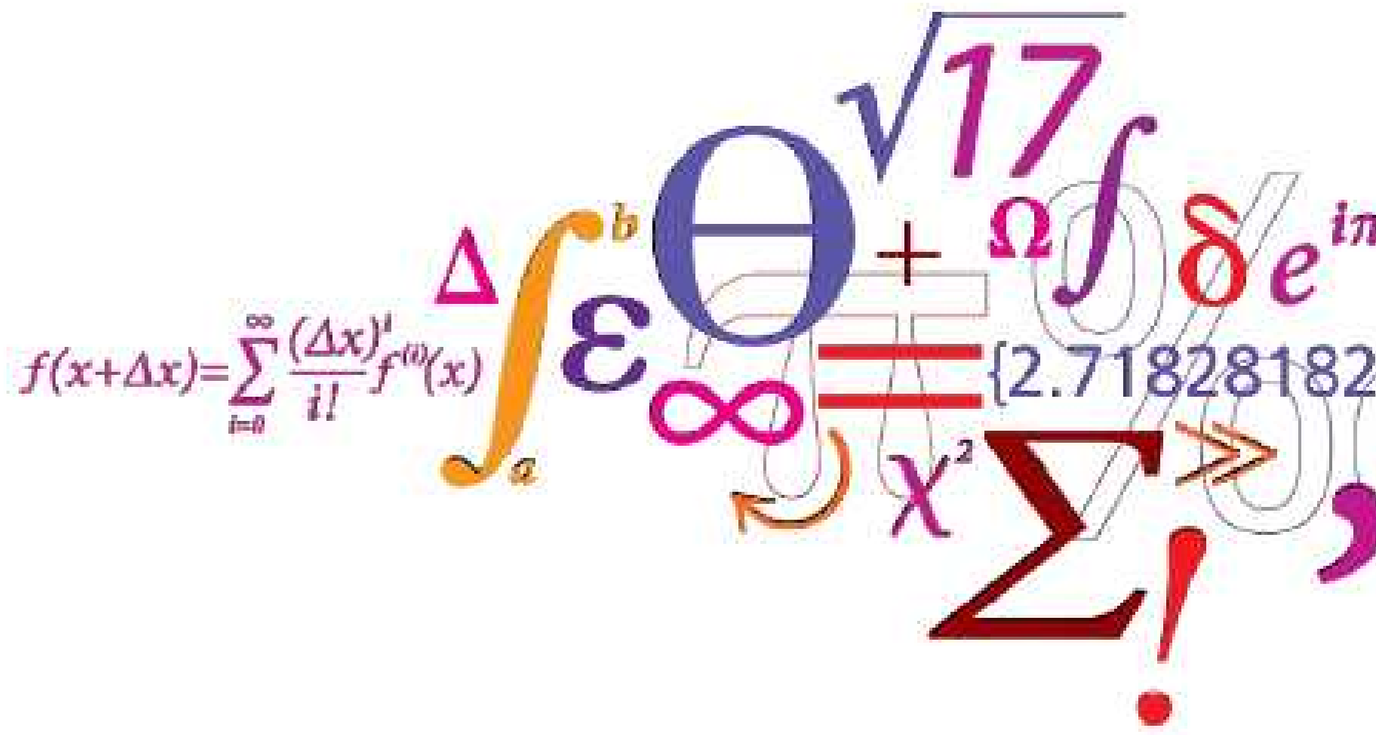
DTU contribution to the CRP

Esben Klinkby,
Bent Lauritzen &
Troels Schönfeldt
DTU Nutech

Peter Willendrup
DTU Physics



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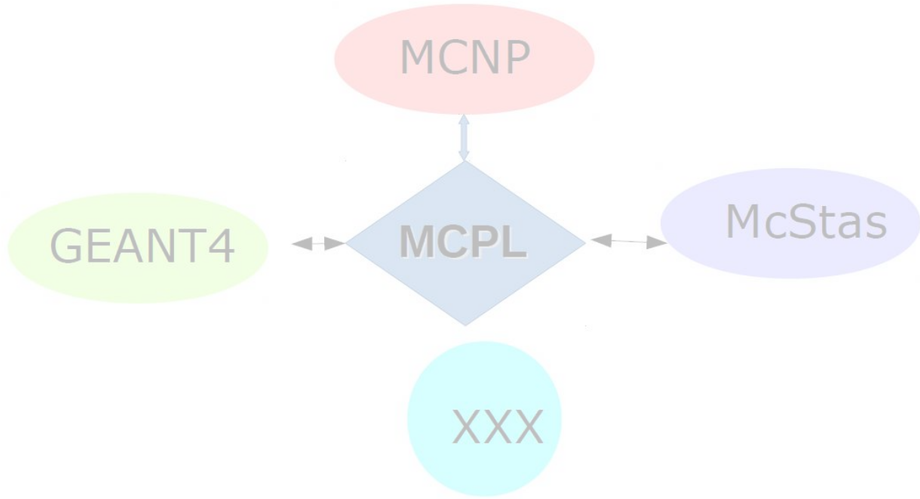
Topics



- 1) Interfacing software: MCNP, McStas, ROOT & Geant4
- 2) ESS moderator design
- 3) New materials - nanodiamonds

$$f(0) = -\frac{2m}{\hbar^2} V R^3 \left(\frac{\sin(qR)}{(qR)^3} - \frac{\cos(qR)}{(qR)^2} \right)$$

1) Software integration: MCNP-McStas

Task 4.1.a.: *Improve interface between neutron transport codes (e.g. MCNP) and modern instrumentation ray-tracing codes (e.g. McStas)*

- The software allowing propagating individual neutrons (i.e., the actual neutron state parameters) from MCNP to McStas and vice versa has been refined, and a production release is made publicly:
- https://github.com/McStasMcXtrace/IAEA-CRP.

