The 30th International Seminar on Interaction of Neutrons with Nuclei (ISINN-30)

Verification of an available cross-section library for neutron interaction with solid deuterium using Monte Carlo simulation

Pham K. T.*, **Nezvanov A.Yu.**, **Muzychka A.Yu.**

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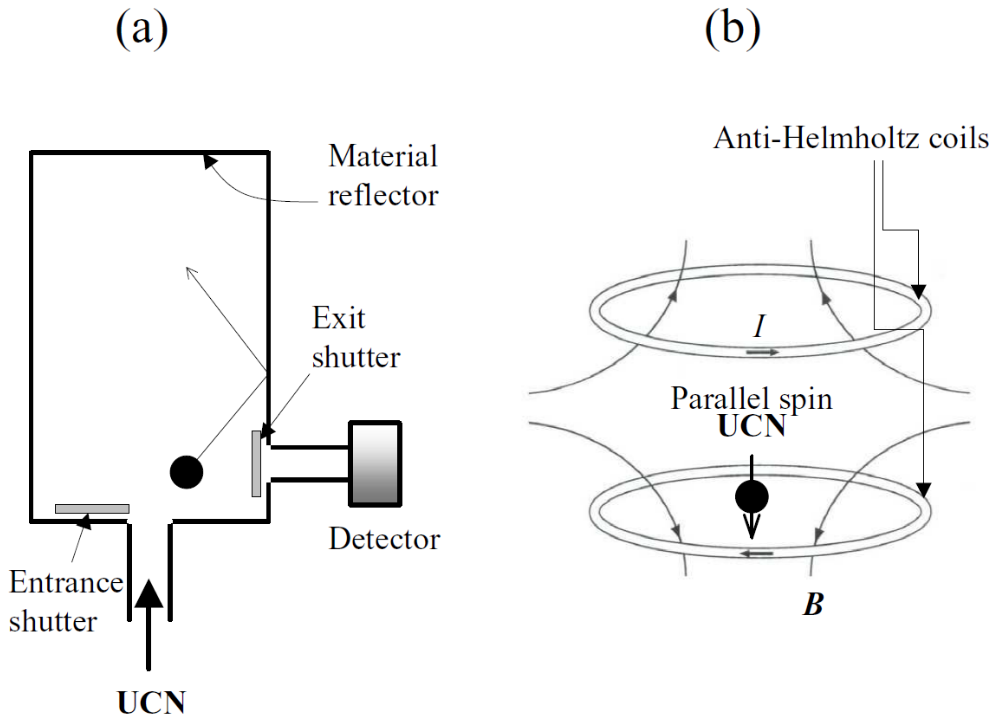
South Sinai Governorate, 14 - 18 April 2024

Ultra Cold Neutrons

UCNs are neutrons whose energy is so low that they are reflected under any angle of incidence and can be contained in traps

Type of neutron	E(ev)	T (K)	Λ (Å)	V (m/s)
Ultra cold	< 10^{-7}	≈(<) mK	> 800	< 5
Very cold	10^{-7} - 10^{-4}	10^{-2} - 10	800 - 30	5 - 130
Cold	(0.1 - 10) x 10^{-3}	10 - 120	30 - 3	130 - 1320
Thermal	(10 - 100) x 10^{-3}	120 - 1000	3 - 1	~ 1320 - 3950
Resonance	> 1		< 0.1	> 4 x 10^{4}

Ref.: G.V. Kulin (ISINN-29). The concept of an UCN source for a periodic pulsed reactor (2023).

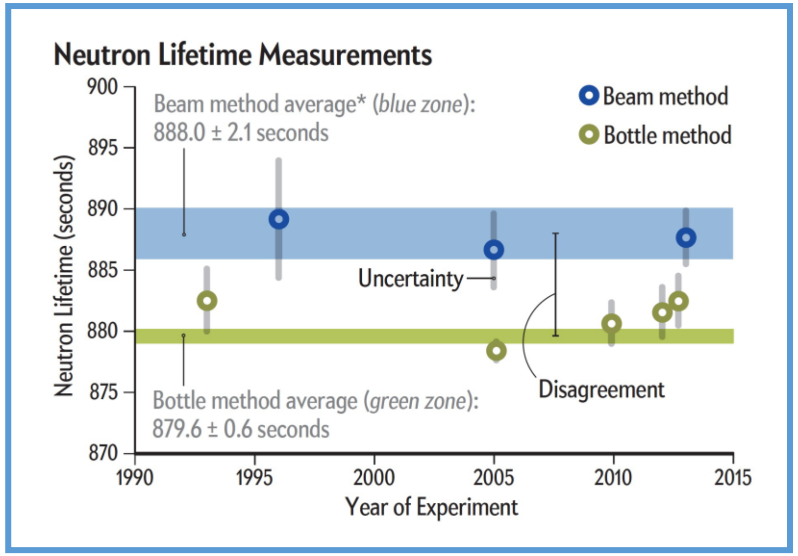


Sketch of UCN traps: (a) A material trap using a material reflector, (b) A magnetic trap.

Ref.: Oh-Sun Kwon (2005), Sogang University. Quasi-elastic scattering of ultracold neutrons (Dissertation).

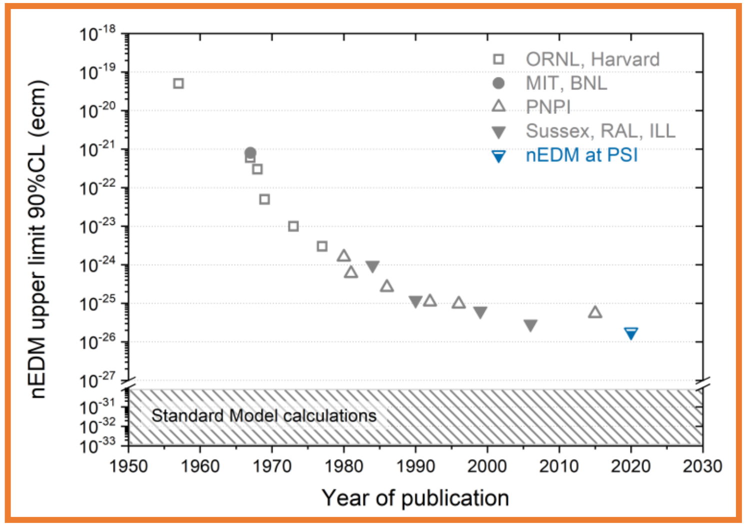
Why UCNs are important tools?

