D. Rochman

Experience from the T6 portable system
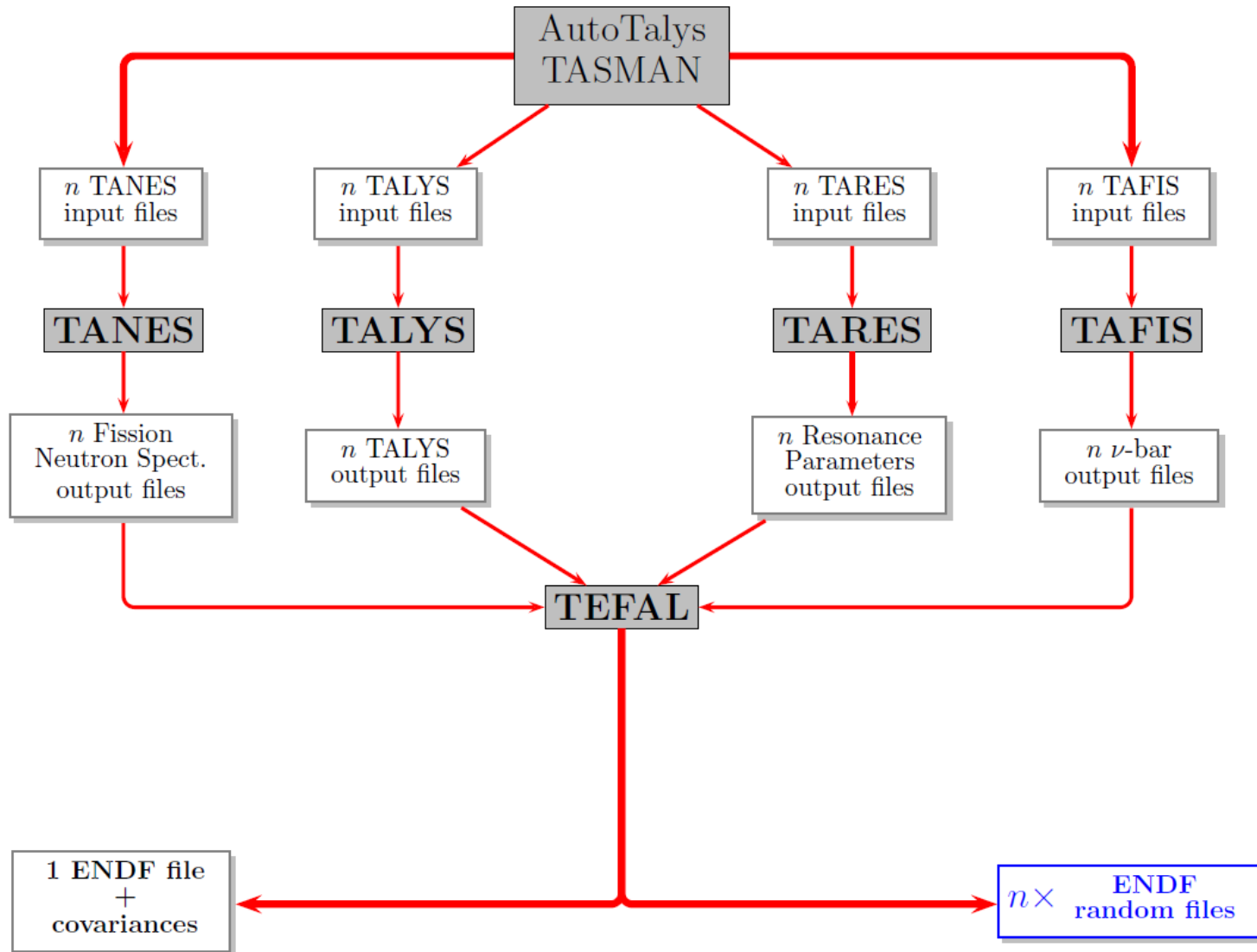
SG49 meeting, NEA, Paris, 27 November 2019

WIR SCHAFFEN WISSEN – HEUTE FÜR MORGEN

- What is T6

- Where was it used, who used it

- Feedback from users

- Future developments

What is T6

- Method: Quality evaluation, production automation, open source

- Support tool box for TENDL (from 2008 to 2019, and beyond)

- Support for TMC, BMC

- Used to produce hundreds, thousands of random[1] files

- Presented in two main papers: NDS 155 (2019) 1, NDS 113 (2012) 2841

- Include more than 6 codes: libraries, scripts, database, text files, tex files, pdf files, c++ files, fortran files…

- Installed at PSI, IAEA, UU, LANL, NRG, TiTech, CEA, AWE (and maybe more)

[1] Definition of random in this presentation:
- random ≠ erratic, blind, fortuitous, orderless, planless, arbitrary
- random = intentionally planned variations (exact uncertainty quantification)

What is T6

- t6.tar: 2.3 Gb
- t6 expended: 19 Gb, 880 000 files
- Necessary additional libraries: 20 Gb, 410 000 files (only for neutrons)

- Production of TENDL-2019 on 300 cpu: 1.5 months

- Tested with different compilers, Linux versions

- Developed now between IAEA (95 %) and PSI (5%)

- Potential users: 10-20

- Potential developers: 1-2

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PSI

I've done some tests on T6 (I running the version used to create TENDL17, according the Arjan). Many nuclides run perfectly well, but do not produce endf files that match TENDL 2017 endf files. Other results crash, giving:

*** AUTOTALYS error: TEFAL crashes for U235

I found the bug. It is in Tares where I give a wrong NLS for MF32. Previous versions of NJOY didn't care, but njoy12.50 is checking this value... I'm going to modify Tares...

