Status of the JEFF project: 2010

A.J. Koning, [1]

Nuclear Research and Consultancy Group NRG,
P.O. Box 25, 1755 ZG Petten, The Netherlands

Abstract

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1 Introduction

The primary objective of the JEFF project is to produce high quality nuclear data libraries for existing and future nuclear energy systems. This rather straightforward objective requires a complex interplay between various working fields: commercial reactor operation, reactor and fuel cycle physics for either existing or future reactors, data library processing and validation, data file evaluation, and theoretical and experimental nuclear physics, see Fig. 1. Depending on the complexity, the total time of such a cycle may take several months to several years, especially if in the latter stages of nuclear data validation, represented by the inner circle of Fig. 1, new needs for differential data improvement emerge, bringing us to the outer circle of Fig. 1 again. In Europe, organizations and infrastructures such as measurement facilities, theoretical and computational nuclear physics groups, nuclear data centers, and reactor physics groups all contribute to provide nuclear data for JEFF that enable efficient development of nuclear technology.

The JEFF project involves evaluation efforts that cover the main nuclear data needs in the fields of fission and fusion applications. This initiative has provided the means for co-operative activities between participating countries while ensuring the most rational and efficient use of available resources. JEFF is an OECD/NEA Data Bank project, and essentially involves only scientists from European countries. The overall structure of the project is depicted in

