IAEA 60 Years
Atoms for Peace and Development

FISPACT-II & TENDL Verification and Validation processes

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Nuclear Data Section

United Kingdom Atomic Energy Authority
Culham Science Centre

Verification and Validation

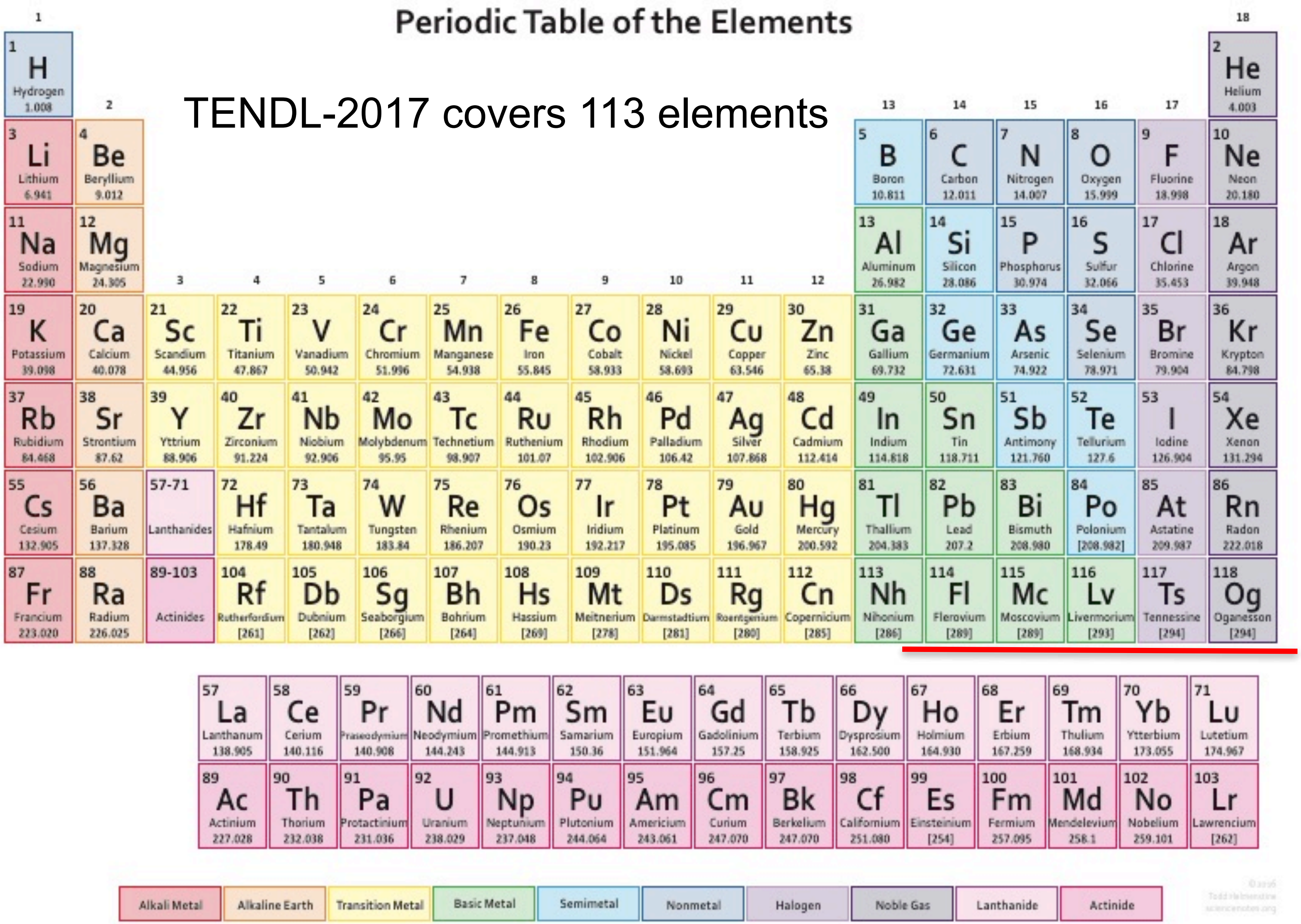
- Validation: have we build the right simulation toolkits?
- Verification: Have we build simulation tools that gives the right answer?

Validation is concerned with checking that the system will meet the needs, while verification is concerned with whether the system is well-engineered, error-free,…

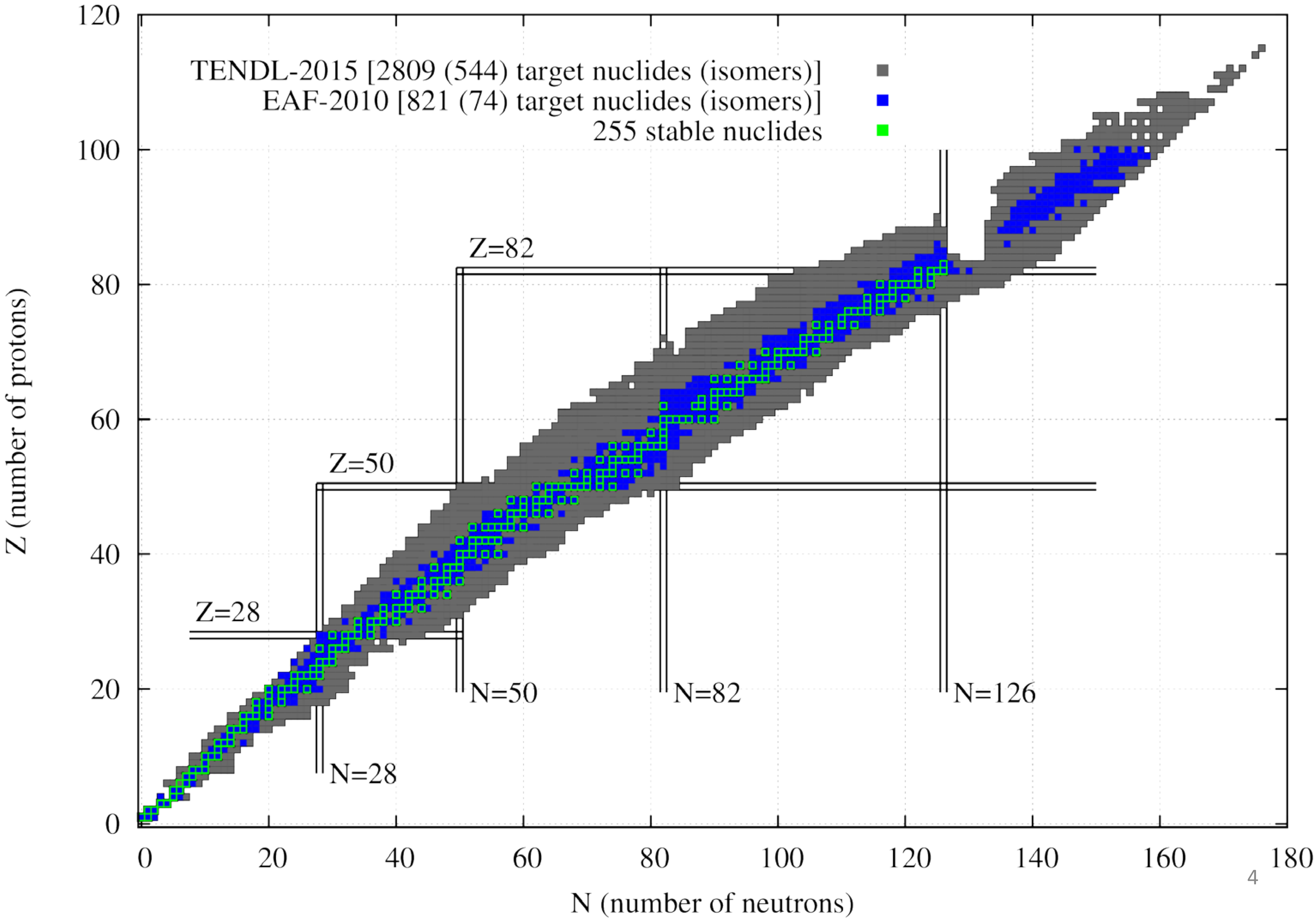
V&V on nuclear data need to be seen as a toolbox, with a wide range of tools: FISPACT-II is one very potent toolbox, with many tools

