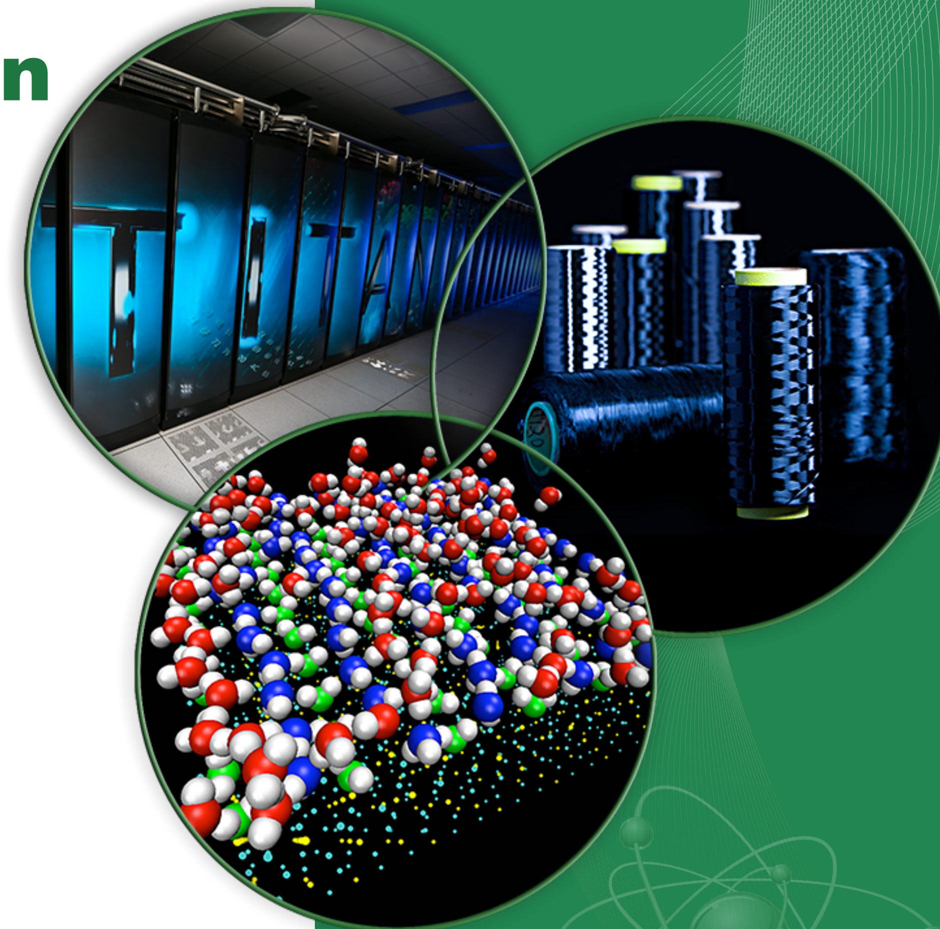
Scattering Kernel Needs for Spallation Sources

WPEC-SG42,

Issy-les-Moulineaux, France

May 19, 2015



F.X. Gallmeier, T. Huegle,
L. Daemon, E.B. Iverson,
W. Lu, I. Remec, I. Popova

ORNL is managed by UT-Battelle
for the US Department of Energy

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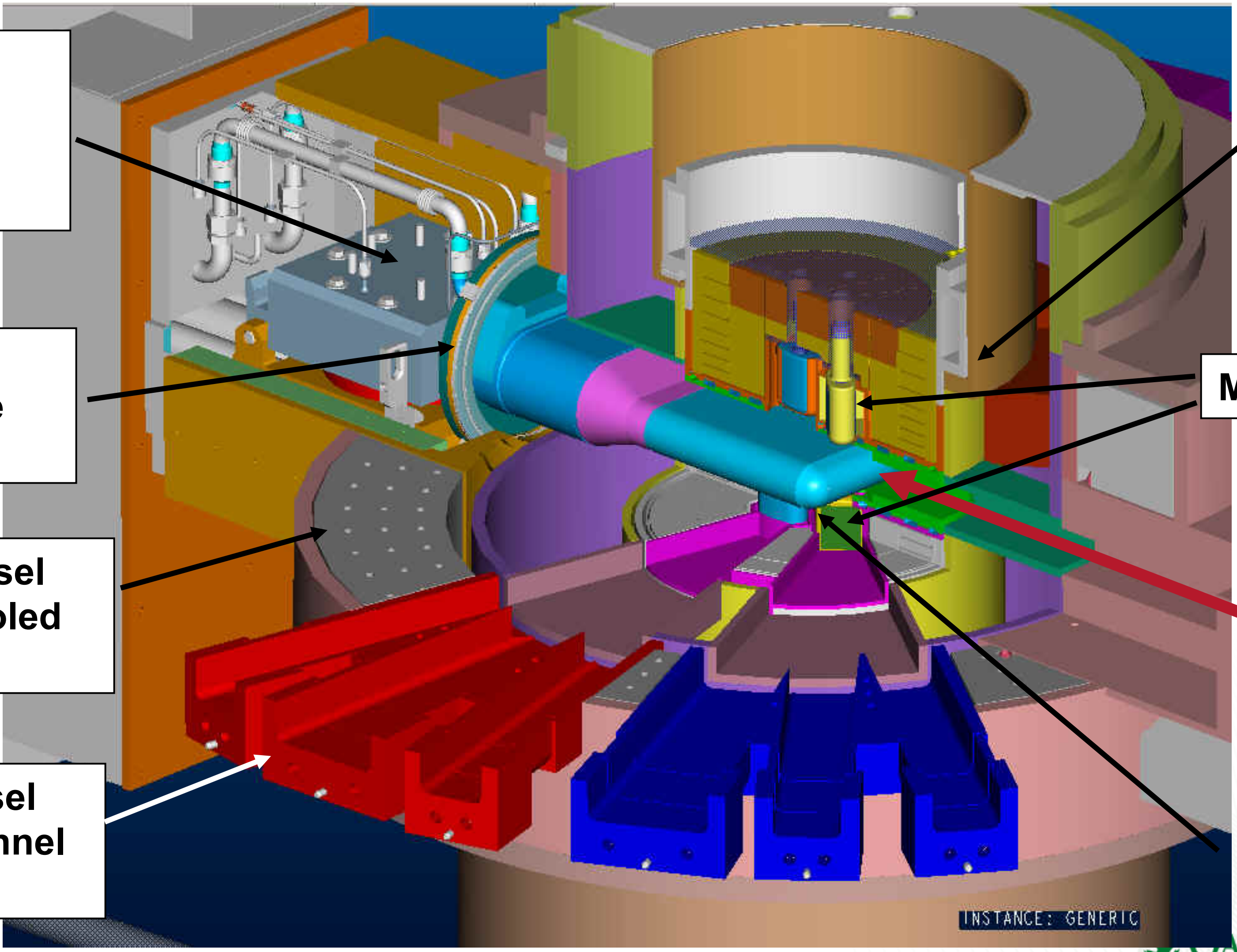
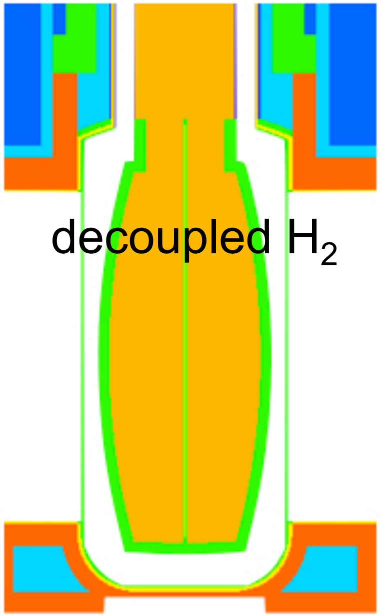
Outline

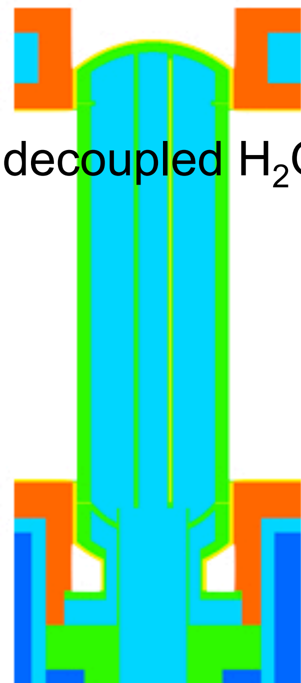
- Spallation Source Moderators
- Spallation Source Needs
- Tooling Needs
- Spallation Source Capabilities for Sab effort