[1] Corresponding author. E-mail address: koning@nrg.eu

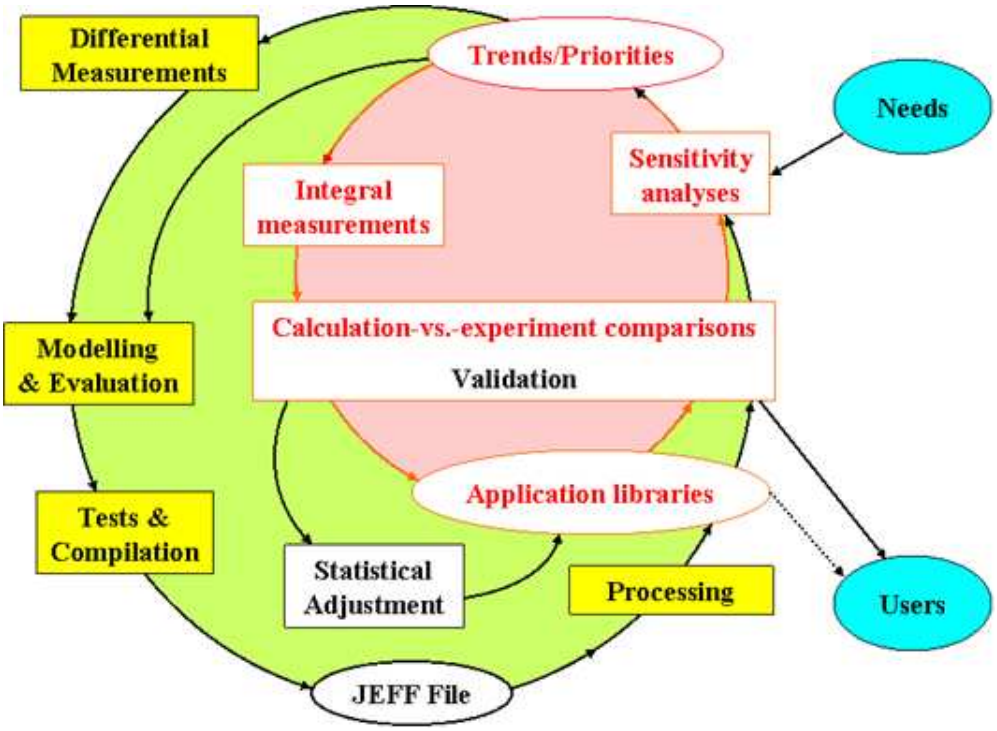

Fig. 1. Life cycle of nuclear data development for JEFF

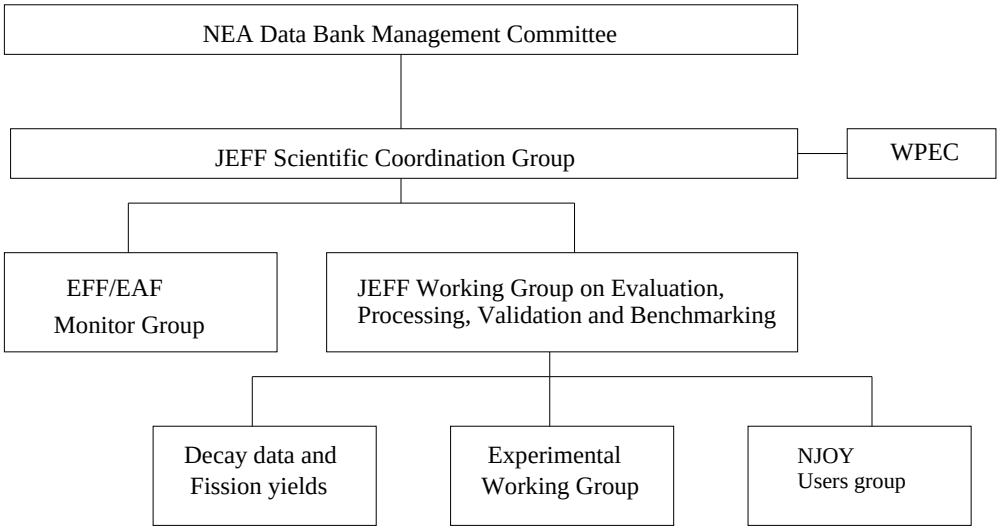

Fig. 2. Organisation of the JEFF project.

Fig. 2. Development of the JEFF libraries is indirectly financed by the voluntary contributions of participating individuals and organizations. Staff at the NEA Data Bank ensure the maintenance of the JEFF library, and twice yearly JEFF meetings bring together experts in all areas mentioned in Fig. 1.

In the computational simulation of nuclear systems, two main classes of nuclear data are required: (1) data describing the transport of neutrons (and

sometimes other particles) interacting with nuclei making up the system, and (2) data describing nuclear changes in system constituents, as a result of fission, fuel depletion (often called burn-up), transmutation, activation reactions or decay. All these data are covered by the JEFF project. For (1), the JEFF general purpose data library is available which contains all cross sections, resonance parameters and other nuclear reaction information entering particle balance calculations. For (2), the JEFF fission yield and decay data libraries are available, as well as a JEFF activation library. An essential ingredient of all these libraries is, or should be, covariance data, which is a measure of the confidence we have in the quality of the nuclear data that come from measurement or theory. These are now being gradually added to all libraries.

While fission energy systems continue to be the main area of application for JEFF, fusion, medical applications, and various non-energy related industrial applications also make use of JEFF data files. The European Fusion File (EFF) project [1] contributes to this initiative through specific tasks on nuclear data evaluations, library production, data verification, development of computer programs and validation of nuclear data through integral experiments.

2 Status of JEFF

The latest large scale release of the JEFF library took place in May 2005 [2], with JEFF-3.1. Since then, a new general purpose library JEFF-3.1.1 was released [3], as well as an upgrade to the activation data library and an update to the fission yield and decay data libraries. In total, JEFF-3.1.1 now consists of the following sub-libraries:

- neutron general purpose library: 381 isotopes
- neutron activation library: 774 isotopes
- thermal scattering law library: 9 materials
- decay data library: 3852 isotopes
- fission yield data library: 19 isotopes
- proton special purpose library: 26 isotopes

In addition, new evaluation efforts are underway to contribute to JEFF-3.2. We outline the most important developments below.

