PAUL SCHERRER INSTITUT

PSI

HORIZON 2020

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SANDA task 4.1: Nuclear reaction code developments and evaluations

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SANDA – general meeting, via remote connection, 9-11 February 2021

Zertifiziertes Managementsystem STARS ISO 9001

Task 4.1

Task 4.1: Nuclear reaction code developments and evaluations
*Task coordinator: **PSI**, partners: **CEA/DAM/DIF, CEA/DEN, PSI, CNRS/IPHC, TUW, UB, UU***

Task 4.1.1: TALYS development

Task 4.1.2: Nuclear reaction evaluation

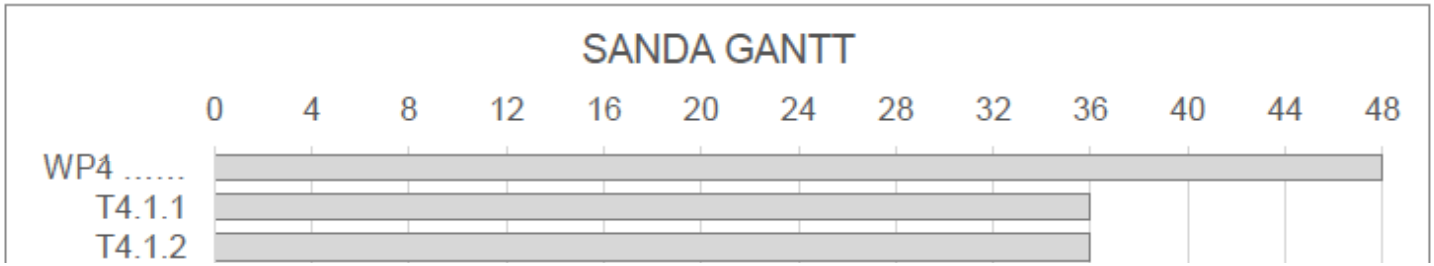

Table 3.1c: List of Deliverables[4]

4.1	Report on code development, methods	4	PSI	R	PU	40
4.2	Report on new nuclear reaction data evaluation	4	CEA	R	PU	48

T0: September 2019

T36: August 2022

T40: December 2022

T48: August 2023

Task 4.1

Task 4.1: Nuclear reaction code developments and evaluations
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Task 4.1.1: TALYS development

Task 4.1.2: Nuclear reaction evaluation

Table 3.2a: List of milestones

Milestones:

M.4.1: availability of TALYS modules (CEA/DAM/DIF): M32
M.4.2: availability of new EMPIRE modules/models (UB): M32
M.4.3: availability of evaluated files for important actinide isotopes (CEA/DEN, CNRS): M32
M.4.4: availability of evaluated files for important fission products (CEA/DEN, PSI): M36

4.1	Availability of TALYS modules	4	32	Short communication
4.2	Availability of new EMPIRE modules/models	4	32	Short communication
4.3	Availability of evaluated files for important actinide isotopes	4	32	Presentation or ENDF file

T0: September 2019

T32: May 2022

T36: August 2022

Subtask 4.1.1: “TALYS development”

- PSI/IAEA:
  - New version of TALYS to be released in 2021 (updated deuteron breakup model)
  - New evaluation tool (T6) developed with various partners

- CEA DAM/CEA DEN/CNRS/IPHC
  - TALYS: Implementation of Engelbrecht-Weidenmüller transformation done .. test and validation underway
  - JLM/QRPA pre-equilibrium based spin rule + Update of QRPA tables
  - Postdoc Work on statistical decay of Fission fragments with TALYS (debugging/implementation/validation in TALYS)

Subtask 4.1.1: “Light elements”

ATOMINSTITUT

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SANDA
WP4

Development of Nuclear Data Evaluation Technique for Light Nuclei

Status of Work performed by
Nuclear Data Group at TU Wien, Austria
H. Leeb, B. Raab, T. Srdinko

Subtask 4.1.1: "Light elements"

