Annual Meeting 2021
WP3

Collaboration with PIK

WP Stefan Mattauch (FZJ), WP Sergey Grigoriev (NRC KI-PNPI)
24.03.2021, online via Zoom

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 871072.

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WP3 overview of the sub tasks (ST):

- **ST 3.1**: High-brilliance cold neutron source; **A. Ioffe** (FZJ)
- **ST 3.2**: Bi-spectral neutron extraction system; **A. Ioffe** (FZJ)
- **ST 3.3**: Development of advanced Very Cold Neutron Source; **O. Zimmer** (ILL)
- **ST 3.4**: General blueprint for the instrumentation at PIK; **N. Kovalenko** (NRC KI-PNPI)
- **ST 3.5**: Prototype of advanced polarized neutron diffractometer DiPol..; **A. Goukassov** (CEA LLB)
- **ST 3.6**: Establ. the scientific infrastructure (SAC, instrum. Subc.) at the ICNR Task; **S. Grigoriev** (NRC KI-PNPI)
- **ST 3.7**: Instrum. specific education and training programs for engineers and scientists; **S. Grigoriev** (NRC KI-PNPI)
- **ST 3.8**: User System; **J. Neuhaus** (TUM)
- **ST 3.9:** Coordination between all tasks; **S. Grigoriev** (NRC KI-PNPI)

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WP3 overview of the sib tasks (ST):

Task	Title/Description	Year 1												Year 2												Year 3												Year 4													
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50
3.	**PIK**																																																		
3.1	High-brilliance cold neutron source																		M												D																				DD		
3.2	Bi-spectral neutron extraction system																		M												D					D														
3.3	Development of advanced very cold neutron source																							MD	→					MD					D	→							D	→				D		
3.4	General blueprint for the instrumentation at PIK																		D																																	
3.5	Prototype of advanced polarized neutron diffractometer for PIK reactor																		M																																D	→	D
3.6	Establishing the scientific infrastructure at the ICNR						M						D																																						
3.7	Instrument-specific education & training programmes for engineers & scientists					M																																												D		
3.8	User system																																																M		D	→	D
3.9	Support strategic coordination of PIK																																																		

Deliverable shifts					
WP	**Deliverable**		**Original due date (month #)**	**Estimated due date (month #)**	**Delay (# months)**
WP3 PIK	*(total # of Del.: 14)*				
	D3.1	Definition of the optimal suite of instruments	M12	M18	6M
	D3.2	Model calculations of VCN yields of converter/reflector VCN source	M24	M30	6M
	D3.8	Prototype of VCN source	M36	M44	6-12M
	D3.12	Prototype of polarized neutron diffracto-meter ready for the installation at PIK	M48	M54?	6M?
	D3.14	Report of the established state-of-the-art user system for PIK	M48	M54?	6M?

Milestone shifts					
WP	**Milestone**		**Original due date (month #)**	**Estimated due date (month #)**	**Delay (# months)**
WP3 PIK	*(total # of Mil.: 8)*				
	M18 (MS3.7)	Decision on converter/reflector VCN source	M24	M30	6M

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High-brilliance cold neutron source :

A **low-dimensional cold moderator for PIK**

TASK 3.2 IN WP3

Participants:

FZJ

NRC KI-PNPI

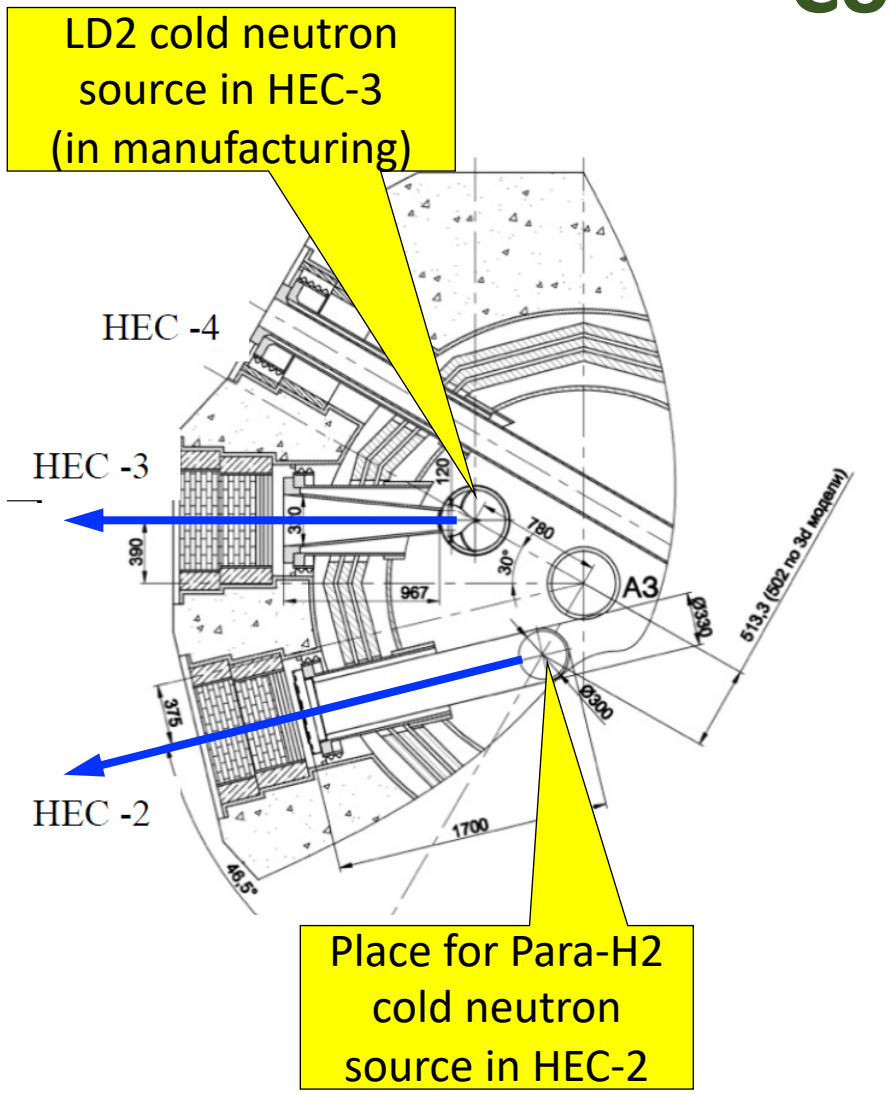
MTA EK (Budapest)

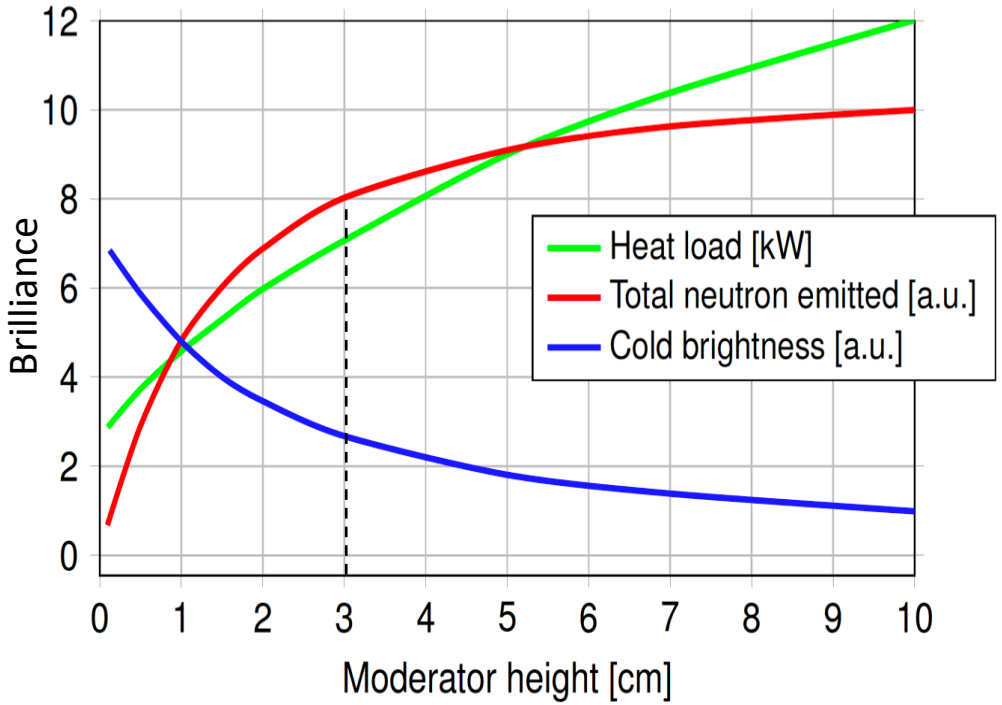
Observers (and active participants!):