2.1 Release of JEFF-3.1.1

Various problems, ranging from small to significant, have been reported since the release of JEFF-3.1. Among the more important feedback for the JEFF-3.1

general purpose file is:

- ^{237}Np underestimation of the thermal capture cross section
- Changes of $\overline{\nu}$ and capture and fission cross sections up to 20 eV for ^{239}Pu
- Need to revise 7 fission product evaluations to satisfy integral fission product inventory experiments.

It was decided to produce an intermediate release, JEFF-3.1.1, at the beginning of 2009 in which these and other corrections are implemented. Meanwhile this library has been validated [3] and has been adopted by French nuclear industry. Several experiments, such as LWR mock-up experiments, PWR and BWR chemical assays and SNF reactivity worth measurements were analysed using both TRIPOLI-4 and APOLLO-2.8 reference calculations, and the conclusion is that, for this software, JEFF-3.1 performs better than other world libraries for analyses of fuel inventory, MOX reactivity and plutonium ageing, and reactivity coefficients such as temperature coefficient and stainless steel reflectors. JEFF-3.1.1 is used worldwide for PWR and BWR calculations, particularly in the new ARCADIA package of Areva-NP.

2.2 Neutron general purpose library

New, updated and extended evaluations produced in Europe during the current mandate period of the JEFF project will be considered for inclusion in the JEFF-3.2 library. The new neutron files that are currently produced, or will be produced in the near future, are shown in Table 1. In addition to this list, the evaluations of important fission products will be revisited. A recent evaluation example for ^{239}Pu by CEA/DAM [4] is given in Fig. 3. Extensive, partly-automated benchmarking tests were undertaken to probe the quality of both the JEFF-3.1 and JEFF-3.1.1 libraries. These studies have included MCNP (NRG, SCK), TRIPOLI (CEA) [5] and APOLLO (CEA) criticality calculations for an unprecedented set of benchmarks. An example is given in Fig. 4, taken from Refs. [6]-[8]. Current-day computer power enables revisions of the JEFF library to be rapidly tested within this scheme. Additional validation is now possible by means of a Monte Carlo approach to the calculation of the effective delayed-neutron fractions [9], and improved thermal scattering law data [11–14]. A wider range of validation exercises is being performed using different methods and codes to study various integral quantities. Apart from reactivity predictions in UO_2-fuelled systems (CEA), JEFF-3.1 has exhibited improvements in isotopic inventory predictions as inferred from post irradiation examination data. Such results are reported in Ref. [3]. Successful multigroup processing of both JEFF-3.1 and JEFF-3.1.1 has been reported recently by ENEA Bologna [10].

Table 1
Neutron evaluations proposed for JEFF-3.2

Nuclei	Energy range and origin
^{50,52,53,54}Cr	0-150 MeV, KIT Karlsruhe
^{55}Mn	0-150 MeV, KIT Karlsruhe
^{174,176,177,178,179,180}Hf	0-20 MeV, SERCO and Birmingham Univ.
^{181}Ta	0-150 MeV, KIT Karlsruhe
^{180,182,183,184,186}W	0-150 MeV, IAEA and KIT Karlsruhe
^{204,206,207,208}Pb	0-200 MeV, NRG update of covariance data
^{209}Bi	0-200 MeV, NRG update of covariance data
$^{235-239}$U	0-30 MeV, CEA/BRC
$^{238-240}$Pu	0-30 MeV, CEA/BRC
^{241}Am	0-30 MeV, CEA/BRC

Fusion-relevant benchmarking is reported in another paper at this conference[1].

2.3 Thermal scattering law library

Revised thermal scattering law data have been produced for all important moderator and structural materials, and these files were included in JEFF-3.1 on the basis of nine evaluations: hydrogen bound in water, zirconium, polyethylene (CH_2) and CaH_2, deuterium bound in D_2O, ^{9}Be, graphite, ^{24}Mg and calcium bound in CaH_2. All files are new evaluations, except ^{9}Be and hydrogen in polyethylene, which are adopted from the JEFF-3.0 library. Many of the evaluations result from an IAEA data development project on thermal neutron scattering [11–14]. Calculations for a variety of temperatures were made with the LEAPR module of NJOY to obtain thermal scattering law data that are accurate over a wider range of energy and momentum transfer. Detailed comparisons with a significant number of measurements of differential and integral neutron cross sections and other relevant data have been performed in order to validate these files on a microscopic scale. The models used for these files are able to describe the experimental data reasonably well.

