CHANDA WP9: Development and validation of new nuclear data evaluation and application capabilities

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Europe should have the computational tools to apply nuclear data in nuclear technology:

- Directly after a (published) new differential measurement or improvement in theoretical models
- Without approximation
- Including uncertainty estimation
- With a proven impact on nuclear safety of both reactors and the fuel cycle

This toolbox should be mature at the end of CHANDA and provide:

- Modern and complete nuclear data libraries
- (Near-)exact uncertainty propagation methods for nuclear data
- Revised sensitivity methods, both deterministic and Monte Carlo
WP9 Partner list

- CIEMAT (Gonzalez) – 6.3 mm: sensitivity/uncertainty of innovative reactor (ESNII)
- CCFE (Sublet) – 11 mm: Processing (PREPRO, NJOY) for reactor and fuel cycle
- CEA –DAM (Bauge) – part of 16.9 mm: covariances and physics extensions of TALYS
- CEA-DEN (de Saint Jean) – part of 16.9 mm: covariance aspects of CONRAD
- CNRS – 5 mm: uncertainties on fuel cycle
- JSI (Kodeli) – 14.9 mm: processing of uncertainty data
- NNL (Mills) – 8.8 mm: fission yields and application to fuel cycle, decay heat
- NRG (Koning) – 10.8 mm: TALYS nuclear model code and uncertainty methodology
- TUW (Leeb) – 7.5 mm: uncertainty methods, extension to angular distributions
- UPM (Cabellos) – 9 mm: uncertainty propagation for back-end of the fuel cycle.
- UU (Pomp) – 10 mm: extension of TALYS with fission yields and neutrons
- IAEA (Capote) – 0 mm: development of physics and uncertainty methods
- NEA (Michel-Sendis, Cabellos) – 0 mm: JEFF connection and accessibility + validation of EXFOR database
Task 9.1: Verification and validation of EXFOR

- NRG, IAEA, NEA
- Verification and validation of EXFOR vs world nuclear data libraries
- Numerical goodness-of-fit and plots (“Atlas”)

- Milestone M9.1: Full quantitative control over EXFOR and automated procedures for evaluators to adopt experimental data (M36)
Databases produced out of EXFOR

- **x4all.x4** (EXFOR format)
  - X4toC4 (done by V. Zerkin, IAEA)
  - **x4all.xc4** (XC4 format)

- Newbase code
  - Reaction database (n, g, p, d, t, h, a, i)
  - EXFOR error statistics

- CENDL, EAF, ENDFB, IRDFF, JEFF, JENDL, TENDL
Global quality and detection of outliers
Statistical Verification and Validation of the EXF0R database: (n,n’), (n,2n), (n,p), (n,α) and other neutron-induced threshold reaction cross-sections
Average deviations of libraries and experiments

Cross-section (mb)

Energy (MeV)

$E_{inc} - E_{1mb}$ (MeV)
Task 9.2: Maintenance and extension of TALYS

- NRG, CEA-DAM, TUW, UU, UB, NNL
- General software management
- Fission yield model (GEF)
- Neutron and gamma decay from fission fragments (GEF)
- Improved composite particle (d, t, h, a) emission
- Optional: TALYS-2.0: Full rewriting in modular Fortran 90/95/03/08
- Optional: inclusion of TASMAN (uncertainty propagation) and TEFAL (ENDF formatting) in TALYS-2.0
- Deliverable D9.3: TALYS-2.0 software package, with all theoretical CHANDA developments implemented (M48)
- CEA-DAM: Post-doc on evaporation from fission fragments starts in March 2015
Fission yield calculations with TALYS +GEF in the fast and high energy range and comparisons to experimental data

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A few words on GEF

The GEF (General Fission) code is developed by Karl-Heinz Schmidt and Beatriz Jurado and described in a recent report
http://hal.in2p3.fr/docs/00/97/66/48/PDF/GEF.pdf

GEF is using **general theoretical ideas** to describe fission **without microscopic calculations**. Hence it is rather **fast** and therefore **good for TMC**.

GEF uses **about 50 parameters** that have been adjusted to fit a large number of systems. **Several parameters and claimed uncertainties** are described in the above report, e.g., position and width of fission channels, shell effects and fragment deformation.

**GEF 2012 is part of TALYS 1.6**: gives yields (pre and post), nubar, nu(A) etc.
• GEFSUB returns \((Z_{ff}, A_{ff}, E_x, J)\) arrays, i.e. for each fission fragment the \(J\)-dependent excitation energy grid, before neutron emission.

• At the end of a “conventional” TALYS calculation, i.e. when the nuclear structure arrays for the actinides can be flushed, a loop over all fission fragments is performed, still inside the same TALYS run, to deplete all excitation energy grids of these fission fragments. This gives:
  • Post-neutron FY for each \(Z,A\)
  • Nu as function of number of neutrons, \(P(\text{n}_{\text{u}})\), fission product, \(\text{n}_{\text{u}}(Z,A)\), and average number of prompt fission neutrons, \(\text{n}_{\text{ubar}}\).
  • The same for gamma’s (and charged particles for high energies)
  • PFNS and PFGS, etc.
  • ......but this time calculated with the full Hauser-Feshbach and pre-equilibrium models of TALYS, including all flexibility for adjustment, optimization and covariances.