Luca Zanini (ESS),

Konstantin Batkov (MAX-IV)

Cold sources at PIK





K.Batkov, 2015

Height = 3cm:

- brilliance – 3x
- Intensity – 0.89 of maximal

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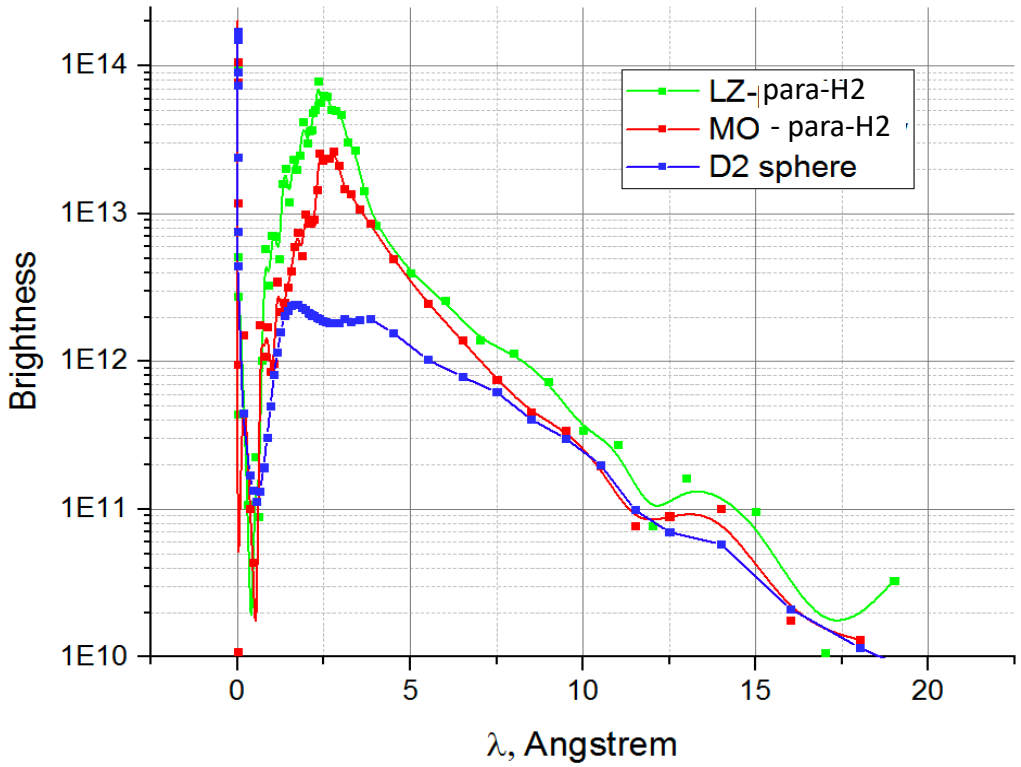
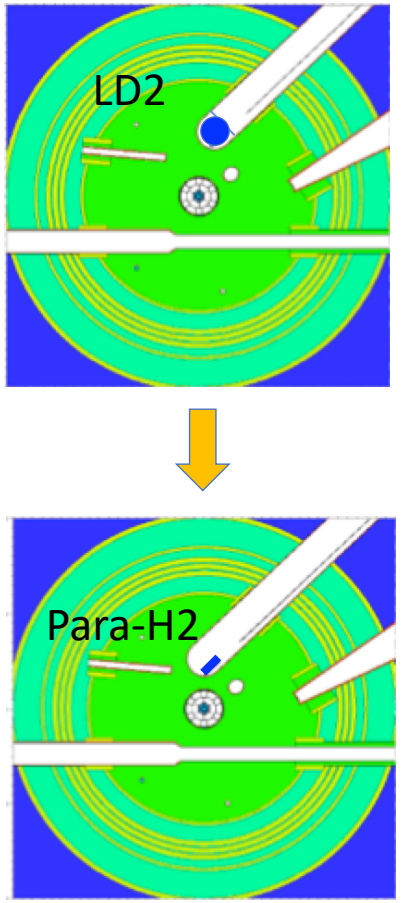
Independent MCNP simulations by 3 groups: PNPI, ESS and FZJ/MAX-IV





Current status:

- agreement on LD2 sphere
- a reasonable agreement on Para-H2
- no gain for Para-H2 above 7Å
- a substantial gain for Para-H2 below 7Å

Next steps:

- Optimization of position in HEC-2
- Diameter and length of HEC-2

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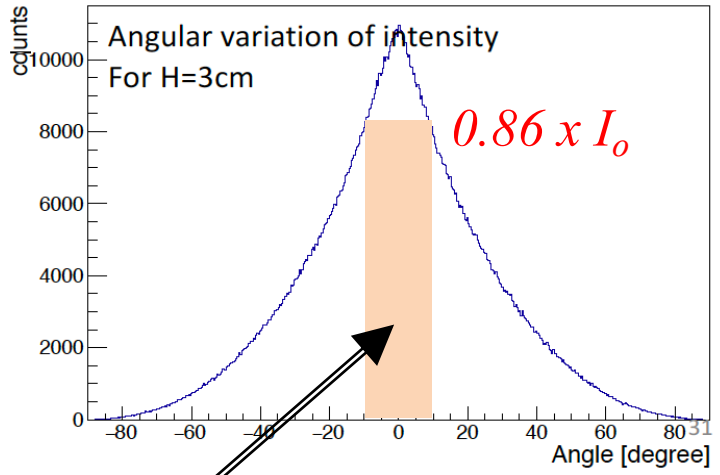
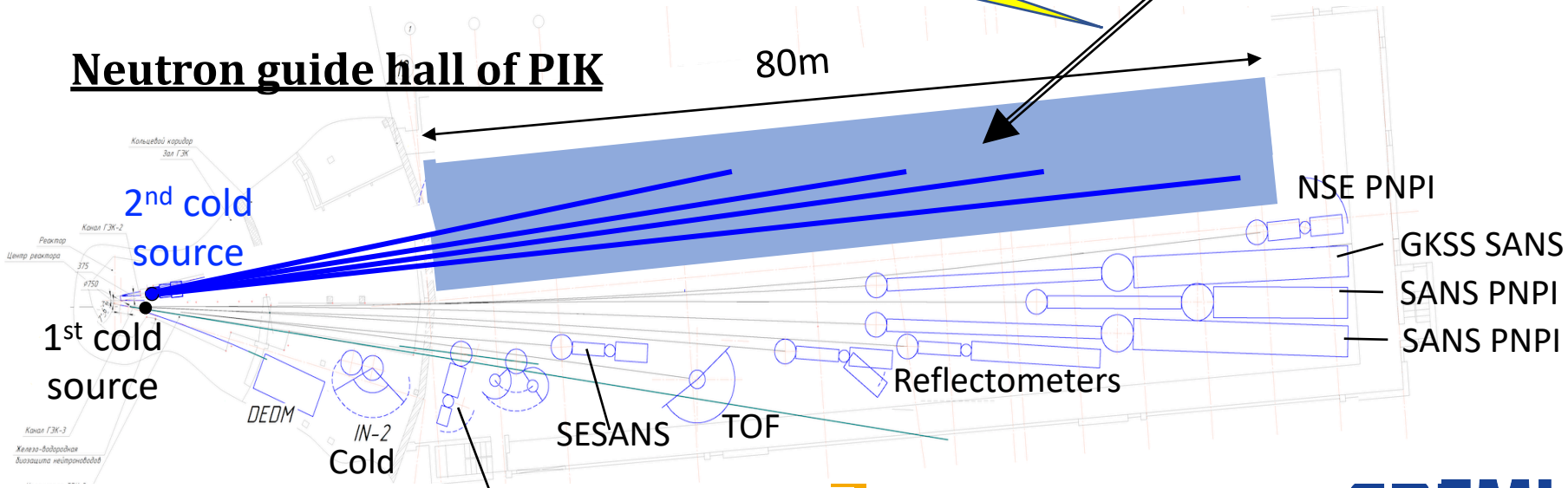
2nd cold source – higher brilliance:

L. Zanini, 2015

Better performance of brilliance-hungry instruments, e.g. SANS, GISANS, reflectometers