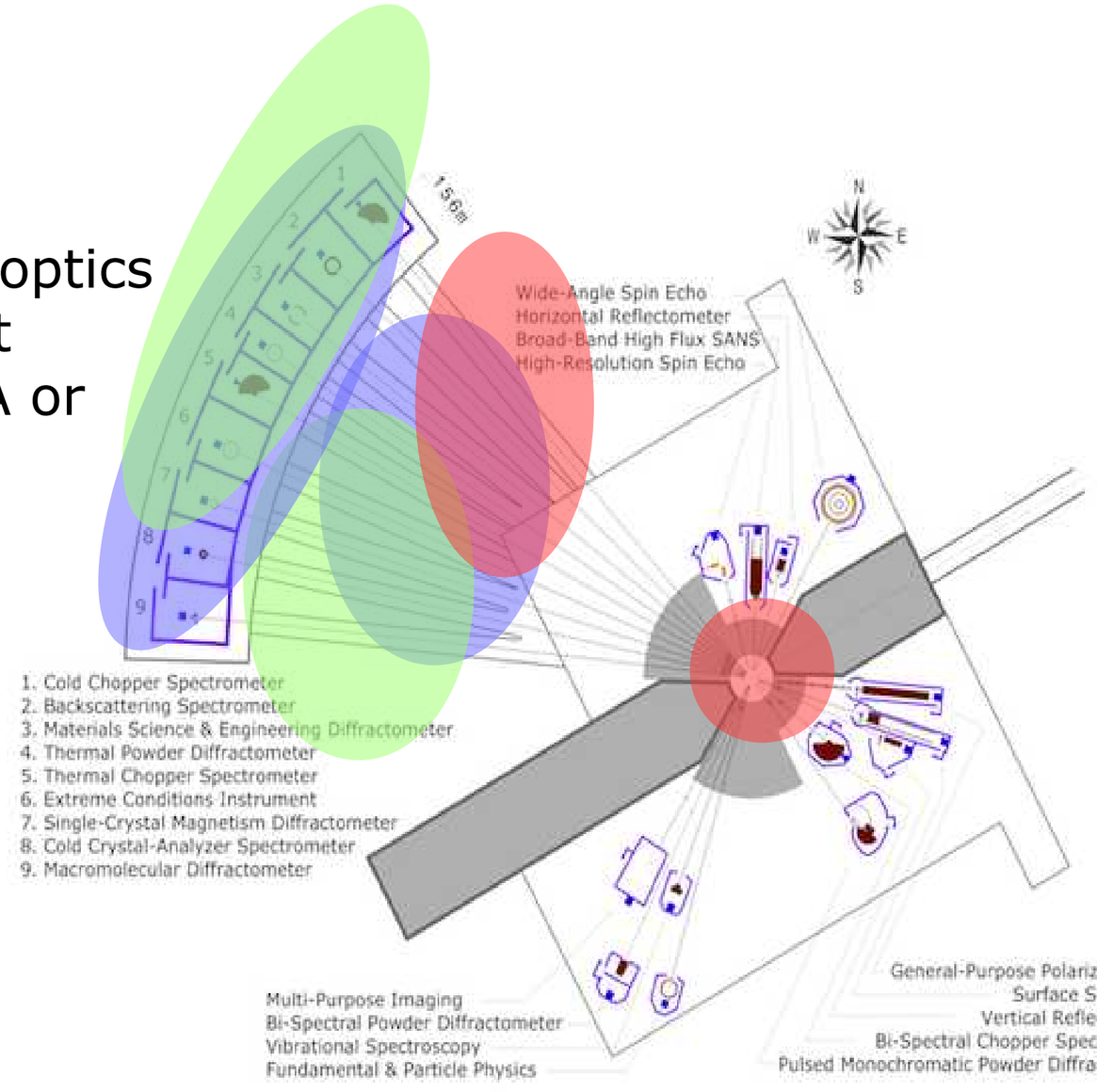
- Contains:
  - The actual software
  - Examples of usage
  - Links to relevant publications
    http://dx.doi.org/10.1016/j.nima.2013.11.071
    http://iopscience.iop.org/article/10.1088/1742-6596/528/1/012032

- Driven in parts by specific facility needs, work is ongoing to expand the scope

1) Software integration: ESS neutron software overview

MCNP: target, moderator, reflector design
McStas: (+g*uide_bot*) for instrument design
GEANT4: for shielding and backgrounds
Vitess & NADS & Particle swarms: shielding & optics
- design documentation for the instrument
MCNP: safety, dose-rates (future use of FLUKA or MARS)
GEANT4: detector design

→ Interfacing is important!
→ MCNP-McStas interface is insufficient
→ A common file format would facilitate 'cradle to grave' simulations, without intermediate loss of information (e.g. through fitting etc)

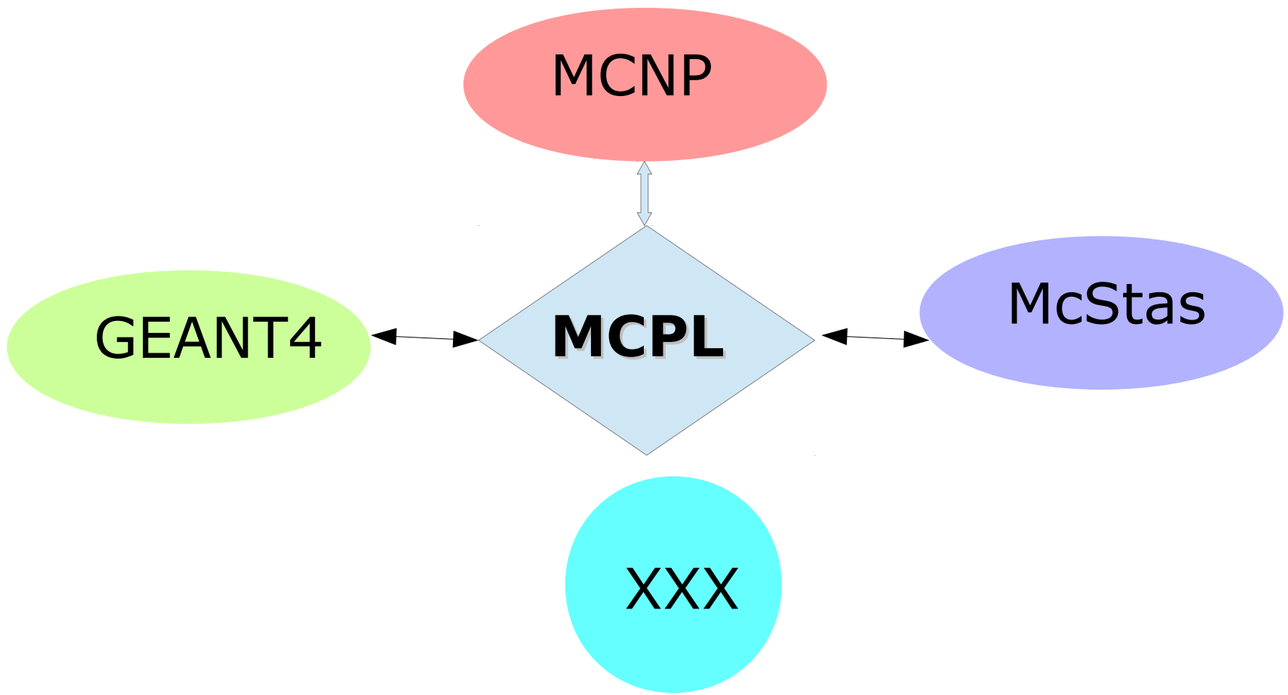


Monte Carlo Particle List: MCPL

4

1) Software integration:
MCPL: MCNP-Geant4-McStas-XXX coupling

- Rather than using converters to read the MCNP SSW format directly from within McStas, an intermediate event format is defined, containing the full event information
- *position, momentum, weight, time, particle ID, custom flags*



- The data format is binary for performance reasons, test-functionality allow the user to view the file content

1) Software integration:
MCPL: MCNP-Geant4-McStas-XXX coupling

```
klinkby@laptop:~/projects/dg_dgcode$ ess_mcpl_tool ./packages/Validation/UnitTests/MCPLTests/data/reffile_skip123.mcpl
Opened MCPL file reffile_skip123.mcpl:

 Basic info
   Format             : MCPL-2
   No. of particles   : 123
   Header storage     : 59 bytes
   Data storage       : 8364 bytes

 Custom meta data
   Source             : "MyMCApp"
   Number of comments : 0
   Number of blobs    : 0

 Particle data format
   User flags         : no
   Polarisation info  : no
   Fixed part. type   : no
   FP precision       : double
   Endianness         : little
   Storage            : 68 bytes/particle

index     pdgcode   ekin[MeV]       x[cm]       y[cm]       z[cm]         ux         uy         uz    time[ms]      weight
    0        2112       1.234           0           0           0          0          1          0           0           1
    1        2112           0           0           0        0.01       0.01          0   -0.99995           0           1
    2        2112       1.234           0           0        0.02       0.02          0     0.9998           0           1
    3        2112           0           0           0        0.03       0.03    -0.99955          0           0           1
    4        2112       1.234           0           0        0.04       0.04          0     0.9992           0           1
    5        2112           0           0           0        0.05       0.05          0   -0.99875           0           1
    6        2112       1.234           0           0        0.06       0.06     0.9982          0           0           1
    7        2112           0           0           0        0.07       0.07          0   -0.99755           0           1
    8        2112       1.234           0           0        0.08       0.08          0    0.99679           0           1
    9        2112           0           0           0        0.09       0.09    -0.99594          0           0           1
```