• Already present in TALYS: JEFF-3.1.1 Radioactive Decay Data File:
  • Independent and cumulative yields
  • Feeding of any isomer, including beta delayed precursors
TALYS-1.6 for $^{234}$U(n,f)

- Pre and post yields
- Neutron multiplicities
- Independent yields

$\bar{\nu} (2 \text{ MeV}) = 2.5250$
$\text{JEF 3.1.2: } 2.6176$

$\bar{\nu} (5 \text{ MeV}) = 2.9714$
$\text{JEF 3.1.2: } 3.0275$

S. Pomp et al., FIESTA 2014, Sept 12, 2014
TALYS-1.6 for $^{234}$U(n,f)

\[ \nu(A) \text{ pre- and post-neutron emission} \]

\[ \nu(A) \text{ at 2 and 5 MeV (post)} \]

See Al-Adili et al., NDS 119, 342 (2014), and PhD thesis Uppsala University 2013.
$^{232}$Th(n,f); $E_n = 9$ to $40$ MeV

V. Simutkin et al., NDS 119, 331 (2014)
I. Ryzhov et al., PRC 83, 054603 (2011)

S. Pomp et al., FIESTA 2014, Sept 12, 2014
Task 9.3: Uncertainty methods

- TUW, CEA-DAM, NRG, CEA-DEN, JSI
- Unified method for experimental and theoretical uncertainties
- Extension to data other than cross sections (notably angular distributions)
- Extension of CONRAD for uncertainty propagation
  - Deliverable D9.1: Report on the procedure for inclusion of angular distributions into the covariance scheme (M24)
  - Deliverable D9.4: Report on CONRAD methodology and comparison with traditional Bayesian methods (M48)
  - Deliverable D9.5: Report on extended procedures for experimental and theoretical uncertainty handling (M48)
  - Milestone M9.4: A method to use Unified Monte Carlo or equivalent covariance method on a routine scale, extended to angular distributions (M48)
From low to high energy nuclear data evaluations
New Development in the CONRAD Code:
UMC and Full bayesian

Cyrille DE SAINT JEAN, Edwin PRIVAS
CEA, DEN-Cadarache,
F-13108 Saint-Paul-lez-Durance, France
What ever is the methodology $\sigma$ and $x$ are considered as random variables (pdf)

Monte-Carlo Sampling is a natural ingredient*

Estimation of Uncertainties with Monte-Carlo during the evaluation process *:

$$p(x \mid y, U) = \frac{\prod_{i=1}^{r} p(x_i, U) \cdot \prod_{i=1}^{u} p(y_i \mid x_i, U)}{\int p(x, U) \cdot p(y \mid x, U) dx}$$

Sample of $p(\tilde{x} \mid M, U) \rightarrow \tilde{x}_k$

For each $\tilde{x}_k$ calculation of Likelihood $\ell_k[p(\tilde{y} \mid M, \tilde{x}_k, U)]$

UMC in the Resonance Range / Unresolved resonance range and Continuum Monte-Carlo data assimilation of nuclear reaction model parameters

Full Bayesian** with Monte-Carlo (taking into account experimental parameters) + marginalization**

Benchmarking with traditional Generalized least square

UMC for Integral experiment as well (see WP12)

*R. Capote and D. Smith, Nucl. Data Sheets 109, 2768 (2008)
** P. Schillebeeck et al., Nucl. Data Sheets (to be published)
Task 9.4: Processing of nuclear data

- CCFE, IJS, UPM
- Invest in knowledge of PREPRO and NJOY to assure that Europe can continue nuclear data processing for reactor and fuel cycle software.
- Milestone M9.2: Standard processing routes for European nuclear data libraries for all reactor codes of interest, especially the European ones (TRIPOLI, APOLOLO, SERPENT, FISPACT) (M36)
CCFE contributions to CHANDA

- WP9 Task 9.4: with retirees, UPM, the IAEA

  - Participate in the development and testing of NJOY-12>032
  - Participate in the development and testing of PREPRO2015 (nearly ready, in testing phase)
  - Maintain the CALENDF-2010 processing code

  - Develop quality assured processing routes (scripts) to assemble Monte Carlo and inventory code systems multifaceted applications libraries

  - Develop, assemble and benchmark a next generation multi applications decay data library: fusion, fission, accelerator, medical, astrophysics..
European Activation SYStem

