Review of project on Improvement of Analysis Codes for NSDD Evaluations

NSDD Scientific Secretary:
Paraskevi (Vivian) Dimitriou

Previous meeting, Oct. 2015

Participants
- Michael Birch
- Tibor Kibedi
- Filip Kondev
- Xavier Mougeot
- Alexander Rodionov
- Balraj Singh
- Sukhjeet Singh
- Jagdish Tuli
- Mark Kellett

Scientific Secretary
- P. Dimitriou

IAEA contacts
- M. Verpelli
- V. Zerkin

Meetings
- 1st Technical Meeting 2014

Links
- NSDD Network
- Nuclear Data Services
- Nuclear Data Section
- IAEA
- NUBASE
- DDEP Homepage

2nd Technical Meeting on Improvement of Codes used for Nuclear Structure and Decay Data Evaluations

5-8 October 2015, IAEA Headquarters, Vienna, Austria

This meeting is a follow-up of the previous first Technical Meeting held from 10-13 June 2014 at IAEA, Vienna (see report INDC(NDS)-0665). The aim is to monitor progress made in the tasks assigned at the previous meeting, discuss and validate the new codes, assess the current status and emerging needs, and revise the list of priorities and assignments accordingly.

Agenda
The Agenda is available here.

Summary Report
The summary report INDC(NDS)-0696 is in preparation.

Presentations

#	Author	Title	Link
1	F. Kondev	RULER - stand-alone version	PDF
2	M. Birch	JGAMUT: ENSDF Adopted Levels, Gammas Assistant Code	PDF
3	B. Singh	JAVA-NDS computer code	PDF
4	B. Singh	Nuclear Data Sheets for A=40*	PDF
5	X. Mougeot	Improvement of analytical calculations of beta spectra	PDF
6	T. Kibedi	NS_Lib - subroutine library	PDF
7	S. Singh	Revised ALPHAD (ALPHAD+RadD)	PDF
8	J. Tuli	Development of Codes on GFORGE	PDF

CODES - 2015	PRIORITY	TASK	NAME	TIMELINE	PRESENT
JAVA NDS	1	FURTHER DEVELOPMENT AND TESTING	CHEN, SINGH	BETA-VERSION END OF NOVEMBER 2015	**OFFICIAL PUBLICATION CODE**
JGAMUT	1	IMPROVEMENT AND TESTING	BIRCH, SINGH	BETA VERSION END OF NOVEMBER 2015	**DONE + RECOIL CORRECTIONS:** ***VALIDATION MAINTENANCE***
VISUAL AVERAGING LIBRARY	1	INCLUDE BARLOW METHOD AND PLOTTING	BIRCH, SINGH	END OF NOVEMBER 2015	**DONE:** ***MAINTENANCE***
BETA SHAPE ANALYTIC	1	IMPROVED TREATMENT OF FORBIDDEN NON-UNIQUE + EC	MOUGEOT	JANUARY 2016 NEXT CODES MEETING	**DONE:** ***ONGOING VALIDATION***
EVALUATION TOOLKIT (EDITOR+CODES)	1	EXPLORE DIFFERENT OPTIONS	ZERKIN	IN PROGRESS-ZERKIN TO START END OF SUMMER 2016	**ENSDF± AVAILABLE** ***ONGOING***

CODE	PRIORITY	TASK	NAME	TIMELINE	PRESENT
R0 (RADd) CODE	1	INCORPORATION IN ALPHAD	SINGH, SINGH	IN PROGRESS FEBRUARY 2016	**DONE:** **NEW ALPHAD-RADD CODE**
NEW R0 TABLES		UPDATE R0 TABLES FOR NEW Q-VALUES, BRANCHINGS AND NUCLIDES	SINGH, SINGH		**NEW R0 TABLES – TO BE PUBLISHED**
ONLINE WEBTOOL	2	MAKE PNPI CHECKING CODES AVAILABLE	ZERKIN	MID-2016	**DONE**
PANDORA	2	ENHANCE CODE	TULI-NSDD NETWORK	CONTINUOUS	**BAND ASSIGNMENT – ZERKIN** ***MAINTENANCE - DEVELOPMENT***
FMTCHK	2	ENHANCE FORMAT CHECKING	NNDC INVOLVE PNPI GROUP	CONTINUOUS	**NNDC (JOHNSON) CONTINUOUS BUG FIXES** ***DEVELOPMENT***