Nuclear landscape: elemental periodic table

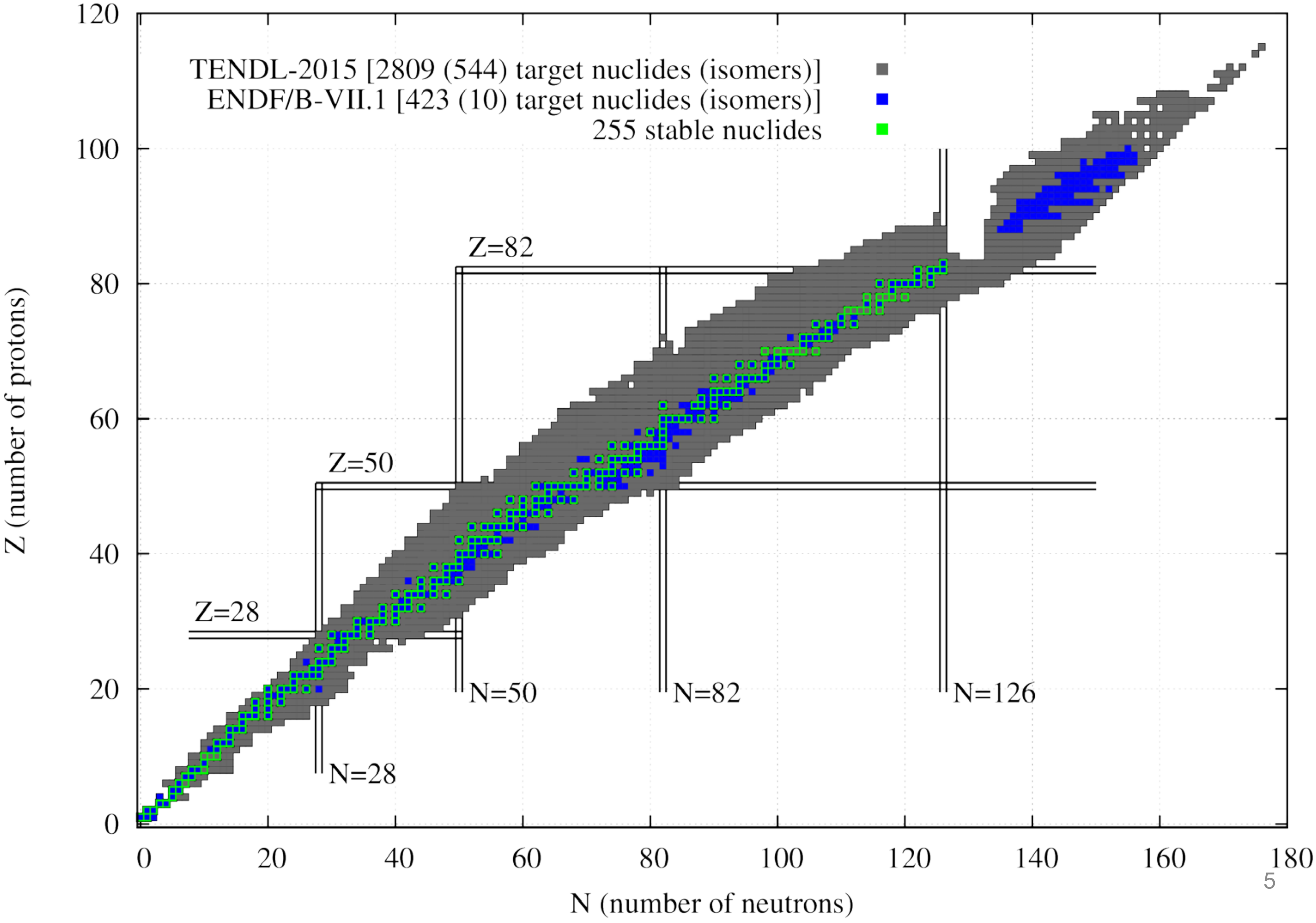
TENDL-2017 covers 113 elements



Nuclear landscape: Isotopic targets



Nuclear landscape: Isotopic targets

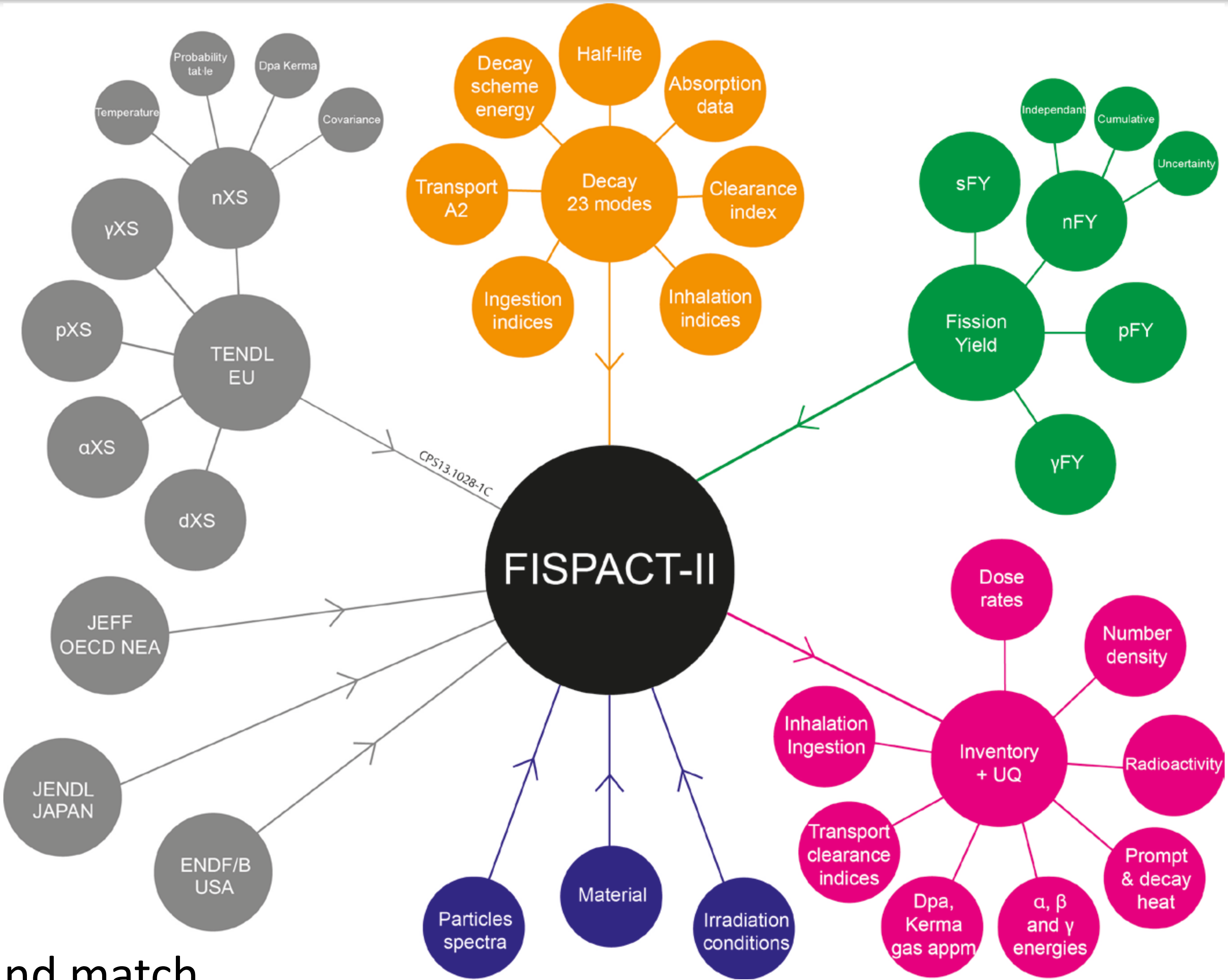


framework

- FISPACT-II is a modern engineered simulation solver for activation-transmutation, depletion inventories and materials science at the heart of an enhanced multi-physics, multi-scale platform that relies on the TALYS collaboration to provide parts of its nuclear data libraries.
- FISPACT-II was designed to be a functional replacement for the earlier code FISPACT-2007 (1987-2007 †) but now includes many enhanced, unique and potent capabilities.
- d, p, α, γ, n-Transport Activation Library: TENDL-2015 from the TENDL collaboration, but also ENDF/B, JENDL, JEFF, CENDL and GEFY
- All nuclear data processing is handled by NJOY (LANL), PREPRO (LLNL) and CALENDF (UKAEA)

FISPACT-II &TENDL, ENDF/B, JENDL, JEFF, CENDL

IAEA 60 Years *Atoms for Peace and Development*

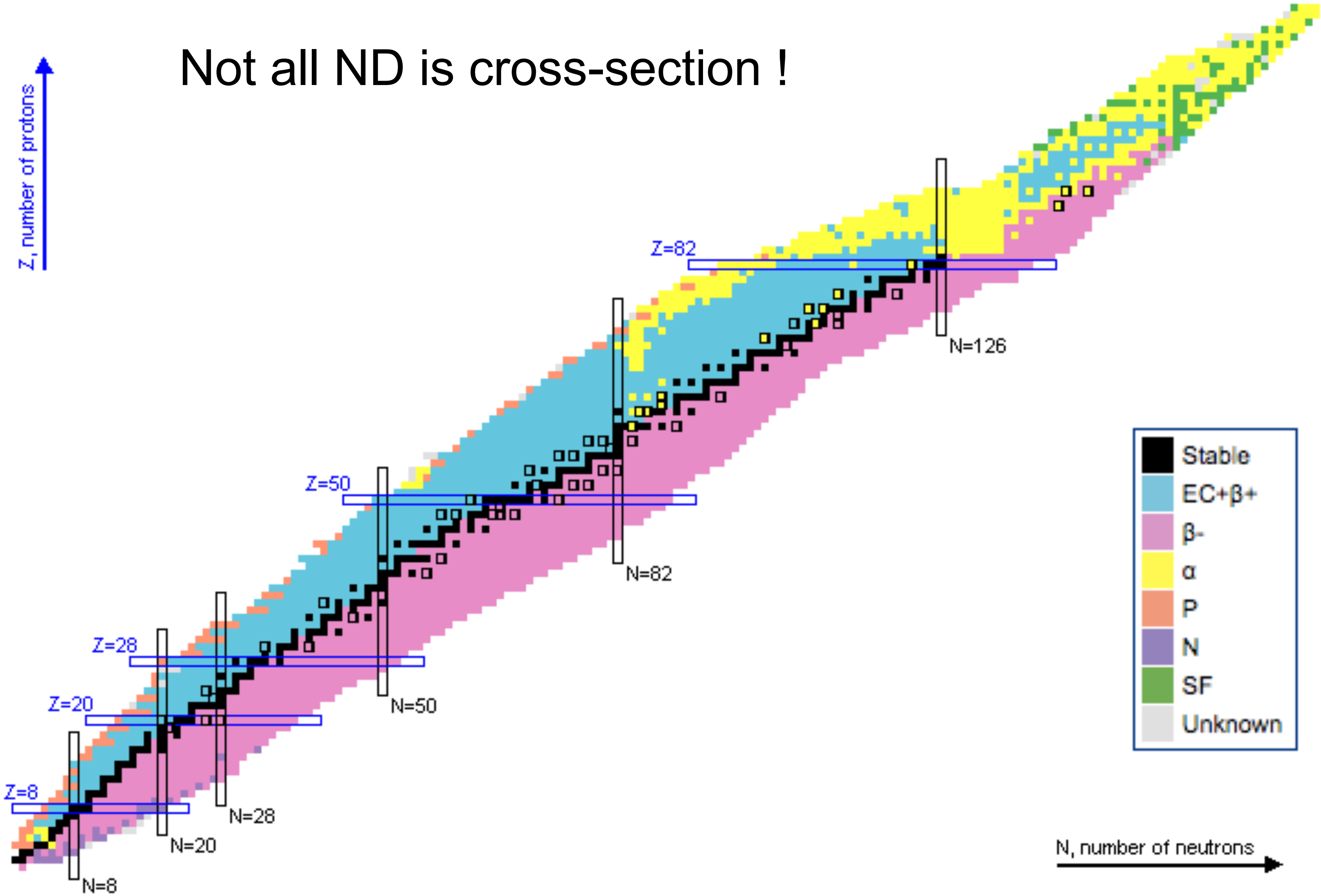


mix and match

Nuclear landscape: decay data

3873 isotopes (23 decay modes; 7 single and 16 multi-particle ones)

Not all ND is cross-section !



FISPACT-II advanced simulations

	FISPACT-II
Solver	Numerical - LSODES 2003
Incident particles	α, γ, d, p, n (5)
ENDF's libraries: TENDL-2015 & GEFY-5.3 ENDF/B-VII.1, JEFF-3.2, JENDL-4.0, CENDL-3.1 (~400 targets each)	✔ XS data (2809 targets) ✔ Decay data (3873 isotopes) ✔ nFY, sFY, otherFY ✔ Hazard, clearance indices, A2
Dpa, Kerma, Gas production, HE radionuclide yields	✔
PKA, primary recoils and emitted particles spectra	✔
Uncertainty quantification and propagation UQP	✔ Variance-covariance
Temperature (from reactor to astrophysics, plasma) 1 KeV ~ 12 million Kelvin	✔ 0, 294, 600, 900 K,…5, 30, 80 KeV
Self-shielding with probability tables **and/or** with resonance parameters	✔ Resolved and Unresolved Resonance Range
Energy range	1.0 10^{-5}eV – 30, 200 MeV, ..1GeV
Sensitivity	✔ Monte Carlo
Pathways analysis, routes of production	✔ multi steps
Thin, thick targets yields	✔

✔ new or unique

Processing steps: three codes

ENDF file

- **NJOY12-099**
  - reconr
  - broadr
  - unresr
  - thermr
  - heatr
  - gaspr
    - groupr
    - purr
    - acer

cross-check

- **PREPRO-2017**
- **linear**
- **recent**
- **sigma1**
- **sixpack**
- **activate**
- **merger**
- **dictin**
- **groupie**

cross-check

- **CALENDF-2010**
  - calendf
  - regroutp
  - lecritp
  - ….

PKA file

ACE file

PT file

Processed ENDF file

Single script for an entire library

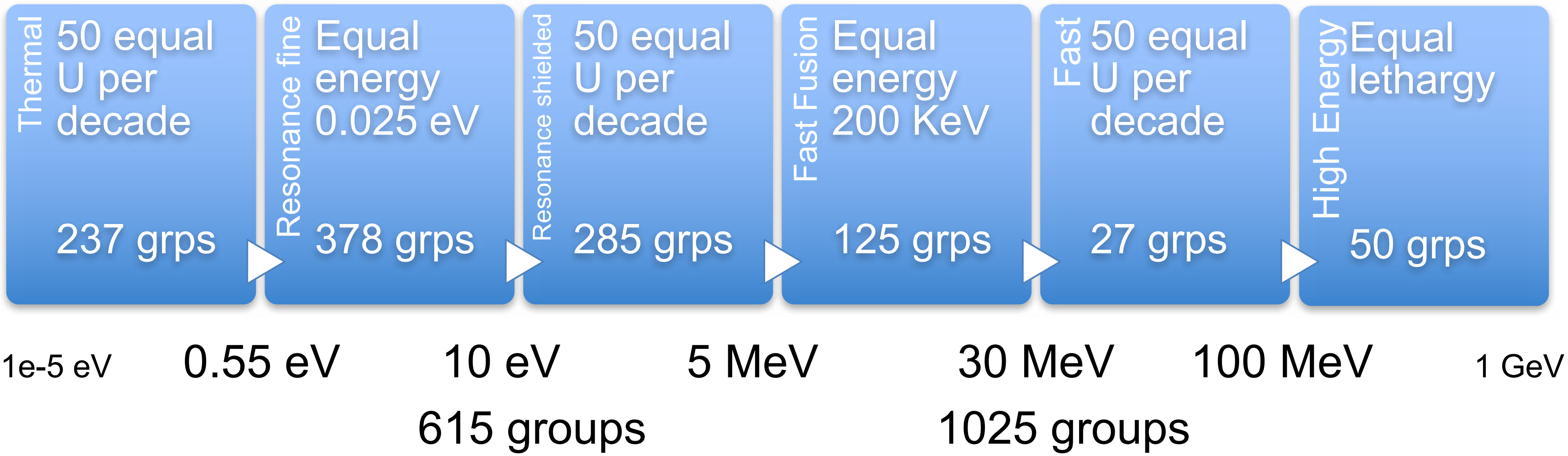
Processing steps: three codes

- **PREPRO-2017**
  - 0 Kelvin run
  - Single temperature pendf, 294 Kelvin to… 100 KeV
  - *SIXPACK*: unique mf3-mt5/mf6 high energy processing
  - *ACTIVATE*: unique mf9 processing
  - Merge NJOY-12 dpa, kerma, pendf responses
  - *GROUPIE* to: 1102 grps @ 1 GeV
    1067 grps @ 200 MeV
    1025 grps @ 30 MeV
    615 grps @ 10 eV
    162 gprs @ 200 MeV (for charge particles)
  - mf-2 processed, but also kept in for further usage

The resulting pendf/gendf "tape" fully comply to the ENDF-6 format frame and many utilitarian process (display, merge, concatenate, etc.) can be performed on such data forms

Group structures

- For all 2809 TENDL target nuclides
- 1102 energy groups for <u>all applications alike</u>

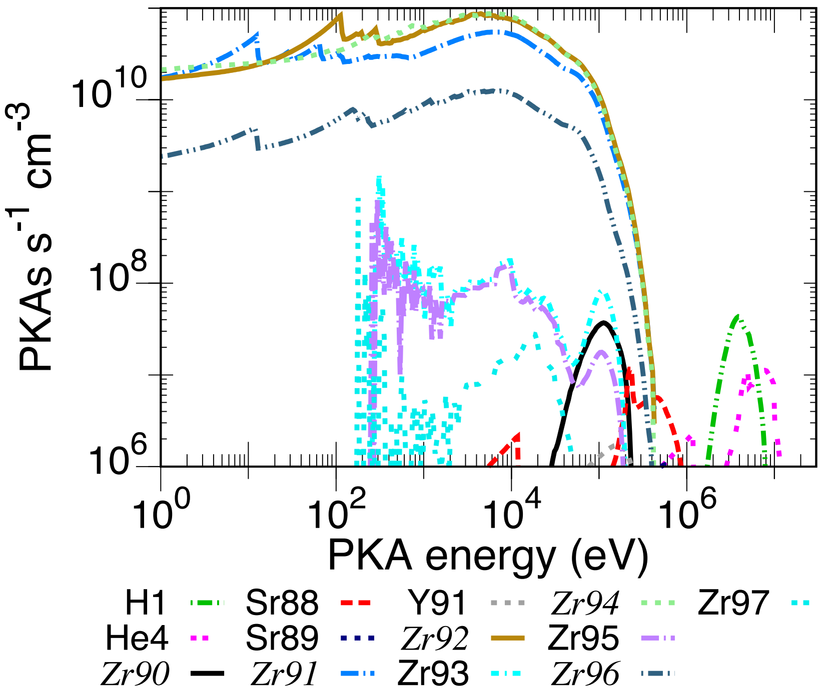


- 237 fine groups for proper 1/E < 0.55 eV
- 378 fine groups in the resonance range < 10 eV
- Resonance shielded data available in the RRR (>0.1 eV) up to the end of the URR for all nuclides IDs
- Fast fine enough structure for accurate threshold reaction rate