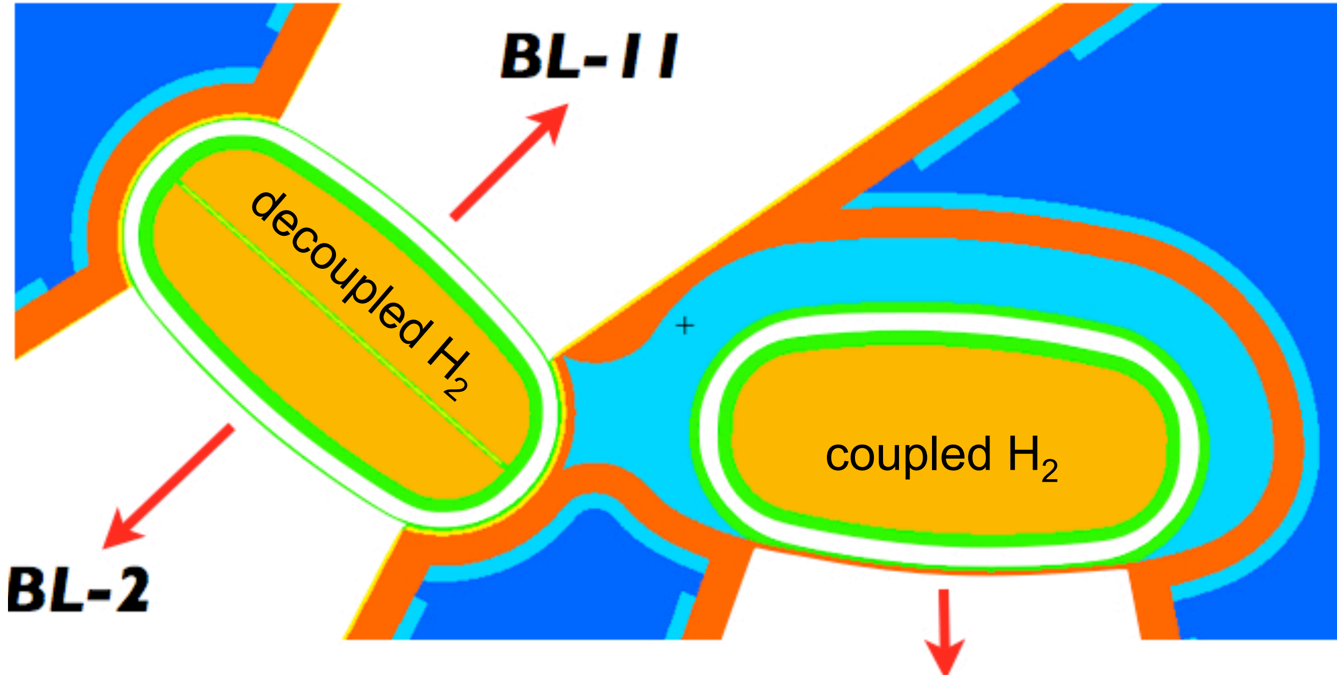
Target Region within Target Monolith



SNS Moderators

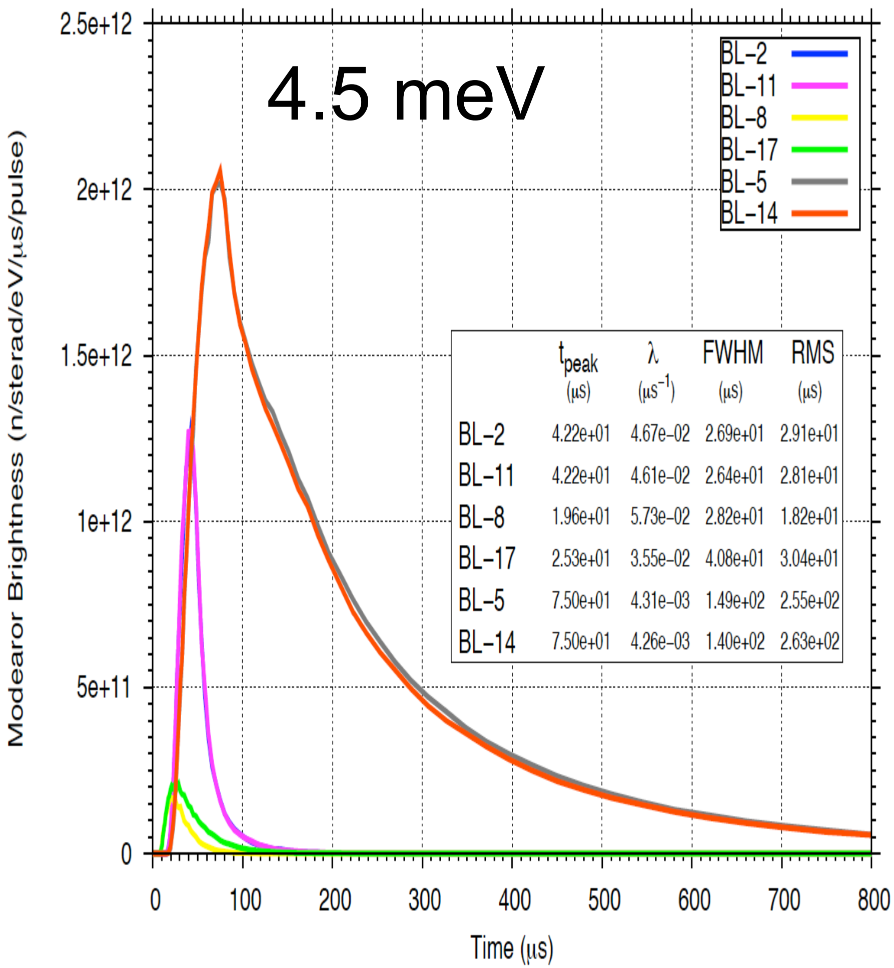




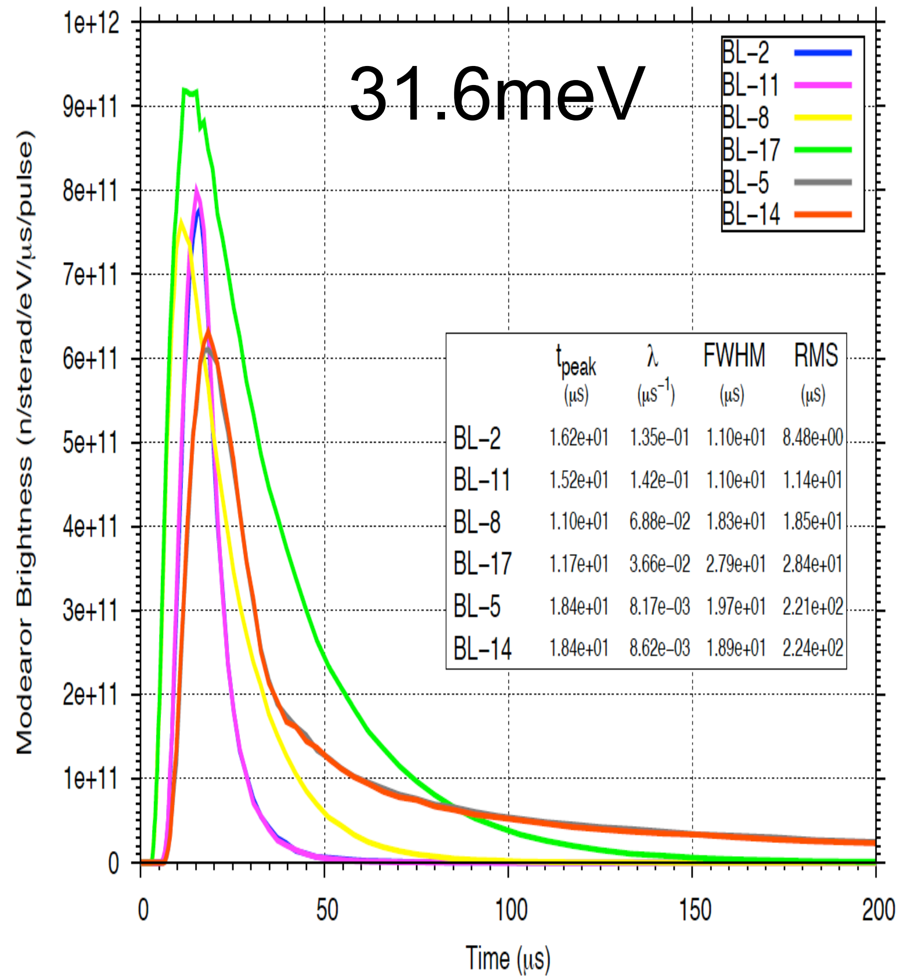


Keen interest in materials offering fast moderation and thermalization to cold and thermal energies with good radiation behavior

SNS Neutron emission-time distributions



	t_{peak} (μs)	λ (μs^{-1})	FWHM (μs)	RMS (μs)
BL-2	4.22e+01	4.67e-02	2.69e+01	2.91e+01
BL-11	4.22e+01	4.61e-02	2.64e+01	2.81e+01
BL-8	1.96e+01	5.73e-02	2.82e+01	1.82e+01
BL-17	2.53e+01	3.55e-02	4.08e+01	3.04e+01
BL-5	7.50e+01	4.31e-03	1.49e+02	2.55e+02
BL-14	7.50e+01	4.26e-03	1.40e+02	2.63e+02