CODE		TASK	NAME	TIMELINE	PRESENT
TRULER **PYRULER**	1	DEVELOPMENT DEVELOPMENT AND TESTING	T. KIBÉDI, F. KONDEV M. BIRCH	BETA VERSION BY JUNE 2016	***ONGOING – TREATMENT OF ASYMMETRIC UNCERTAINTIES***
ND_LIB	1	DEVELOPMENT AND TESTING	KIBÉDI	NEXT CODES MEETING	***DONE***
BRICCEMIS	1	DEVELOPMENT	T. KIBÉDI	IN PROGRESS REPORT AT NEXT CODES MEETING	***ONGOING – ASYMMETRIC UNCERTAINTIES AND ATOMIC DATA FORMAT IN ENSDF***
LOGFT	2	WARNING MESSAGES FOR UNPHYSICAL INPUT DATA AND ASSIGNMENT OF UNCERTAINTIES	NNDC	PENDING	***??***

NSDD 2017, INDC(NDS)-0733

T-RULER: a new code written by Kibedi to treat uncertainties by means of the distribution functions obtained via the Monte Carlo method.

- can handle asymmetric uncertainties,
- uncertainty limits: fixes ranges for <0.5, <+0.5,....,
- two methods for deducing mean values and uncertainties from distribution function,
- clear policy needed on uncertainties in order to continue work.

Recommendation: this approach is reasonable, and should be agreed and endorsed by the network so that a beta version is completed and made available for validation.

BrIccEmis: is in the process of being developed to calculate the atomic radiation database. As soon as (a) this on-going work has been completed, (b) the Monte Carlo treatment of the uncertainties has been endorsed, and (c) an agreed format has been adopted in ENSDF for the resulting atomic data, the code will be finalized and released, and an appropriate paper prepared for publication (estimated finish by the end of 2017).

Proposed format for atomic data: 'MA', 'MX', E(TOT), I(TOT), etc. - option should be added to display atomic radiation data on the web. Add a flag in the ENSDF file to signal when the decay scheme is incomplete, and that BrIccEmis should not be run.

The above format was agreed and adopted by the network (related to Action #25, Annex 4),

BetaShape code (Mougeot, LNHB, CEA Saclay): modelling of EC transitions is missing, and forbidden non-unique transitions are handled as allowed (as in the LOGFT code).

Work is in progress to model EC transitions and improve the treatment of non-unique forbiddenness that will include nuclear structure effects. Otherwise the code gives improved spectra and average beta energies, based on more advanced calculations and consideration of the experimental beta shape factors

Recommendation: LOGFT needs to be replaced with a more advanced code, and the subcommittee was pleased to learn that Mougeot is carrying out a systematic analysis of his BetaShape results - this analysis effort merits future discussion.

PANDORA: enhancement of code is still required. LBNL to consider working on PANDORA (see Annex 4, Action #4).

NewGTOL: code written by PNPI (Russia) to handle singular matrices in conditions when GTOL fails to furnish results. Needs to be tested by experienced evaluators before any recommendations can be made. Available as part of the MyEnsdf web tool on the IAEA-NDS website.

MyEnsdf Web tool: All checking codes (Russian) are available on this web tool. NewGTOL is also there to test. An additional section for non-ENSDF analysis/utility codes is included where useful codes for evaluators can be made available. Access to MyEnsdf Web tool for those only wanting to run the codes is made free without a password

Editors: There is a need for an ENSDF editor that is publicly available and can be fully supported and maintained.

EVP editor: is continuously developed. It is obtainable upon request from A. Sonzogni (NNDC-BNL).
Tree-editor: The subcommittee supports the efforts of Zerkin at IAEA-NDS.
Recommendation: an expert evaluator works closely with Zerkin to implement all required features. LBNL is willing to provide the expertise.

Formats:

Formats for continuous data (proposal by Sonzogni):
Recommendation: a more thoroughly worked out proposal should be prepared for a format for continuous data accompanied by an example (see Annex 4, Action 26).

Goals for this meeting

- Follow-up on progress from TM Codes 2015 and NSDD 2017
- Discuss new codes (Java-Ruler, Consistency checking by Jun Chen)
- Validation procedure for codes (ready for release)
- Formats for atomic radiation data and continuous data
- Dissemination

So that at NSDD 2019:

- Present final validated codes for use with examples/exercises
- Final proposals for formats for adoption
- Improved editors

Thank you!