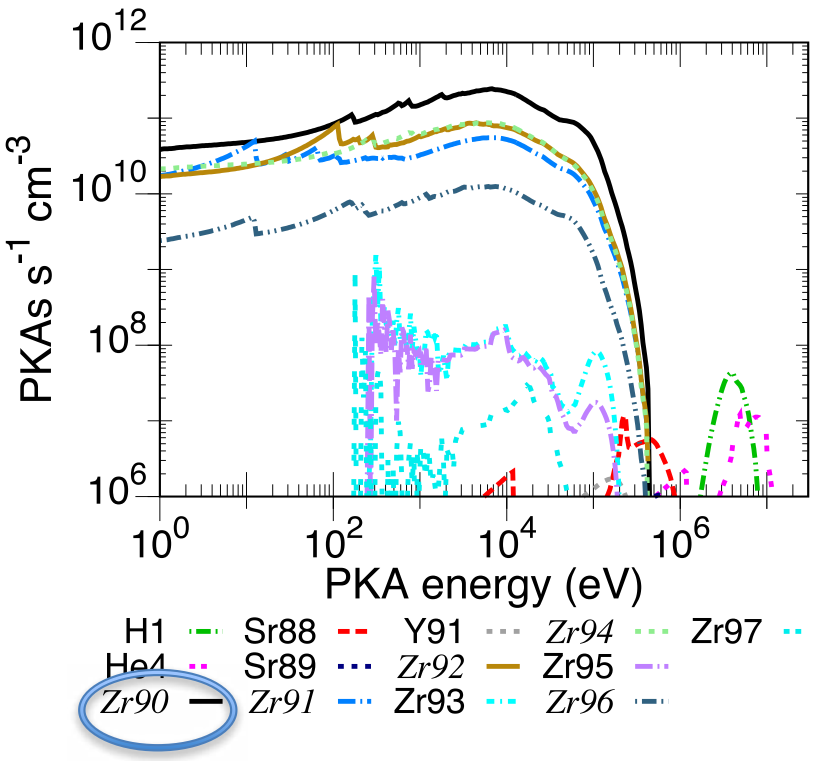
NJOY12 updates for Zr isotopes

*/ ident up69
*/18aug2016
*/ - groupr
*/   - the dimension limit of 3 in getmf6 for iyss, izss and jjss means
*/   we're assuming no more than a ground state plus two isomers for
*/   a given ZA. Recent files may exceed this limit

Before < 3 isomer limit



After < 6 isomers



Verification and Validation V&V

Typically these are divided into differential & integral:

- Differential
  - C/E with the latest EXFOR database
  - C/C with other ENDF's files
  - SACS: Statistical Analysis of Cross Section
- Integral
  - Activation-transmutation; activity, gamma, decay heat
    - FISPACT-II validation suite (~500 reaction rates, thousands of integral E, time dependent, fast system)
  - MACS and RI: Maxwellian-averaged cross sections and astrophysical reaction rates, resonance integrals
  - Decay heat and inventories predictions for fission events

FISPACT-II resources

- FISPACT-II and libraries are subject of various validation reports:
  - CCFE-R(15) 25 Fusion decay heat
  - CCFE-R(15) 27 Integral fusion
  - CCFE-R(15) 28 Fission decay heat

CCFE

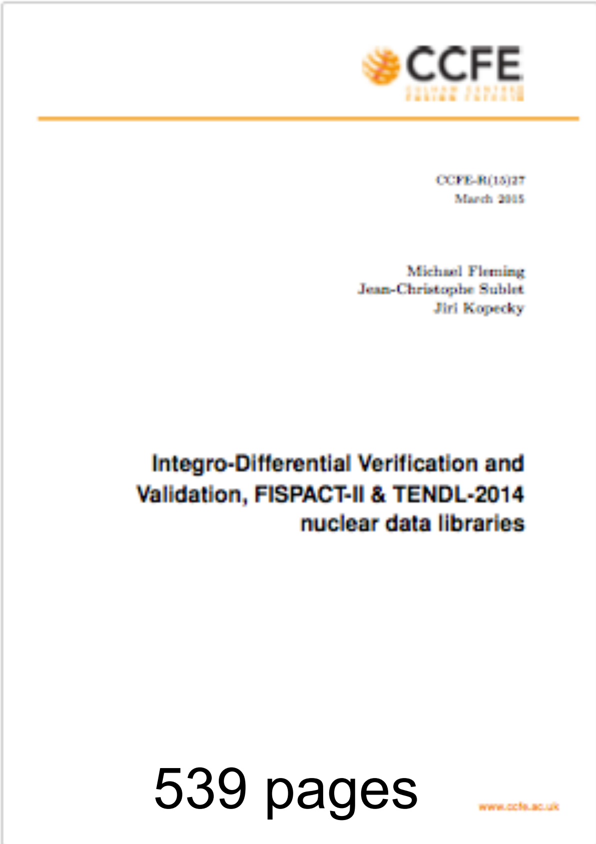
CCFE-R(15)28
June 2015

Michael Fleming
Jean-Christophe Sublet

Validation of FISPACT-II Decay Heat and Inventory Predictions for Fission Events

www.ccfe.ac.uk

458 pages



CCFE

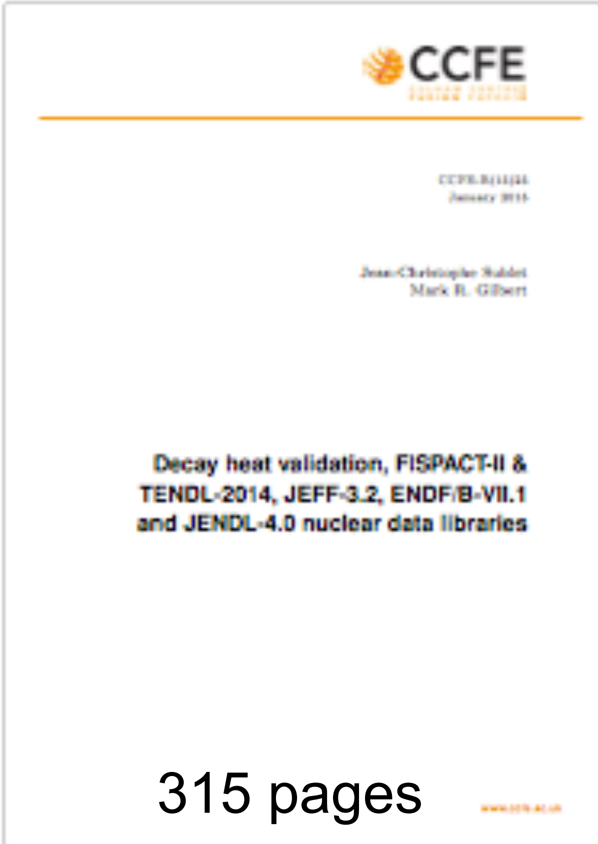
CCFE-R(15)27
March 2015

Michael Fleming
Jean-Christophe Sublet
Jiri Kopecky

Integro-Differential Verification and Validation, FISPACT-II & TENDL-2014 nuclear data libraries

www.ccfe.ac.uk

539 pages



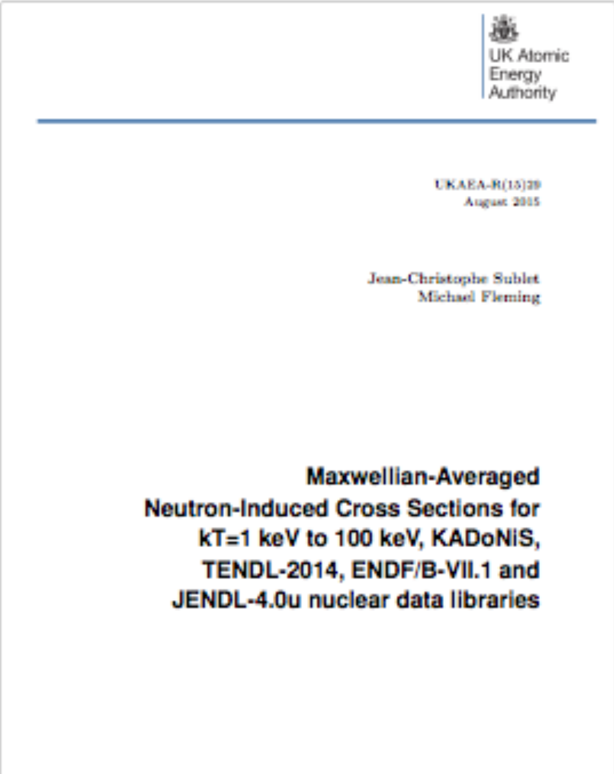
CCFE

Decay heat validation, FISPACT-II & TENDL-2014, JEFF-3.2, ENDF/B-VII.1 and JENDL-4.0 nuclear data libraries

315 pages

FISPACT-II resources

- FISPACT-II and libraries are subject of various validation reports:
  - UKAEA-R(15) 29 Astro s-process
  - UKAEA-R(15) 30 RI/therm/systematics
  - UKAEA-R(15) 35 Summary report



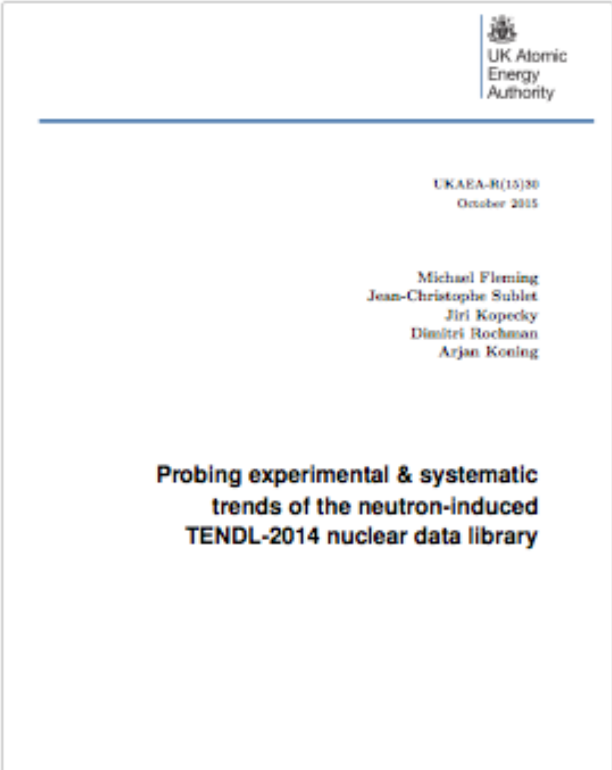
UK Atomic Energy Authority

UKAEA-R(15)29
August 2015

Jean-Christophe Sublet
Michael Fleming

Maxwellian-Averaged Neutron-Induced Cross Sections for kT=1 keV to 100 keV, KADoNiS, TENDL-2014, ENDF/B-VII.1 and JENDL-4.0u nuclear data libraries

417 pages



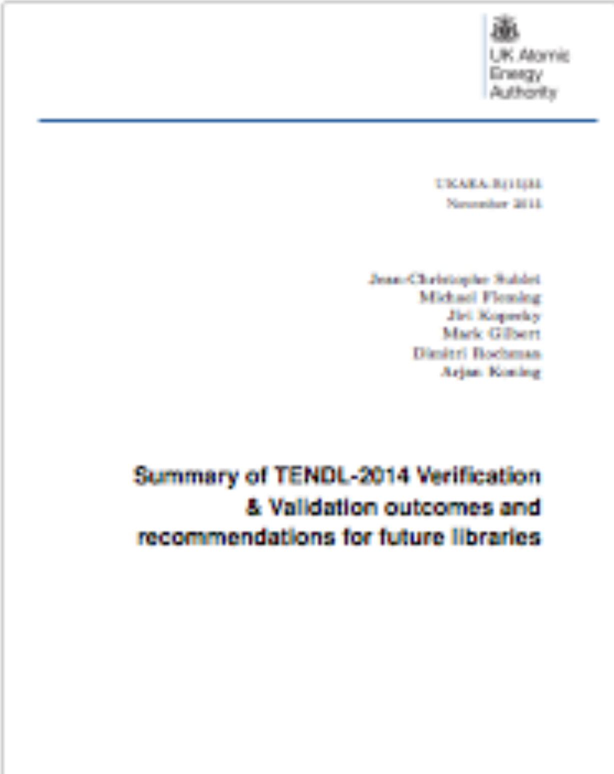
UK Atomic Energy Authority

UKAEA-R(15)30
October 2015

Michael Fleming
Jean-Christophe Sublet
Jiri Kopecky
Dimitri Rochman
Arjan Koning

Probing experimental & systematic trends of the neutron-induced TENDL-2014 nuclear data library