One rectangular moderator covers the half of the PIK guide hall





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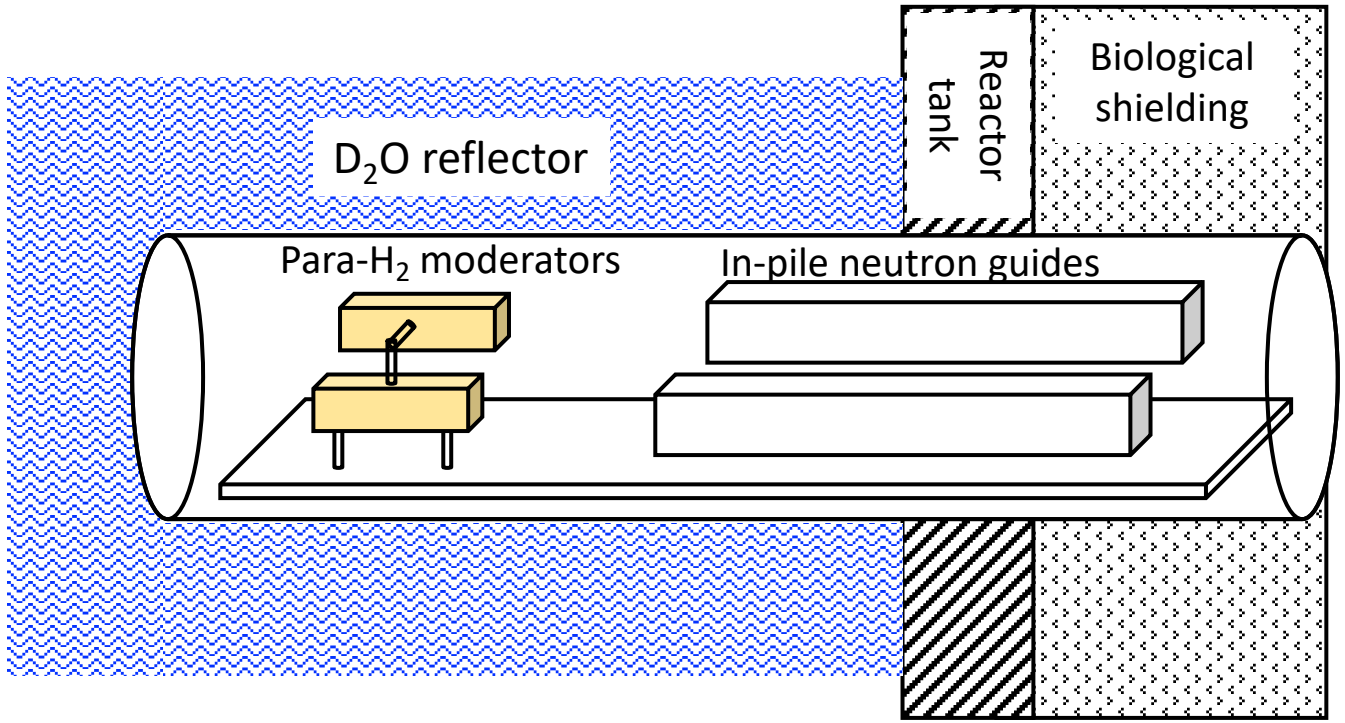
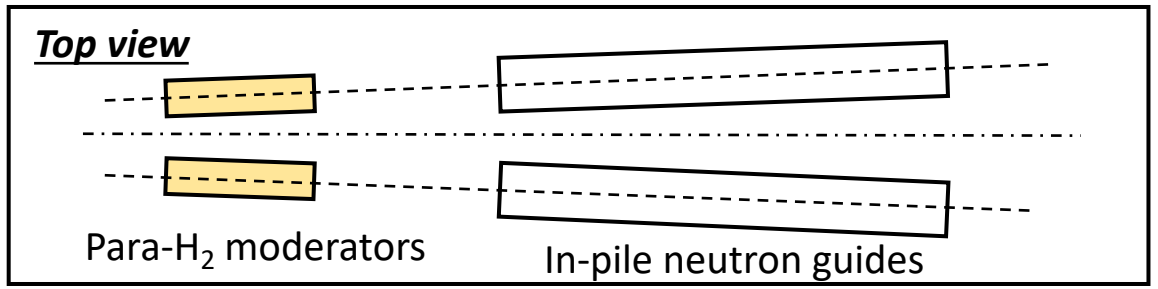
Design for Para-H2 moderators in the beam tube





A. Ioffe, FZJ

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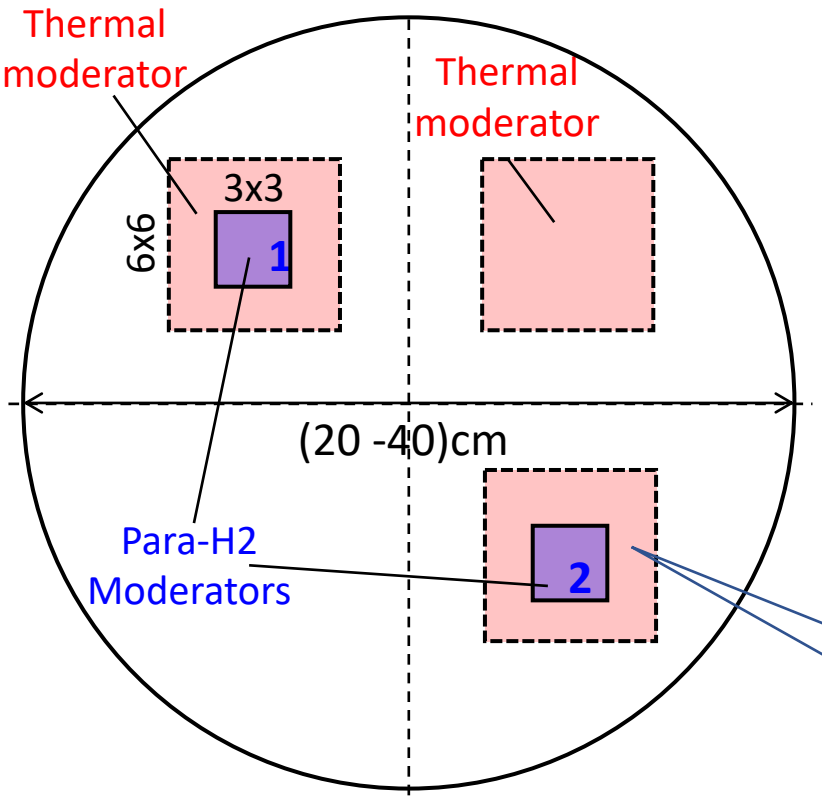
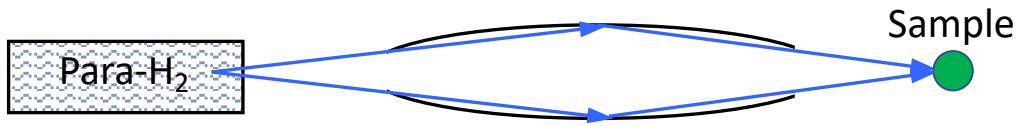
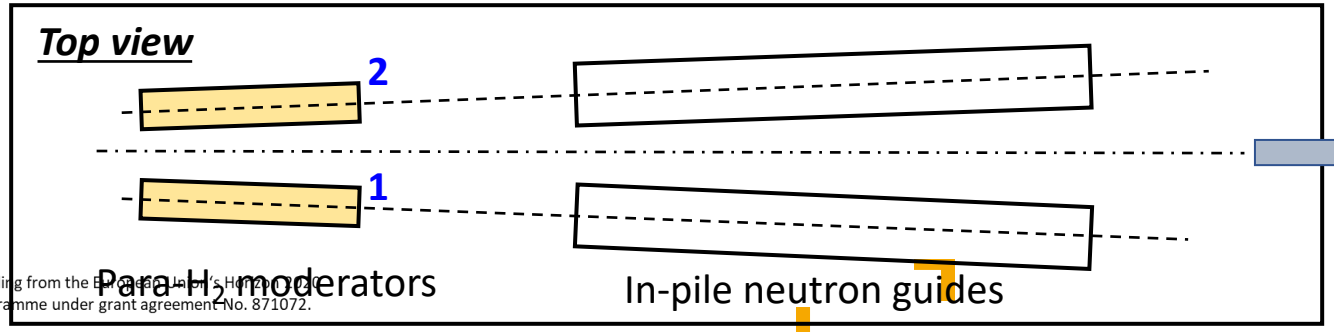
Pair of para-H2 moderators in the beam tube



- Cold neutron guides on 2 levels => simpler and better optics
- Thermal neutron guide for mono-instruments



Bi-spectral illumination!