- Search for the neutron electric dipole moment (EDM)
- Measurement of the neutron lifetime
- Measurement of angular correlation coefficients of neutron beta decay
- Search for neutron-antineutron oscillations
- Quantization of neutron sates in gravitational field and search for new interactions
- Non-stationary quantum mechanics and neutron optics



Neutron lifetime measurements

Ref.: https://www.scientificamerican.com, modified



The history of neutron EDM limits

Ref.: Abel, C.; et al. (2020)

Status of UCNs development in the world

TRIUMF (Canada)
He source tested

NC-State (USA)
D2 source waiting for deployment

ILL (France)
Turbine source running
He source operating

Mainz (Germany)
D2 source operating

ESS (Sweden)
D2 source planned (2nd Workshop on UCN and VCN Sources, 8-9 May 2023)

PSI (Switzerland)
D2 source operating

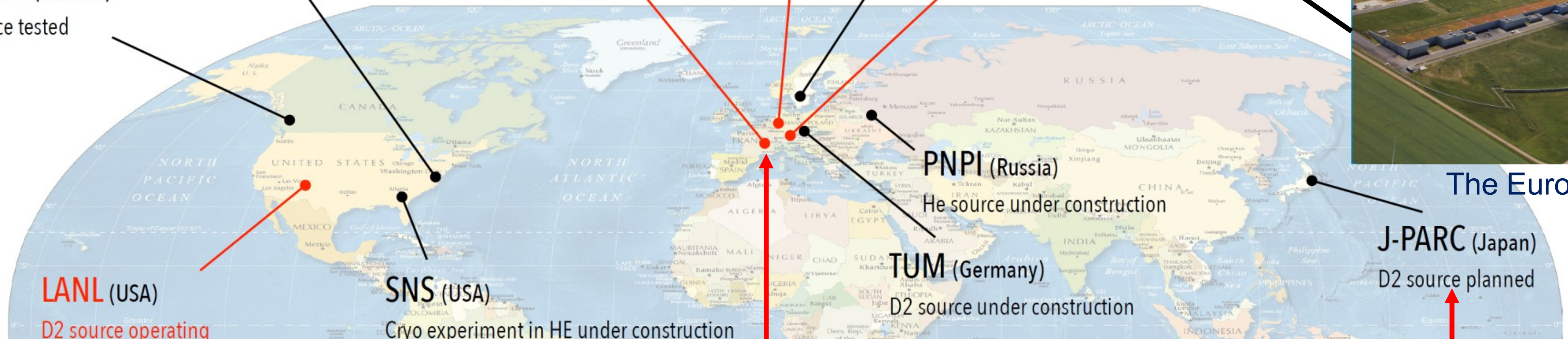
PNPI (Russia)
He source under construction

TUM (Germany)
D2 source under construction

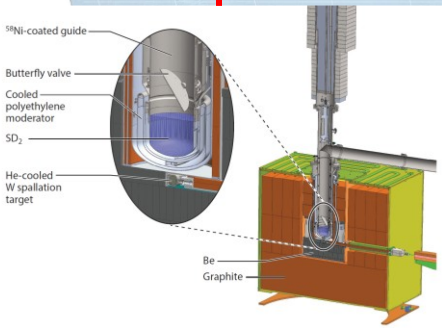
J-PARC (Japan)
D2 source planned

LANL (USA)
D2 source operating

SNS (USA)
Cryo experiment in HE under construction

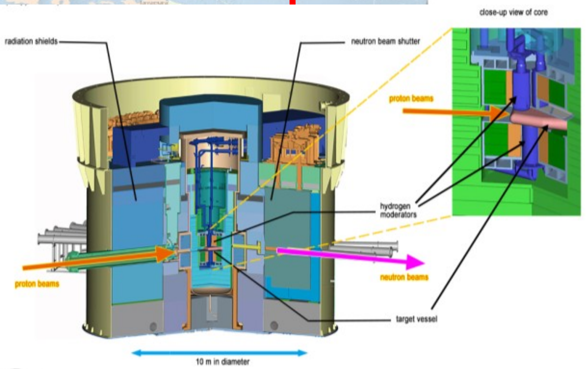


The European Spallation Source is under construction*



Engineering visualization of UCN sources in LANSCE

The reactor hall of the Laue-Langevin Institute - Grenoble, France



Cross-sectional view of pulsed neutron source in J-PARC

Ref.: G.V. Kulin (ISINN-29). The concept of an UCN source for a periodic pulsed reactor (2023). *https://europeanspallationsource.se/about

Some published articles on low energy neutron sources

PTEP

Prog. Theor. Exp. Phys. **2016**, 013C02 (22 pages)
DOI: 10.1093/ptep/ptv177

Pulsed ultra-cold neutro
a Doppler shifter at J-PA

S. Imajo[1,*], K. Mishima[2], M. Kitaguchi[3], Y
T. Oda[6], T. Ino[2], H. M. Shimizu[3], S. Yamas

Sci|Post

SciPost Phys. Proc. 5, 004 (2021)

UCN, the ultracold neutron source - neutrons for particle physics

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Nuclear Instruments and Methods in Physics Research A 1062 (2024) 169215

Contents lists available at ScienceDirect

Nuclear Inst. and Methods in Physics Research, A

journal homepage: www.elsevier.com/locate/nima

ELSEVIER

Full Length Article

Check for updates

An intense source of very cold neutrons using solid deuterium and nanodiamonds for the European Spallation Source

Nicola Rizzi[a], Ben Folsom[b], Mina Akhyani[c], Mads Bertelsen[d], Peter Böni[e], Yannick Beßler[f], Tomasz Bryś[d], Amalia Chambon[a], Valentin Czamler[g], Bent Lauritzen[a], Jose Ignacio Márquez Damián[d], Valery Nesvizhevsky[g], Blahoslav Rataj[d], Stavros Samothrakitis[h], Valentina Santoro[d], Ha Shuai[i], Markus Strobl[h], Mathias Strothmann[f], Alan Takibayev[d], Richard Wagner[g], Luca Zanini[d,*], Oliver Zimmer[g]

REVIEW OF SCIENTIFI

Performance of the Los Alamos Na
solid-deuterium ultra-cold neutron

A. Saunders,[1] M. Makela,[1] Y. Bagdasarova,[1]
T. J. Bowles,[1] R. Carr,[3] S. A. Currie,[1] B. Filip
K. P. Hickerson,[3] R. E. Hill,[1] J. Hoagland,[2] S. Hoedl,[4] A. T. Holley,[2] G. Hogan,[1] T. M. Ito,[1,3]
Steve Lamoreaux,[1,6] Chen-Yu Liu,[7] J. Liu,[3,8] R. R. Mammei,[9] J. Martin,[3,10] D. Melconian,[11]
M. P. Mendenhall,[3] C. L. Morris,[1] R. N. Mortensen,[1] R. W. Pattie, Jr.,[2] M. Pitt,[9] B. Plaster,[12]
J. Ramsey,[1] R. Rios,[13] A. Sallaska,[4] S. J. Seestrom,[1] E. I. Sharapov,[14] S. Sjue,[1,4]
W. E. Sondheim,[1] W. Teasdale,[1] A. R. Young,[2] B. VornDick,[2] R. B. Vogelaar,[9] Z. Wang,[1]
and Yanping Xu[2]

167

ns at the

Andreas Frei
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E-mail: andreas.frei@tum.de

Some published articles on low energy neutron sources

Nuclear Instruments and Methods in Physics Research A 823 (2016) 47–55

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

ELSEVIER

UCN sources at external beams of thermal neutrons. An example of PIK reactor

E.V. Lychagin [a], V.A. Mityukhlyaev [b], A.Yu. Muzychka [a], G.V. Nekhaev [a], V.V. Nesvizhevsky [c,*], M.S. Onegin [b], E.I. Sharapov [a], A.V. Strelkov [a]

On the new possibility of pulse accumulation of UCN in a trap

A.I. Frank[a,1], G.V. Kulin[a,2], M.A. Zakharov[a,]

[a] Joint Institute for Nuclear Research, Dubna, Russia

Technical Physics, 2022, Vol. 67, No. 6

Superfluid helium based ultracold neutron source for the PIK reactor

© *A.P. Serebrov, V.A. Lyamkin, A.K. Fomin, M.S. Onegin*

St. Petersburg Nuclear Physics Institute, National Research Center Kurchatov Institute, Gatchina, Russia

e-mail: serebrov_ap@pnpi.nrcki.ru

Frank A. I., Kulin G. V., Rebrova N. V., Zakharov M. A. P3-2021-22

On the Possibility of Creating a UCN Source on a Periodic Pulsed Reactor

The possibility of creating a UCN source on a periodic pulsed reactor is considered. It is shown that the implementation of the principle of time focusing, based on nonstationary neutron diffraction, and the idea of pulse filling of the trap for UCN allows us to create a sufficiently intense source of UCN on a pulsed reactor of a moderate power.