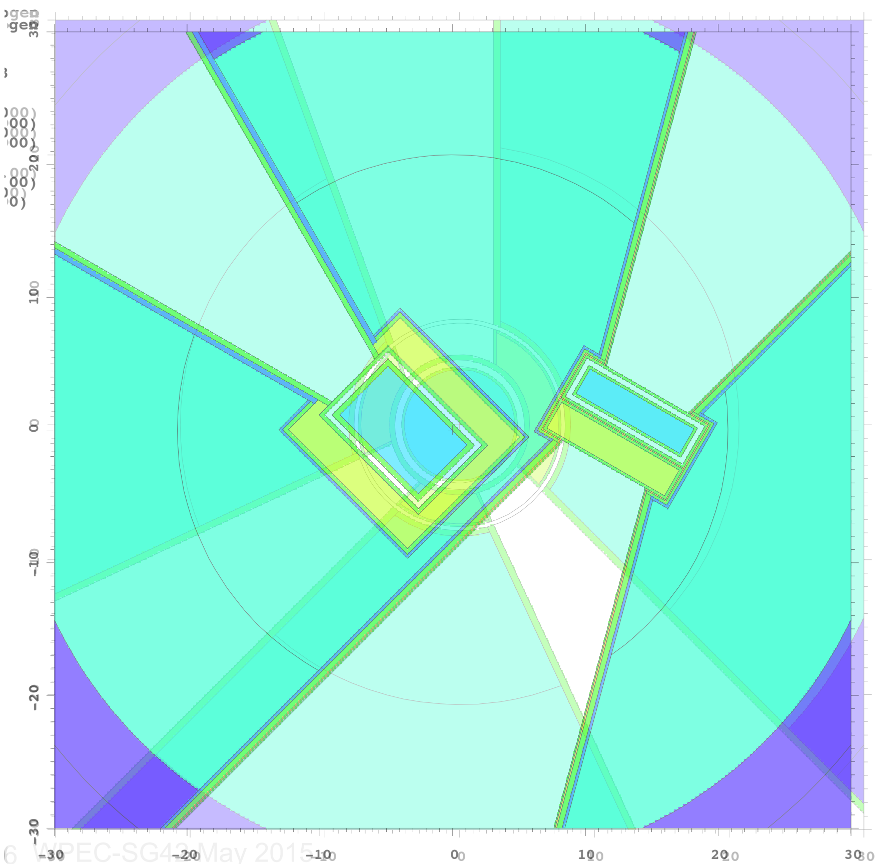


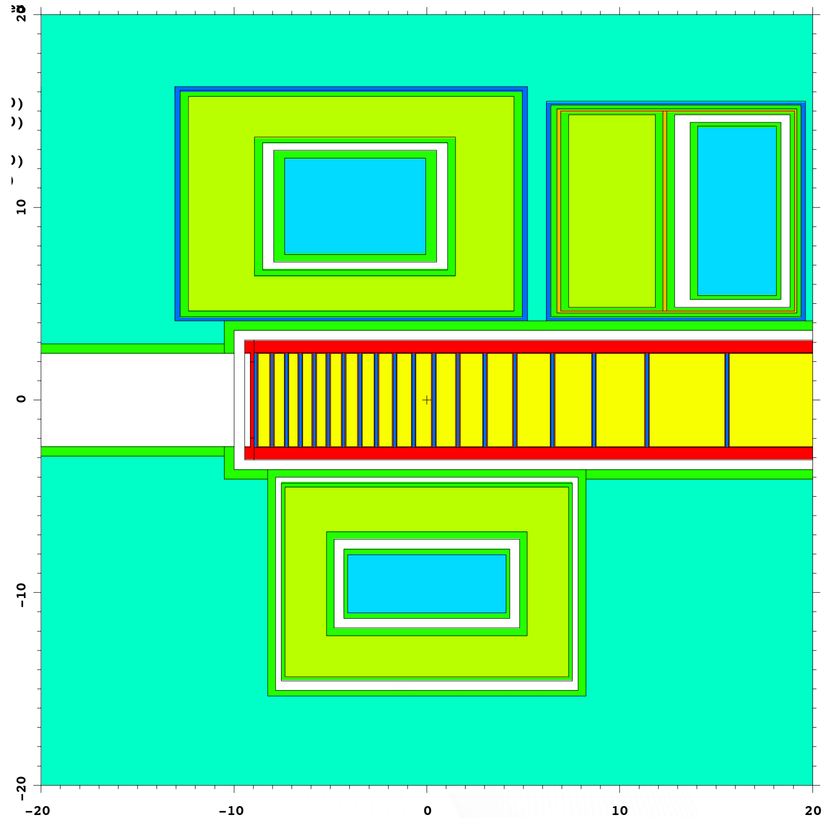
	t_{peak} (μs)	λ (μs^{-1})	FWHM (μs)	RMS (μs)
BL-2	1.62e+01	1.35e-01	1.10e+01	8.48e+00
BL-11	1.52e+01	1.42e-01	1.10e+01	1.14e+01
BL-8	1.10e+01	6.88e-02	1.83e+01	1.85e+01
BL-17	1.17e+01	3.66e-02	2.79e+01	2.84e+01
BL-5	1.84e+01	8.17e-03	1.97e+01	2.21e+02
BL-14	1.84e+01	8.62e-03	1.89e+01	2.24e+02

Narrow pulses, suppressed tails

Second Target Station (STS)- TDR Baseline Configuration

Coupled para-hydrogen moderators in the upstream positions





Decoupled para-hydrogen and water moderators at top downstream position

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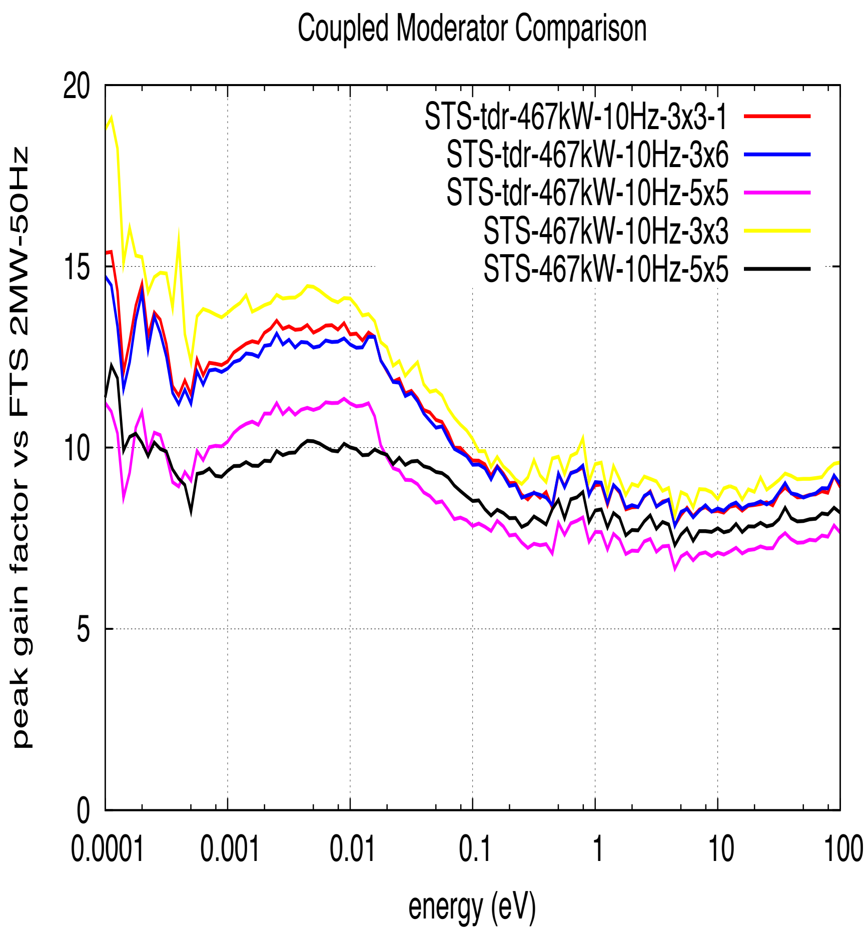
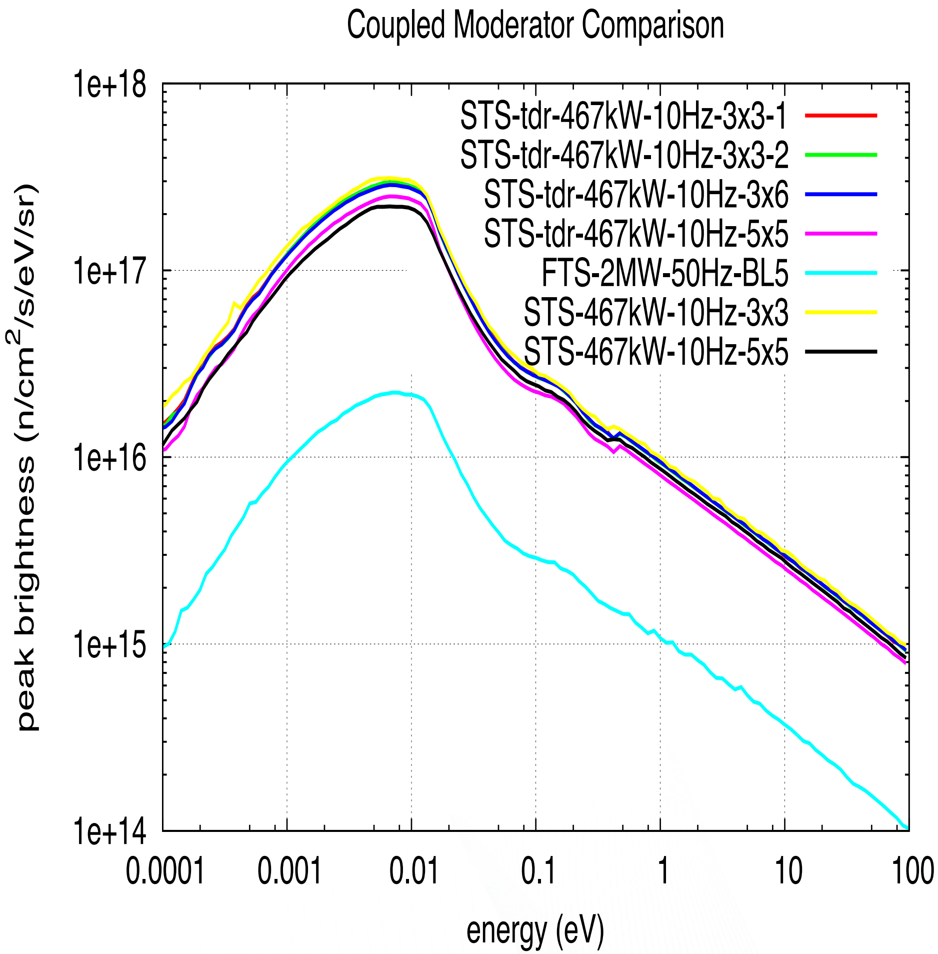
STS Coupled cold moderator performance