A. Ioffe, FZJ

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Bi-spectral extraction design

TASK 3.2 IN WP3

PARTICIPANTS:

FZJ

NRC KI-PNPI

MTA EK (BUDAPEST)

Neutron scattering for condensed matter research

Q-resolution

↓

Diffraction

↓

High-resolution techniques:

- Small-angle scattering
- Reflectometry
- Imaging

→

Biology
Chemistry
Nanoscience
Engineering

↓

High Q-resolution requires severe collimation of neutron beams, down to 1mrad.
⇒ significant intensity losses
⇒ to enhance brightness (cf. synchrotrons)

E-resolution

↓

Spectroscopy

↓

Wide Q-range:

- neutron beams with wide λ–range
- High intensity both of thermal and cold spectra

⇒ To compose beams from thermal and cold neutron source (bi-spectral extraction)

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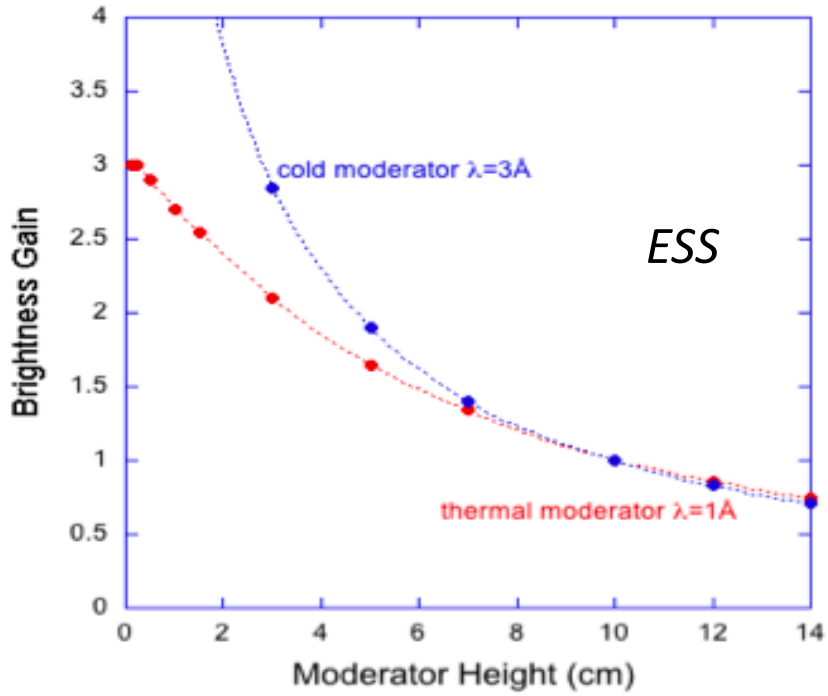
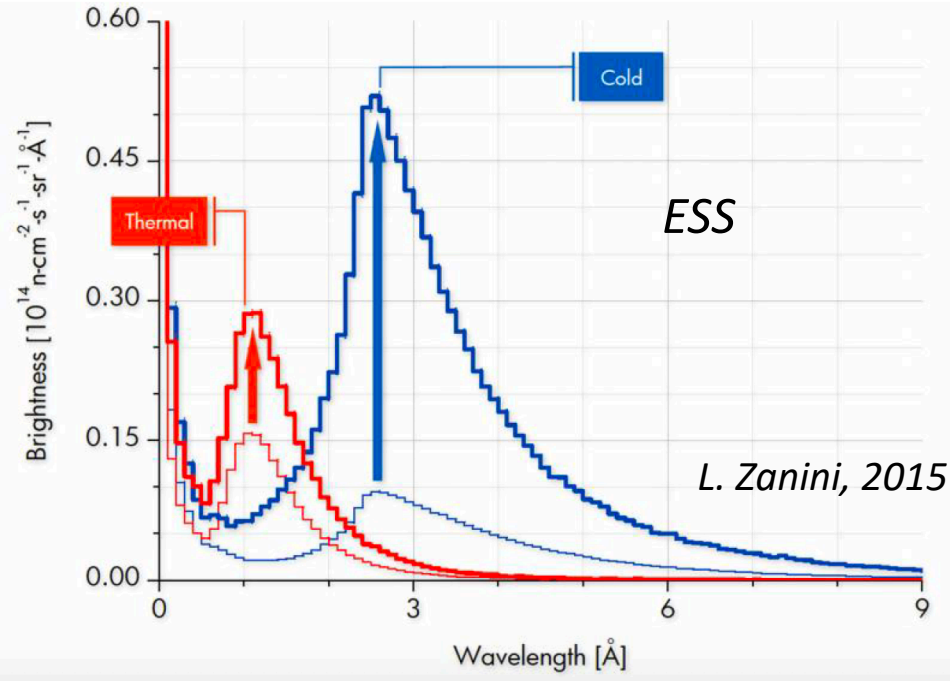
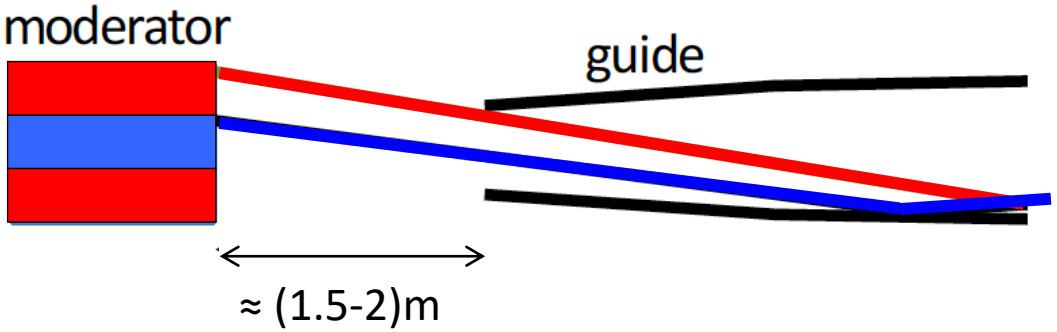
Low-D cold neutron source

Bi-spectral extraction: about 5 times higher flux at (0.8-2)Å





Acceptance
by neutron guide:



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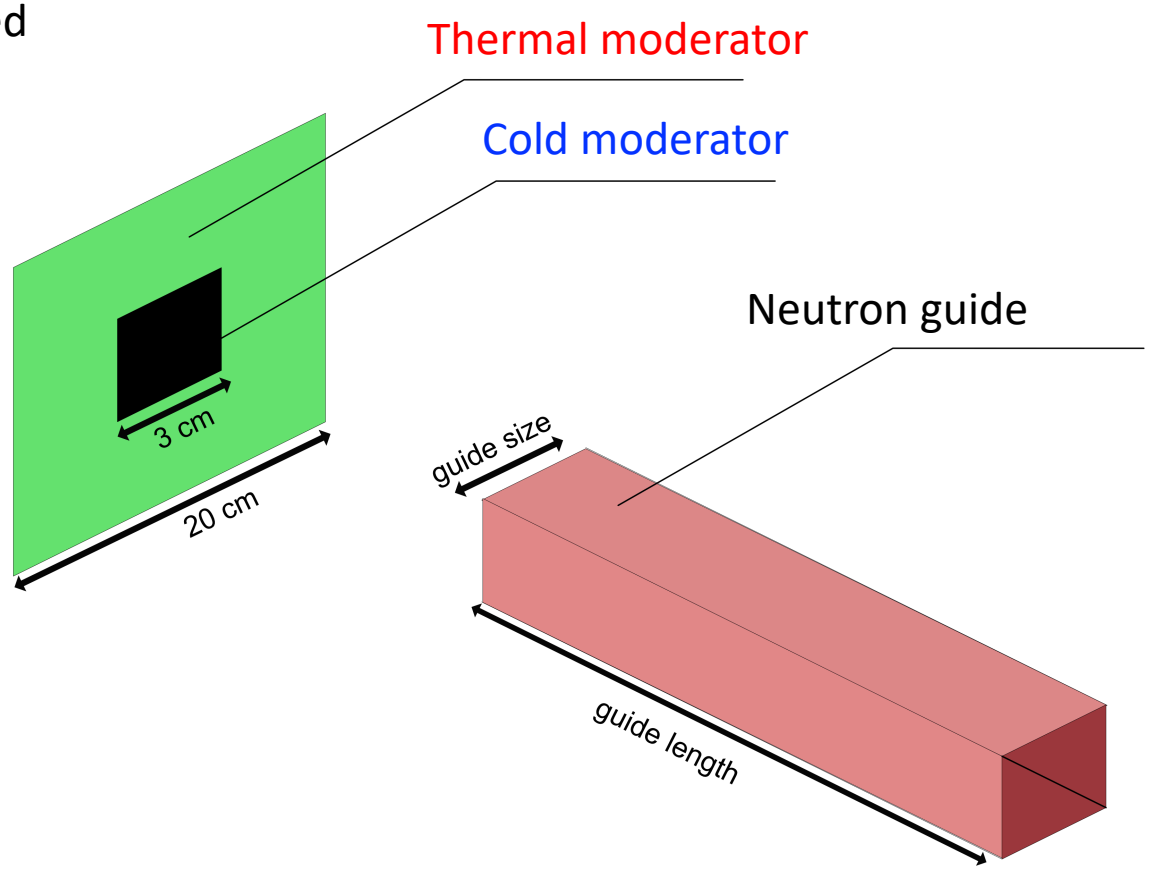
The problem