- Developed within the software framework of the ESS Detector Group – Thomas Kittelmann is the main developer
- Core software (written in c) is stable but some examples + documentation are missing. Expected “release” by autumn 2016. Until then, contact me and/or Thomas for instructions
- First use-case: Geant4 – MCNPX comparisons: arXiv:1509.03036

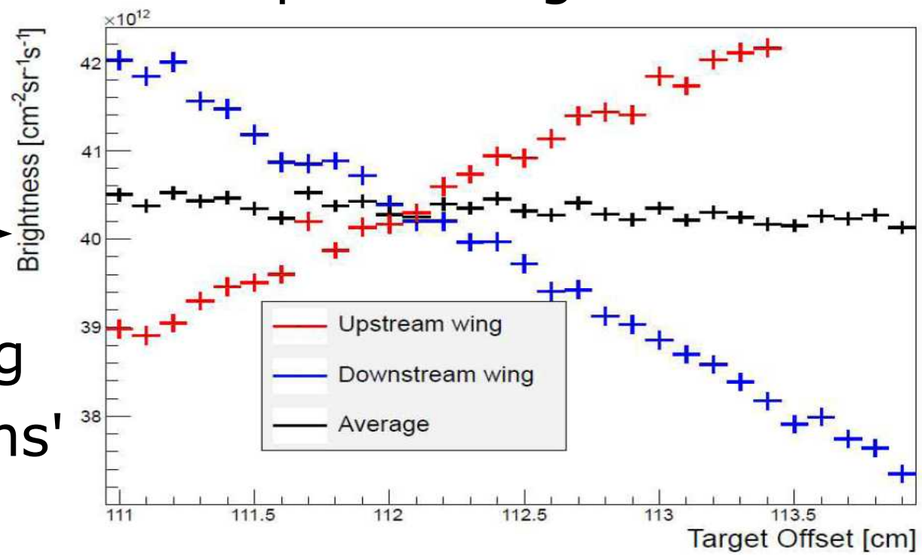
1) Software integration: mctal2root & ssw2root

Task 4.1.e: *Event post-processing*

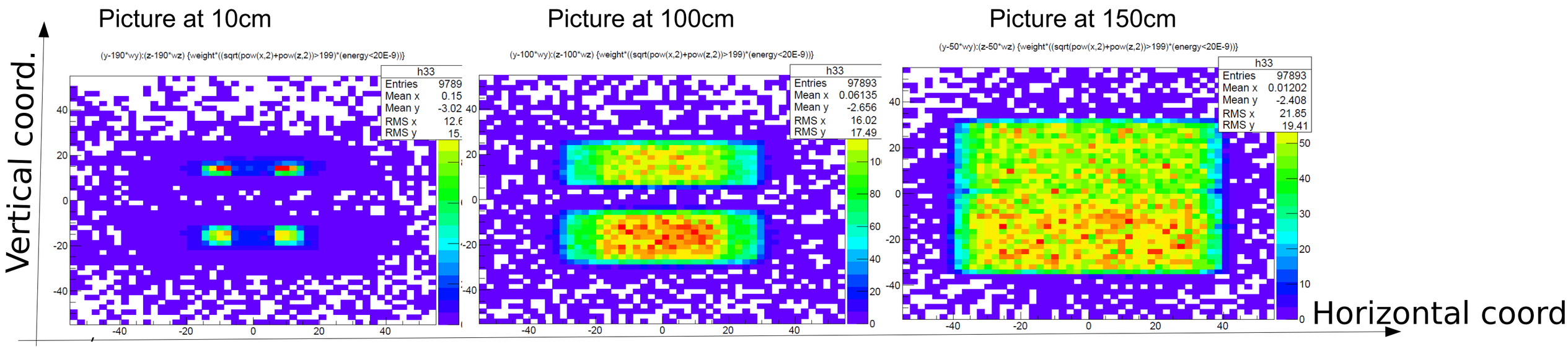
A prototype of the MCNP-root toolset for event post processing has been developed, and is available to the collaboration. These tools are made available from the website: https://github.com/McStasMcXtrace/IAEA-CRP.

Example of usage is shown in the next slides

The software is stable and validated with recent releases of MCNP and ROOT. Future release of MCNP and ROOT software require the event processing tools to be updated.



- `mctal2root`: make MCNP tally available in ROOT format → layout, fitting
- `ssw2root` : hands over individual neutrons crossing a surface→ useful to 'follow the neutrons'



2) Moderator design

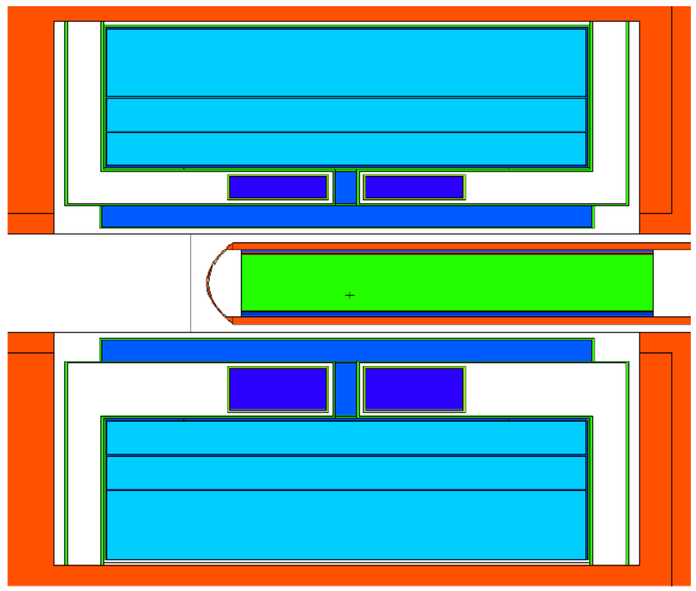
Task 4.3: *Design and/or Deploy New Cold Moderators to Improve Performance of member facilities*

→ Involvement in design of ESS moderators - see talk of Luca Zanini for details

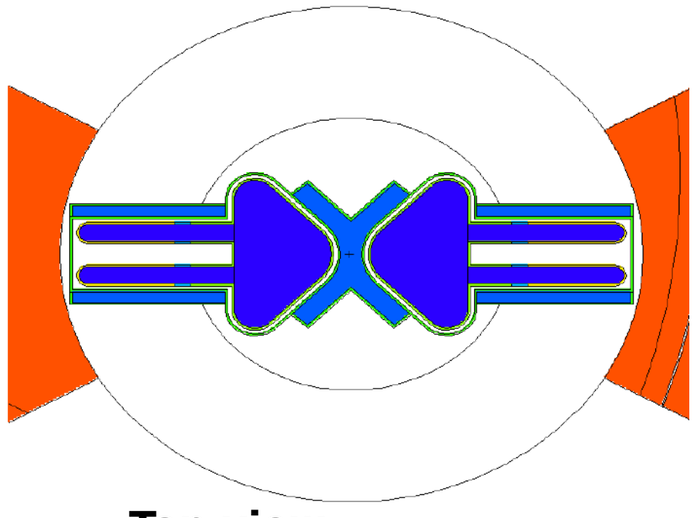
Final decision in spring 2015 => butterfly design

=>flat moderator adopted to meet the needs and constraints of the ESS.