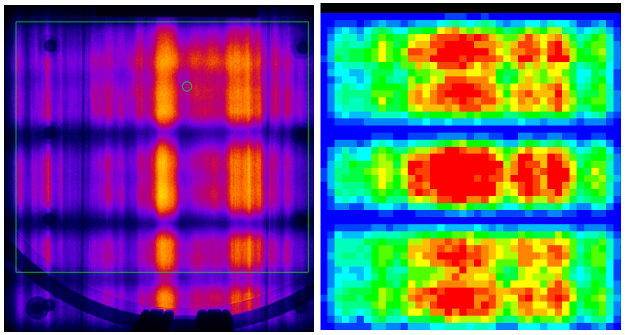
- The TDR configuration maintains the gains seen in the single moderator optimization studies

Material alternatives to H_2O and lq. H_2?

- Interest in moderator, pre-moderator and reflector materials
- For moderator and pre-moderator:
  - Higher hydrogen density
  - Richer low-energy inelastic modes
- For moderator:
  - Colder neutron spectra (VCN, feeding UCN)
- Constraints
  - Heat removal
  - Radiation resistance
- Candidates
  - (Methane), ammonia, hydrides, MOFs

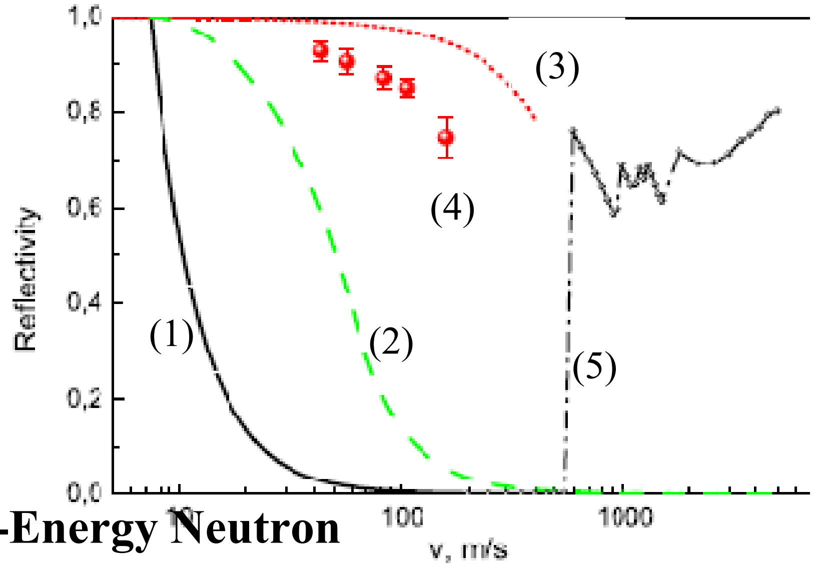
Small Angle Scattering to be added to scattering kernel?

- Diffusor for neutron beams to smooth gaps in divergence profiles



CG1 measured and simulated neutron distribution at guide exit

- Reflector enhancements by small angle scattering diamond nano-powder



Application of Diamond Nanoparticles in Low-Energy Neutron Physics

Materials **2010**, *3*, 1768-1781; doi:10.3390/ma3031768

Valery Nesvizhevsky [1,4,*], Robert Cubitt [1], Egor Lychagin [2,4], Alexei Muzychka [2,4], Grigory Nekhaev [2,4], Guillaume Pignol [3], Konstantin Protasov [3] and Alexander Strelkov [2,4]

Single Crystal Scattering

- Implemented Single Crystal Model from MCSTAS code into MCNPX. Model describes diffraction on mosaic crystals in kinematical theory.
- Not perfect for perfect crystals such as silicon, which would have to be described in dynamical scattering theory.
- Physics effects:
  - Highly transparent material for neutrons (especially when cooled to suppress inelastic scattering)
  - Bragg scattering at select energy/angle conditions
- Adds complexity to problem setup: single crystal must be oriented