The investigation has been performed at the Frank Laboratory of Neutron Physics, JINR.

Journal of Neutron Research 24 (2022) 145–166 145

DOI 10.3233/JNR-220007

IOS Press

Development of UCN sources at PNPI

Anatolii Serebrov * and Vitaliy Lyamkin

Petersburg Nuclear Physics Institute, Gatchina, Russia

E-mail: serebrov_ap@pnpi.nrcki.ru

Some tasks on the concept of the source

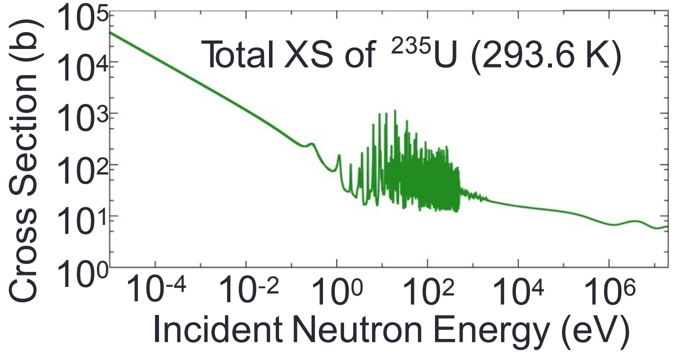
As part of the work on the concept of the source, priorities will be:

- Analysis of possible candidate materials for use as UCN converter, considering the specifics of the planned source.
- Modeling of the converter, calculation of the UCN output from it and optimization of its geometry.
- Participation in the formation of technical requirements and in the design of a UCN converter unit.

Evaluated nuclear data and Nuclear data processing systems

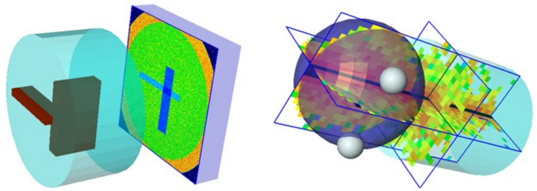
Evaluated Nuclear Data
(**JENDL, ENDF/B, JEFF, …**)

Nuclear Data Processing



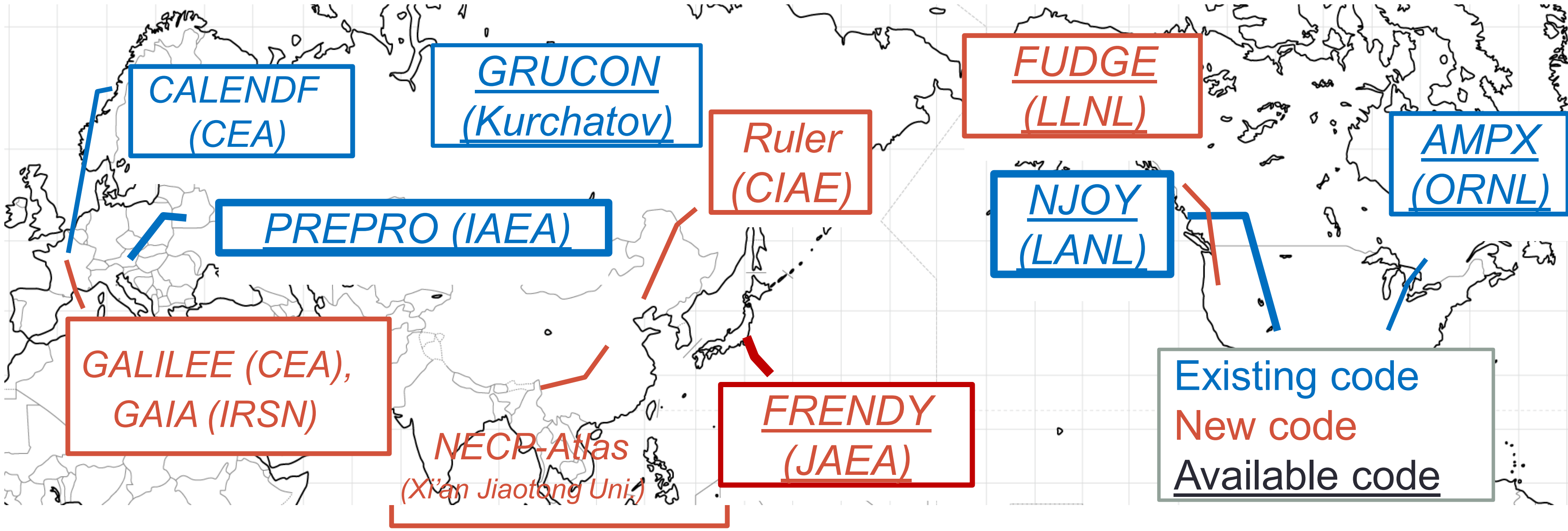
Cross Section (XS) Library

Transport Codes



Ref.: PHITS development team, Apr. 2023. https://phits.jaea.go.jp/

[Nuclear data processing system development in the world]



Ref.: D. Brown, "The New Evaluated Nuclear Data File Processing Capabilities," *INDC(NDS)-0695*.

PHITS and ACE format

Particle and Heavy Ion Transport code System

Capability

Transport and collision of nearly all particles over wide energy range using Monte Carlo method

neutron, proton, ions, electron, photon etc

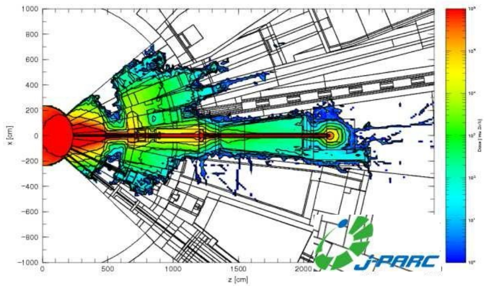
10^{-5} eV to 1 TeV/n

All-in-one-Package

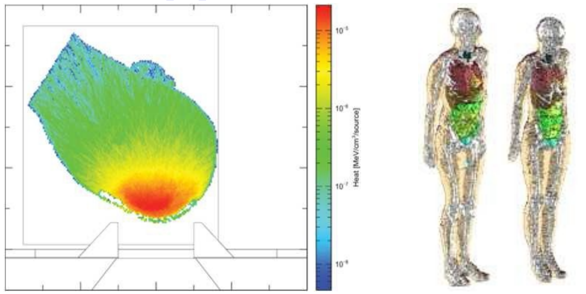
All contents of PHITS (source files, binary, data libraries, graphic utility etc.) are fully integrated in one package