Validation of tools => indirect experimentalverification of the flat moderator concept, carried out through collaboration between CRP partners: J-PARC, ESS & DTU

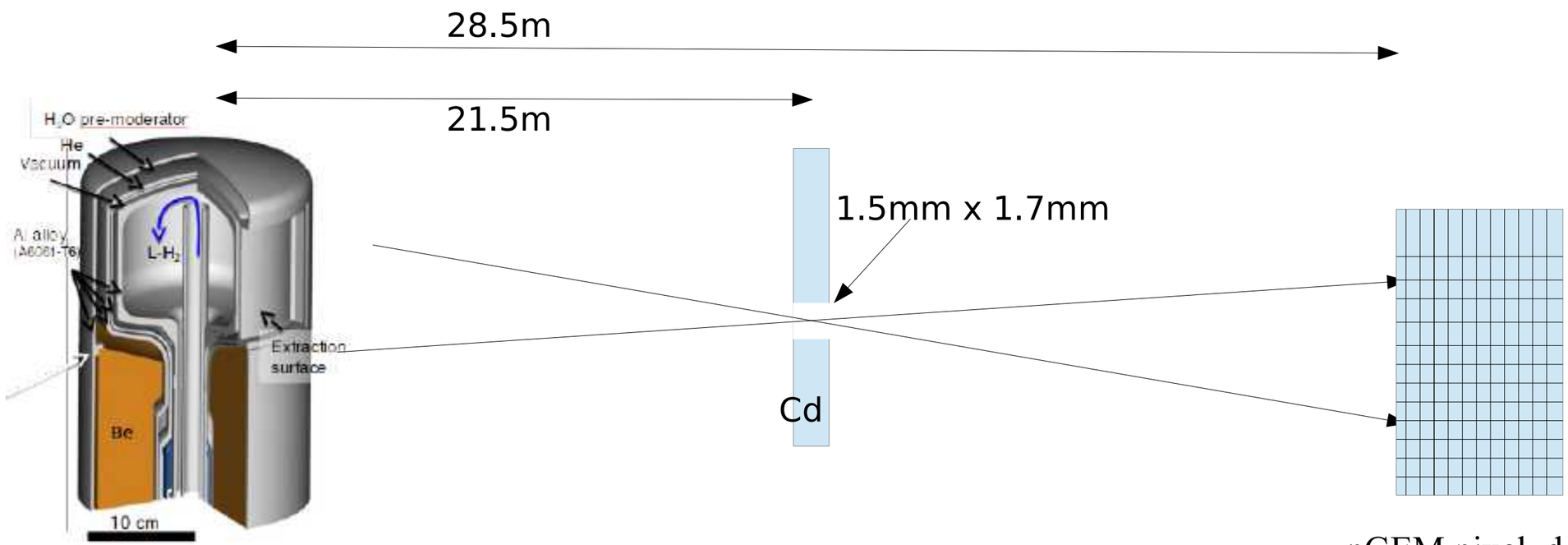


Side view



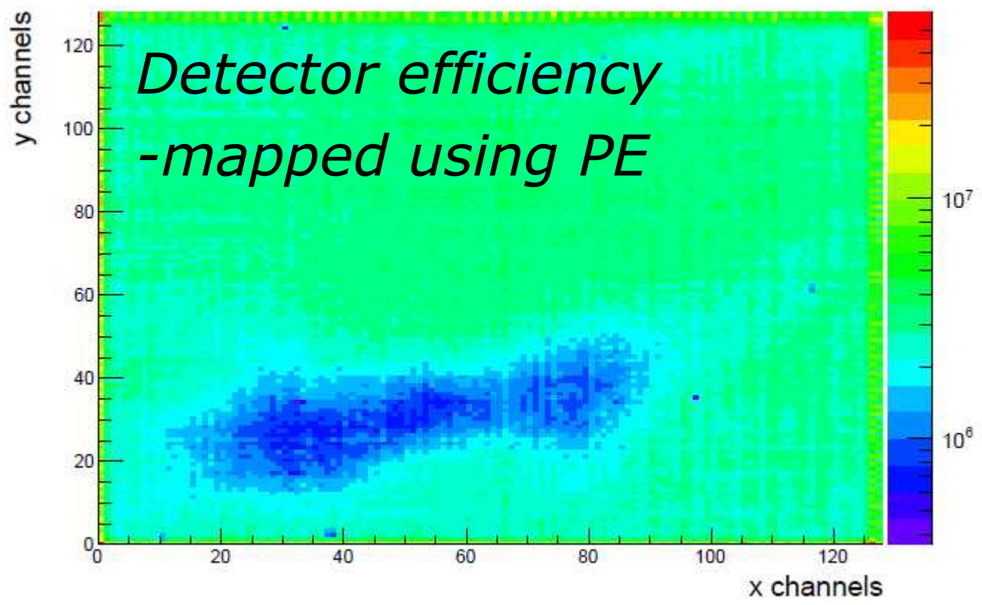
Top view

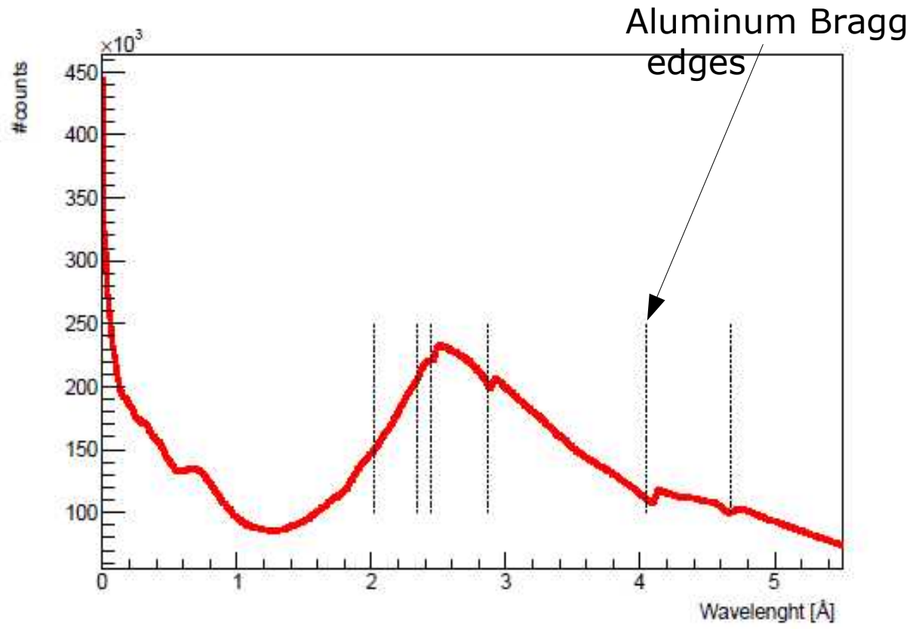
2) Moderator design: validation of the flat moderator