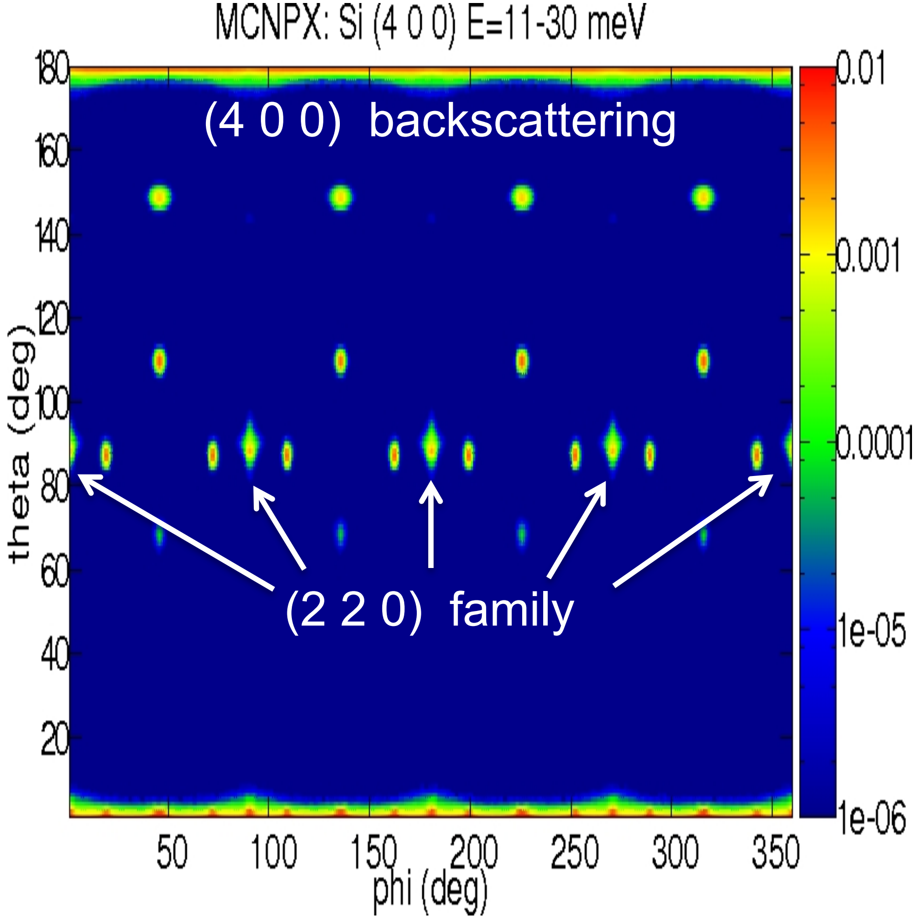
Single Crystal Model Implementation

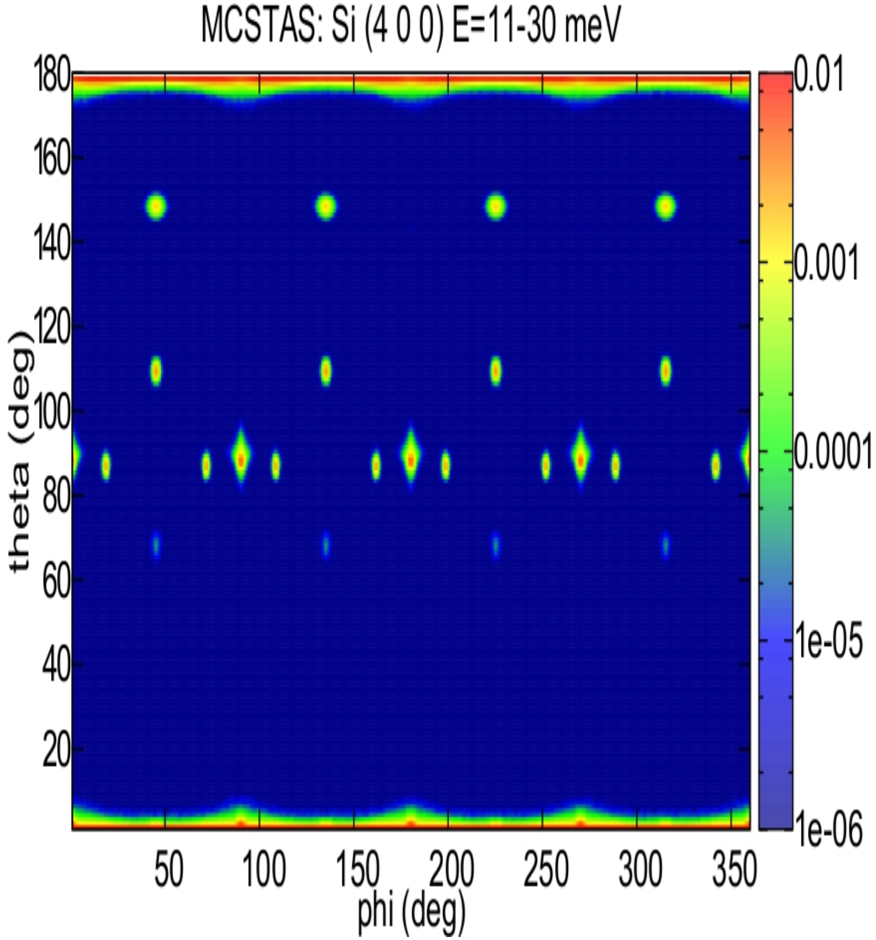
- Single crystal model provides coherent elastic scattering information:
  - scattering cross section calculated by searching listings of crystallographic planes and summing probabilities of Bragg diffraction at given energy and flight direction,
  - one Bragg condition is sampled for scattering
- Scattering kernel (for poly-crystalline structure) provides inelastic incoherent scattering (phonon-interactions):
  - table lookup of scattering cross section
  - scattering energy and direction sampled from tabulated distributions

Single Crystal Model Needs

- Needs: Inelastic scattering for neutron monochromator and filter materials such as
  - Copper
  - Sapphire
  - Graphite
  - Heusler
  - Beryllium
- At different temperatures

Single Crystal: MCNPX-McStas





- 1 mm^3 Si crystal oriented with (4 0 0) crystallographic plane on Z-axis and irradiated by pencil beam on Z-axis
- Tallied with spherical detector at 1 meter distance

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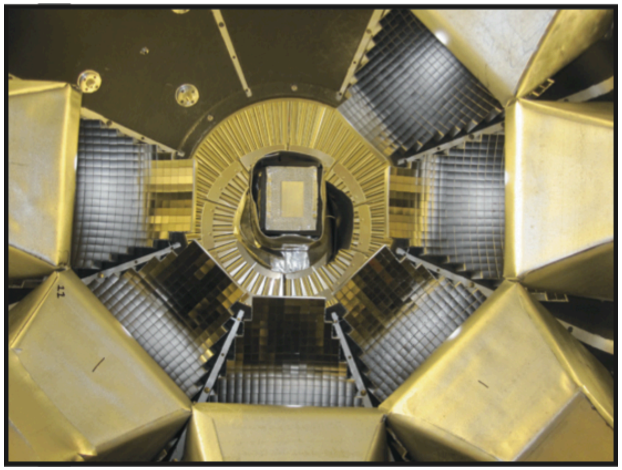
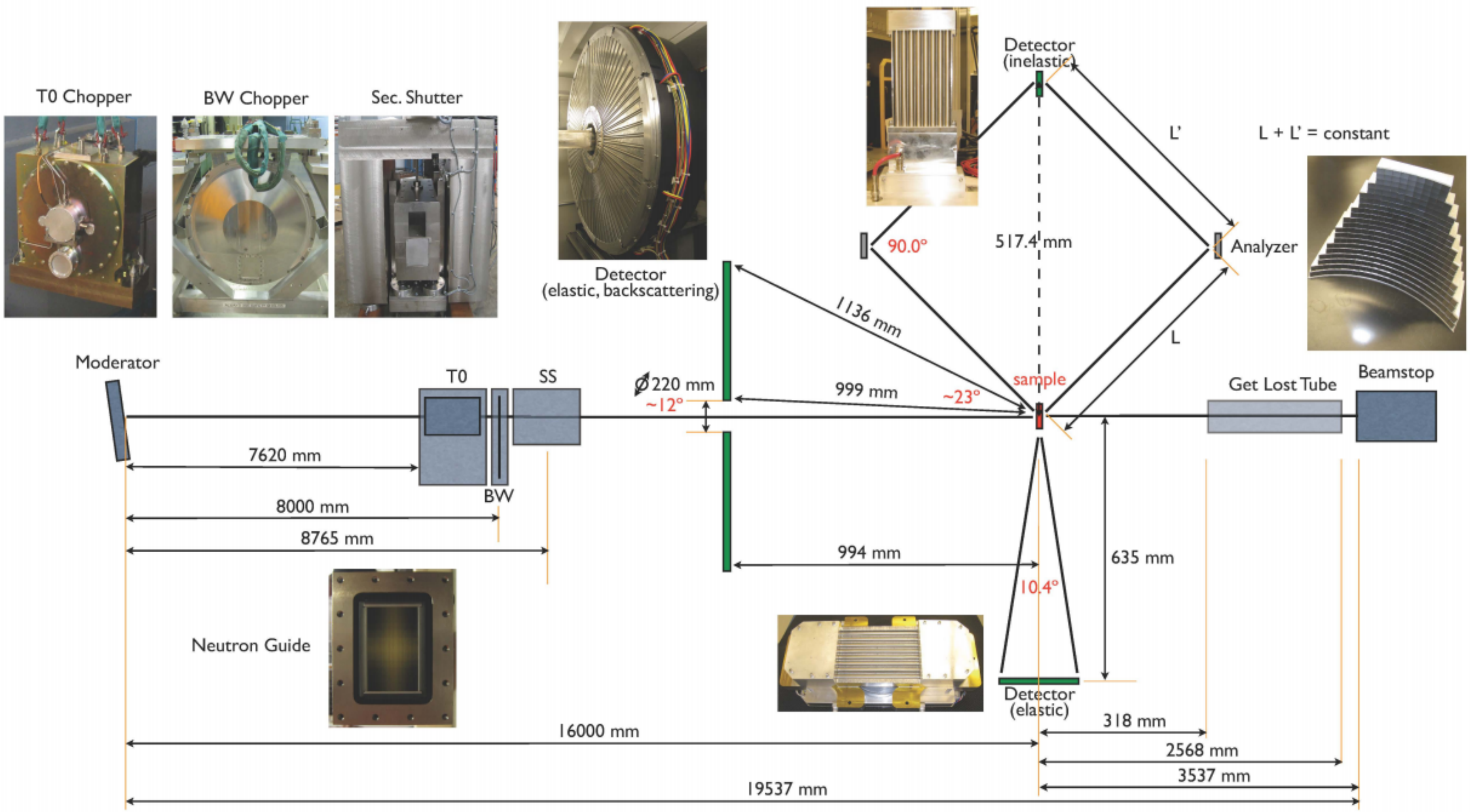
The VISION instrument