99 pages



UK Atomic Energy Authority

UKAEA-R(15)35
November 2015

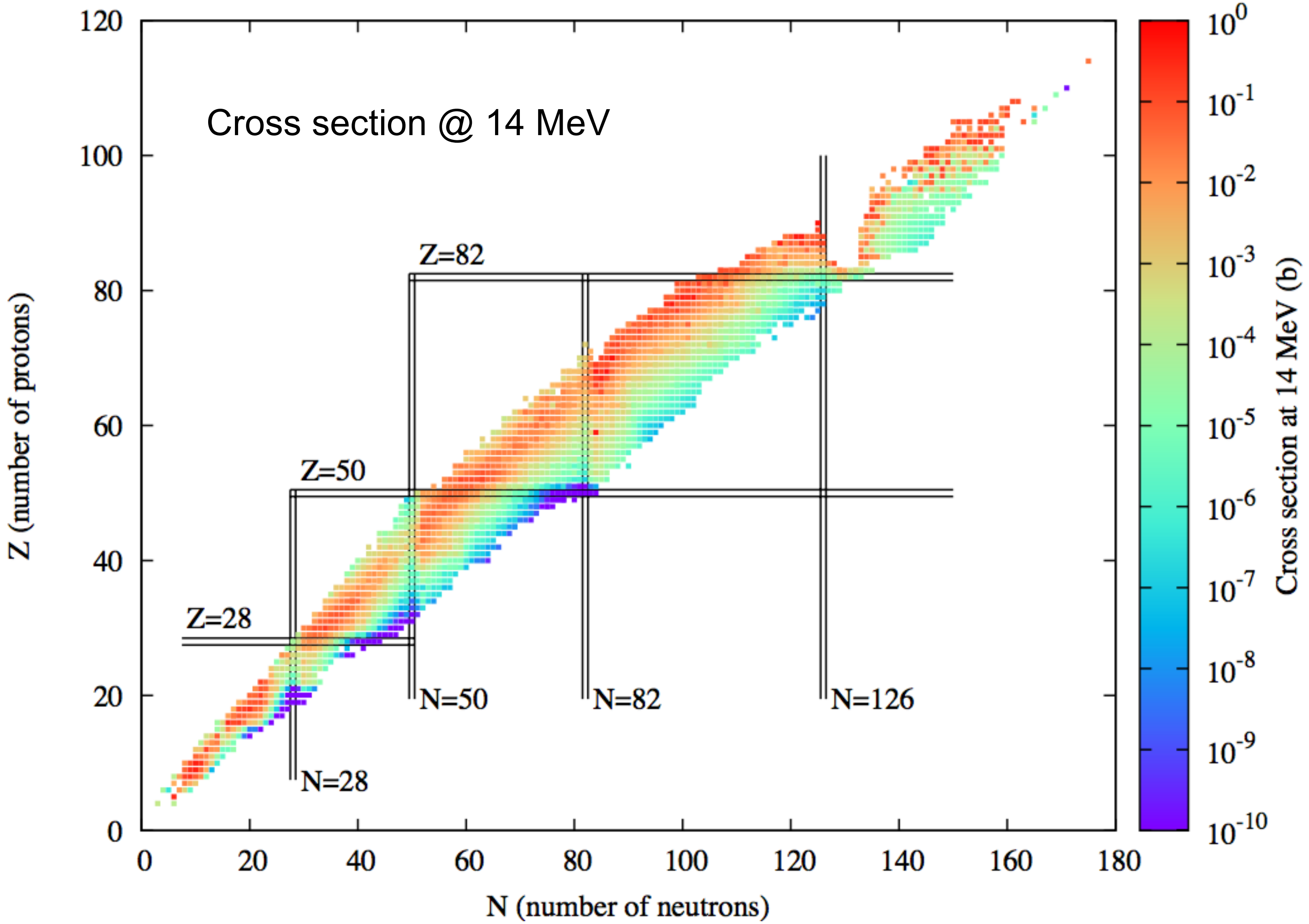
Jean-Christophe Sublet
Michael Fleming
Jiri Kopecky
Mark Gilbert
Dimitri Rochman
Arjan Koning

Summary of TENDL-2014 Verification & Validation outcomes and recommendations for future libraries

38 pages

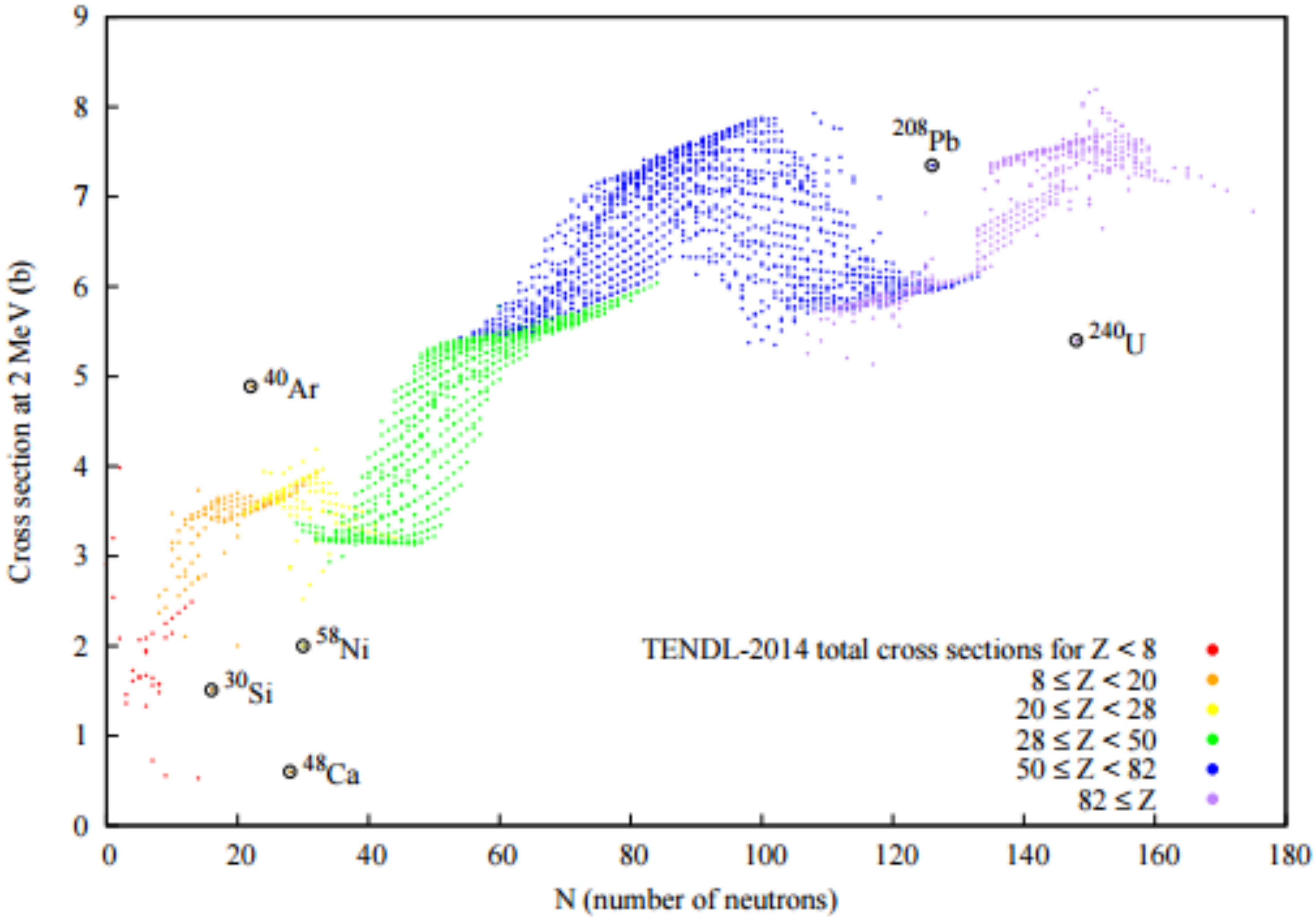
V&V: Global checks on nuclear data

- Global checks and new visualisation methods developed to provide verification over the massive data-set



Global trends

- Trends (here in total) help find programming glitches after various effects (shell, high-energy resolved resonances, etc.) have been taken into account



V&V: Global checks on nuclear data

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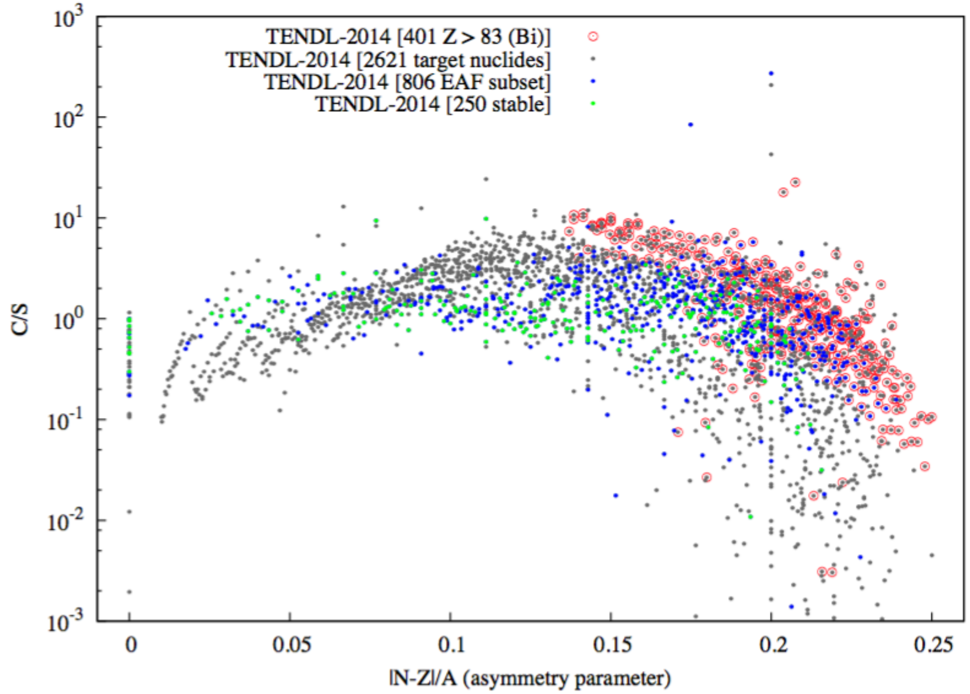
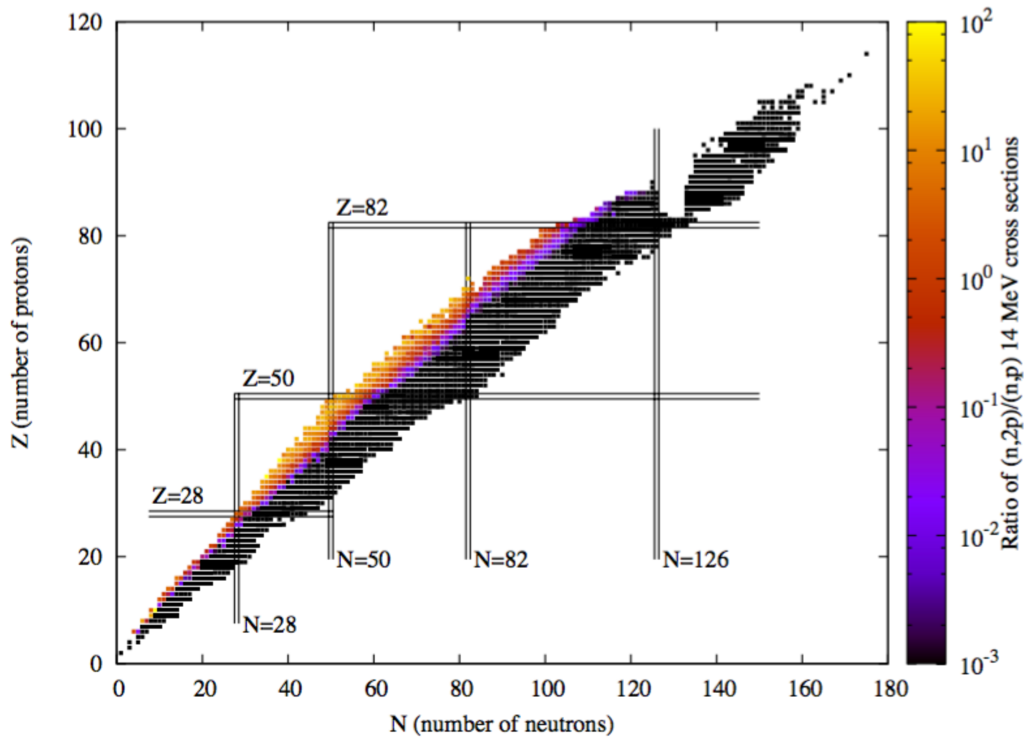


Asymmetry

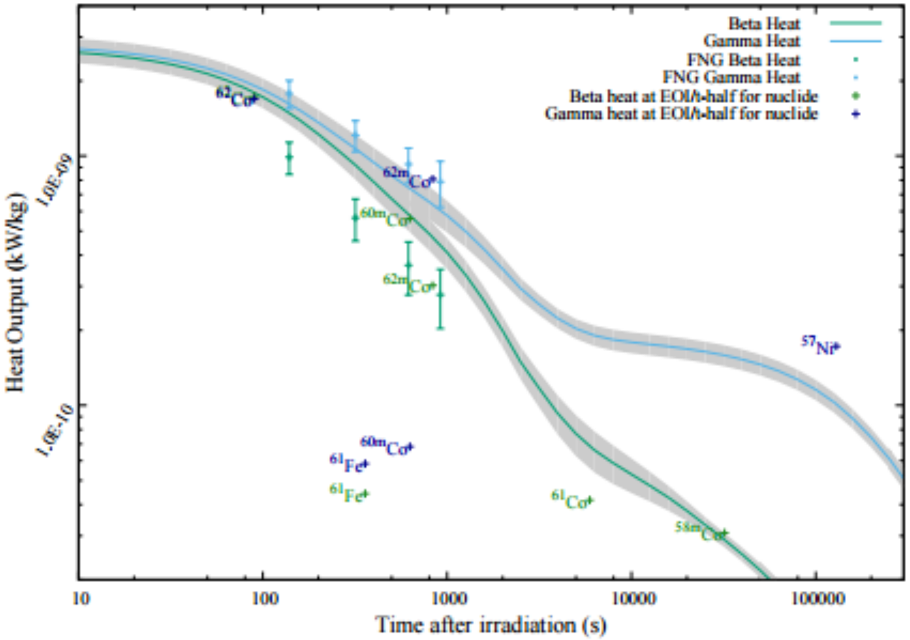


Cross section ratio @ 14 MeV

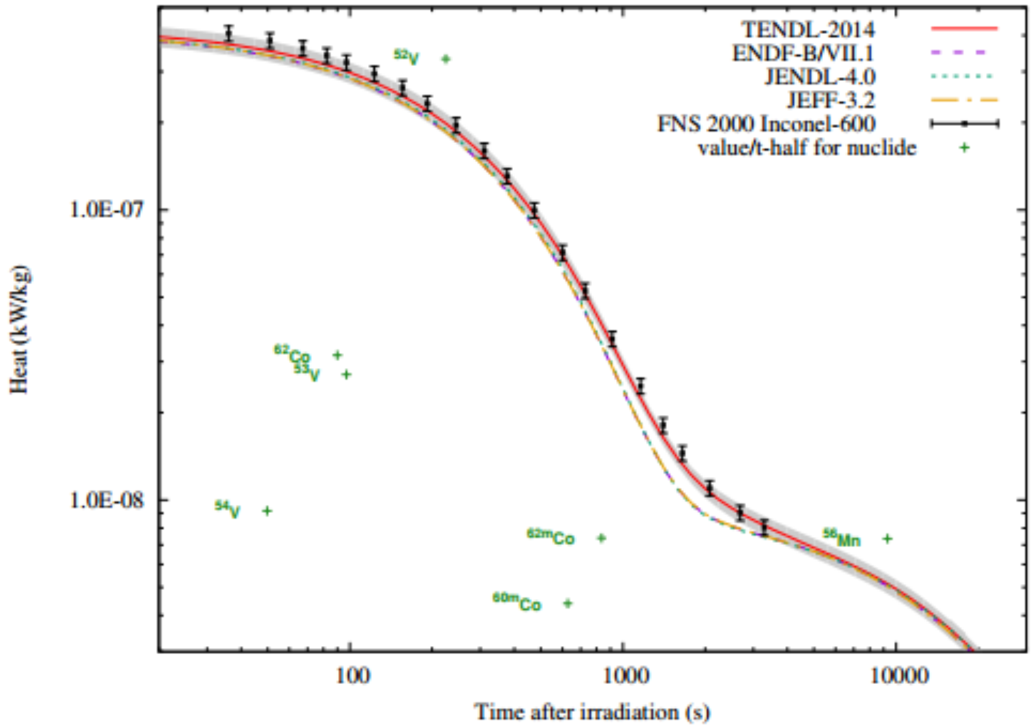
(n,2p) dominates p-rich, not in systematics