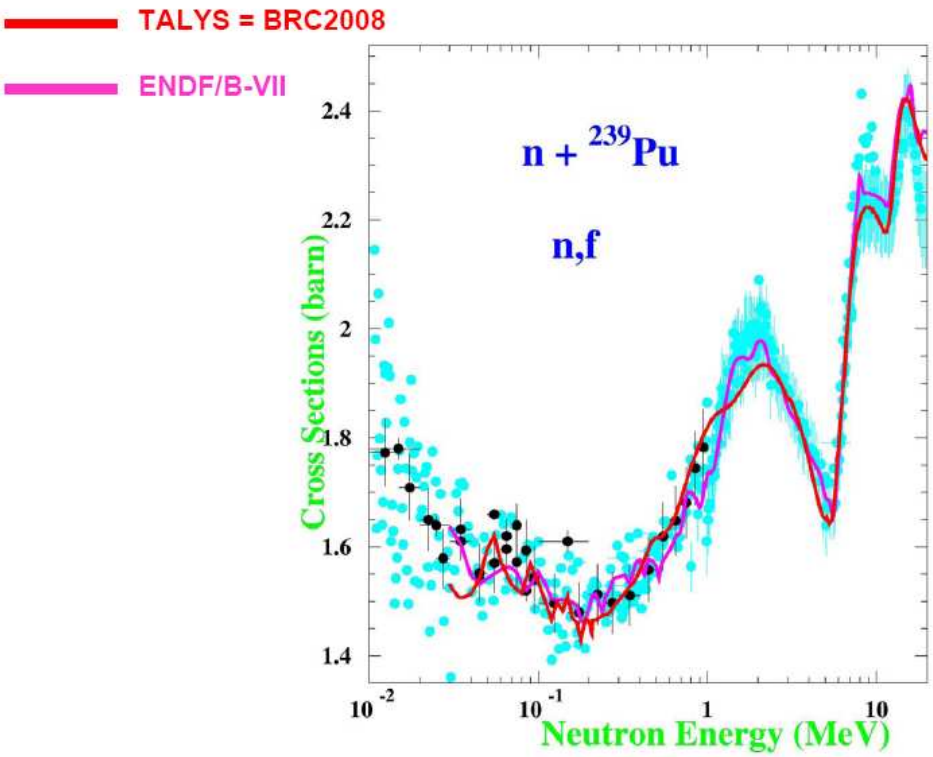

Fig. 3. Evaluated ^{239}Pu(n,f) cross section compared with experiment. Figure taken from [4].

2.4 Fission yield and radioactive decay data libraries

A complete description of the contents and performance of the JEFF-3.1.1 radioactive decay data and fission yield library is available [15].

The fission product yield libraries JEFF-3.1/NFY&SFY include independent and cumulative yields for the neutron-induced fission of ^{232}Th, ^{233,234,235,236,238}U, ^{237,238}Np, ^{238,239,240,241,242}Pu, ^{241,242m,243}Am, ^{243,244,245}Cm and the spontaneous fission of ^{242,244}Cm and ^{252}Cf [16]. These data are a development of UKFY3 [17]. The main changes with respect to earlier libraries include an extended experimental database, calculation of the cumulative yields using the JEFF-3.1 decay data, improved calculation of uncertainties in the yields, improved adjustment to the physical constraints and the inclusion of new ternary yield data for ^{3}H and ^{4}He [18].