Available in free of charge by submitting application form via PHITS website

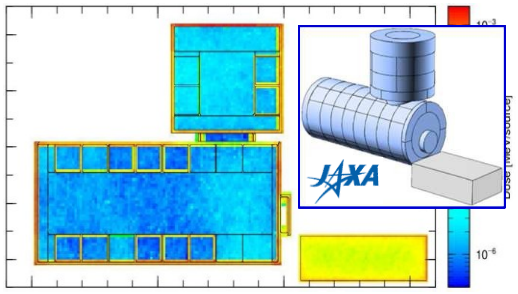
Applications



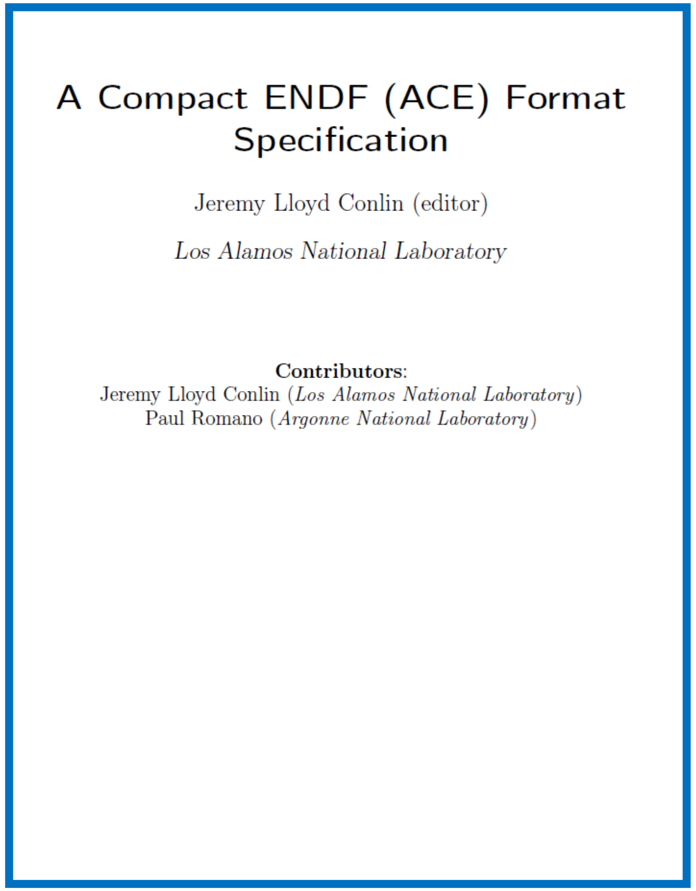
Accelerator Design



Radiation Therapy & Protection



Space & Geoscience



A Compact ENDF (ACE) Format Specification

Jeremy Lloyd Conlin (editor)

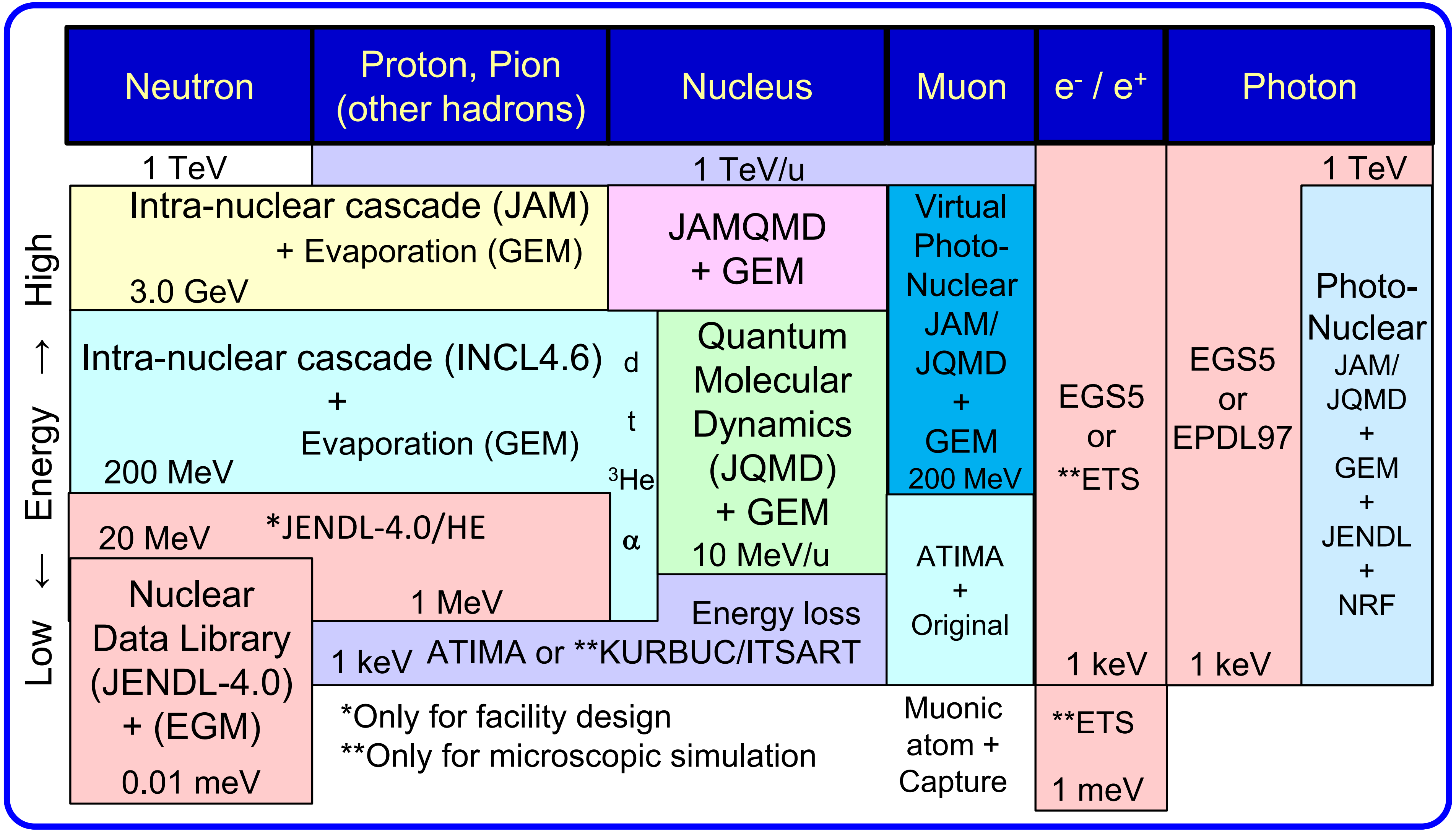
Los Alamos National Laboratory

Contributors:
Jeremy Lloyd Conlin (*Los Alamos National Laboratory*)
Paul Romano (*Argonne National Laboratory*)

Current version is only for continuous neutron and thermal scattering law (TSL) data