- It is possible to mix T and C neutrons without additional optics?
- Spatial profile is ok
- Divergence profile must be smoothed



- (0.5-8)Å band
- 2 m from source to optics
- $m = 3$

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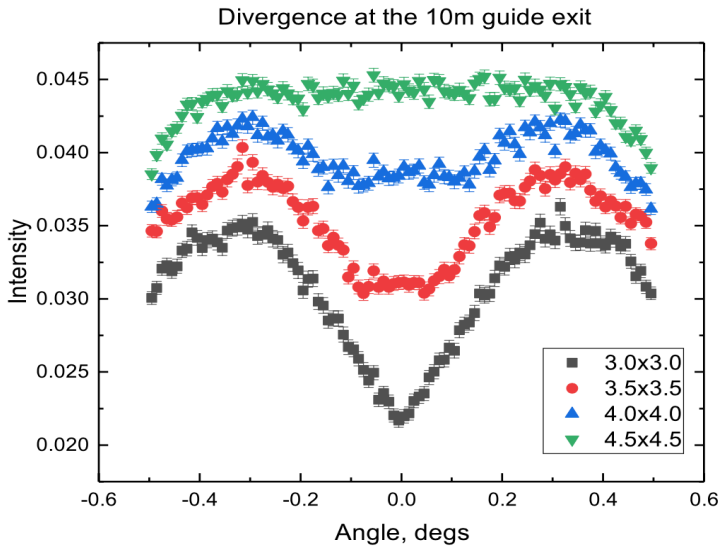
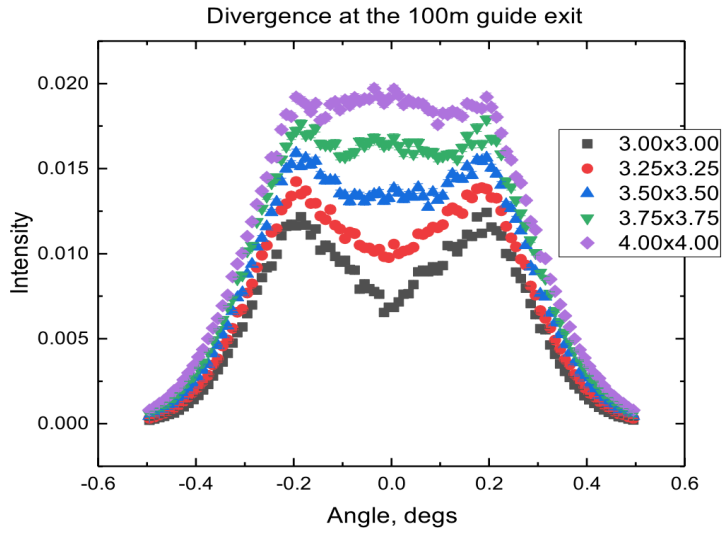
Divergence profile

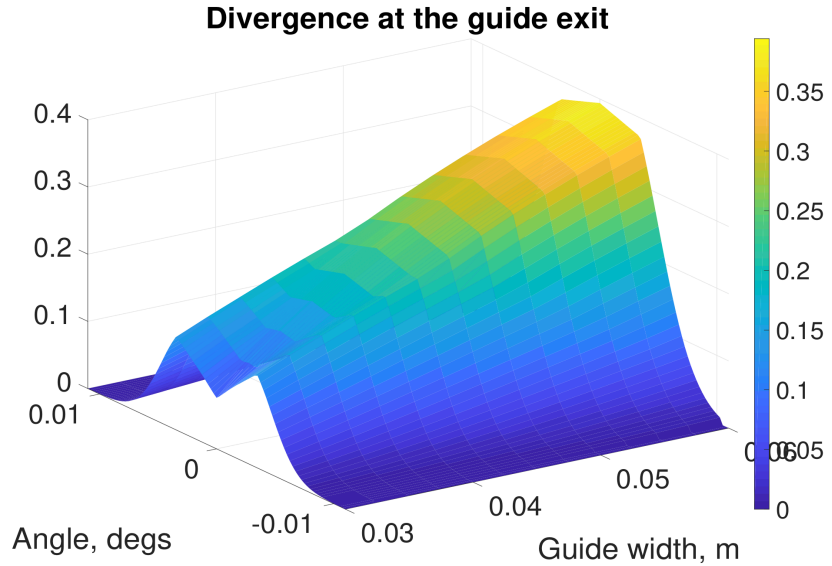
P. Konik, A. Ioffe, FZJ





VITESS simulations for full 0.5-8 Å band

- It is possible to mix T and C neutrons without additional optics
- Spatial profile is ok
- Divergence profile must be smoothed



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Next steps

- More complex source geometries
  - Round source
  - Half-transparent source
- More complex guide geometries
  - Ballistic, elliptic, parabolic guides
- Bi-spectral source geometry parametrization:

  => to fit into general source-instrument description being developed for task 3.4.

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Development of advanced Very Cold Neutron Source

TASK 3.3 IN WP3

A. Aleksenskii, A. Dideikin, M. Dubois, G. Gorini, Zs. Kókai, E. Lychagin, J.I. Márquez Damián, A. Muzychka, V. Nesvizhevsky, A. Nezvanov, A. Nekhaev, V. Santoro, A. Shvidchenko, A. Strelkov, K. Turlybekuly, A. Vul, L. Zanini, O. Zimmer

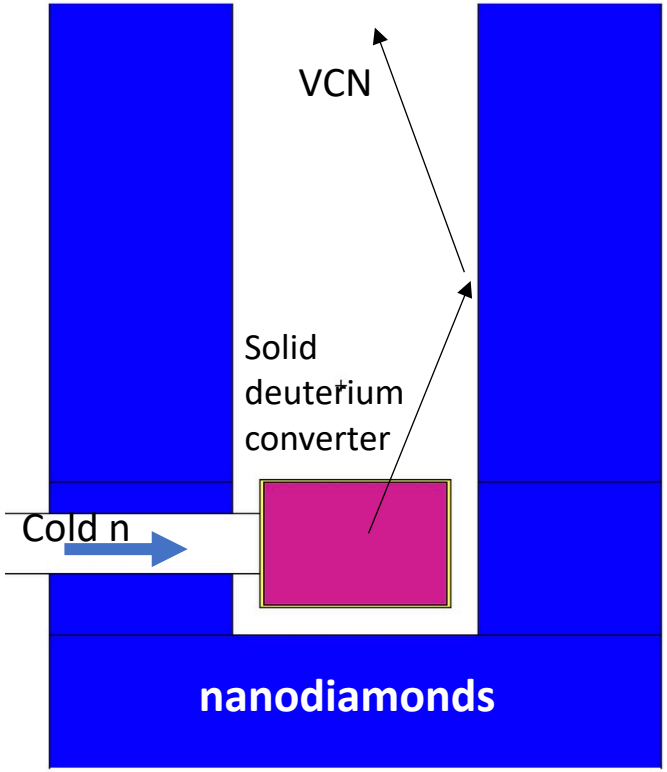
University Milano-Bicocca, Italy
IOFFE Physico-Tehnical Institute, Russia
Institut Laue-Langevin, Grenoble, France
European Spallation Source, Lund, Sweden
Joint Institute for Nuclear Research, Dubna, Russia