nGEM pixel detector,
Pixel size ~1mm^2,
timing resolution ~1ns

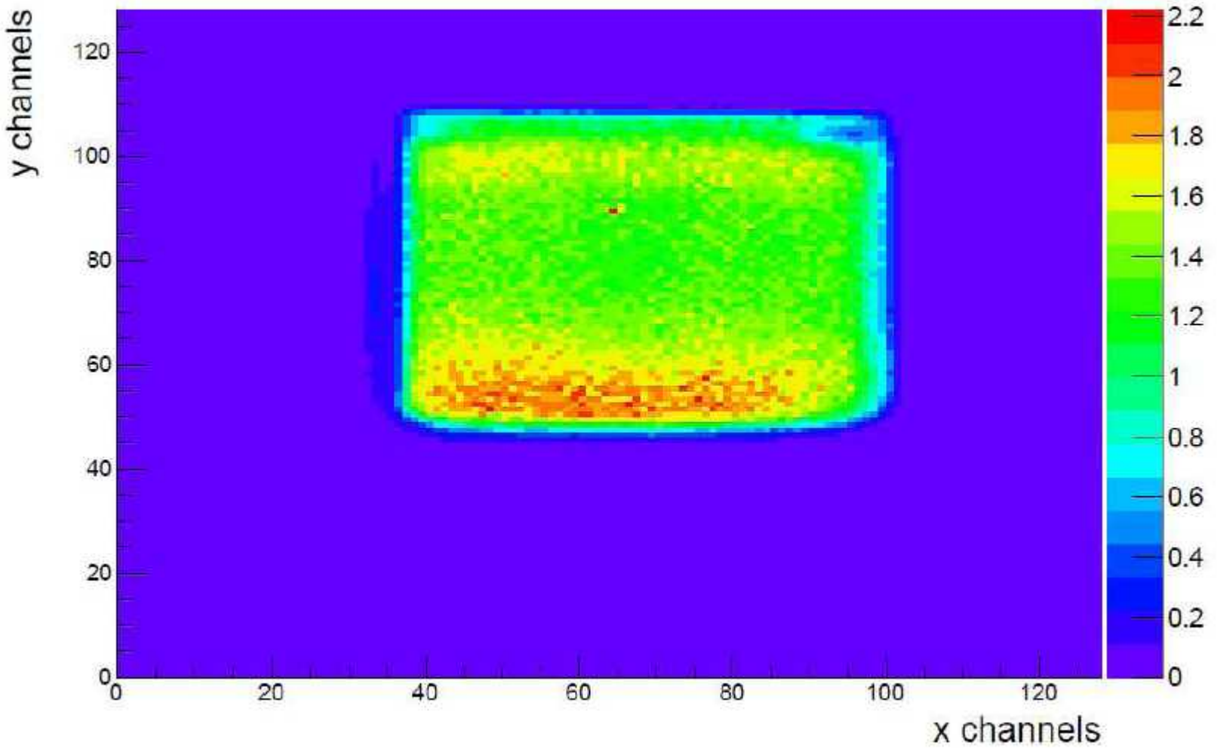
→ Imaging experiment performed in April 2015, measuring the spectral brightness of the coupled JSNS moderator.



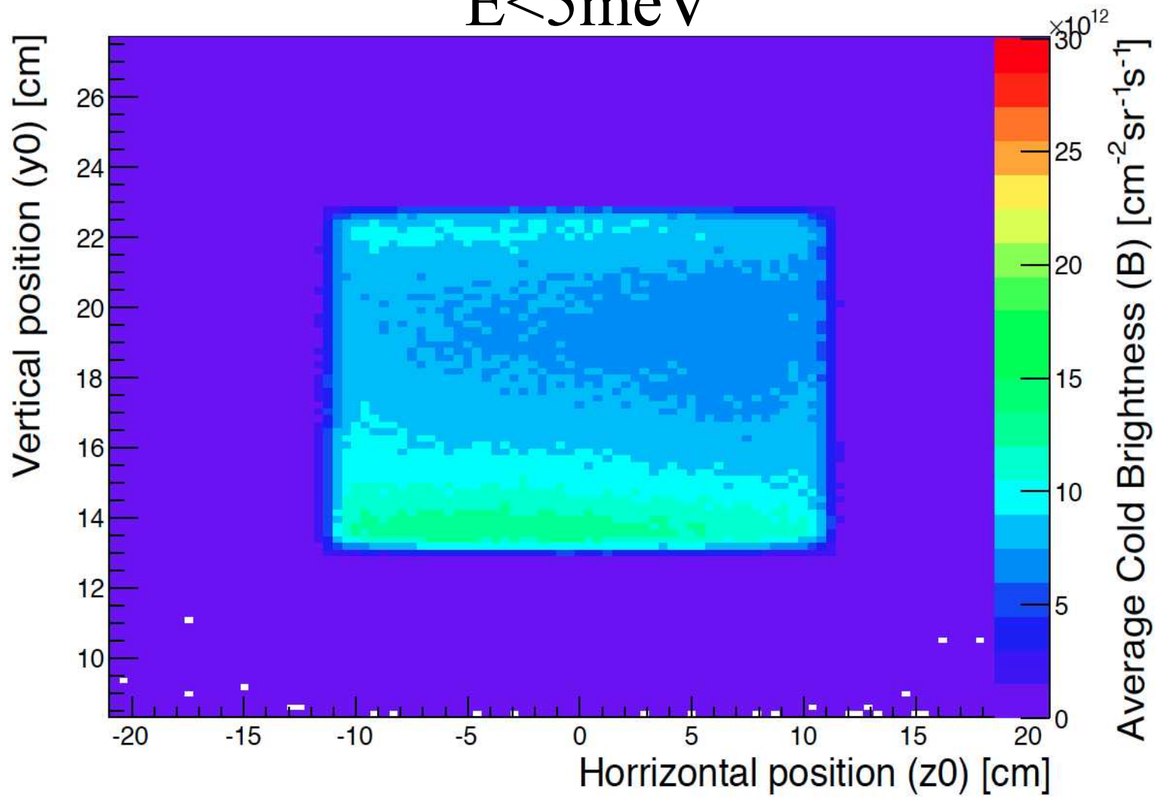


2) Moderator design: validation of the flat moderator

E<5meV



E<5meV



Measurement at J-PARC

Simulations of ESS ~TDR moderator

→ An interesting result in it's own right.
→ Validation of simulation tools
=> We are confident that the flat moderator serves the instruments at ESS well

Publication is pending – draft exists

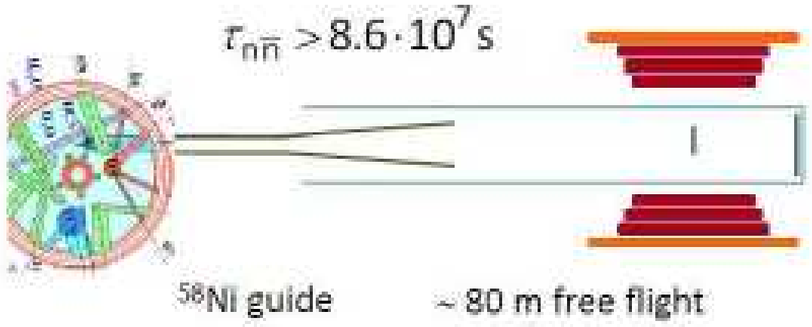
3) Nanodiamonds: Motivation

Task 4.3: *Identify and Characterize New Materials and Geometries Suitable for use in Neutron Moderation Systems*