The decay data library JEFF-3.1/RDD contains 3852 nuclides from the neutron to ^{272}Rg. The Decay Data sub-group of the JEFF Project decided that a completely new start should be made in the construction of this library compared with previous versions. NUBASE-2003 contains fundamental nuclear properties, and formed the basis for identification of isotopes to be included in the decay data library [19]. Three evaluated libraries from within Europe

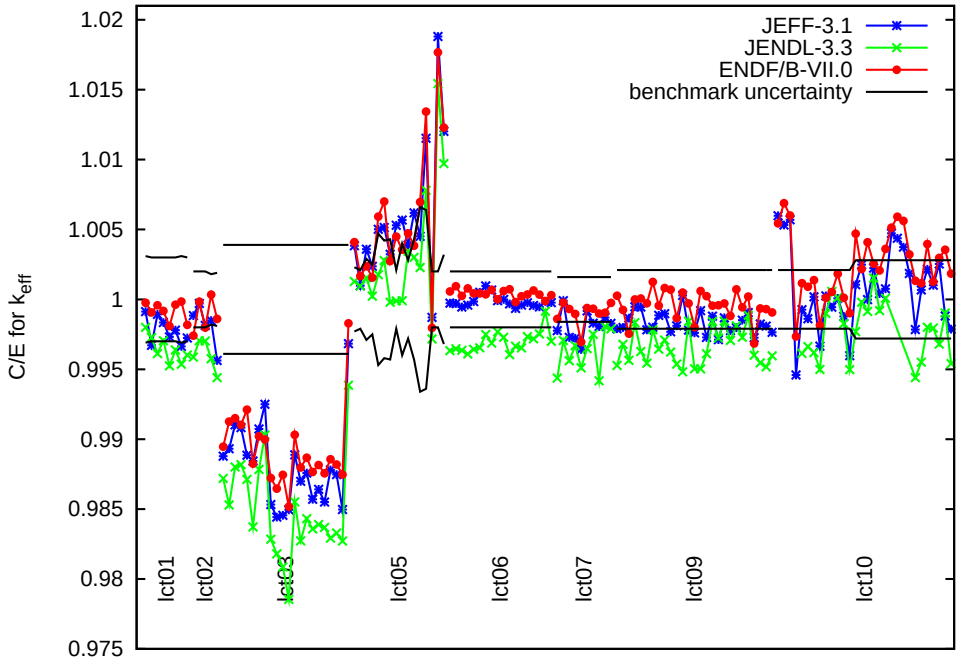

Fig. 4. Performance of JEFF-3.1 for various low enriched U thermal criticality benchmarks compared with other libraries.

were used to replace individual NUBASE files for almost 600 nuclei. Two libraries originated from the UK (UKPADD-6.4 and UKHEDD-2.4, sub-sets of Refs. [20,21]) and the third from the Decay Data Evaluation Project (DDEP) [22] overseen by the Laboratoire National Henri Becquerel (LNHB) at CEA Saclay, France. Files were also selected from the ENSDF library that contains decay data identified with basic nuclear structure data [23]. Approximately 900 fission product files were selected from ENSDF for which sufficiently consistent data were present to allow calculations of energy balance to better than 2%. The most recent revision (JEFF-3.1.1/RDD) includes a further 60 new isotopic evaluations from the UK (included in UKPADD-6.7 [20]) and following the first decay heat benchmarking studies of JEFF-3.1, a further 29 nuclei, originally taken from NUBASE, had their mean energies updated with values measured by Greenwood et al. [24] using a Total Absorption Gamma-ray Spectrometer (TAGS). Further TAGS studies are ongoing, as recommended by WPEC sub-group 25 [25], and values from these will be incorporated into future versions as appropriate.