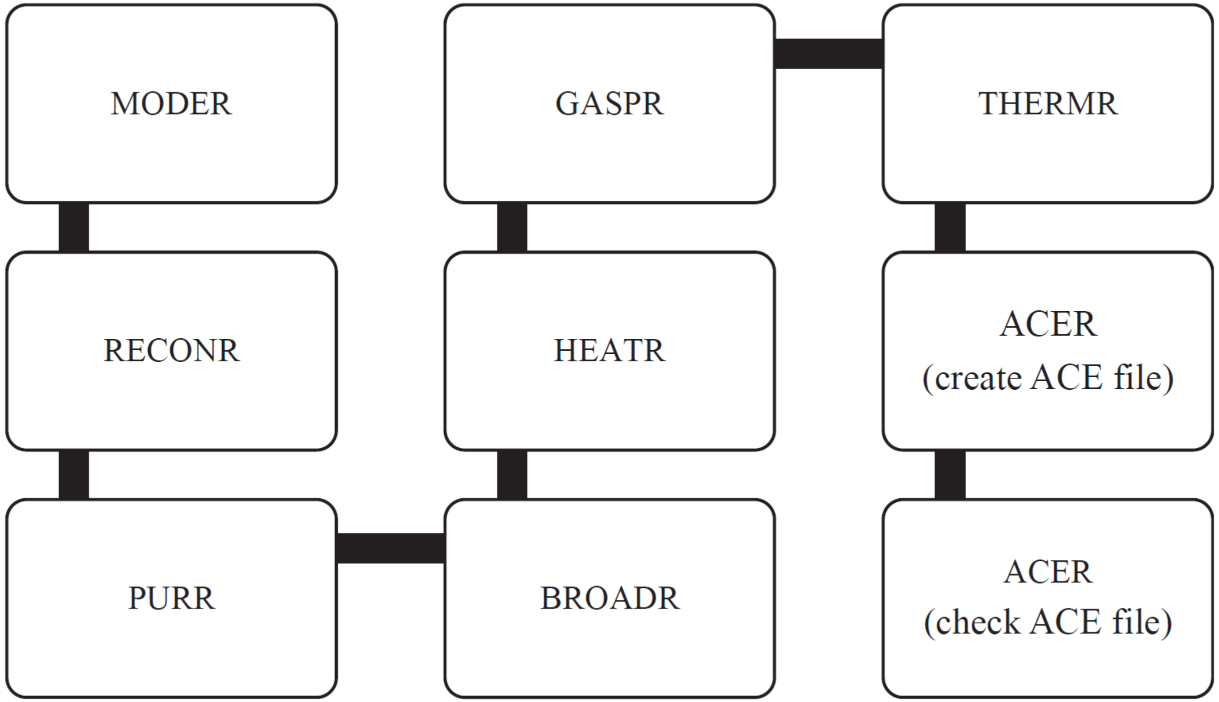
Ref.: PHITS development team, Apr. 2023.
https://phits.jaea.go.jp/

Map of Models Recommended to Use in PHITS



Ref.: PHITS development team, Apr. 2023.
https://phits.jaea.go.jp/

Nuclear Data Processing Code (NJOY2016)



Flow diagram of NJOY2016 processing for ACE format library construction

Ref.: K. Ouadie et al. / Nuclear Engineering and Technology 49 (2017) 1610e1616

```
2.0.1                        1001.710nc                   ENDFB-VII.1
0.999167 2.5301E-08 12/17/12      3
The next two lines are the first two lines of 'old-style' ACE.
  1001.80c    0.999167  2.5301E-08   12/17/12
H1 ENDF71x (jlconlin)  Ref. see jlconlin (ref 09/10/2012  10:00:53)      mat 125
      0         0.      0         0.      0         0.      0         0.
      0         0.      0         0.      0         0.      0         0.
      0         0.      0         0.      0         0.      0         0.
      0         0.      0         0.      0         0.      0         0.
  17969      1001     590         3       0         1       1         0
      0         1       1         0       0         0       0         0
      1         0    2951      2954    2957      2960    2963      4352
   4353      5644    5644      5644    6234      6235    6236      6244
   6245      6245    6246     16721       0     16722       0         0
      0         0       0         0       0     16723   16724     16725
1.00000000000E-11   1.03125000000E-11   1.06250000000E-11   1.09375000000E-11
1.12500000000E-11   1.15625000000E-11   1.18750000000E-11   1.21875000000E-11
1.25000000000E-11   1.28125000000E-11   1.31250000000E-11   1.34375000000E-11
1.37500000000E-11   1.43750000000E-11   1.50000000000E-11   1.56250000000E-11
1.62500000000E-11   1.68750000000E-11   1.75000000000E-11   1.81250000000E-11
1.87500000000E-11   1.93750000000E-11   2.00000000000E-11   2.09375000000E-11
2.18750000000E-11   2.28125000000E-11   2.37500000000E-11   2.46875000000E-11
2.56250000000E-11   2.65625000000E-11   2.75000000000E-11   2.84375000000E-11
2.93750000000E-11   3.03125000000E-11   3.12500000000E-11   3.21875000000E-11
3.31250000000E-11   3.40625000000E-11   3.50000000000E-11   3.59375000000E-11
```

ACE Header with beginning of XSS array for ^{1}H

Ref.: Conlin, Jeremy Lloyd, Romano, Paul (2019). A Compact ENDF (ACE) Format Specification

Theoretical basic for the sD_2 TLS library (1/3)

It is based on the neutron scattering kernel for sD_2 proposed by Granada J.R.

The main characteristics of Granada's model including:

- The lattice's density of states
- The Young-Koppel quantum treatment of the rotations
- The internal molecular vibrations
- The elastic processes involving coherent and incoherent contributions are fully described, as are the spin-correlation effects

epl A Letters Journal Exploring the Frontiers of Physics

June 2009

EPL, **86** (2009) 66007

doi: 10.1209/0295-5075/86/66007

www.epljournal.org

Neutron scattering kernel for solid deuterium

J. R. Granada[a]

Centro Atómico Bariloche and Instituto Balseiro, Comisión Nacional de Energía Atómica 8400 S.C. de Bariloche (RN), Argentina

$$S(\mathbf{Q},\omega)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\mathrm{d}t\,e^{-i\omega t}$$

$$\times\left\langle\sum_{l,l'}\sum_{\nu,\nu'}\overline{a^{*}_{l\nu}a_{l'\nu'}}\exp\{-i\mathbf{Q}\cdot\mathbf{R}_{l\nu}(0)\}\exp\{i\mathbf{Q}\cdot\mathbf{R}_{l'\nu'}(t)\}\right\rangle,$$

The intermediate scattering function $\chi(Q,t)$

Theoretical basic for the sD_2 TLS library (2/3)

$$\chi(\mathbf{Q},t) = 4b_c^2\, j_0^2(Qr/2)\{I(\mathbf{Q},t) - I_s(\mathbf{Q},t)\} + v(\mathbf{Q},t)\cdot I_s(\mathbf{Q},t), \quad (1)$$

$$\chi(\mathbf{Q},t) = \chi(\mathbf{Q},0) + \chi(\mathbf{Q},t\neq 0), \quad (2)$$

$I_s(Q, 0)$ = 1

$I(Q, 0) = |F(Q, 0)|^{2*}$

$$\chi^{el}(\mathbf{Q},0) = \{4\, b_c^2 j_0^2(Qr/2)\, |F(\mathbf{Q})|^2 + v(\mathbf{Q},0) - u(\mathbf{Q})\} \times \chi^{vib}(\mathbf{Q},0). \quad (3)$$

For o-D_2: $v(\mathbf{Q},0) = 2\,[b_c^2 + b_i^2] + [b_c^2 + 1/2\, b_i^2]\, j_0(Qd)$,

For p-D_2: $v(\mathbf{Q},0) = 2\,[b_c^2 + b_i^2] + [b_c^2 - b_i^2]\, j_0(Qd)$,

Minor approximation neglecting small energy-dependent second-order effects due to spin and structural correlations

$$\chi^{el}(\mathbf{Q},0) = 4b_c^2\, j_0^2(Qr/2)|F(\mathbf{Q})|^2\chi^{vib}(\mathbf{Q},0) \quad \text{(Elastic Coherent)} + 2(1+\alpha)\, b_i^2\chi^{vib}(\mathbf{Q},0) \quad \text{(Elastic Incoherent)} \quad (4)$$

d (= 0.74 Å) being the interatomic distance
j_0 the spherical Bessel function of order zero

|F(Q,0)| is the lattice structure factor corresponding to the arrangement of molecular centers

v(Q,t) contains all the complexity associated to the molecular rotations with definite parity for each (ortho, para) molecular species