- Indirect geometry (white incident beam, fixed final energy)
- High flux (~5x10^7 neutrons/cm^2/s) and high throughput
- Broadband (-2 to 1000 meV at 30Hz, 5 to 500 meV at 60 Hz)
- Constant dE/E throughout the spectrum (~1.5%)
- Elastic line FWHM ~150 µs
- Backscattering diffraction bank Q range 1.5 to 30 Å^{-1}



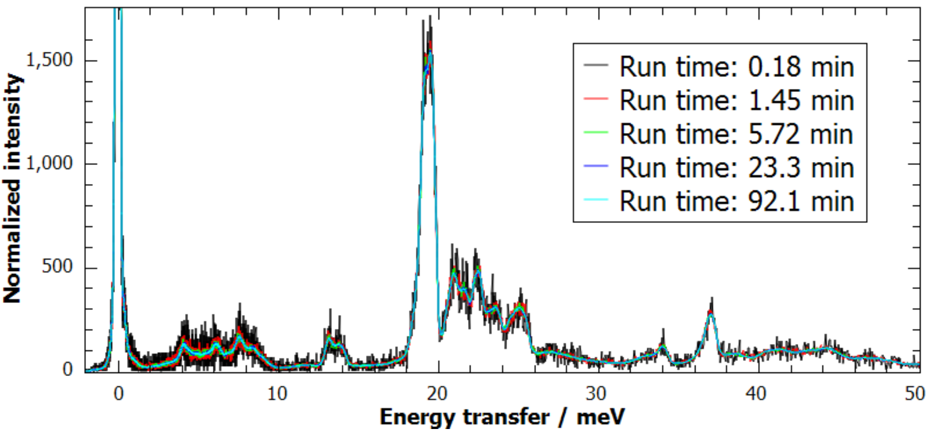


DGE
oratory

VISION is unique for its…

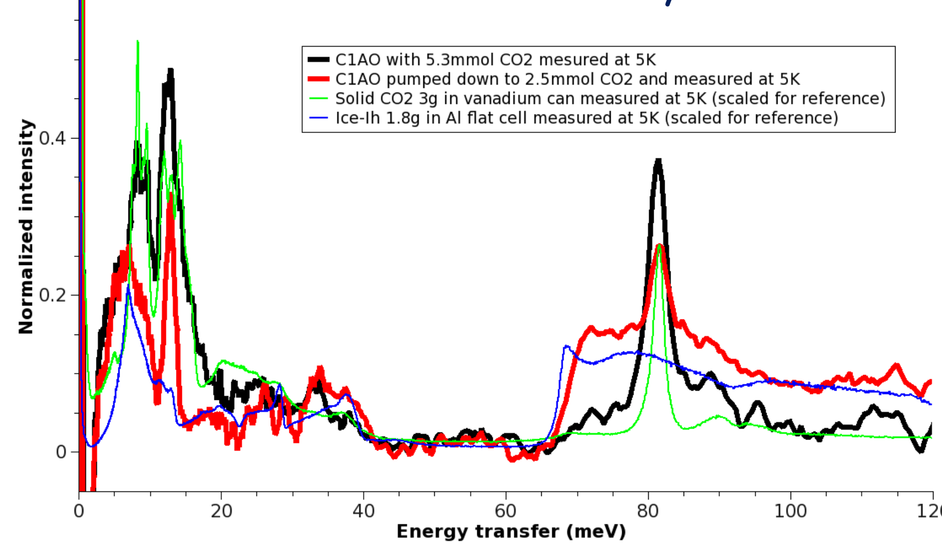
❑ High-throughput

INS spectra in minutes.
VISION has the highest data rate (millions of events per second) among all neutron beamlines in the world.



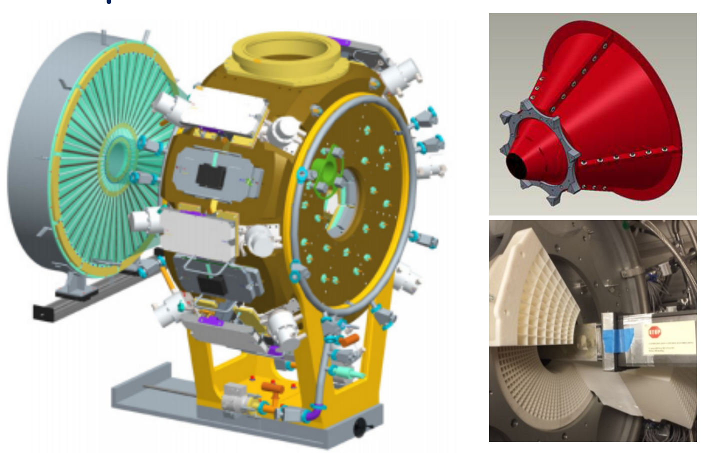
❑ High-sensitivity

INS of a few millimoles of CO_2 and H_2O adsorbed on the surface of catalysts



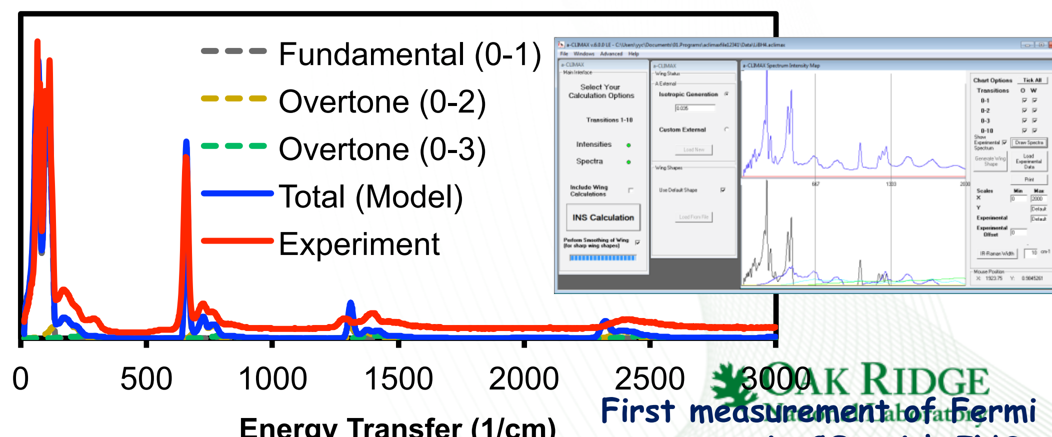
❑ Simultaneous measurement of INS and diffraction

Not only how atoms move and but also where they are.
Ideal for phase transition and chemical reactions.



❑ Integrated modeling capability

The aClimax software and INS calculation based on first-principles modeling



First measurement of Fermi resonance in CO_2 with INS

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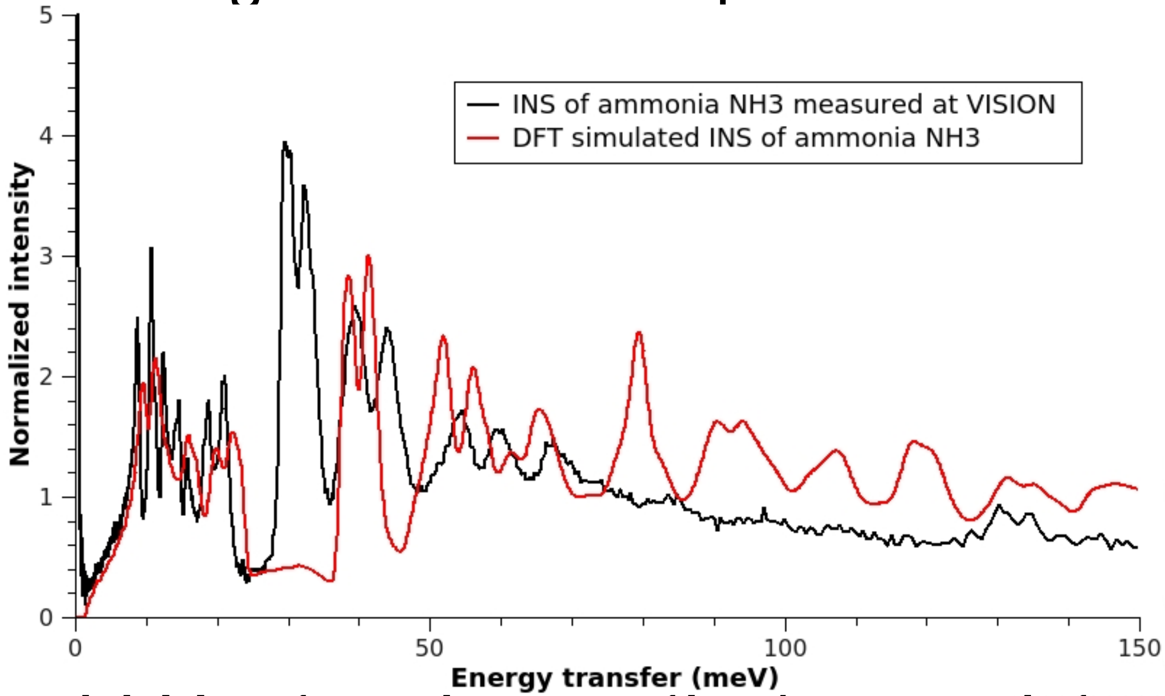
VISION vs Raman/Infrared: complementary tools for vibrational spectroscopy