Some of the initial decay heat calculations were carried out [26] using WIMS, TRAIL and FISPIN10 with JEFF-3.1 based libraries [27] and concerning measurements of the decay heat from irradiated PWR assemblies [28]. This included 20 measurements with cooling times between 2.4 and 8.2 years for irradiations between 25 and 40 GWd/t. Assemblies came from the San Onofre, Point Beach and Turkey Point reactors. The stainless steel cladding from San Onofre did not have a measured value for the cobalt impurity and, as this

Reactor	Assembly	Enrichment (%)	Irradiation (GWd/t)	Cooling (d)	Measured heat* (W)	JEF-1 C/E	JEF-2.2 C/E	JEFF-3.1 C/E
WEPCO	C-52	3.397	31.914	1635	724	1.04	0.98	0.97
WEPCO	C-52	3.397	31.914	1635	723	1.04	0.98	0.97
WEPCO	C-56	3.397	38.917	1634	921	1.04	1.01	1.00
WEPCO	C-64	3.397	39.384	1633	931	1.04	1.01	1.00
WEPCO	C-66	3.397	35.433	1630	846	1.03	0.97	0.96
WEPCO	C-67	3.397	38.946	1629	934	1.03	1.00	0.99
WEPCO	C-68	3.397	37.057	1630	874	1.04	1.00	0.99
Turkey Point	D-15	2.556	28.430	962	1423	1.05	1.05	1.04
Turkey Point	D-15	2.556	28.430	2077	625	1.02	1.03	1.01
Turkey Point	D-22	2.556	26.485	963	1284	1.06	1.06	1.05
Turkey Point	D-34	2.556	27.863	864	1550	1.07	1.06	1.05
Turkey Point	B-43	2.559	25.595	1782	637	0.99	1.00	0.98
Mean ; Standard Deviation					WEPCO	1.04 ± 0.01	0.99 ± 0.02	0.98 ± 0.02
					Turkey Point	1.04 ± 0.03	1.04 ± 0.03	1.02 ± 0.03
					All Zr-4	1.04 ± 0.02	1.01 ± 0.03	1.00 ± 0.03

Fig. 5. Comparison of PWR assembly decay heat measurements with calculations using the JEF(F) libraries

results in 10 to 20% of the heat in these cases, they could not be used for validation. Experimental decay heats and FISPIN results are compared in Fig. 5 for several JEFF files.

More extensive decay heat validation of the JEFF-3.1.1 libraries have been performed for newly available results from Swedish BWR and PWR assemblies[29] and results for a fission pulse are included in JEFF Report 20 [15].

2.5 Activation library

The JEFF-3.1/A activation data library in ENDF-6 format [30] is based on the European Activation File EAF-2003 [31]. The JEFF-3.1/A library contains 12617 excitation functions involving 774 different targets from ^{1}H to ^{257}Fm, atomic numbers Z=1 to 100, in the energy range 10^{-5} eV to 20 MeV. An uncertainty file is also provided that quantifies the degree of confidence placed in the data for each reaction channel. Cross section validation exercises against both experimental data and systematics enable a comprehensive assessment of the data. The SAFEPAQ-II software [32] is used to apply a series of adjustments to the original source data. A very important set of modifications concerns renormalization and branching using experimental or systematic data. A total of 3225 reactions (26% of all the reactions) have been changed in this manner, which was a challenging task as the source contains non-threshold reactions with energy-dependent branching ratios.

The particular version of EAF which will be adopted as the JEFF-3.2/A activation data library will be chosen when the JEFF-3.2 library is released. Assisted by TALYS and automation scripts, EAF-2007 [33] contains 65565 excitation functions, five times more than its predecessor. More importantly, more reaction channels have been improved by normalization to high quality experimental data. This holds to an even larger extent for EAF-2010.

2.6 Special purpose proton library

The JEFF proton library contains data for 26 evaluated isotopes. Data are based primarily on theoretical analyses with TALYS [34], in which the nuclear model parameters have been adjusted to reproduce the existing experimental data, after which dedicated formatting software produced the full ENDF-6 data files. Valuable experimental data were provided by the EU FP5 HINDAS project for several materials of key importance to accelerator applications. This has resulted in files that provide a complete representation of the nuclear data needed for transport, damage, heating, radioactivity and shielding applications for protons with energies up to 200 MeV.

