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PROPOSAL FOR A NEW WPEC SUBGROUP ON THERMAL SCATTERING LAW : MEASUREMENT, EVALUATION AND APPLICATION

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WPEC meeting, NEA, Paris, 18-22 May 2015

Context

The motivation for the subgroup is the recent interest throughout the world on revisiting and revising the existing thermal neutron scattering data in the existing cross section libraries such as the ENDF, JEFF, JENDL, …

- Many questions emerge from the **WPEC SG-40** (CIELO) related to the impact of the thermal scattering data on criticality benchmarks
- Investigation and production of covariance matrices are also key issues for TSL data files. Definition of a new format for covariances is an important topic for **WPEC SG-38**
- TSL covariances matrices are key ingredients for the activities of **WPEC SG-39** related to the use of Integral Data Assimilation procedures for improving nuclear data files

List of thermal scattering law data files in ENDF-6 format

The major libraries contain a limited number of existing TSL data files

Material number	JEFF-3.1.1	ENDF/B-VII	JENDL-4.0
1	H(H20)	H(H2O)	H(H2O)
2		Para Hydrogen	Para Hydrogen
3		Ortho Hydrogen	Ortho Hydrogen
7	H(ZrH)	H(ZrH)	H(ZrH)
8	H(CaH2)		
11	D(D2O)	D(D20)	D(D2O)
12		Para Deuterium	Para Deuterium
13		Ortho Deuterium	Ortho Deuterium
26	Be metal	Be metal	Be metal
27		Be(BeO)	Be(BeO)
28		O(BeO)	
31	Graphite	Graphite	Graphite
33		Liquid Methane	Liquid Methane
34		Solid Methane	Solid Methane
37	H(CH2)	H(CH2)	
40		Benzine	Benzine
45		Al metal	
52	Mg metal		
56		Fe metal	
58		Zr(ZrH)	Zr(ZrH)
59	Ca(CaH2)		
75		O(UO2)	
76		U(UO2)	
Number of materials	**9**	**20**	**14**

Over the last 40 years new methodologies for measuring and evaluating double differential cross sections have emerged. Better-measured and evaluated data are produced nowadays ⇒ **not available in the ENDF libraries**

Kick off meeting : 18-19 may

A kick off meeting was organised at the NEA for evaluating the motivation and the interest of the nuclear data community

The kick off meeting has grown to a large event ⇒ 16 presentations and more than 20 participants

Three mains topics were covered

- **Experimental activities** in large-scale facilities and “compact” neutron sources
- **Theory, Evaluation and Covariance activities** : Ab Initio and Molecular Dynamic calculations
- **Data testing and Benchmaking activities** using MCNP, SERPENT and TRIPOLI codes

Three main needs emerge from the discussions

- Needs for **reactor applications**
- Needs for **cold moderator applications**
- Needs for materials used as **neutron monochromators and filters** for neutron scattering instruments

LEAPR module of NJOY and new generation of evaluation tools

TSL data available in the major ENDF libraries were produced with LEAPR with experimental phonon spectrum

New generation of evaluation and processing codes are needed for applications which are sensitive to double-differential data

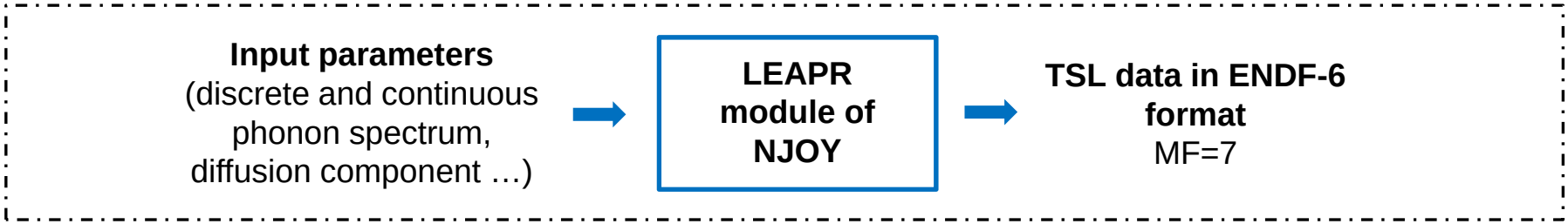
Two « new » approaches were discussed:

- **Ab Initio DFT calculation** with the Vienna Ab initio Simulation Package (VASP) is able to provide reliable TSL data ⇒ predictive approach used at the North Caroline University, production of covariance matrix is under investigation

- The « gaussian incoherent approximation » of LEAPR can also provide improved TSL data by using phonon spectrum obtained from **molecular dynamics simulations** based on « phenomenological » potentials ⇒ the GROMACS code was used by the Bariloche team for improving TSL data for light and heavy water (CAB model), covariance matrix can be produced with « standard » techniques based on Monte-Carlo and Bayesian methods

⇒ Advantages and limitations of the different models and codes will be discussed in the frame of this new sub-group

Link with the WPEC SG-38 activities (new format)



Input format for LEAPR and restructuration of the code:

- Accumulation of options (iel, ncold parameters) for producing TSL data
- Crystalographic data are in the source code of LEAPR
- …

⇒ Restructuration of the code is needed to get a modern, flexible and generic evaluation/processing tool ⇒ on-the-fly calculations of TSL data for producing application libraries ? automatic generation of α and β grids according to the thermal cut-off energy ? …

Format MF=7 and Covariance files

- A modernisation of the format is needed ($S(\alpha,\beta) \Rightarrow S_s(q,\omega)$, …)
- Definition of concise methods for storing and communicating the covariance matrix

Link with the experimental database EXFOR

⇒ How to test and improve TSL data ?

- **Integral experiments** are sensitive to various nuclear data
- Direct comparison with **experimental total cross section** is easy but not enought
- Direct comparisons with **double-differential data** are difficult ⇒ the simulation of the experimental set-up with Monte-Carlo codes are often impossible (missing experimental information)

This issue has to be discussed at AIEA in order to propose long term solutions for storing and communicating precise experimental information, MCNP inputs … (solutions already exist for criticality, propagation and reactor benchmarks with ICSBEP, SINBAD and IRPHE)

Detailed time schedule

year	period	activities
2015	May	Start of SG activities at the NEA: • Review of the experimental facilities and on-going work • Review of the existing/new "evaluation methodologies" • Review of the existing Evaluated Nuclear Data File in ENDF-6 format • Selection of the benchmarks of interest ☑
	May-June	Collect evaluation in ENDF-6 format ☐
	June- Dec.	• Processing and Benchmarking • Status/performance of available data ☐
2016	Jan-May	Begin to reflect on the generation of covariance data ☐
	May	Status of the one-year activity: • Presentation of the experimental programs • Presentation of the benchmark results • Review of the methodologies for producing covariance data • Needs for improving the evaluation
	May-July	Collect experimental data of interest for covariance ☐
	July-Dec.	Applied methodologies for producing covariance data ☐
2017	May	Status of the two-year activities: ☐ • Presentation of the experimental results • Presentation of the covariance data • Presentation of the improved evaluations
	May-Dec.	Begin to reflect on the nuclear data format ☐
2018	Jan-May	Monte-Carlo and deterministic uncertainty propagation work ☐
	May	Status of the three-years activities ☐ Proposal for a draft version of the final report that includes recommendation for future experimental works, evaluations and covariance

Kick off meeting 18-19 May 2015

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Compilation of existing TSL data:

- **CAB**, Bariloche
- **ILL**, Grenoble
- **North Caroline University**
- **IKE**, Stugart
- …

+ LEAPR model parameters ?

Define a set of dedicated ICSBEP benchmarks (light water, heavy water, grafite …)?

Comparison with differential data