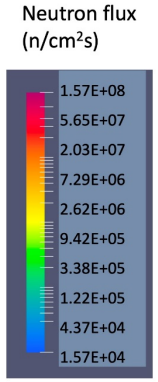
Monte Carlo modeling for prototype VCN experiment

Zs. Kókai, J.I. Márquez Damián, V. Santoro, L. Zanini (ESS)

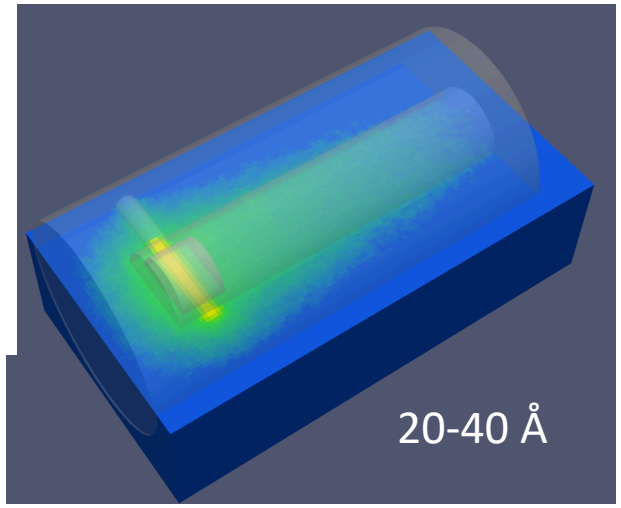
- A model of elastic scattering including SANS (parametrized from experimental data from Teshigawara et al.) Bragg scattering and inelastic scattering has been implemented in MCNP.
- MCNP model of prototype experiment with VCN converter (solid deuterium or liquid hydrogen) with nanodiamond reflector under study.
- First simulations show very promising gain factors.

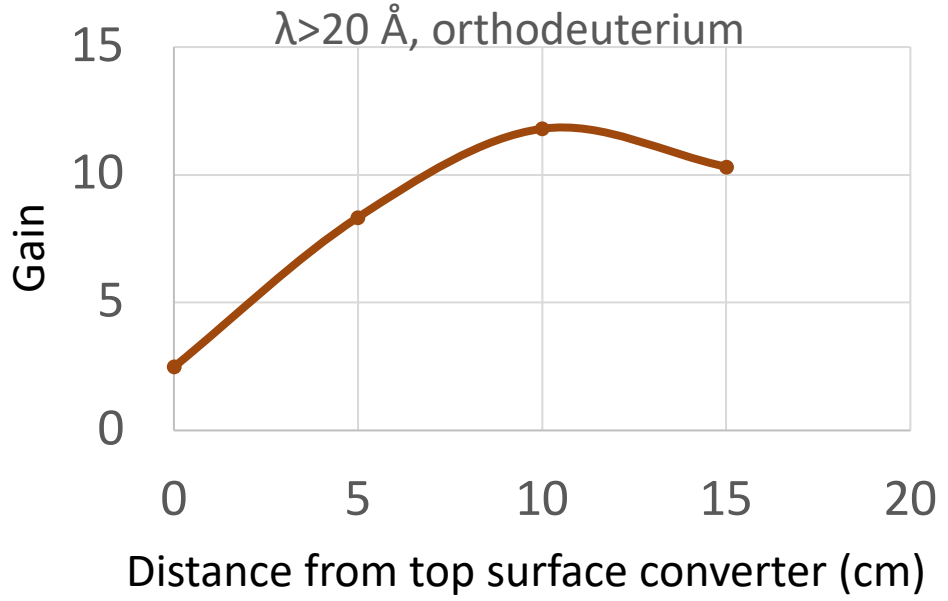
MCNP model





Neutron flux





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Achievements / highlights

- Investigation of nanodiamond powders, experiments (nSANS, xSANS, etc.)
- Many SANS measurements of different type with nanodiamond powders (raw, fluorinated, deagglomerated, separated) has been performed. The data are currently analysed.
- Different technologies of powder purification have been tested with NAA and prompt-gamma analysis. We have selected a suitable one for the production of quite pure powder for the main experiment installed at an external neutron beam. Further purification from metals would be required for using it in intense neutron fields. Also, we probably found a possibility to decrease nitrogen contamination in nanodiamonds.
- To perform the main experiment, 1 kg of deagglomerated and purified nanodiamond powder has been produced in PTI. The first portion of this powder has been sent to UCA for fluorination.

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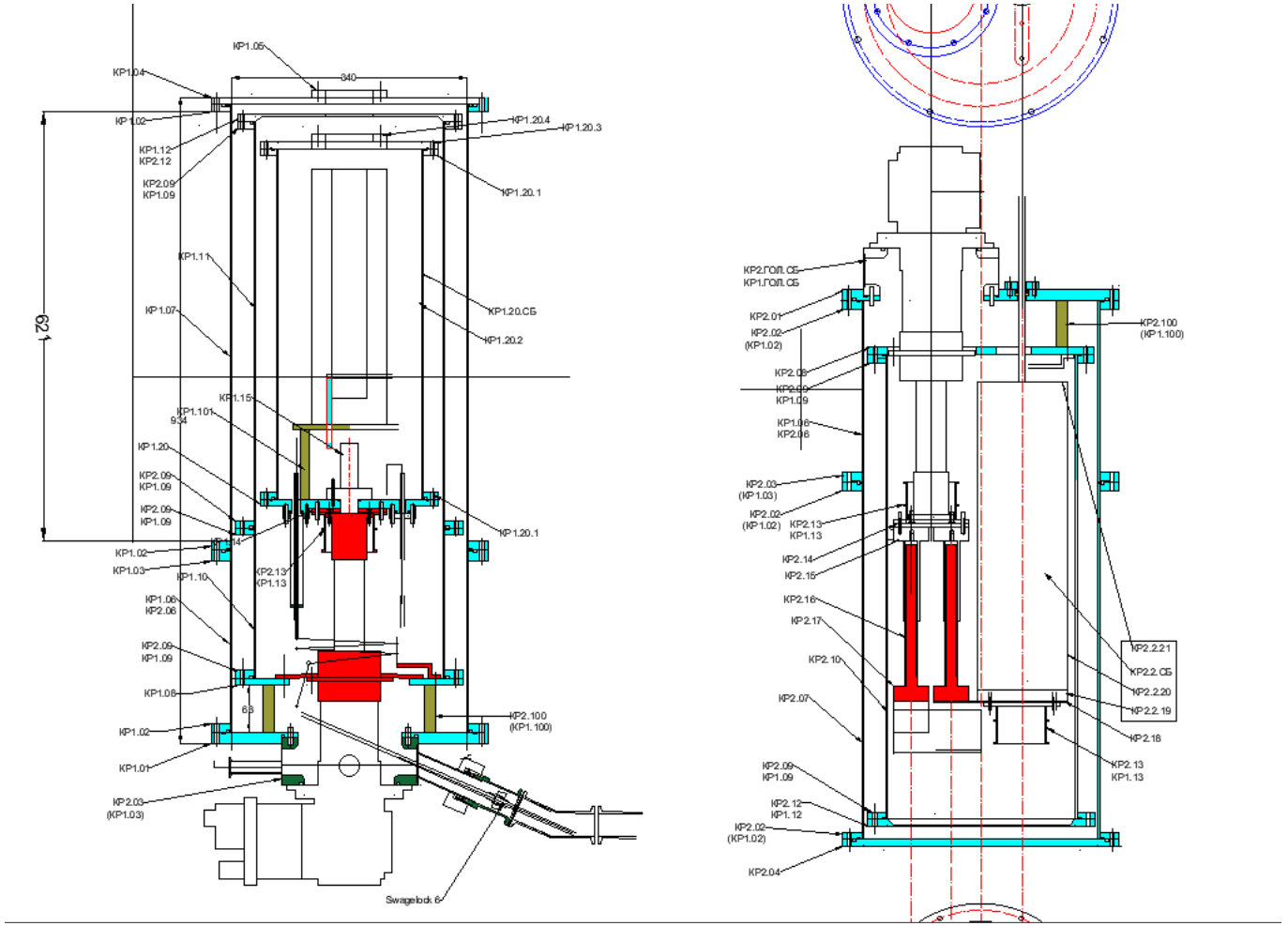
Achievements / highlights

- Manufacture of the para-ortho converter, design of cryostat

The development of the para-ortho converter for solid deuterium and the design of a suitable cryostat have been started at Dubna.