Validation – decay heat

- Integral “effective “cross sections are inferred from post-irradiation measurements such as gamma-decays or calorimetric data



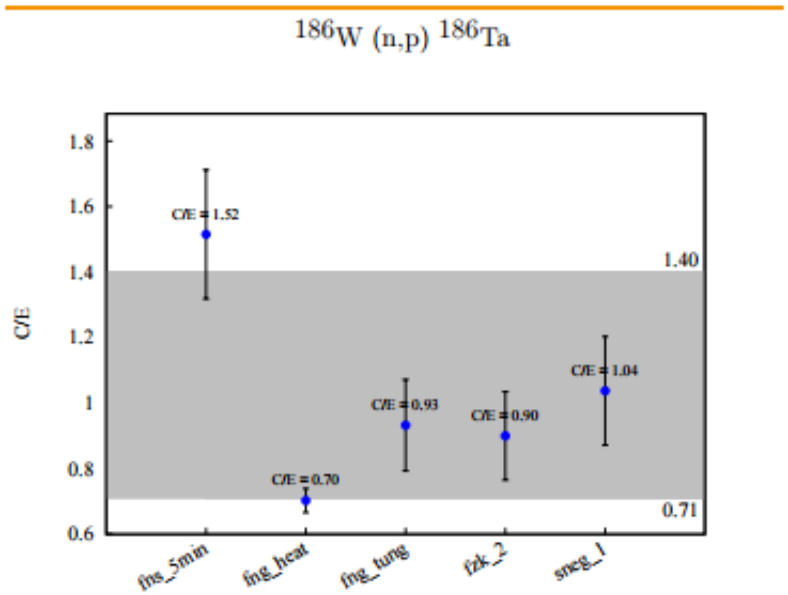
Spectroscopic heat from ENEA FNG campaign

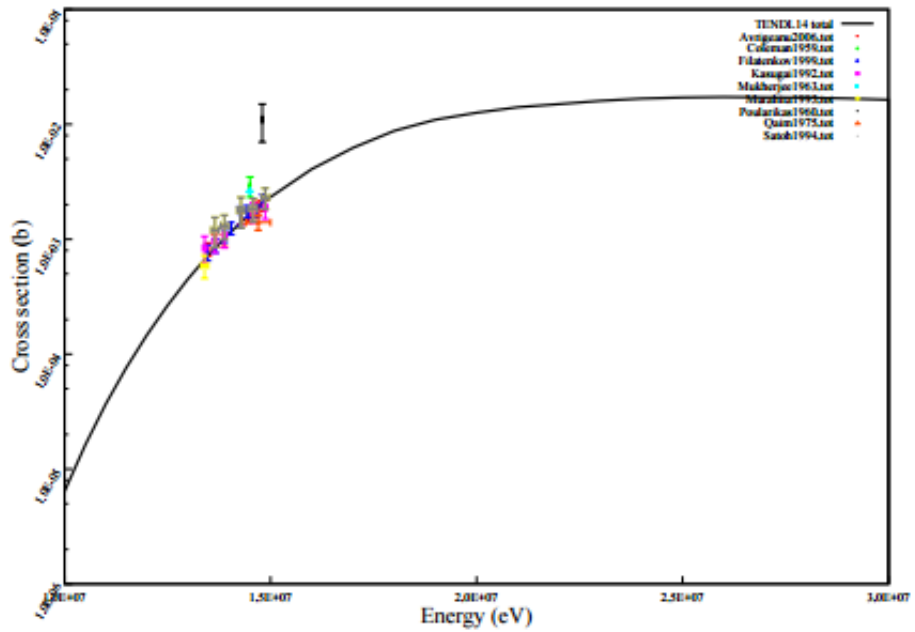


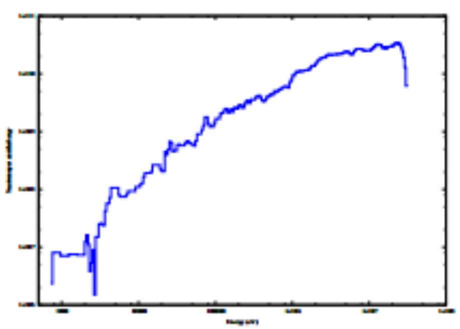
Total heat calorimetric measurements from JAEA FNS campaign

Multi-faceted validation

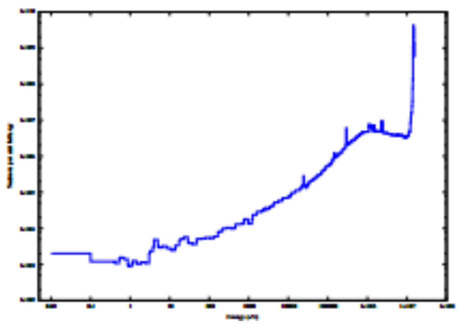
- The best approach is to use multiple experiments from different systems, covering int. and diff. experiments



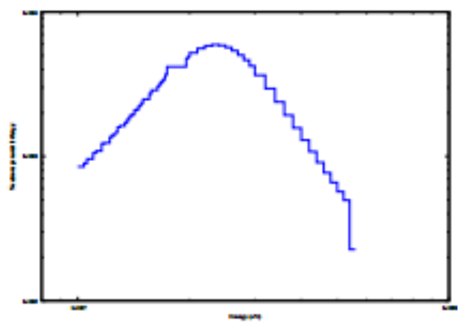




Spectrum >100 MeV

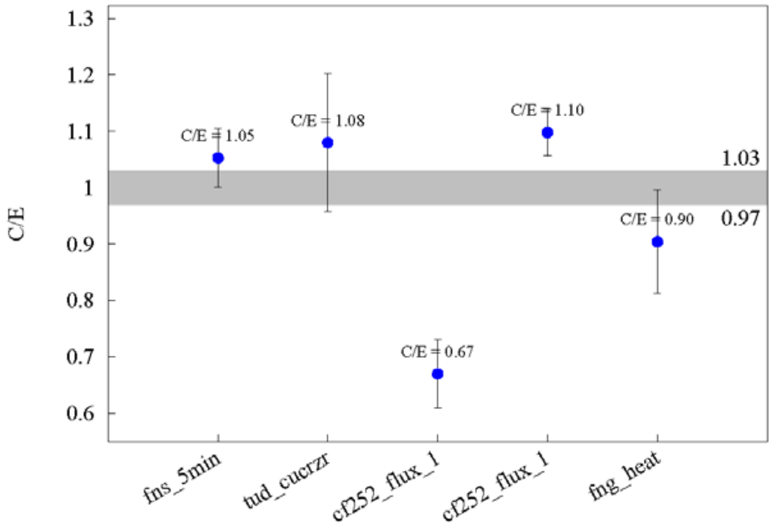


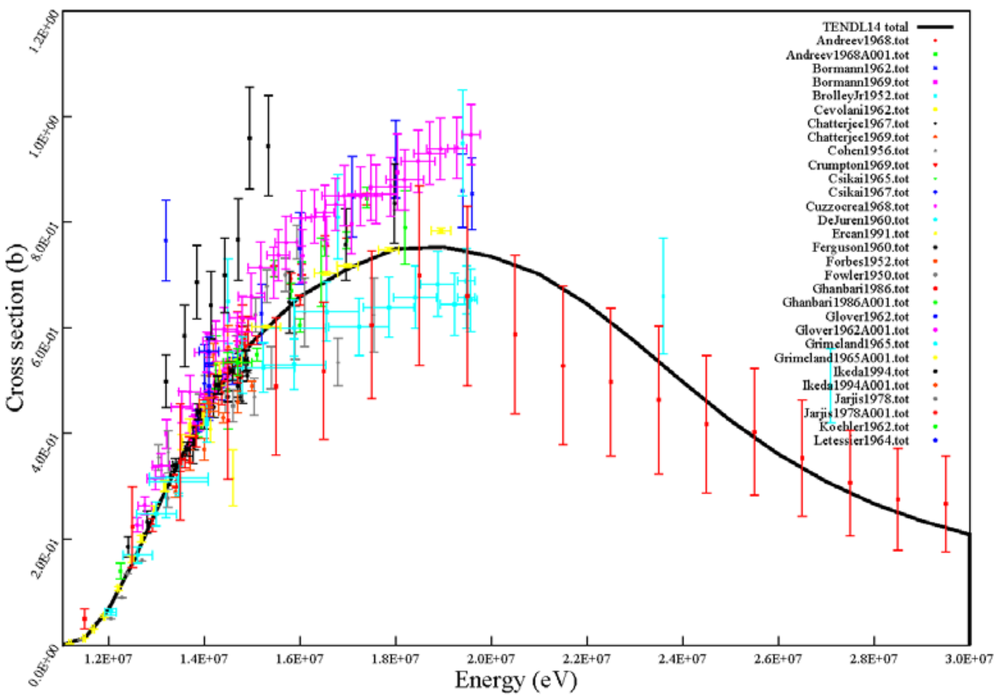
Total heat FNS



D-Be gamma exp

Integro-differential 65Cu (n,2n) 64Cu





Not all integrals..
Not all differentials..

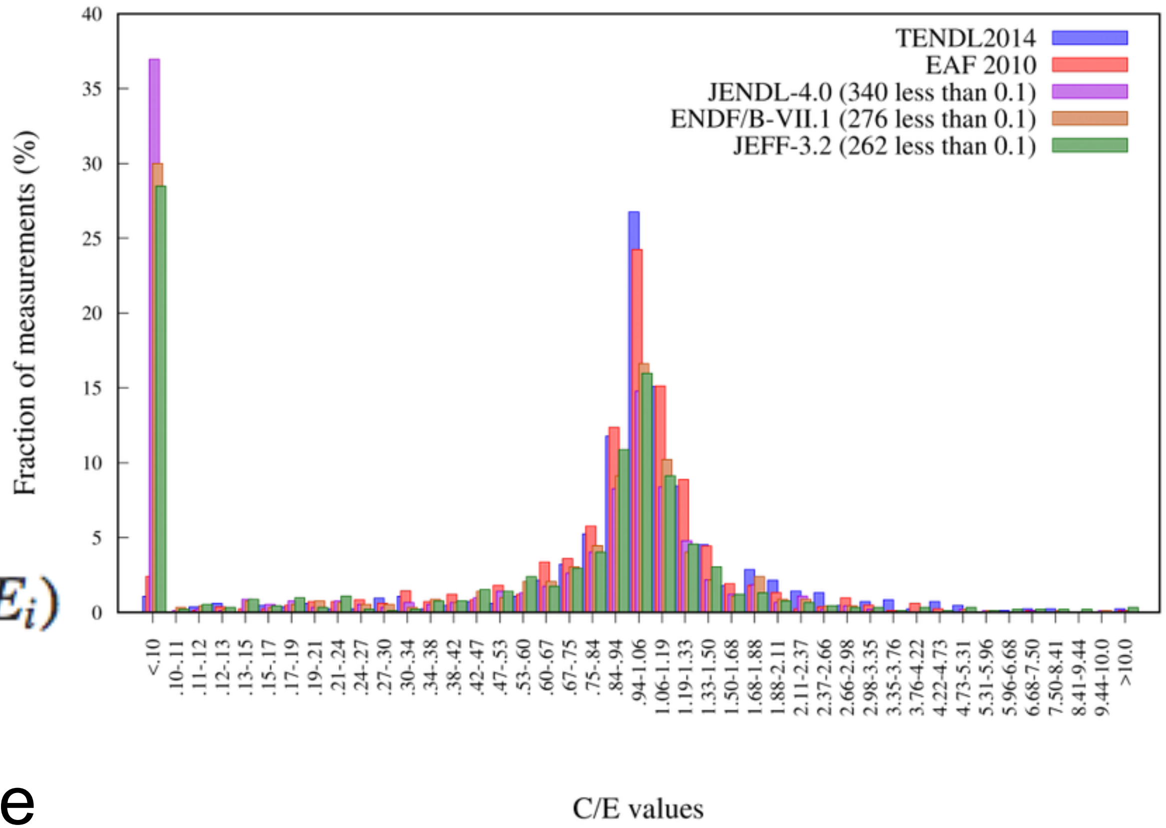
are as reliable, so the importance of the covariances

Integro-differential results

- TENDL has outperformed all libraries, **including EAF**, which is *tuned* to these experiments!