- Nanodiamond reflectors could potentially boost the performance of ESS instruments.
- Nanodiamond research is closely followed at DTU/ESS, but so far, we have little to contribute the to field
  - Samples shipped to CRP partners
  - Example: reflectors for nnbar search
  - First look towards simulations

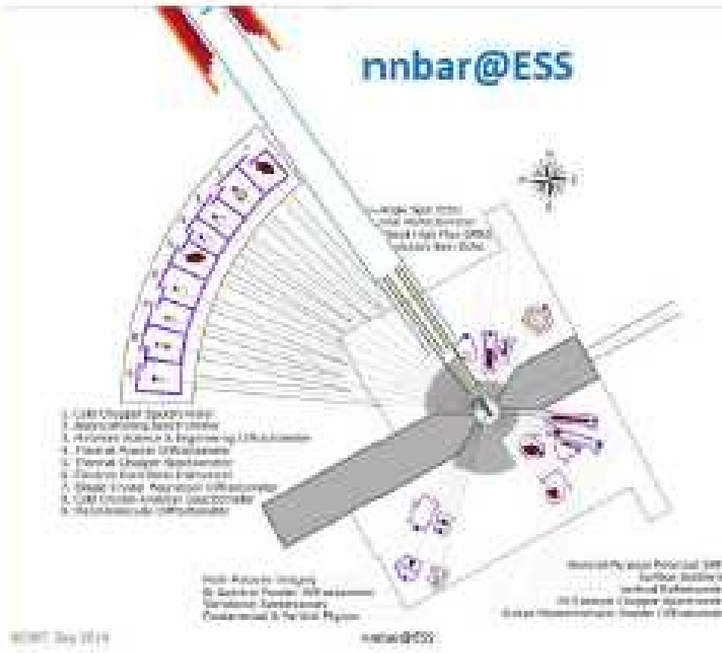
3) Nanodiamonds: Motivation - nnbar

nnbar at ILL

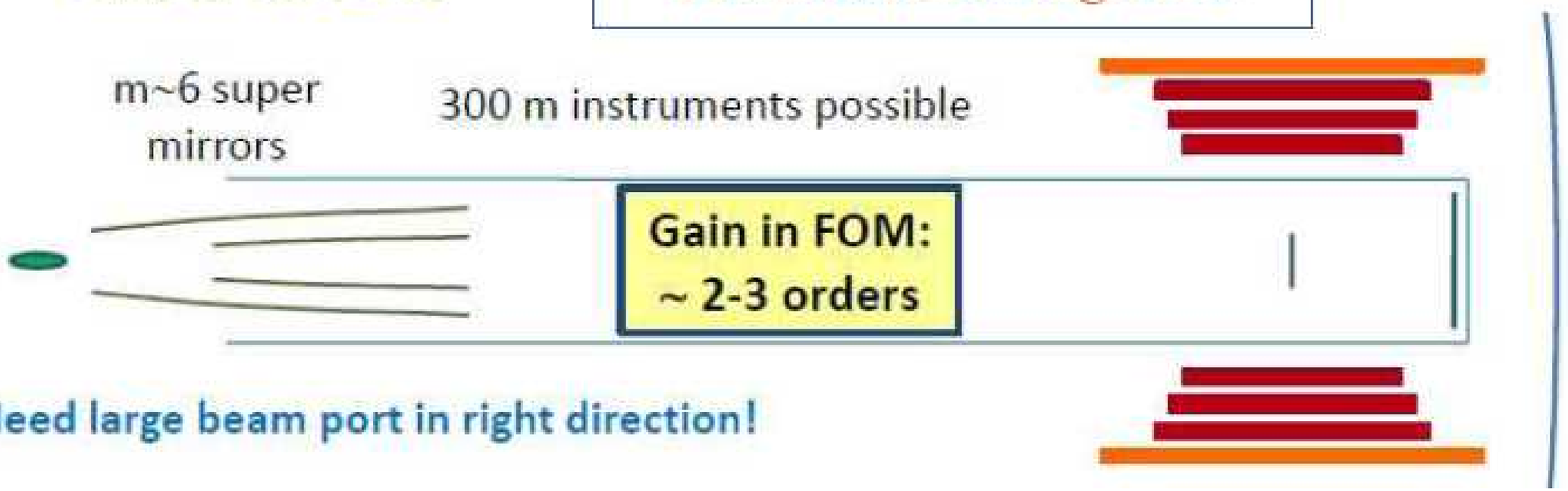


- **Pros**
- Part of initial facility layout
- Pulsed source
- Increased instr. length
- Increased running time
- Better neutron optics
- Placed closer to the source