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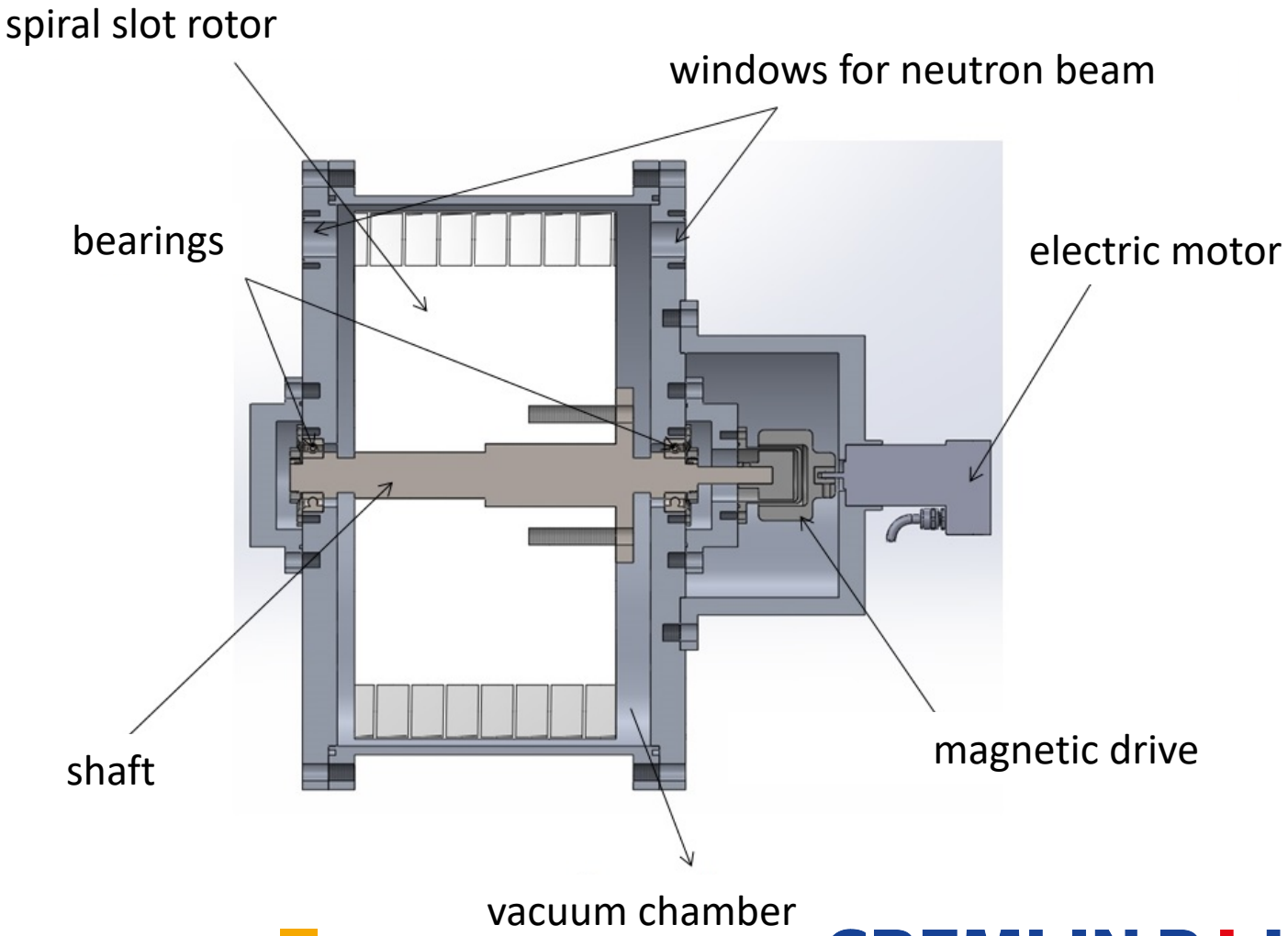
Achievements / highlights

Development and manufacture of the VCN Selector

The development of the selector has started. First CAD models of the device have been produced.



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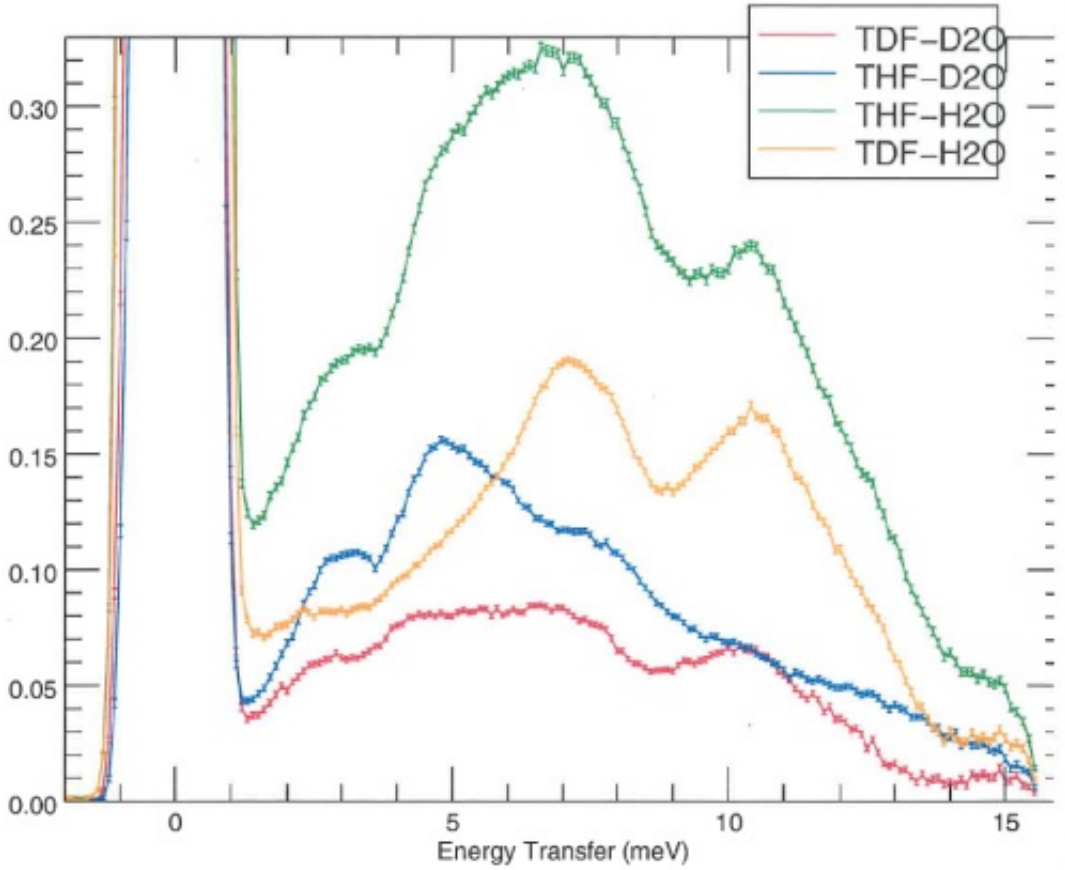
Experiments for determination of S(q,ω) of promising novel materials for moderation to Very-Cold Neutrons

- First measurements of inelastic neutron scattering on various clathrate hydrate compounds have been performed, using the time-of-flight instrument IN5 at ILL
- Further experiments are planned to be performed in ILL's next two reactor cycles in 2021



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General blueprint for the instrumentation at PIK