I(Q,t) contains the contributions due to all molecular centers in the system

u(Q) is the molecular structure factor

χ^{vib}(Q,0) is the Debye-Waller factor

α = 1/4 for o-D2,
−1/2 for p-D2, and
0 for n-D2

Theoretical basic for the sD_2 TLS library (3/3)

The incoherent approximation for the inelastic term

$$I(\mathbf{Q}, t \neq 0) \cong I_s(\mathbf{Q}, t \neq 0) \quad (5)$$

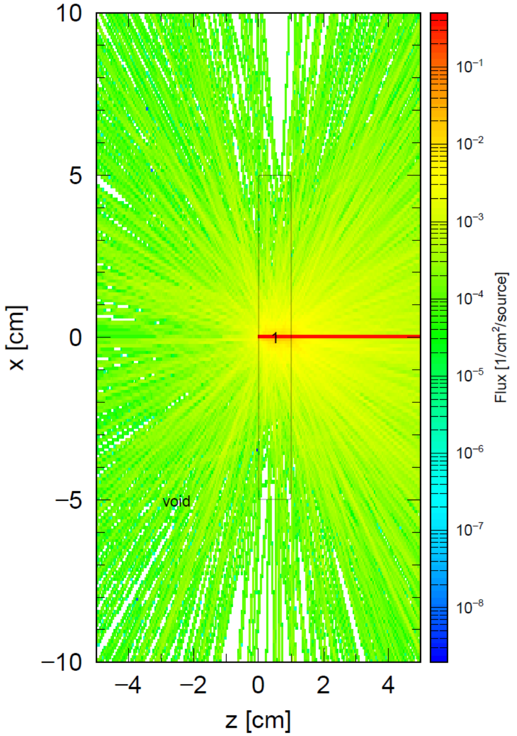
$$\chi^{inel}(\mathbf{Q}, t) = v(\mathbf{Q}, t) \cdot I_s(\mathbf{Q}, t) \cdot \chi^{vib}(\mathbf{Q}, t) \quad (6)$$

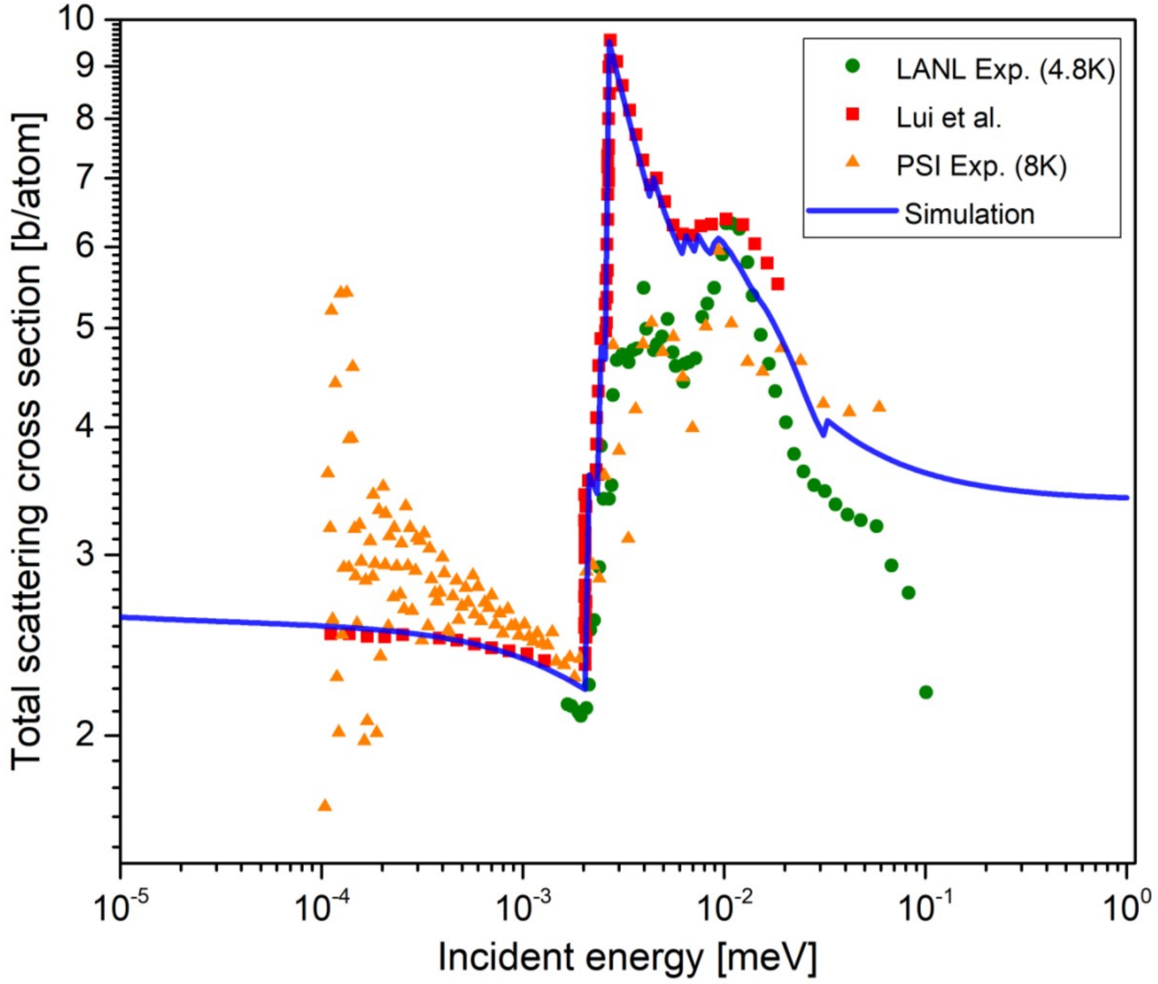
v(Q,t) contains all the complexity associated to **the molecular rotations** with definite parity for each (ortho, para) molecular species.

$\boldsymbol{I_s(Q,t)}$ is the self-contribution of the molecular centers determined by the dynamics of the lattice in the case of solid systems

Simulation results and comparison (1/4)

Simulation configuration	
Material	(Ortho) sD_2
Source type	Point
Layer radius (cm)	5
Thickness (cm)	1
Type of particle	Neutron
Beam direction	Cos (θ) = 1
Temperature (K)	5





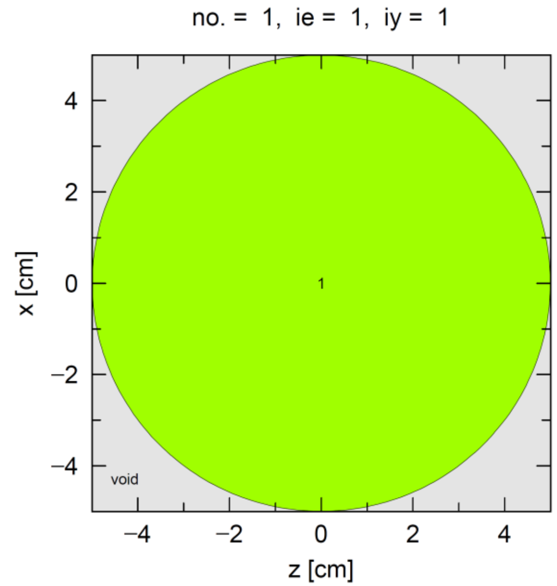
Total scattering cross section per atom for sD_2 at 5 K as a function of incident energy