- **Cons**
- Fast neutron background

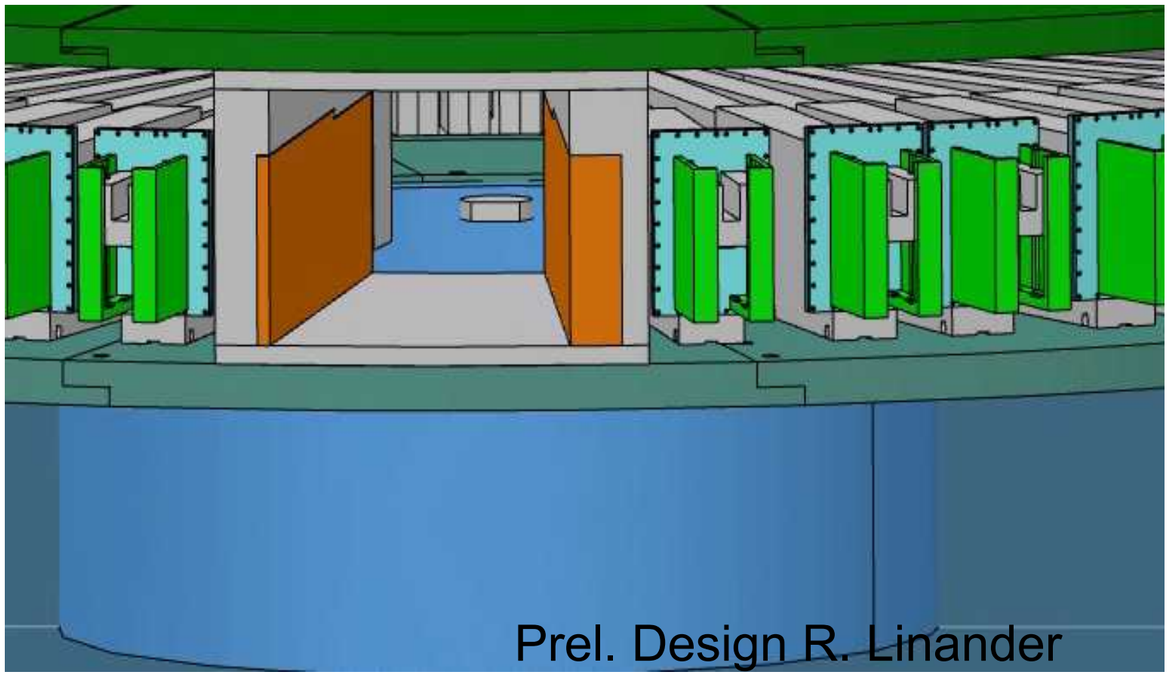


nnbar at ESS

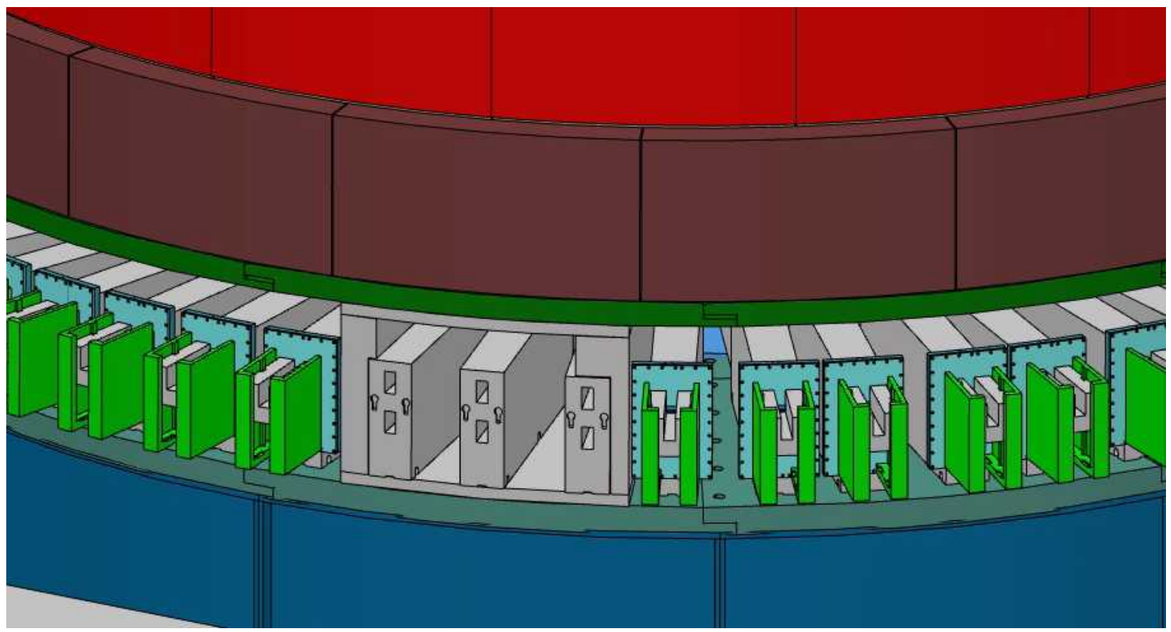


Need large beam port in right direction!

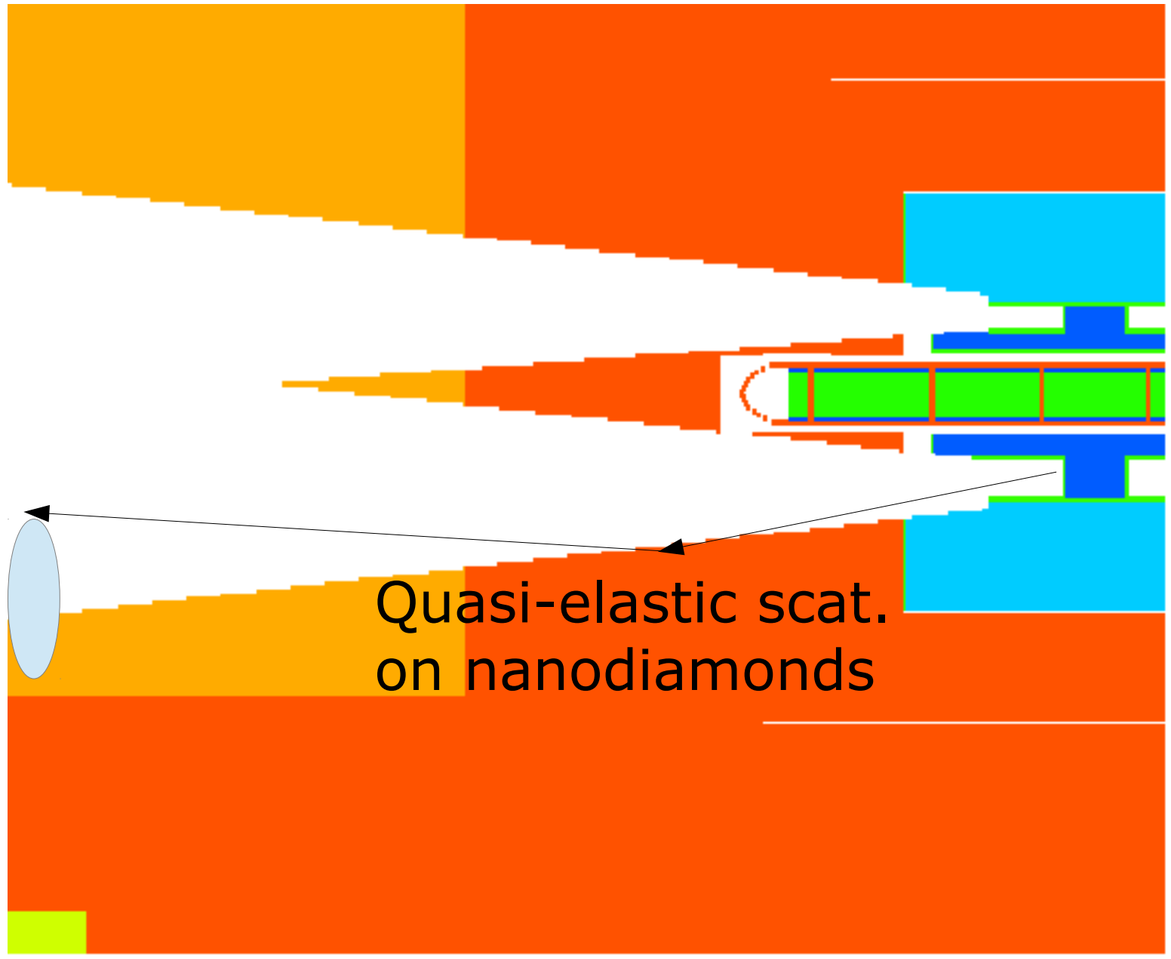
3) Nanodiamonds: Motivation - nnbar



3-5 years running



- Not a scattering instrument => loose requirements on collimation
- Benefits from large extraction area => view both moderators to increase integrated neutron intensity
- Quantification of gains, requires simulations



3) Nanodiamonds: First look toward simulations

- Work started to implement the shown formalism into a McStas module.
- However, I learned that Matt Frost and Yuri Kamyshkov similar effort are also working on this topic, and are more advanced
- Decided to await a stable release, and couple this code to McStas/MCPL
- Also, it would be very useful to have a MCNP implementation – a kernel

$$f(\theta) = -\frac{2m}{\hbar^2} V R^3 \left(\frac{\sin(qR)}{(qR)^3} - \frac{\cos(qR)}{(qR)^2} \right) \quad (1)$$