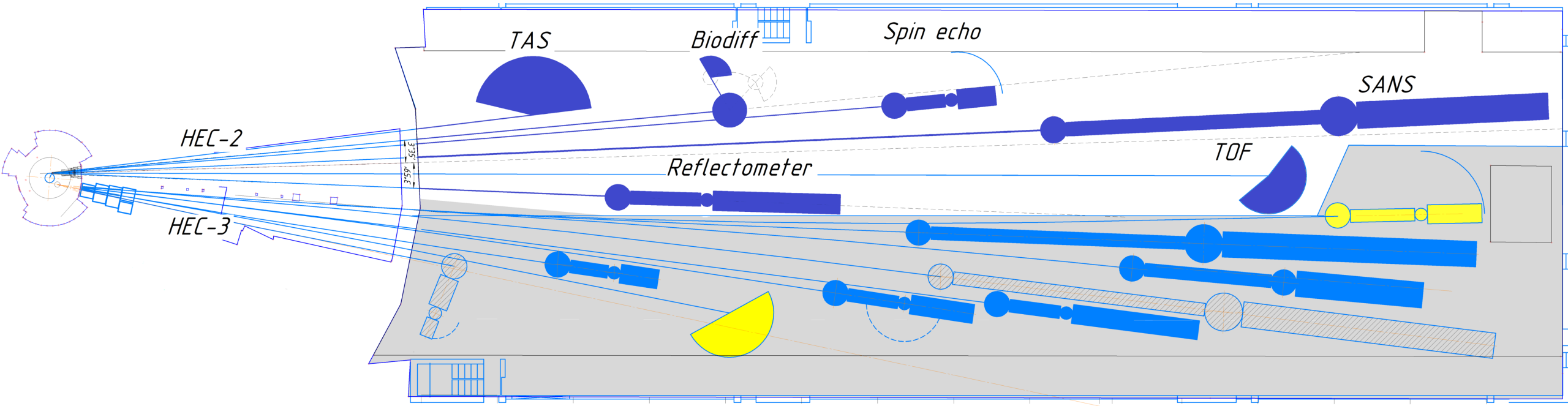
TASK 3.4 IN WP3

N. KOVALENKO

NRC KI-PNPI

Achievements / highlights

- The ‚blueprint' of the neutron guide hall



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Prototype of advanced polarized neutron diffractometer DiPol

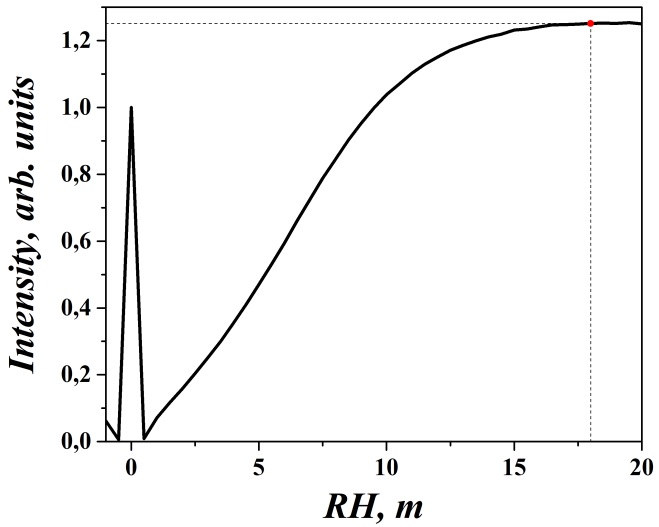
TASK 3.5 IN WP3

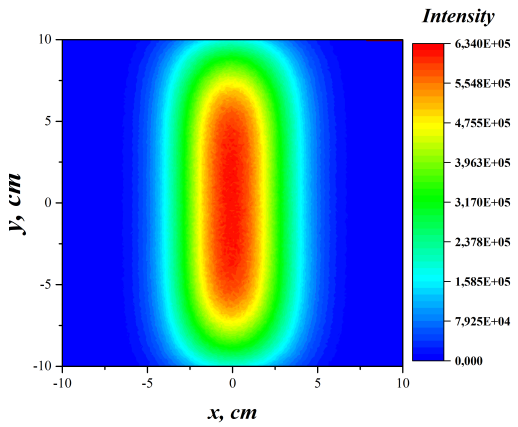
A. GUKASSOV

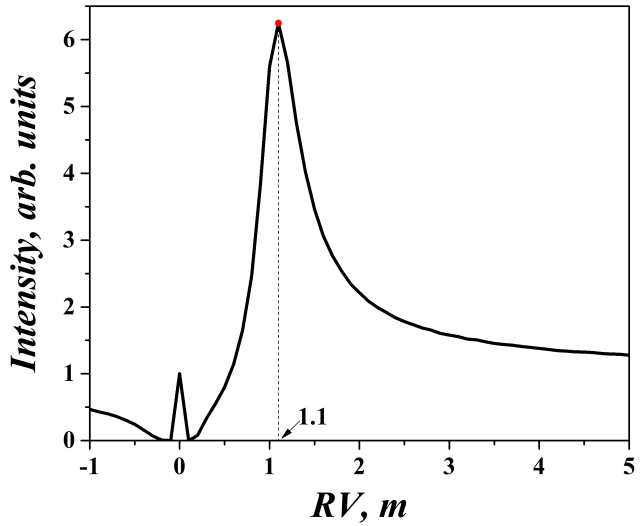
CEA-LLB

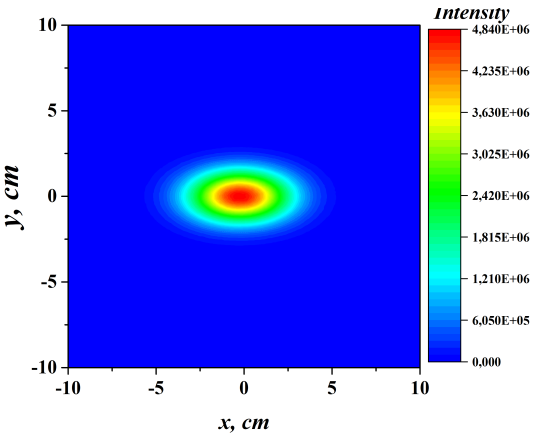
Achievements / highlights

- MCSTAS model of prototype
- Simulation of prototype
- Presented in Subcommittee; -> recommendation to install DIPOL at thermal beam and not hot channel! -> PNPI is taking care of this









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Next actions

- We have to prepare by July 2021 (M18) a report on a full scale simulation of the prototype and start a design of first elements.
  - That means, that the better approach to the simulation we need to take the neutron flux at the detector for the evaluation of the best focusing parameters of the monochromator and the polarizing and analysing units.
  - plan to start the design of the monochromator stage
  - start the modelling and design of the radiation shielding.

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3.6 Establish the scientific infrastructure (SAC, instrument Subcommittees) at the ICNR

3.7 Instrument specific education and training programs for engineers and scientists

3.9 Coordination between all tasks

TASK 3.6, 3.7 AND 3.9 IN WP3

S. GRIGORIEV

NRC KI-PNPI

Achievements / highlights in 3.6

- The kick-off meetings of the 6 subcommittees have been organized within two last months of 2020. These are subcommittee on neutron diffraction, neutron spectroscopy, LSS, CNS and neutron optics, Fundamental physics with neutrons, Neutron detectors. Due to corona pandemic all meeting had been held in the on-line format. The meeting of the SAC of WP3 (Cooperation with PIK) is postponed and is planned for the 12th of April 2021 in on-line format.

Next actions in 3.6

- We plan to arrange 1 additionally meeting of WP3 SAC and 2 meetings for each of 6 SubCommittees: in total 2 + 12 meetings.
- We plan to hold one of them in online format and another one in face-to-face format

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Achievements / highlights in 3.7

- Petersburg Institute of Nuclear Physics (NRC "Kurchatov Institute") had held the III School "Simulation methods of instrument design: McStas-course" on 14 - 18 September 2020 in Peterhof, near Saint-Petersburg,
- The IX School of Polarized Neutron Physics "FPN-2020" had held on December 10-11, 2020 at NRC KI - PNPI jointly with St. Petersburg State University, in Gatchina, Russia

Next actions in 3.7

- We plan to arrange 2 similar schools within 2021 in September and December

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Achievements / highlights in 3.9

- actions of Subcommitee for detectors of WP3 with actions of WP7 for neutron detectors,
- actions of the Subcommitee for diffraction of WP3 with actions of leader of the Task 3.5,
- actions of the Task 3.7 (Education) with actions of the Task 3.6 (Subcommittee).
- actions of the Task 3.1, Task 3.2 and Task 3.3 with actions of the Subcommitte on the Neutron optics and moderators,
- actions of the Task 3.4 with actions of the Subcommittee on Difraction, of SC on LLS, of SC on Spectroscopy.

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User System

TASK 3.8 IN WP3

J. NEUHAUS

TUM

Member of the Helmholtz Association

CREMLIN PLUS
Connecting Russian and European Measures
for Large-scale Research Infrastructures

JÜLICH
Forschungszentrum

Achievements / highlights task 3.8, user system PIK

- Analysis of existing user office systems is ongoing
- Exchange of experience on best practice of user operation
- Definition of requirements specific to the PIK neutron source
- Challenge to hire qualified personell for implementation phase not yet successful

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Next actions
task 3.8, user system PIK

- Finalize the analysis of user systems.
- Selection of a software solution, or solution framework to implement a user system at PIK
- Detailing specification on the local requirements of work flows and institutional and leagal boundaries.

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Thank you for your attention

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