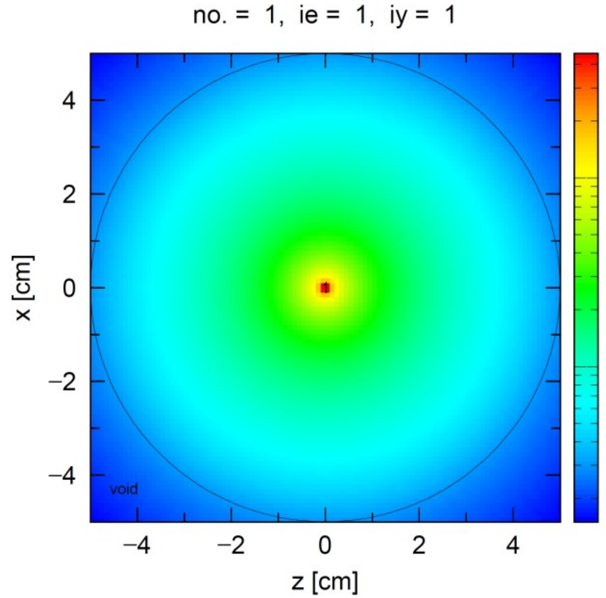
$$\sigma = \frac{\ln(I_0/I)}{\rho d}$$

I_0 and ***I*** are the transmitted intensities for the empty and full sample cells,
ρ: the density, and
d: the thickness of the sample cell.

Simulation results and comparison (2/4)