ATOMINSTITUT

Nuclear Data Evaluation for Light Nuclear Systems

TU WIEN

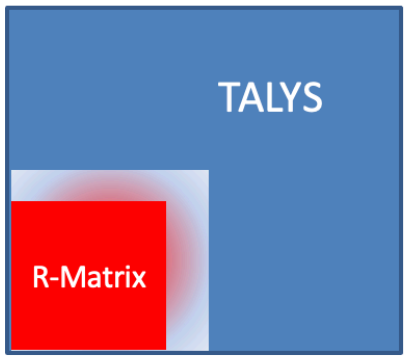
Status: evaluations of reactions of light nuclei are not satisfactory at present

Problems: microscopic theories not sufficiently accurate for evaluation
mean-field techniques not applicable, of limited use only at high energies
reliable uncertainty estimation in resonance region is still not established

Objective: development of a consistent evaluation technique for light nuclear systems

Method: Unified Bayesian Evaluation Procedure

Prior: generated from TALYS (stat. model) and GECCCOS (R-matrix description)



Evaluation update based on observables based on modified GLS technique for large scale evaluations proposed by Schnabel&Leeb

Uncertainty information: determination of covariance matrices including model defects based on Gaussian processes for resonance and high-energy region using the prior covariance matrix of the unified Bayesian evaluation procedure

$$A_0(E,E') = f(E,E')A_0^{RMat}(E,E') + \left[1 - f(E,E')\right]A_0^{TALYS}(E,E')$$

Subtask 4.1.1: "Light elements"

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Status of work performed

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main work performed in 2020

1) Modification of moduls of GENEUS to accommodate various types of observables (integral, differential cross sections, …) considering all subchannels associated with the same compound nucleus
   - solved for integral and most angle differential data,
   - some open problems for double-differential data

2) Automatic determination of a consistent set of observables with regard to sum rules, integral relations and other dependencies
   - solved for integral and angle-differential data,
   - further work required for double differential and breakup data

3) Implementation of the Large Scale Bayesian GLS algorithm developed at TU Wien
   - a prototype of an extended module for GENEUS is under construction, but its completion requires the completion of point 2).

4) Construction of a module for the generation of the prior information based on calculations with TALYS and GECCCOS in terms of the Large Scale GLS algorithm
   - at present only preparatory analytical work has been performed
   - numerical implementation is envisaged for this year.

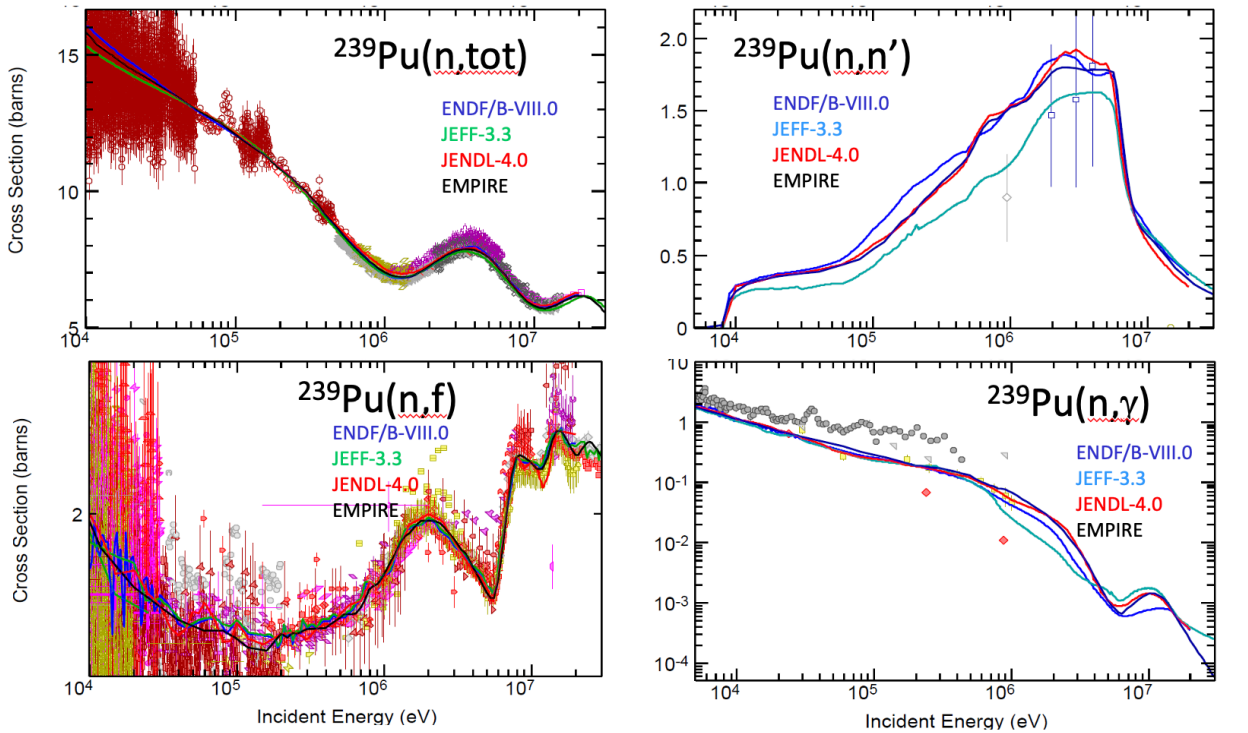
Apart from these points there are efforts to develop a proper data system allowing for efficient storage and in- and output of experimental, intermediate and evaluated data.