Arjan, Pu9 ?

After debugging, I think there is a bug in NJOY (ERRORR) for Multi Level Breit Wigner (MLBW). In TENDL, following the (good) advice of JC, we dropped Reich Moore (RM) in 2013 and switched to MLBW. Today, I've produce two similar files in MLBW and RM and process them with NJOY. The one with RM is giving me what I expect, and the one with MLBW

 I have already checked the ENDF files for TENDL2015 for Th232 and I also see some extrange behaviour. For example if I see the MF 3 MT 5 (p,x) and MF 3 MT 37, some energy points are repeated or missing (when you compare with the same ENDF file available in TENDL2015 web page without the individual reaction channels). So maybe using this files as basis will lead to some extrange behaviour in ACE files.

Just talked witrh Steven, and he shopwed me the files are ijndeed wrong.
At leats I see it in Er168 and it may be a problem in every TENDL file. It looks loke the elastic peak has been folded into the spectra of MF6/MT5. You only see this with > 30 MeV tests and

Now... The bad one is that there is a BIG bug in stellarrate.f subroutine, in the integration procedure of the MACS. I found it out comparing TALYS astrorate.g output with the small code I wrote to estimate the MACS with the RRR.

I guess these are both more NJOY issues than TALYS errors, but maybe you can build a workaround in the TENDL files or send corresponding bug reports/fixes to some responsible people behind NJOY...

Most ridiculous TEFAL error ever:
TALYS and TEFAL say: above mass 216 there is fission, so we need nubar, pfns, etc.
W216 has no nubar in any library, so TEFAL starts searching until if finds the lowest Z,A combination with a nubar in a library. That is Th227 in JEFF3.2.

That looks good. But first of all: stop the presses, the photonuclear library for TENDL-2015 is wrong and should be changed. I discovered a terrible bug in the production system which affects the photonuclear data library. I am going to reproduce it, hoping

Recently we found a new problem on the ACE file of TENDL-2017 neutron sub-library. Please see the attached file about this new problem. If you have any questions, please tell me.

The secondary neutron spectrum data of mt=5 in TENDL-2017 are incorrect at 30MeV.

The calculated neutron spectra with 40 MeV neutrons are shown in Fig. 3 with the measured ones [6]. The calculated neutron fluxes with TENDL-2017 unphysically increase near 30 MeV, while those with

Bug found in TENDL data: wrong particle yields. Wait until TENDL 2012 (December)

I am having similar difficulties with TENDL 2015.

After writing a download script for TENDL-2017 (link to tendl-2017 script) and getting an NJOY with Boron 10 (link to issue) I started trying to use TENDL-2015

I have written a openmc-get-tendl-2015-data script (link to tendl-2015 script) which downloads the ace files and converts them to h5 (based on the nndc and JEFF scripts).

Problems on TENDL-2015 neutron sub-library and its ACE file

Konno, Chikara; Tada, Kenichi

The nuclear data library TENDL-2015 up to 200 MeV is being used as a standard nuclear data library worldwide, particularly in Europe. We found out the following three problems in the ENDF and ACE files in TENDL-2015 neutron sub-library; (1) no unresolved resonance data in most of the ACE files, (2) no secondary γ data in most of the ACE files, (3) No high-energy γ peaks in the capture reaction of a lot of the ENDF files. We examined effects of these problems and the followings were demonstrated; (1) insufficient self-shielding correction, (2) wrong γ spectra in neutron-γ coupling calculations and wrong DPA cross section data. Secondary γ data of the capture reaction and ACE files in TENDL-2015 neutron sub-library should be revised.

General observations

- First comment: the more we produce, the more bugs we distribute

- Second comment: in T6, problems can be related to T6, but also to ENDF format, to PREPRO, to NJOY, to MCNP, …

- Many users of TENDL: many aspects which are tested. Therefore more problems found

- Open new possibilities (complete ENDF/text files for charged particles): more troubles

- Difficult to create a priority list (who pays ?): who says what is important ?

- Avoid latest "computer environment" packages: for portability, only simple scripts, commands.

Need to do

- Improve cross sections and stop code changes

- Better (simple) makefile

- Simplify, simplify and simplify
  - Remove all unnecessary features
  - Think about running it on a VAX system (or even Windows)

- Separation of database, manuals and codes

- More tests, improved QA (the TENDL production is actually our QA test)

- Separate production and development versions

- Is it ready for Gitlab, Docker ? How far do we want to go ?

Conclusions

- More than 10 years of developments for T6 (20 for TALYS ?)

- Not portable enough (not perfect), but portable enough (it works)

- Not ready for Gitlab (too big, too messy ?)

- Still, it is one of the most advanced systems in our field regarding portability.

- Needs better QA and structures,