- Legacy libraries miss 1/3 of the channels

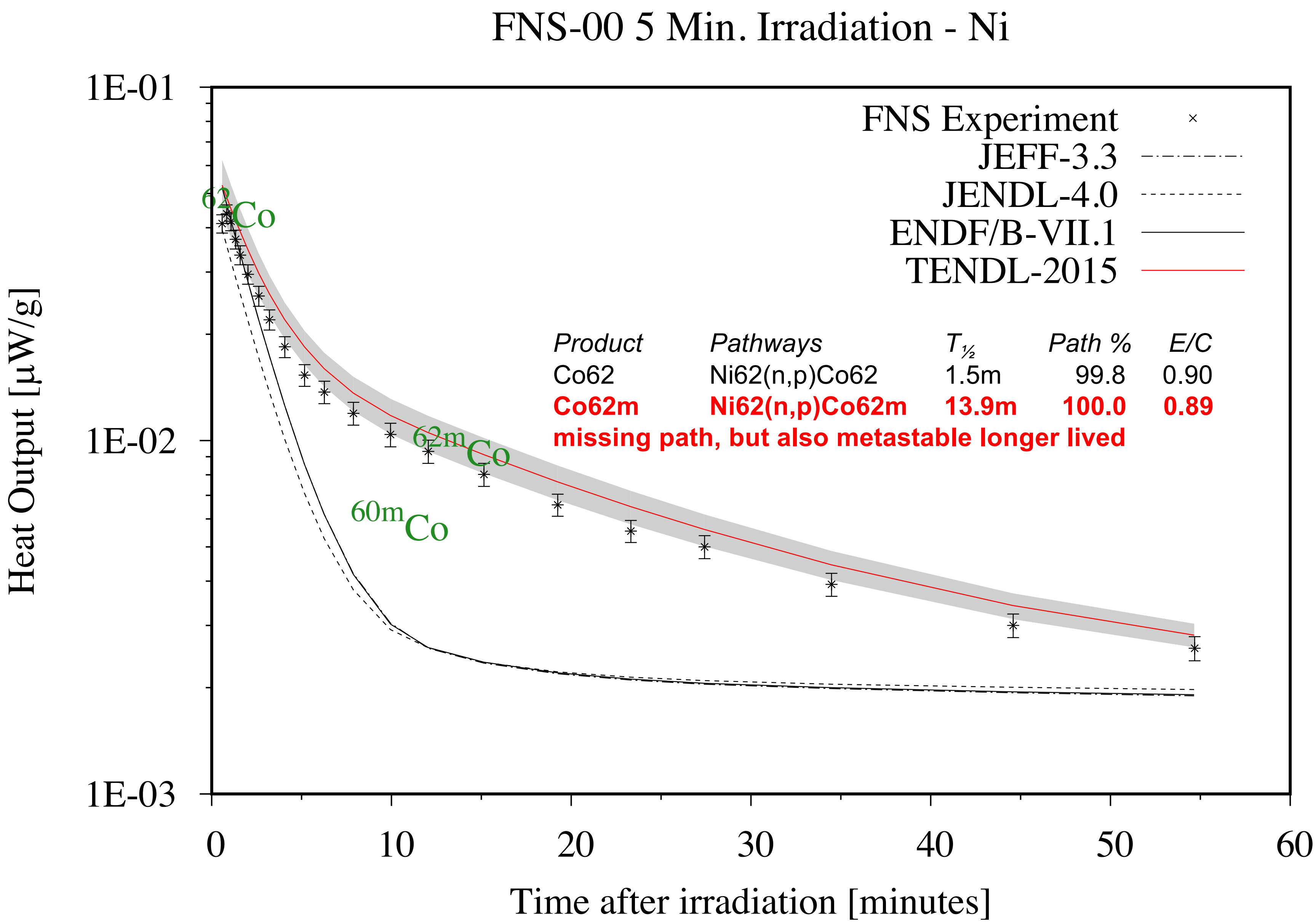
$$\mathrm{Log}\left(\overline{C/E}\right) = \frac{1}{n}\sum_{i=1}^{n} \mathrm{Log}\left(C_i/E_i\right)$$



- EAF mean = **0.850** while TENDL = **0.993** – asymmetry implies underestimations

Decay power: FNS JAERI

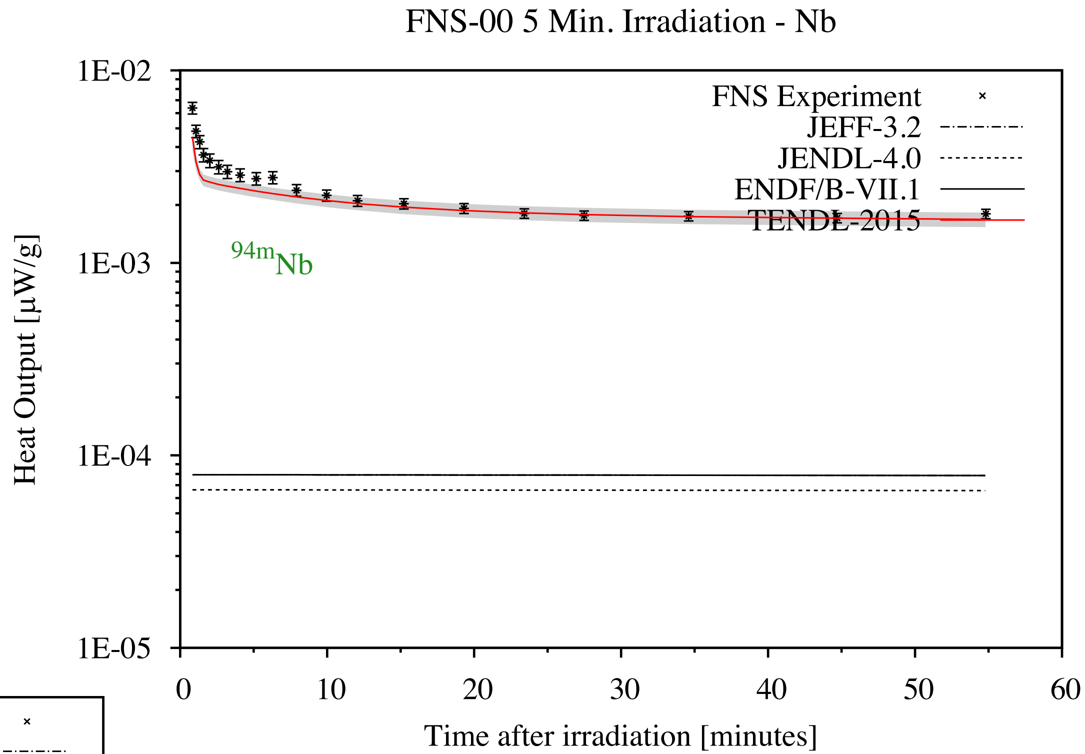
Random walk uncertainty

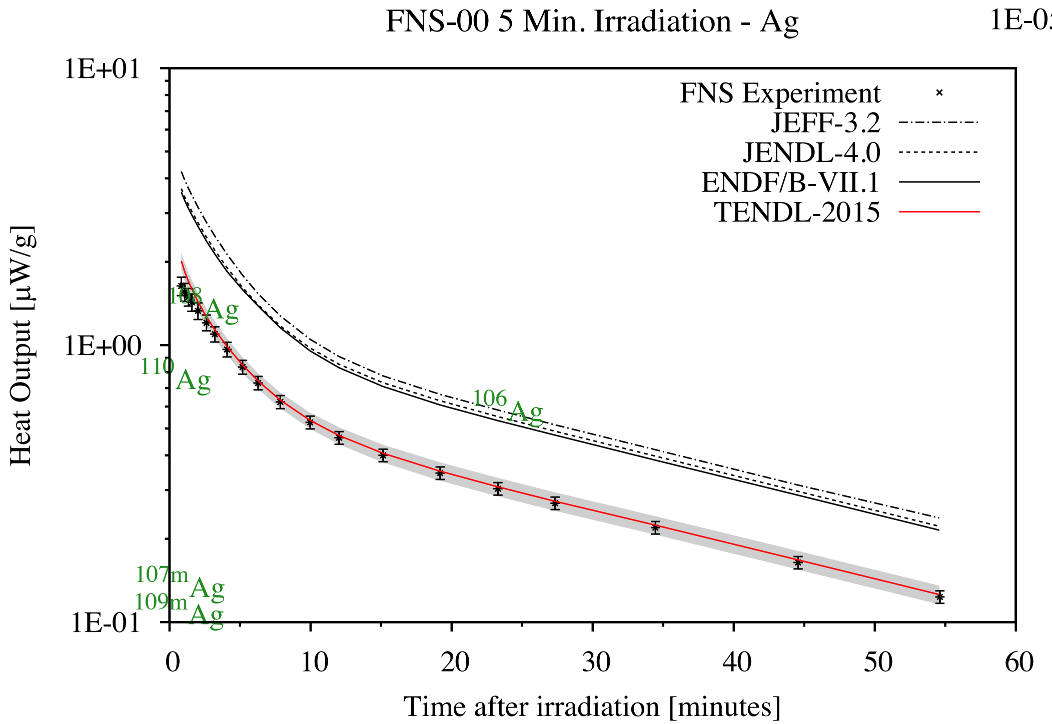


Decay power: FNS JAERI

When you do not account for isomer production channels….

The responses are missed entirely !!