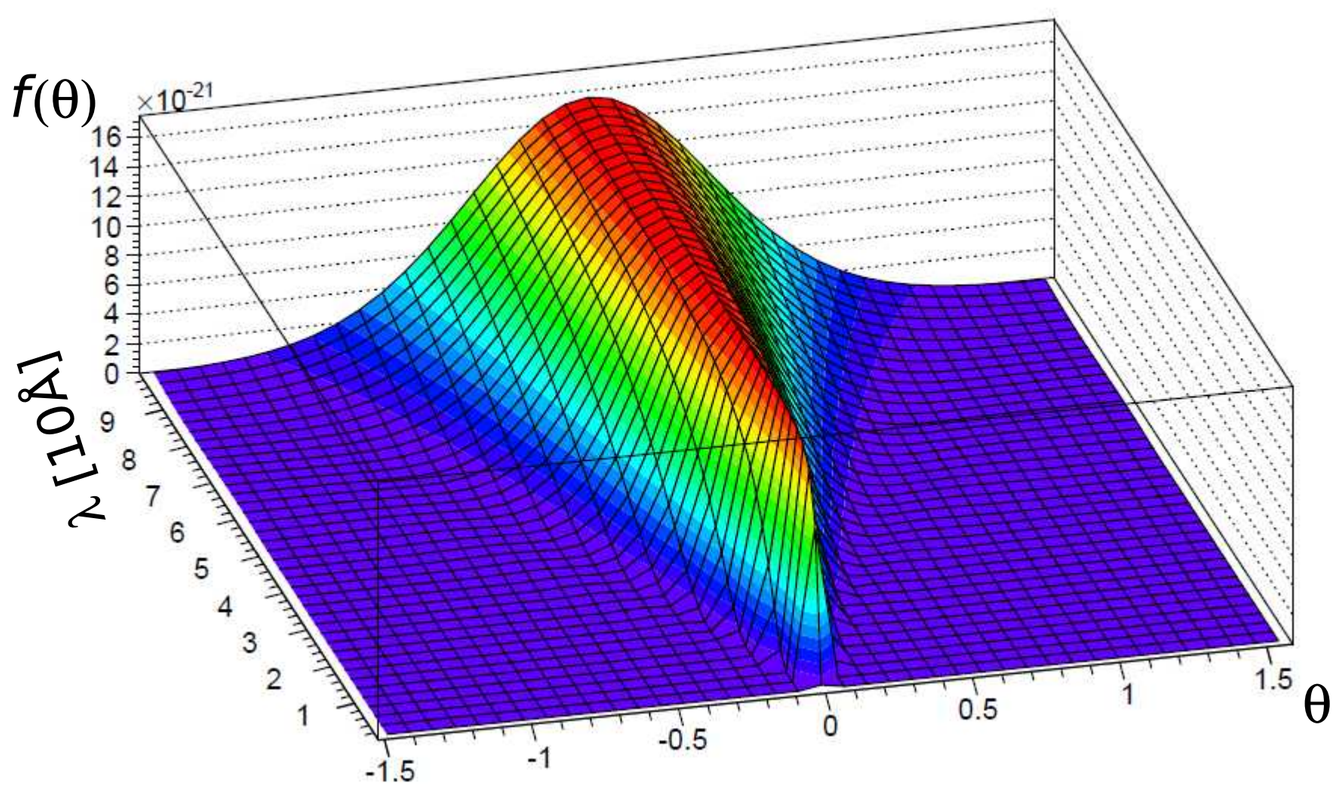
where $q = 2k\sin(\theta)$ is the transferred momentum. The total elastic cross-section is therefore equal to

$$\sigma_s = \int |f|^2 \, d\Omega = 2\pi \left| \frac{2m}{\hbar^2} V \right|^2 R^6 \frac{1}{(kR)^2} I(kR) \quad (2)$$

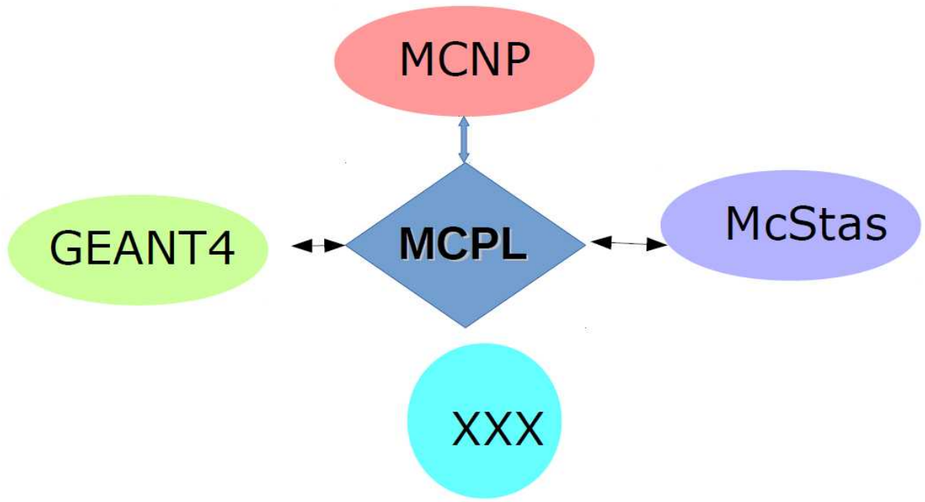
where

$$I(kR) = \frac{1}{4} \left(1 - \frac{1}{(2kR)^2} + \frac{\sin(4kR)}{(2kR)^3} - \frac{\sin^2(2kR)}{(2kR)^4} \right). \quad (3)$$

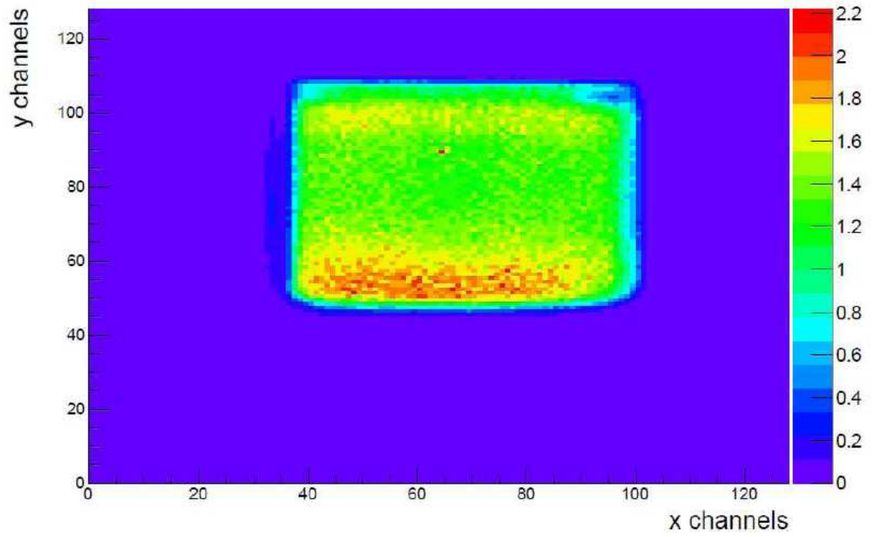
*Nucl. Instr. and Meth. in Phys. Res. **A** 595 (2008) **631–636***



Conclusions



- MCNP-McStas-ROOT interface further developed
- MCPL event format introduced to increase usefulness
  → development ongoing



- Flat moderator validated through experiments

- First look into nanodiamonds simulations
  → McStas/MCPL description underway

$$f(0) = -\frac{2m}{\hbar^2} V R^3 \left(\frac{\sin(qR)}{(qR)^3} - \frac{\cos(qR)}{(qR)^2} \right)$$