VISION (INS)	Raman/Infrared
Measures dynamics of nuclei (direct)	Measures response of electrons (indirect)
Weighted by neutron scattering cross section	Weighted by polarizability or dipole moment
Easy to simulate/calculate	Difficult to simulate/calculate
No selection rules	Selection rules apply
No direct dependence on band gap	Band gap dependent
High penetration (bulk probe)	Low penetration (surface probe)
Easy access to low energy range (librational and translational modes)	Energy cutoff 200~400 cm^{-1}
Q trajectories in the (ω,Q) map	Gamma point

VISION recent measurements

- Liquid and solid NH_3 at various temperatures
  – No existing DOS data prior to these experiments
  – Simple molecular structure, however, abinitio simulations not in agreement with experiments



- Liquid H_2 at various ortho/para mixtures

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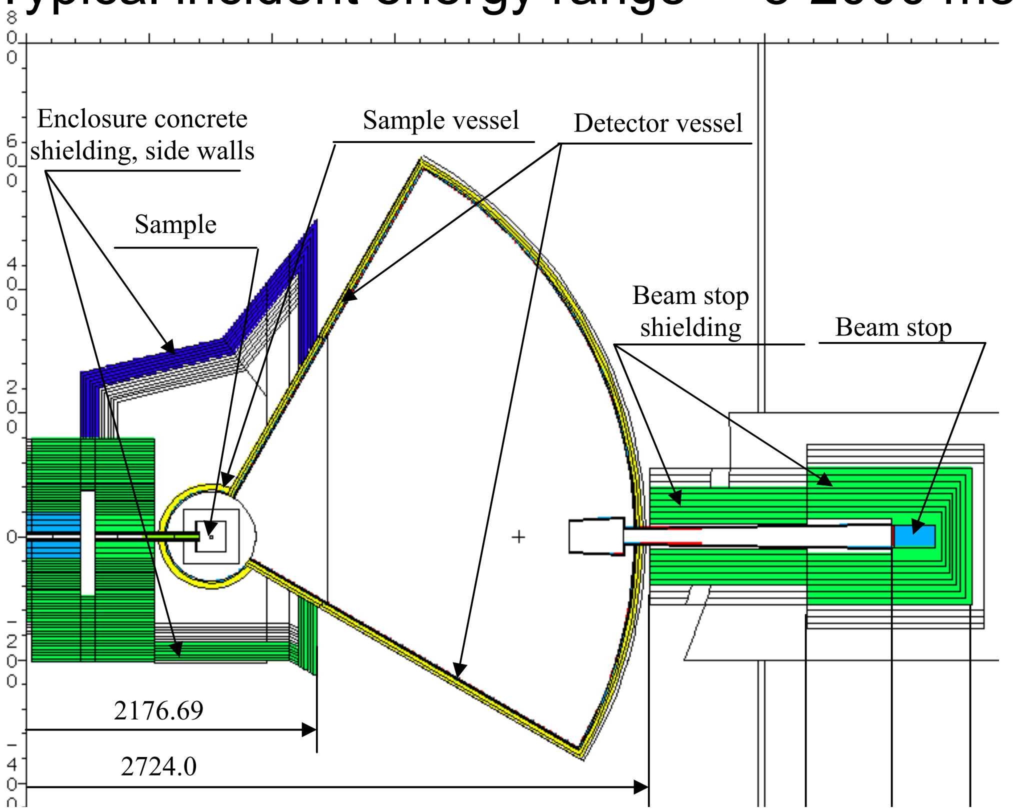
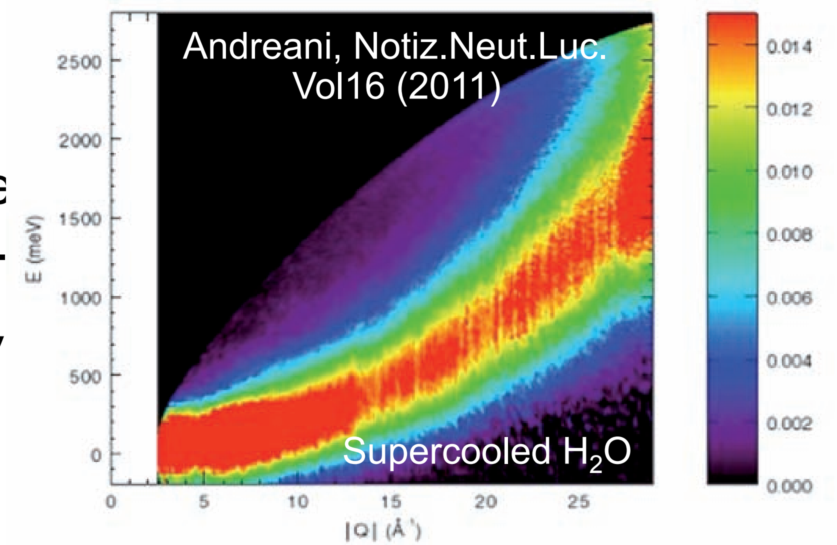
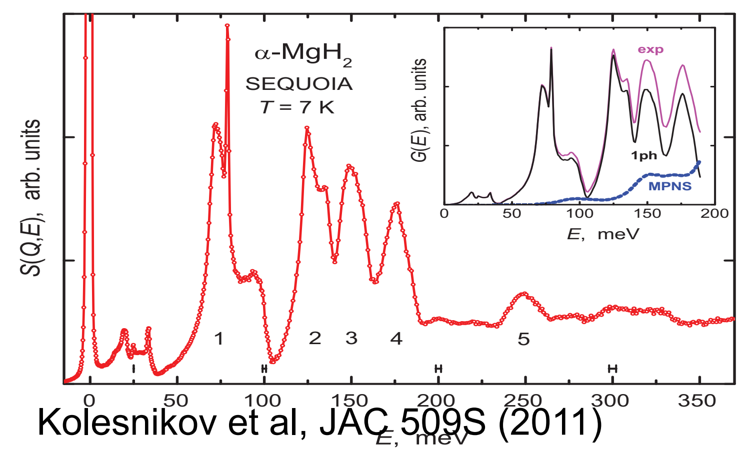
SEQUOIA: Fine-resolution Direct-geometry Chopper Spectrometer

Source-sample distance 20.0
Mean sample-detector distance 5.53 m
Angular coverage: Horizontally -30 to 60 de
Vertically: +/- 18 deg.
Range of energy resolution (% E_i) 1-3
Typical incident energy range 8-2000 meV





Scattering from water at 3 eV incident energy. The scattering is centered at the proton recoil energies.



Kolesnikov et al, JAC 509S (2011)

Fig. 1. The dynamical structure factor $S(Q,E)$ of the α-MgH_2 powder sample (open circles) as a function of the energy loss ($E > 0$) or gain ($E < 0$) of the inelastically scattered neutrons measured at 7 K with the SEQUOIA spectrometer at ORNL, USA. The

Para-H_2 Total Cross Section Measurement

- Bi-product of NPDGamma parity violation measurement
- Discrepancy asks for re-calibration of para-H_2 kernel
- Has impact on optimization of liquid H_2 moderators (increased transparency below 2 meV neutron energy)

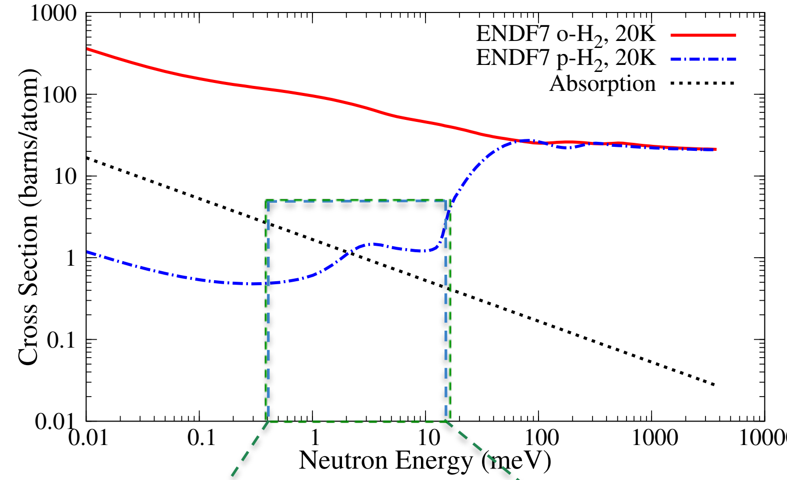


FIG. 1. Parahydrogen and orthohydrogen scattering cross sections at 20 K from ENDF-VII [33] and the absorption cross section [34].