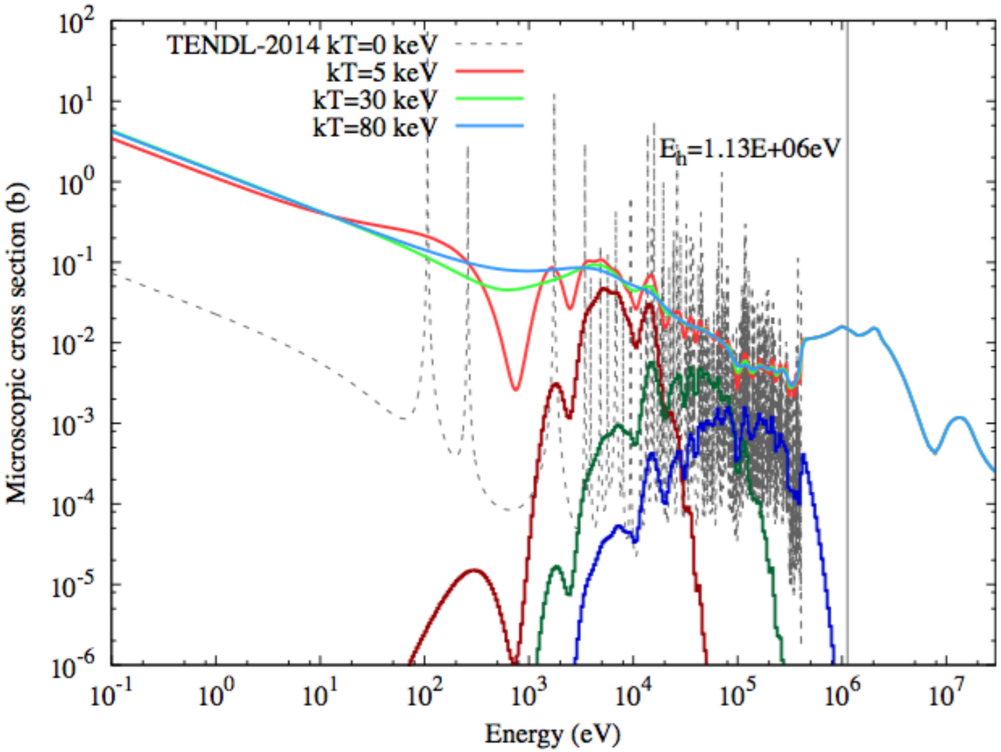


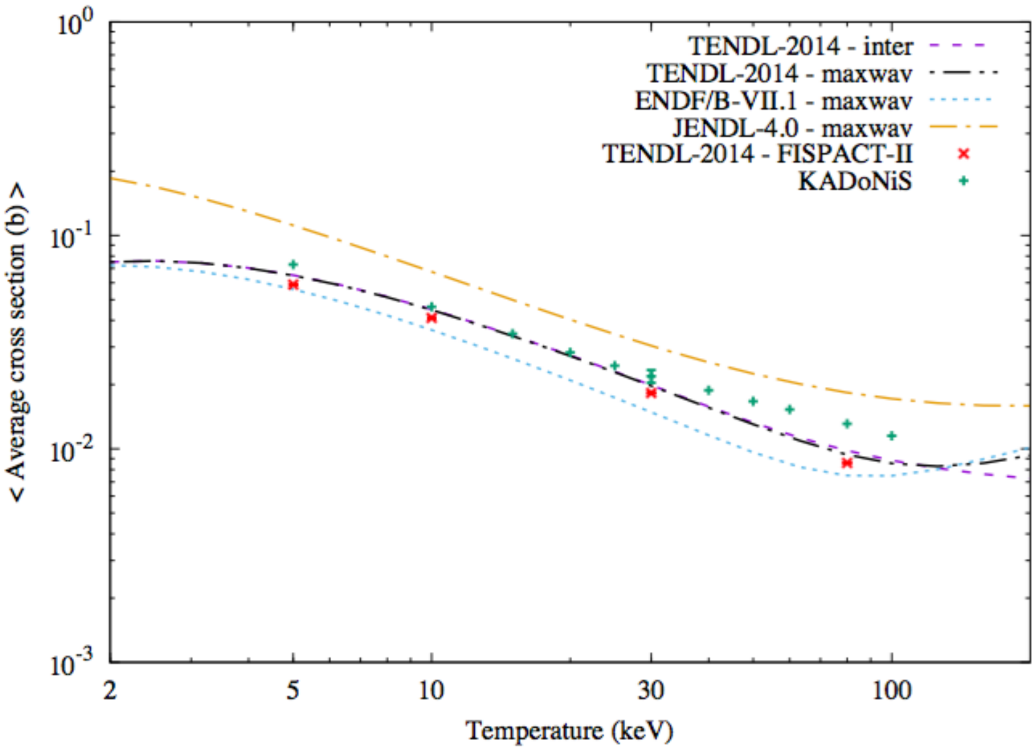
Hunt for the isomers, the short lived…

Most are lost in seconds, minutes…

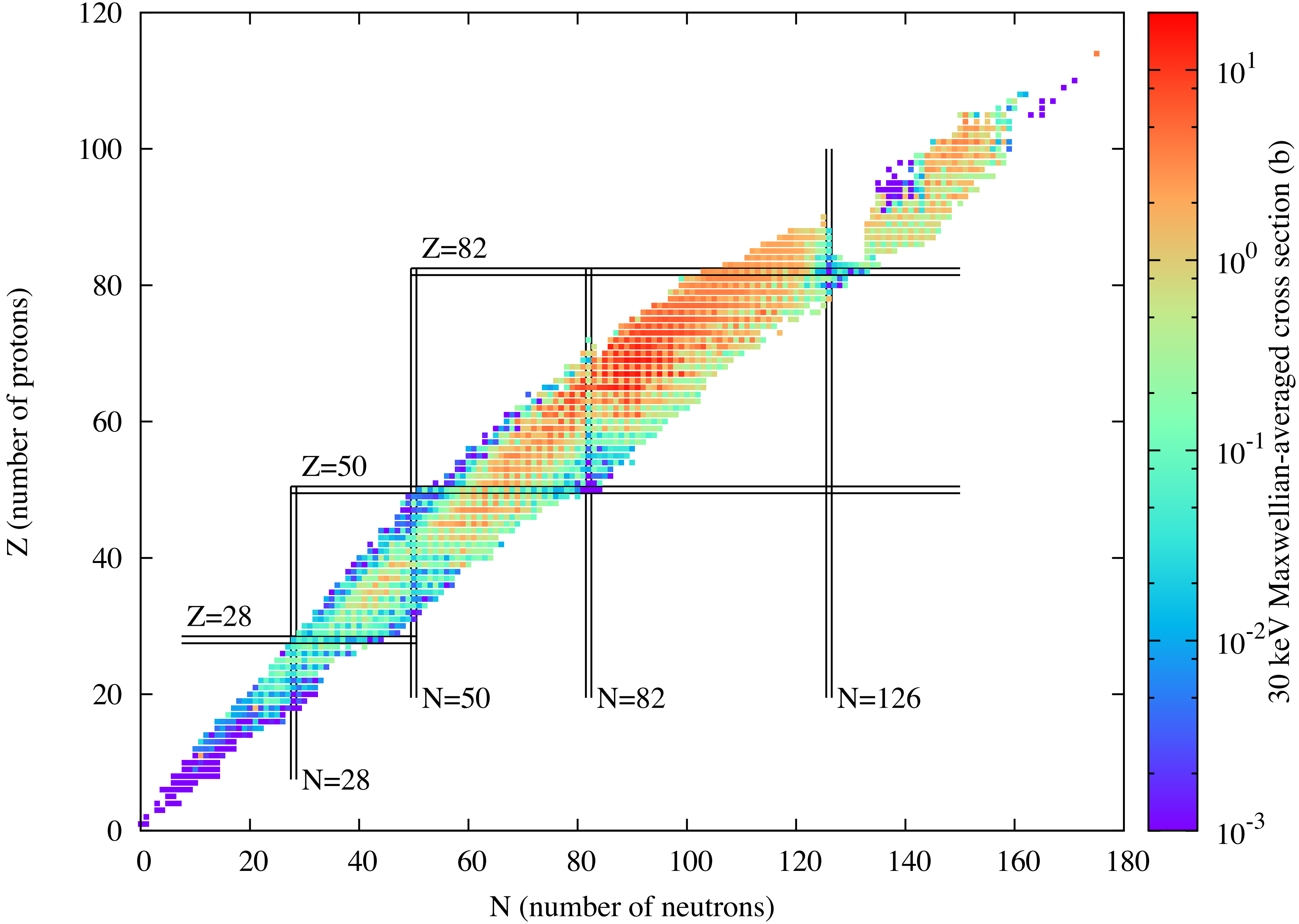
T-dependence: *s*-Process Nucleosynthesis

- AGB stars forge elements above Fe through neutron capture with kT=1-100keV, precisely in resonance ranges!
  - Many experiments give data of use in benchmarking – subject of report UKAEA-R(15)29
  - Left: microscopic σ(E) and RR(E), Right: RR(kT) against exp. (Sn122)



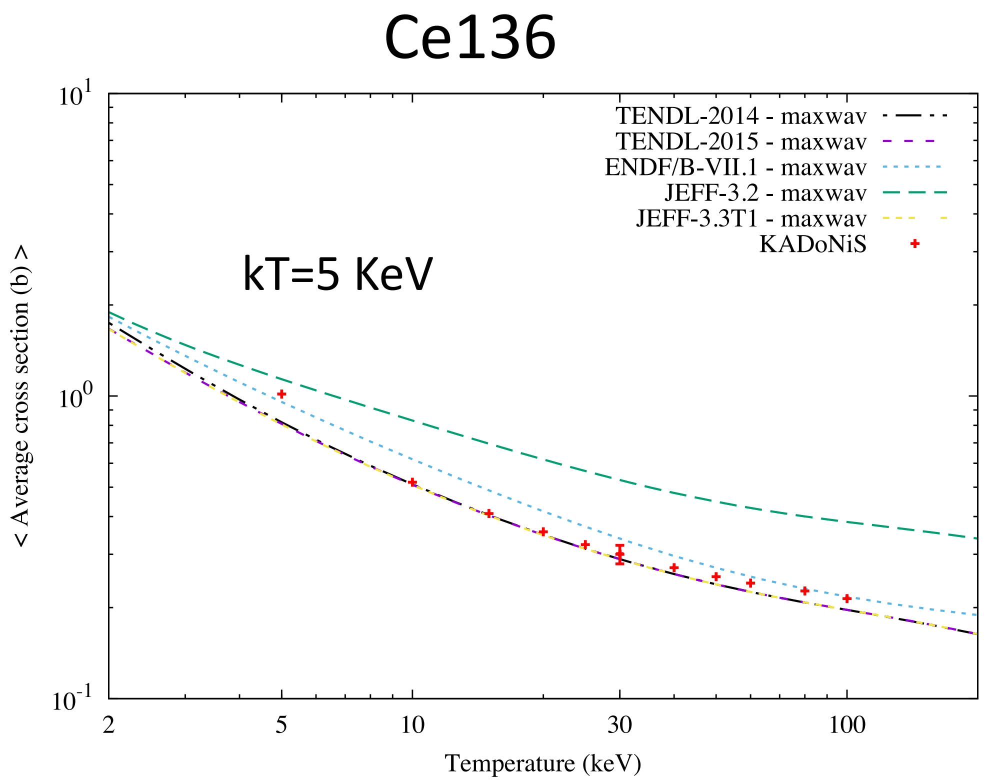


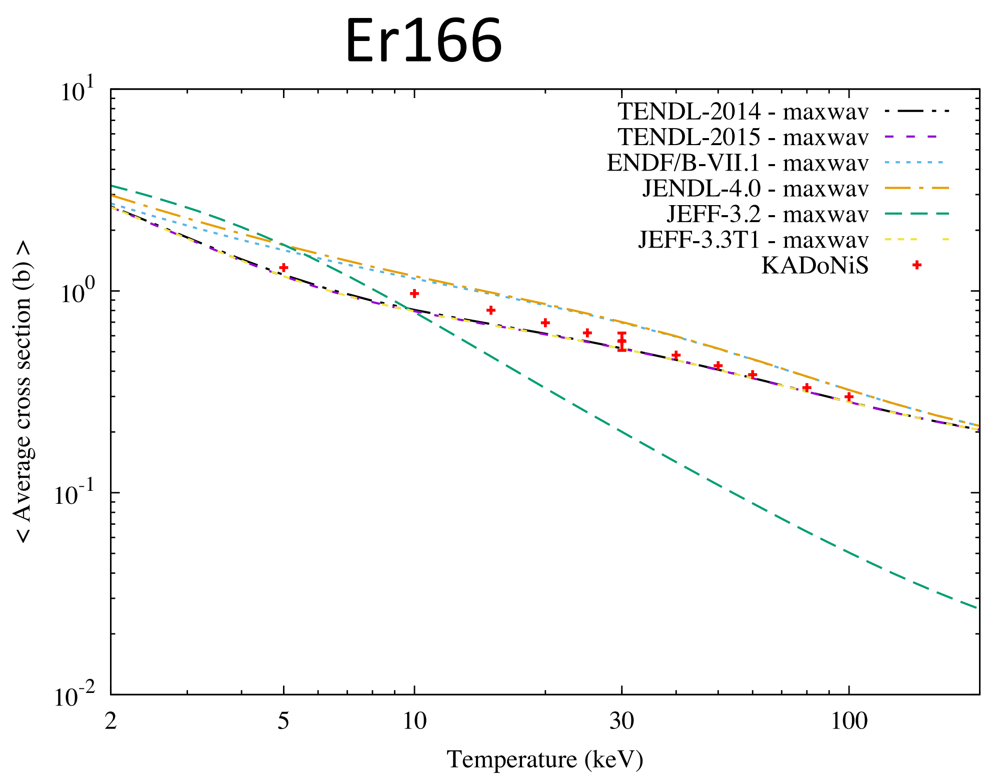
kT= 30 keV Maxwellian



New MACS for TENDL15

- Some nice improvements, adoption of data, for example:

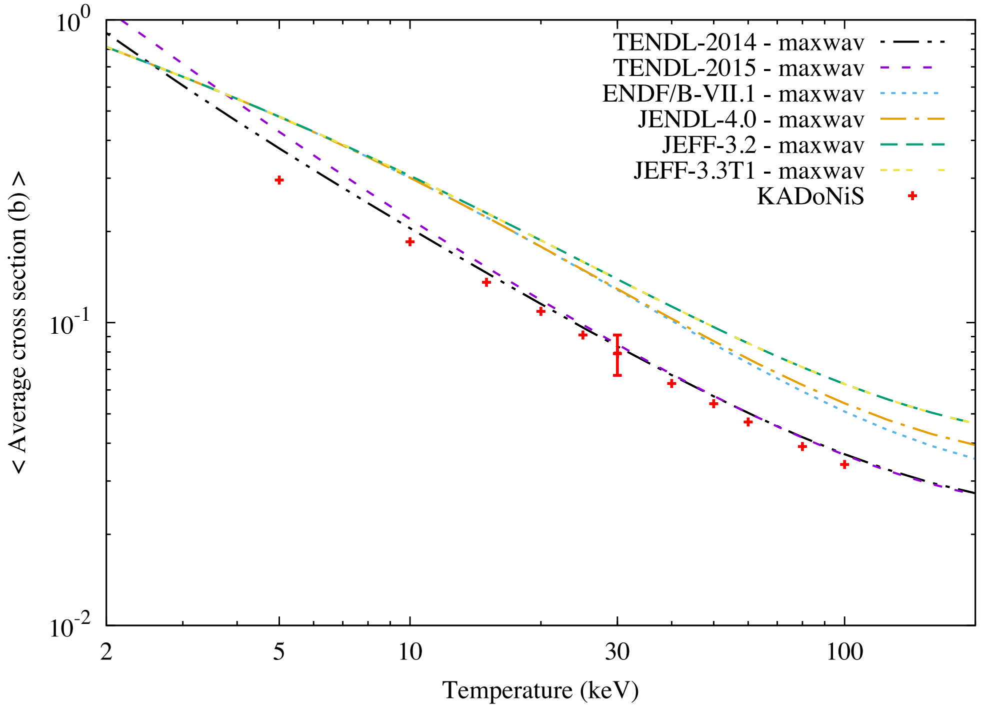




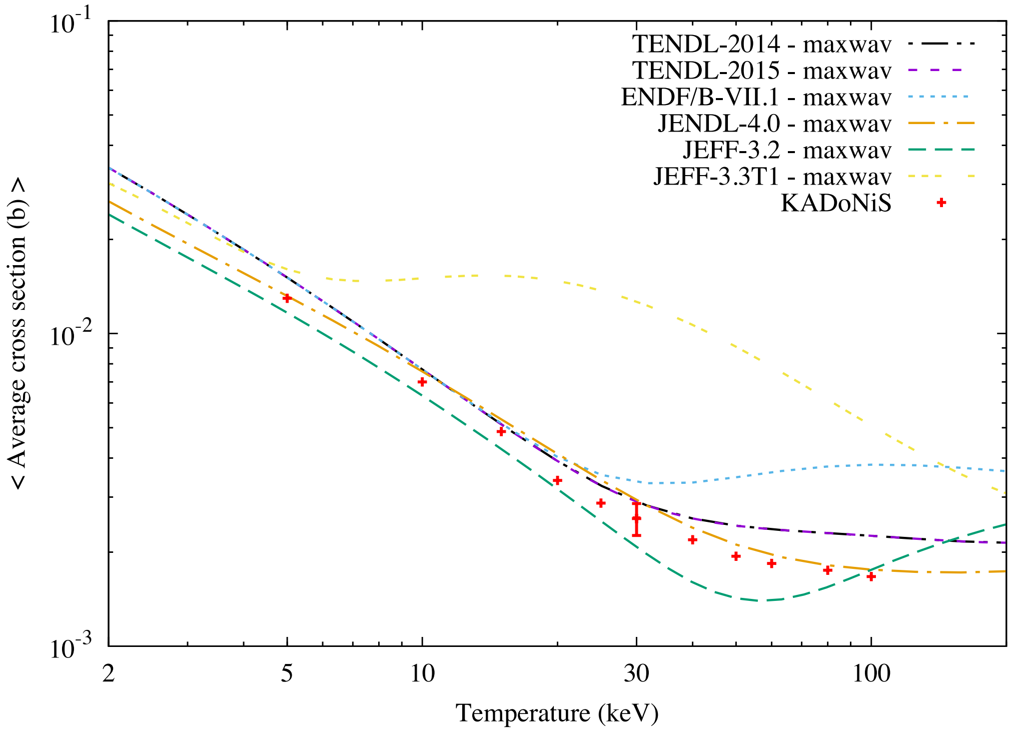
New MACS for TENDL15

- Some outstanding issues, questions to be addressed:
  1. How much faith to place in these data?
  2. What can be drawn, and how, from TENDL?