EASY-II

Astrophysics
Fusion
Burnup
Material Science
Activation
Pile

Source terms
Depletion
Fission
Criticality
Shielding

Source

Fusion

Burnup

Material Science

Activation
Pile

Source

Depletion
Fission
Criticality
Shielding

Medical
Transmutation

\[
\frac{dN_i}{dt} = -N_i(\lambda_i + \sigma_{ca}) + \sum_{j=1}^{\text{species}} N_j(\lambda_{ij} + \sigma_{ij})
\]
• FISPACT-II new capabilities:
  ▪ Robust processing steps: NJOY, PREPRO and CALENDF
  ▪ Any ENDF-6 formatted library can now be used for simulations: TENDL-2014, ENDF/B-VII.1, JENDL-4.0 and JEFF-3.2
  ▪ Uncertainty quantification and propagation – if given in the data file
  ▪ Pathways analyses for any response function

• EASY-II with TENDL (or other capable library) has the ability to use transmutation and fission yields of arbitrary incident neutron energy (< 200 MeV)
  ▪ Potentially required for correct beta feeding leading to emitted neutrino spectrum from any sources: reactor, accelerator, astrophysic

• TENDL-2014 based Ace style transport libraries for MCNP, SERPENT, openMC but also Pendf style for TRIPOLI
Benchmarks to the Iron Cross Sections and on the Impact of Fe Scattering on Integral Benchmarks

A. Trkov, G. Žerovnik, I. Kodeli

International Atomic Energy Agency
Jožef Stefan Institute
Integral iron benchmarks

• Identification of ICSBEP criticality benchmarks, sensitive to iron cross sections:
  • Fast spectrum.
  • Thermal spectrum (to a certain extent if iron/steel is one of main materials).

• Re-evaluation of SINBAD shielding benchmarks:
  • 34 benchmarks are relevant for iron cross section benchmarking.
  • The available experimental data is of varying quality.
  • OKTAVIAN Fe, TUD Iron slab, JANUS phase I, and some others have been found useful for validation of iron cross section data.
Impact of Fe scattering on integral benchmarks

• A new patch for NJOY to process ang. distrib. (MF=4) in RML format.

• Different iron ENDF files have been tested:
  • ENDF/B-VII.1
  • ENDF/B-VII.1 template with new ORNL resonance parameters
  • ENDF/B-VII.1 template with new ORNL resonance parameters and angular distributions
  • Same as above but with thinned angular distributions

• Testing on ICSBEP iron benchmarks -> no significant impact on $k_{eff}$.

• Number of data points for MF=4 can be reduced ~80 000 -> ~500.

• Still to be verified on deep penetration problems.
Task 9.5: Uncertainties in fuel cycle data

- NNL, CCFE, CIEMAT, UPM, CNRS, JSI
- Full (Total) Monte Carlo inventory calculations
- Sensitivity profiles of inventory and decay heat parameters to cross sections, fission yield and decay data
- Apply this to modern (GEN-IV) reactor design
- Isotopic content and criticality safety uncertainties after burn-up with EVOLCODE
- Deliverable D9.2: Report on sensitivity/uncertainty analysis for an up-to-date reactor design (M36)
- Milestone M9.3: Capability to perform exact uncertainty calculations for nuclide inventory (M36).
Contribution of CIEMAT to Task 9.5 (1/3)

- Involvement of 6.3 person-month.
- Delivery date: Month 36.
- Use of the EVOLCODE simulation system (validated extensively over the past 10 years) for:
  
  - The calculation of the isotopic content and criticality safety parameters along the burn-up.
  - Development of a methodology for performing sensitivity/uncertainty analyses for the criticality safety parameters.
  - Sensitivity analysis of inventory and decay heat parameters on the cross sections, fission yields and decay data with the hybrid method.

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Contribution of CIEMAT to Task 9.5 (2/3)

The calculations will be made for one of the (following three) ESNII reactor concepts. The work will exploit the synergies between CHANDA and the ESNII_PLUS project, of which CIEMAT is also part.

ASTRID sodium-cooled fast reactor

MYRRHA: Multi-purpose hybrid research reactor for high-tech applications

ALFRED lead-cooled fast reactor

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Contribution of CIEMAT to Task 9.5 (3/3)

• ACAB code is capable of obtaining sensitivity profiles of cross sections, fission yield and decay data.

• Complete integration of ACAB in the EVOLCODE system for isotopic evolution estimations.

• Some checks are needed to ensure that the required features work well in the integration.

• In parallel, ESNII_PLUS activities include a benchmark calculation of the ASTRID sodium-cooled fast reactor core characterization:
  - Neutronic characteristics of the core: $k_{\text{eff}}$, kinetic parameters, power distributions
  - Criticality safety coefficients: Doppler constants, coolant void worths, control rods reactivity worths

• CIEMAT has participated in this activity, gaining useful experience in this up-to-date reactor concept. Clear synergies with CHANDA to be exploited.
Conclusions

WP9 is well underway
Some problems with personnel:
• CEA-DAM postdoc starts in March 2015
• NRG looking for successor of Dimitri Rochman
No problems expected for timely delivery of milestones and deliverables