Simulation configuration	
Material	(Ortho) sD_2
Source type	Point isotropic
Sphere radius (cm)	5
Type of particle	Neutron
Initial energy (meV)	20.4
Temperature (K)	5






```
 sod2.05t    1.996800  4.3087E-10   08/13/21
* solid ortho-deuterium @ 5K - European Spallation Source     *            mat 128
  1002         0.      0         0.      0         0.      0         0.
     0         0.      0         0.      0         0.      0         0.
     0         0.      0         0.      0         0.      0         0.
     0         0.      0         0.      0         0.      0         0.
 4437672         3        65       200         5        -1         2        63
       0         0         0         0         0         0         0         0
       1       111       220   4430411   4430445         0   4430478   4430588
 4430697         0         0         0         0         0         0         0
       0         0         0         0         0         0         0         0
       0         0         0         0         0         0         0         0
                 109  1.00000000000E-11  1.78000000000E-11  2.50000000000E-11
  3.50000000000E-11  5.00000000000E-11  7.00000000000E-11  1.00000000000E-10
  1.26000000000E-10  1.60000000000E-10  2.00000000000E-10  2.53000000000E-10
  2.97000000000E-10  3.50000000000E-10  4.20000000000E-10  5.06000000000E-10
  6.15000000000E-10  7.50000000000E-10  8.70000000000E-10  1.01200000000E-09
  1.23000000000E-09  1.50000000000E-09  1.80000000000E-09  2.03000000000E-09
  2.27700000000E-09  2.60000000000E-09  3.00000000000E-09  3.50000000000E-09
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  3.38000000000E-08  3.65000000000E-08  3.95000000000E-08  4.27570000000E-08
  4.65000000000E-08  5.00000000000E-08  5.69250000000E-08  6.25000000000E-08
  6.90000000000E-08  7.50000000000E-08  8.19720000000E-08  9.00000000000E-08
  9.60000000000E-08  1.03500000000E-07  1.11573000000E-07  1.20000000000E-07
  1.28000000000E-07  1.35500000000E-07  1.45728000000E-07  1.60000000000E-07
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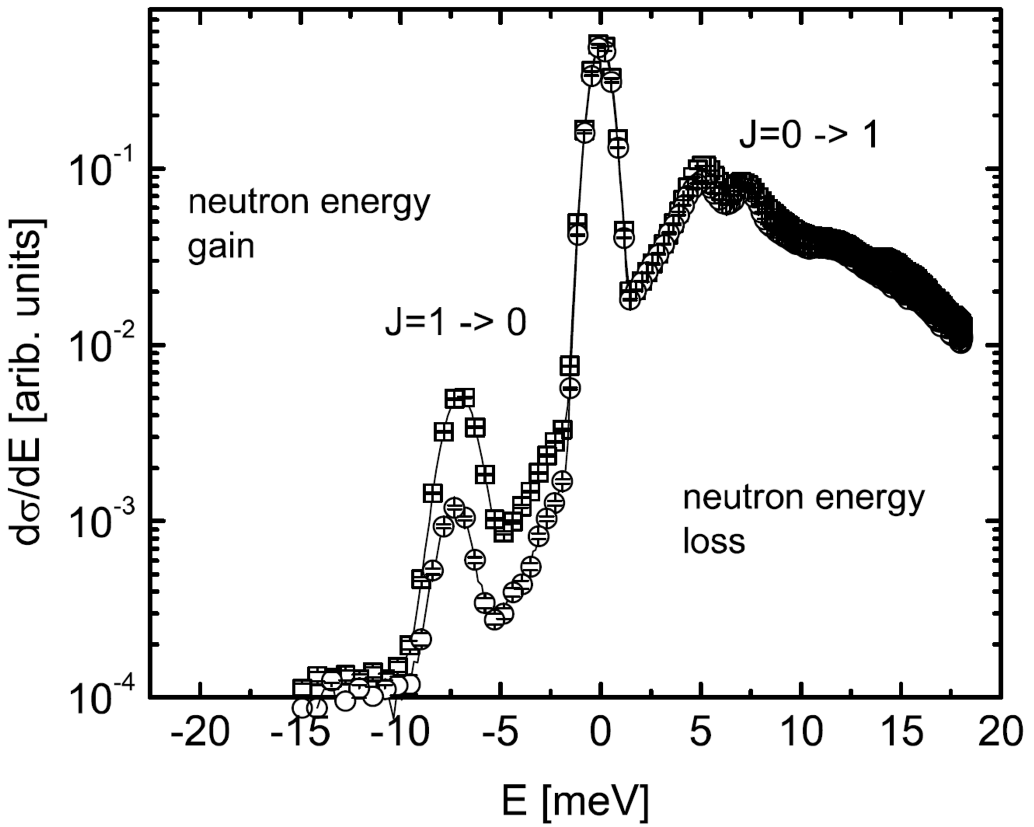
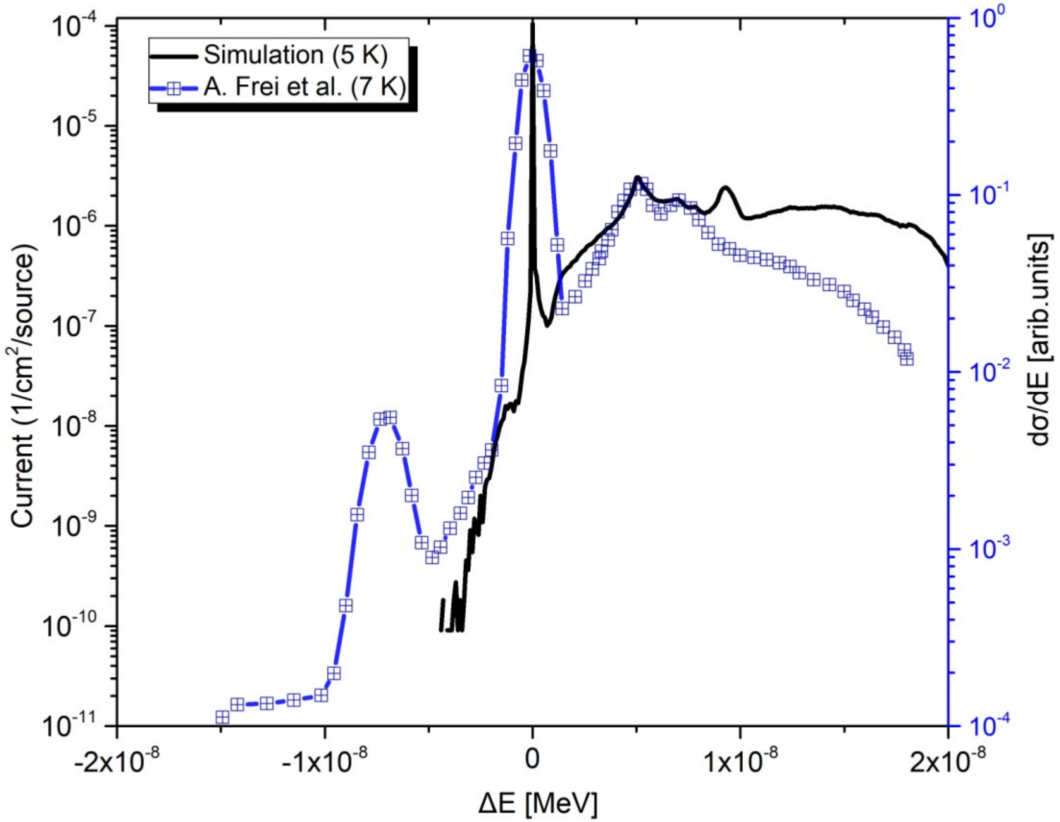
Simulation results and comparison (3/4)



An example of a dynamical neutron cross-section of solid D_2 at T = 7 K. Comparison of two ortho-concentrations C_0 = 66.7% (□) and C_0 = 98% (○). Initial energy of the thermal neutrons is E_0 = 20.4 meV.



A comparison between simulation result with A. Frei's result.

Note: The TLS library used for the simulation was developed for pure ortho-D_2 at 5 K

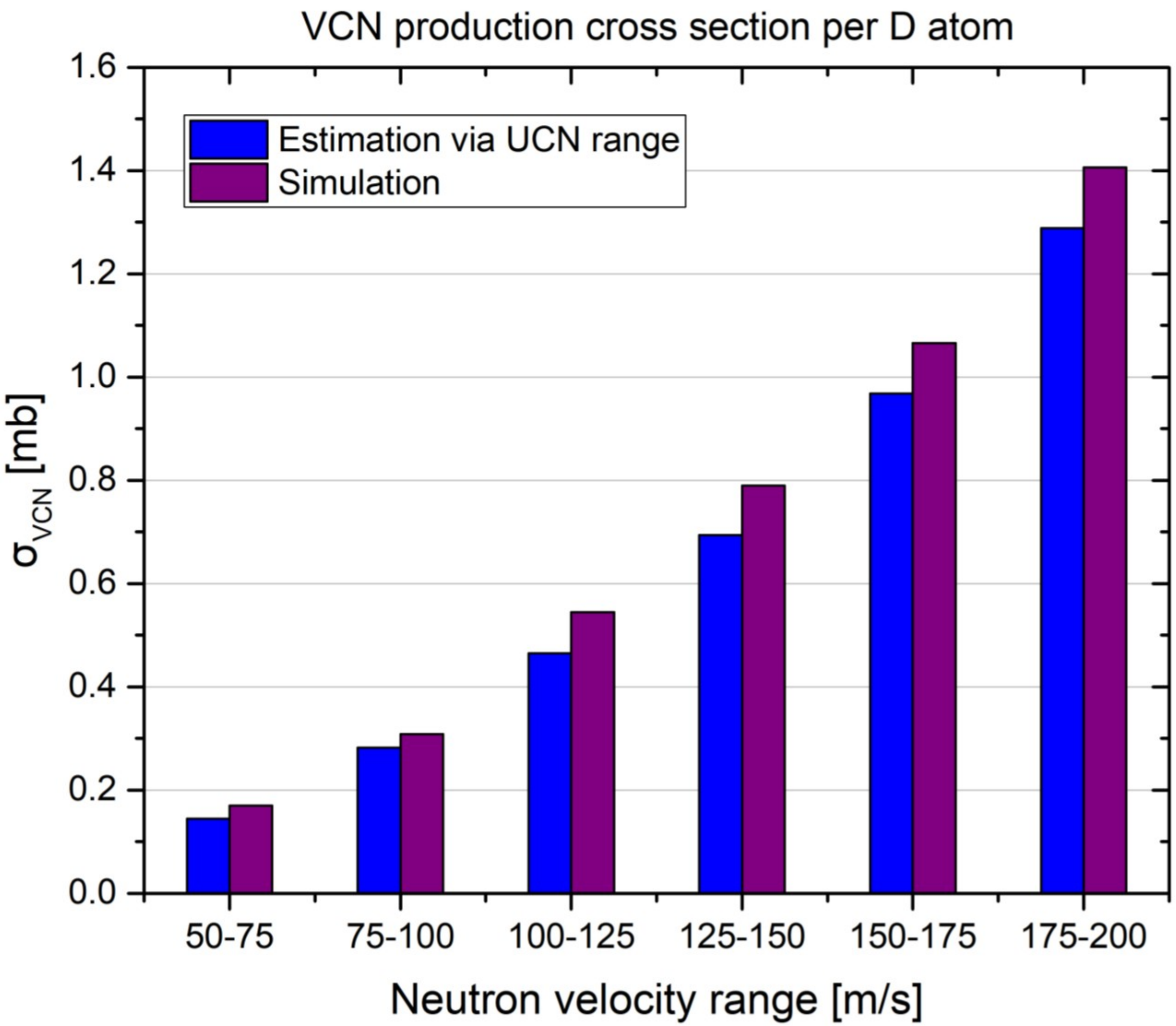
Ref.: A. Frei et al.. doi: 10.1209/0295-5075/92/62001

Simulation results and comparison (4/4)

E_0 (meV)	Velocities (m/s)	Energy (MeV)	VCN production cross section (mb)
20.4	50	1.3068E-10	1.6991E-01
	75	2.9402E-10	3.0807E-01
	100	5.2270E-10	5.4464E-01
	125	8.1672E-10	7.9014E-01
	150	1.1761E-09	1.0660E+00
	175	1.6008E-09	1.4058E+00
	200	2.0908E-09	

VCN production cross-section approximation: $\sigma_{VCN} = \sigma_{UCN}\left(\frac{V_{VCN}}{V_{UCN}}\right)^3$

$V_{UCN} = 5.3567$ m/s (150 neV); σ_{UCN} = **0.75E-7** b.
$[0, V_{VCN}]$ – the VCN production range.



Next tasks

1. Study and generate multi-group cross section (MGXS) libraries for converter materials using NJOY or FRENDY

2. Perform assessments on the applicability of new generated libraries through simulation calculation using GEANT4 and compare with published results

3. Calculate cross section for the generation of UCNs

Conclusion

- Low-energy neutrons have been an extremely productive tool for the investigation of fundamental interactions
- Many projects and researches on the development of low-energy neutron sources are being implemented actively in the world
- The limitation applies of the available library to the range of neutron energies from 10^{-2} to 10^{3} meV was reconfirmed
- The investigation on the generation of VCN with velocities from 50 - 200 m/s using the available library was conducted
- Some tasks were planned for the further research

THANK YOU
FOR YOUR ATTENTION!