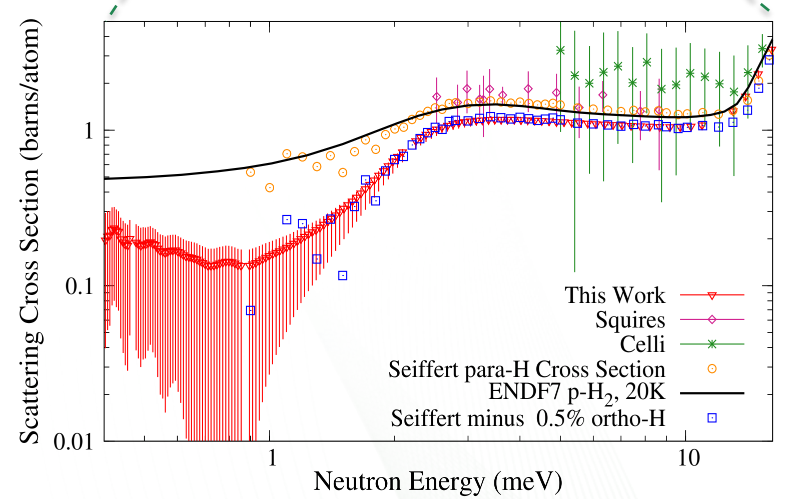


FIG. 7. (color online) The scattering cross section extracted in this work (triangles), Squires [32] (diamonds), Celli [27] (stars, some points omitted), Seiffert [31] (circles), ENDF-VII (black), and subtraction of a 0.5% admixture of orthohydrogen from Seiffert (squares).

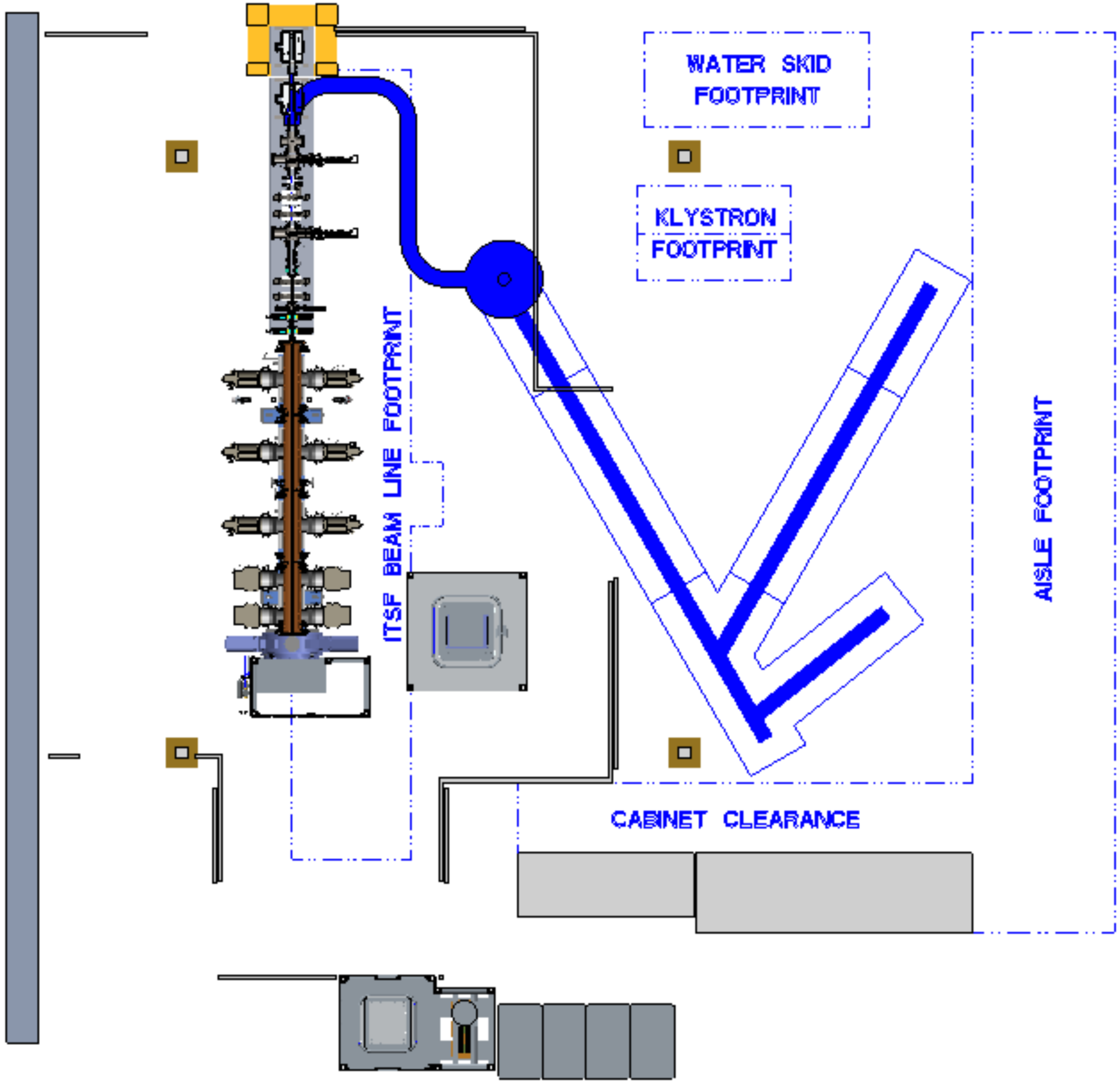
New measurement of the scattering cross section of slow neutrons on liquid parahydrogen from neutron transmission

K. B. Grammer,[1,*] R. Alarcon,[2] L. Barrón-Palos,[3] D. Blyth,[2] J. D. Bowman,[4] J. Calarco,[5] C. Crawford,[6] K. Craycraft,[1,6] D. Evans,[7] N. Fomin,[1] J. Fry,[8] M. Gericke,[9] R. C. Gillis,[8] G. L. Greene,[1,4] J. Hamblen,[10] C. Hayes,[1] S. Kucuker,[1] R. Mahurin,[11,9] M. Maldonado-Velázquez,[3] E. Martin,[6] M. McCrea,[9] P. E. Mueller,[4] M. Musgrave,[1] H. Nann,[8] S. I. Penttilä,[4] W. M. Snow,[8] Z. Tang,[12,8] and W. S. Wilburn[12]

arXiv:1410.2177v3 [nucl-ex] 24 Apr 2015

Moderator Test Facility in Development

- Using RFQ test stand as proton source of 2.5 MeV H^- pulsed at 1-60 Hz and pulse widths 1 ms - 1µs
- Sending beam into a lithium target
- Having moderators in wing-configuration
- Testing new and "old" moderator concepts for STS
- Testing large volume para-hydrogen and high-brightness moderators for emission spectra and emission time distributions



SECTION VIEW THROUGH UPPER BEAM LINE

Meeting with W. Bernnat (IKE): sends his regards

- Reworked numerous thermal data:

Be-05K-IKE.ace	H2O-s_04K.ace	Sab_al_70K.ace	oD2_10Ksolid_inc.ace
Be-100K-IKE.ace	H2O-s_113K.ace	Zr_90_293K.ace	oD2_17Ksolid_coh.ace
Be-10K-IKE.ace	H2O-s_165K.ace	Zr_90_77K.ace	oD2_17Ksolid_inc.ace
Be-20K-IKE.ace	H2O-s_218K.ace	Zr_91_20K.ace	oD2_g_70K.ace
Be-30K-IKE.ace	H2O-s_248K.ace	Zr_92_50K.ace	oD_5Ksd_coh.ace
Be-50K-IKE.ace	H2O-s_273K.ace	Zr_92_77K.ace	oD_5Ksd_inc.ace
Be-77K-IKE.ace	H2O-s_30K.ace	Zr_94_20K.ace	oH2_g_20K.ace
Bi_209_293K.ace	H2O-s_77K.ace	Zr_96_293K.ace	pD2_g_200K.ace
Bi_209_50K.ace	Pb_206_50K.ace	Zr_96_50K.ace	pD2_g_40K.ace
Bi_209_77K.ace	Pb_206_77K.ace	cold_xs_IKE	pD2_g_70K.ace
CH4l_91K.ace	Pb_207_50K.ace	oD2_05Ksolid_coh.ace	pH2_s_05K.ace
CH4s_50K.ace	Pb_208_293K.ace	oD2_05Ksolid_inc.ace	pH2_s_06K.ace
D_liquid	Pb_208_50K.ace	oD2_08Ksolid_coh.ace	pH2_s_13K.ace
H2O-l_400K.ace	Sab_al_06K.ace	oD2_10Ksolid_Coh.ace	xd_e71_s

Contact person: Michael Wohlmuther (PSI): michael.wohlmuter@psi.ch