Subtask 4.1.1: "EMPIRE developments"

- UB:
  - Full and consistent model calculations for the neutron induced reaction data on $^{238-242}$Pu isotopes for the incident energy range 0.01-30 MeV. These model calculations will represent the starting point for new evaluations performed by an IAEA collaboration.

UB –Task 4.1

Preliminary model calculations for n+ ^{239}Pu cross sections



Subtask 4.1.2: “Nuclear reaction evaluation”

- PSI/IAEA/CEA DAM/CEA DEN
  - Preparation of new evaluations, to be submitted for JEFF-4 and TENDL

- CEA DAM/CEA DEN/CNRS/IPHC
  - Work on ^{238}U evaluation is scheduled for may/june (related to IPHC measurements+CEA-DEN collaboration)
  - 1st results on ^{239}Pu uncertainties with MCMC (towards a reference calculation).
  - PhD work started at IPHC and CEA DAM/DEN (measurements+evaluations)

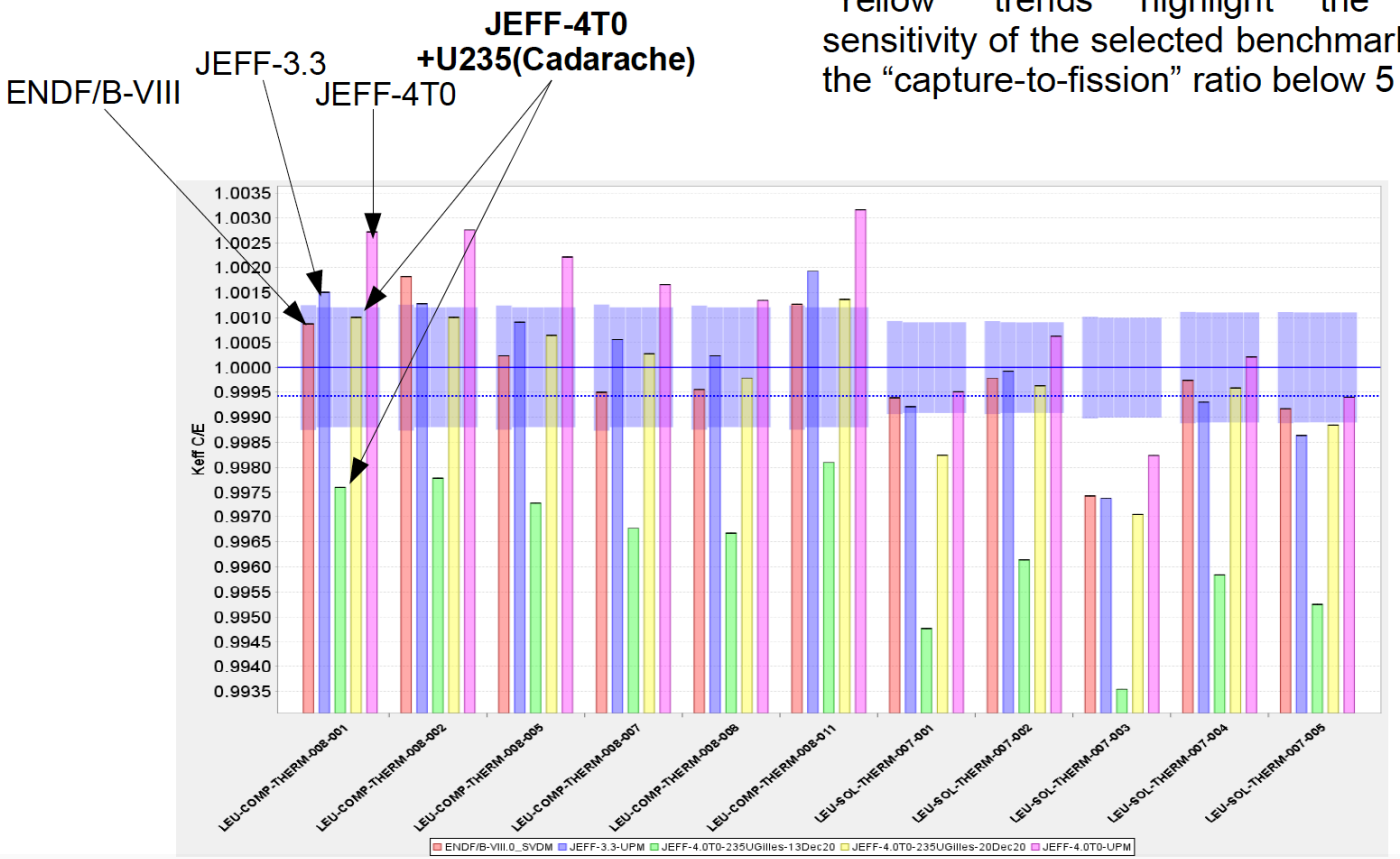
Subtask 4.1.2: “Nuclear reaction evaluation”

Contribution from CEA/DES Cadarache

New resolved resonance parameters for U235 with the CONRAD code

Integral feedbacks from Oscar Cabellos (Universidad Politecnica de Madrid)

The differences between the “Green” and “Yellow” trends highlight the high sensitivity of the selected benchmarks to the “capture-to-fission” ratio below 5 eV.



Subtask 4.1.2: "Nuclear reaction evaluation"

UPPSALA UNIVERSITET

Summary of UU work in NFRP-2018-4 Activity line Evaluation & Uncertainties (UU_eval)

Objectives