For all other isotopes, users have the possibility to use data from TENDL [35]. Further data collections available from TENDL are a complete 200 MeV deuteron library and proton and deuteron activation libraries up to 60 MeV for 1170 nuclides.

3 Outlook: JEFF-3.2

With the release of the intermediate library JEFF-3.1.1 and associated validation for the nuclear industry, the release of JEFF-3.2 has been postponed. There is no firm timetable and completion target date for the preparation of the JEFF-3.2 library, but a release is still planned in 2010. For this release and for subsequent JEFF file releases, specific items to be addressed include the following:

- *Revision and test of FPs*: the JEFF project needs to exploit the FP evaluations undertaken as part of WPEC and for ENDF/B-VII, for the selection of those data files that best reproduce the European integral measurements of FP capture. In addition, gamma production data for fission products will be addressed to enable a more precise prediction of energy deposition in control rods and moderators.
- *More emphasis on minor actinides*: transmutation scenarios, GEN-IV systems and deep-burn designs require the accuracy of some minor actinide data to approach those of the major actinides.
- *Inclusion of more covariance data*: the availability and quality of covariance data is clearly inadequate. Various activities are addressing this matter, and the JEFF project should benefit from these initiatives.
- *TALYS-1.2* will be used in many future evaluations.
- *New proton and deuteron libraries*: these data will be primarily based on TALYS.

- *Adoption of EAF-2010 as new activation library*: includes an energy extension to 60 MeV, which is required for the IFMIF fusion programme.
- *Update of the decay data and fission yield libraries*: inconsistencies will be corrected and additional spectral data will be included for specific radionuclides. In a new European nuclear data project, ANDES, it will be investigated as to what extent uncertainty information can be added to these libraries.
- *Thermal scattering law data* will undergo further testing.
- *More complete gamma production data*: presence of gamma production data in all libraries is still rather random - a more systematic approach to the production of gamma data is needed, and this issue will be taken up in future releases of JEFF.
- *NJOY extensions required for JEFF processing*: a special NJOY users group [36] has been launched inside the JEFF project.
- *CONRAD*: new, modern modular software developed by CEA, Cadarache, for the analysis of nuclear data [37] will provide a natural interface between the resolved and unresolved resonance region and fast neutron range in neutron data evaluations.

Specific neutron evaluations that will be renewed or updated:

- *Revision and validation of* $^{235-239}U$ to solve remaining deficiencies, especially for fast HEU systems.
- *New evaluations of Cr, Mn, Ta and W isotopes* are, or will be, available from the EFF fusion project.
- *Revised evaluations for Pb, Bi and Am* using IRMM measurements, TALYS, and new covariance methods.

We foresee validation and benchmarking activities on the following:

- *Criticality studies by means of Monte Carlo*: large-scale validation of the ICSBEP criticality data is planned that will be based on MCNP and TRIPOLI, and well-automated procedures within the JEFF project.
- *Integral experiments with deterministic methods*: codes such as ERANOS and SCALE are being used to test the JEFF-3.1 library for fuel inventory, reactivity variation, and FP integral experiments.
- *14-MeV shielding benchmarks*: LLNL, FNS, OKTAVIAN, FNG, TUD benchmarks will be tested for new JEFF library releases, especially on the basis of the Monte Carlo codes.
- *Activation benchmarks.*
- *Decay heat benchmarks.*
- *IRPHE benchmarks* on larger reactor systems.

4 Conclusions

After the releases of JEFF-3.1 and JEFF-3.1.1, the JEFF-3.2 nuclear data library is currently under development. Concerted efforts have been expended on all of the general and special purpose libraries to achieve overall improvements over a range of simulations for nuclear technology applications. Covariance data deserve particular attention for the coming releases. Remaining deficiencies pose new challenges to, and incentives for, the further development of the JEFF library. Proposed future objectives have been listed in this paper, and need to be realised in order to meet users' demands and needs.

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