1. Develop and implement methods for treating model defects in the fast energy range for the stable Cr isotopes.
   - Method developed and implemented in a ND evaluation pipeline using Gaussian Processes in both the parameter domain[1] and observable domain (not reported)
2. Develop and implement methods for consistent and automatic treatment of discrepant experimental data.
   - Method developed and implemented in ND evaluation pipeline using Marginal Likelihood Optimization
3. Production of a data files for ^{50,52,53,54}Cr using the above-mentioned methods combined with methods and data developed in other activities within the project.
   - To be completed using the developed methods outlined above.

[1]G. Schnabel, H. Sjöstrand, J. Hansson, D. Rochman, A. Koning, and R. Capote, "Conception and software implementation of a nuclear data evaluation pipeline," *arXiv:2009.00521 [nucl-ex, physics:nucl-th, physics:physics]*, Sep. 2020, Accessed: Sep. 14, 2020. [Online]. Available: http://arxiv.org/abs/2009.00521.

Plans/conclusions

- All participants have started their work, with slight delays (PhD work with experimental data)

- Very good collaboration between partners, and with outside collaborators (other evaluator communities, JEFF, TENDL, IAEA, ENDF)

- Participations to (online) meetings and support for future library releases

- First milestone in May 2022 (no delay for now)
- First deliverable in August 2022 (no delay for now)

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