Zr95

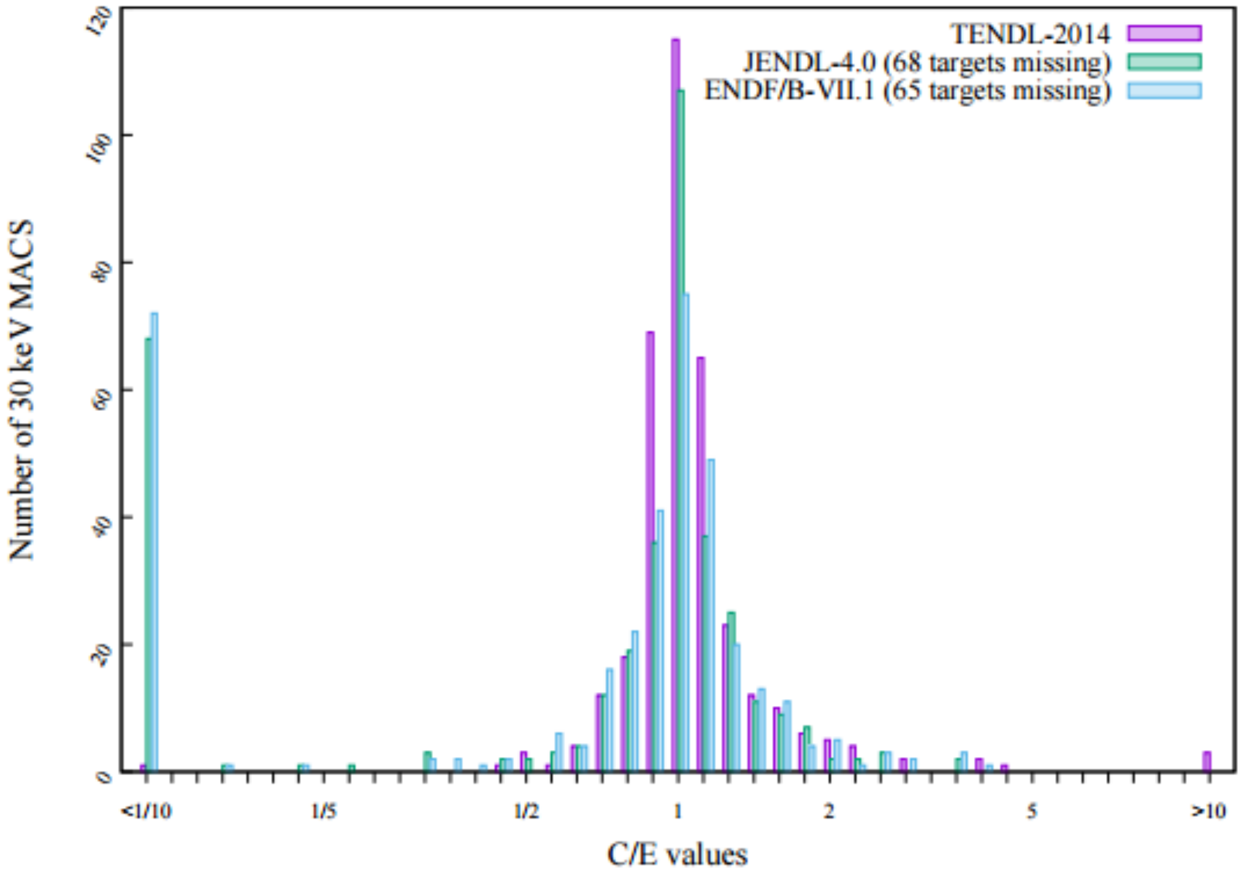


Bi209



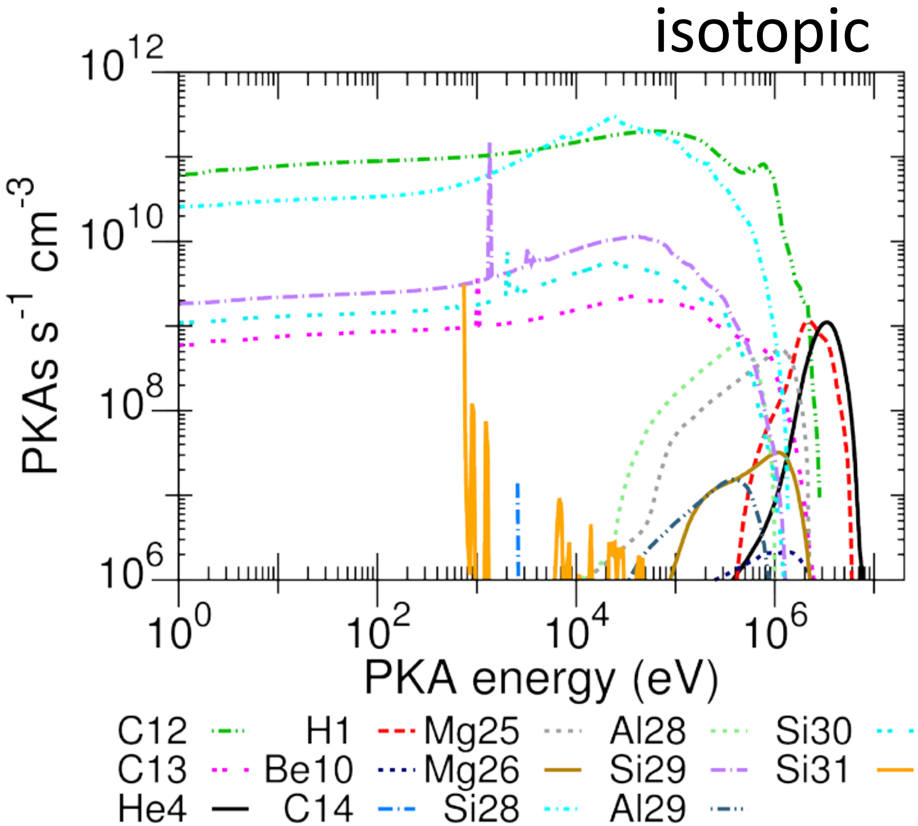
KADoNiS feedbacks (357)

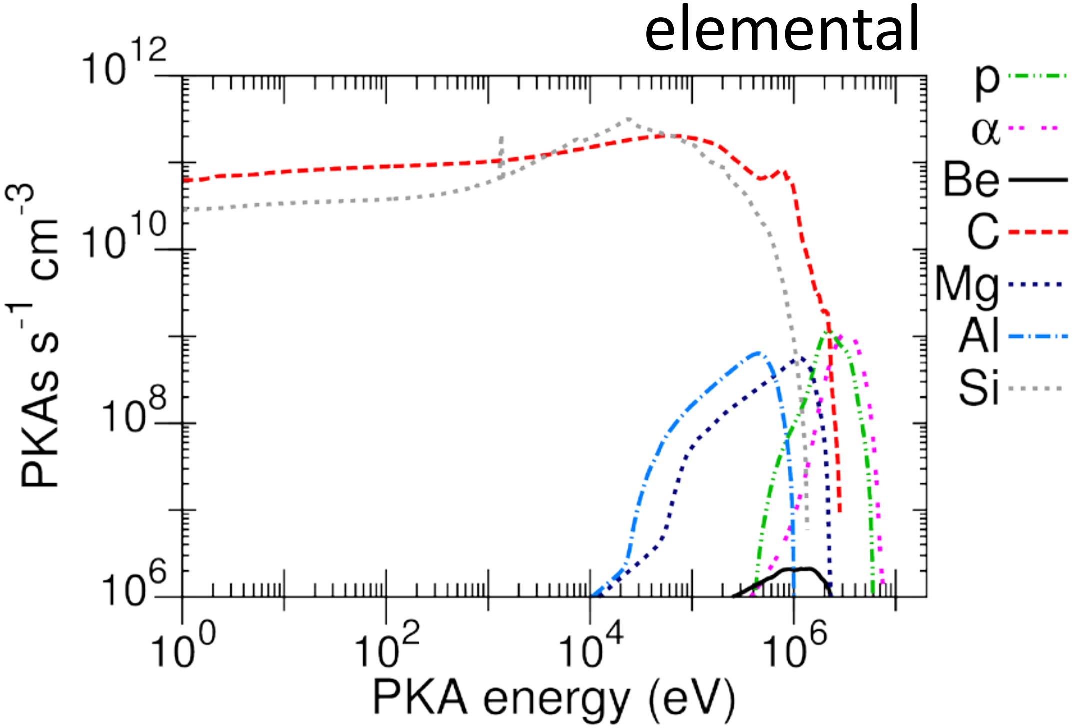
- About 20% of the channels are not in ENDF/B or JENDL or JEFF although TENDL of course includes all
- TENDL based on intelligent 'borrowing' of best resonance parameter descriptions + HFR so as good as legacy libraries



New Verification: n-prod matrices PKA spectra

- PKAs in SiC under PWR conditions:

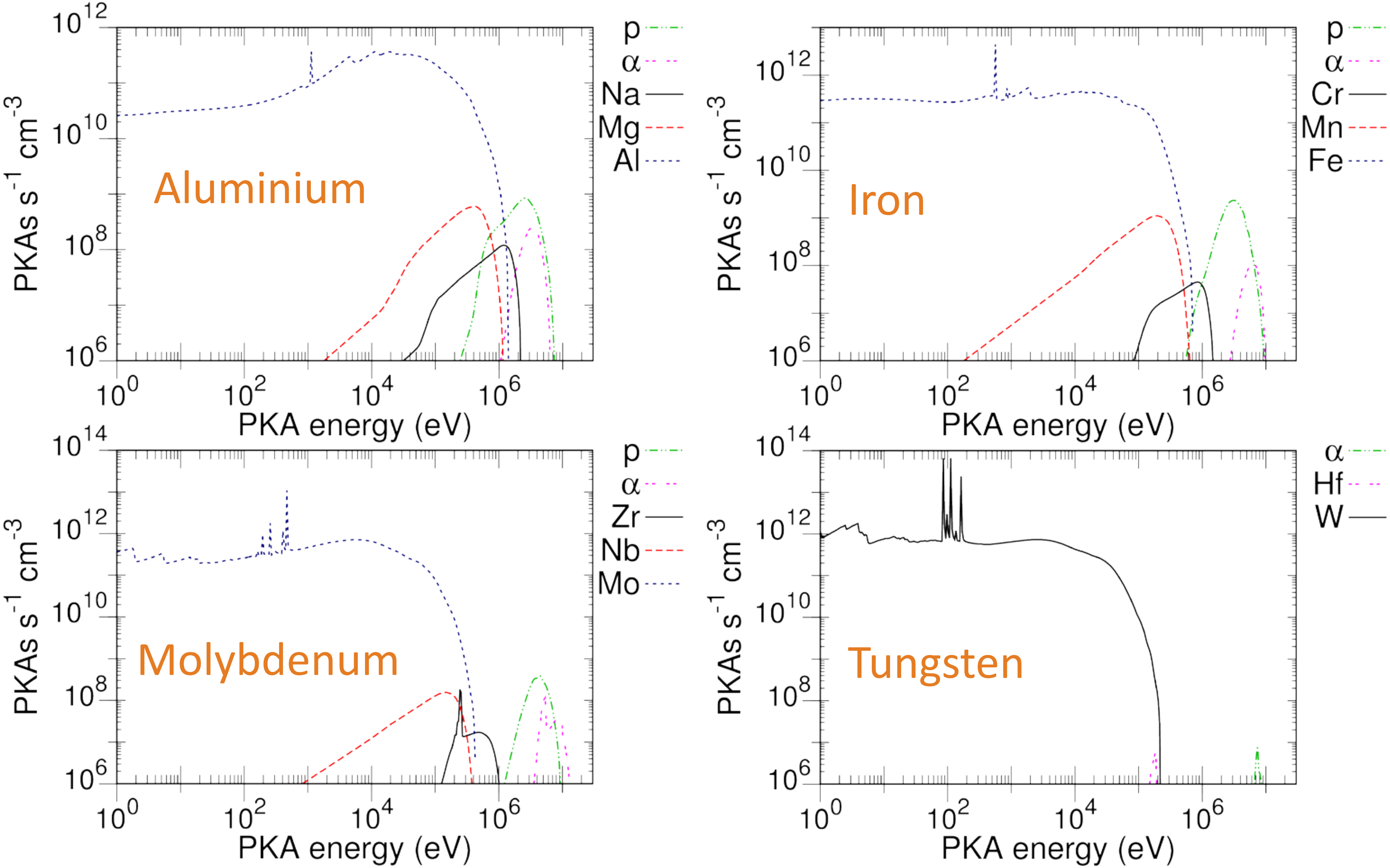




- Primary knock-on atom (PKA) evaluations using TENDL and SPECTRA-PKA*
- Necessary as input into materials modelling of radiation damage creation and evolution

Variation in primary damage with material

- PKAs in different elements under PWR conditions:



FISPACT-II web site

- http://fispact.ukaea.uk/

UK Atomic Energy Authority

FISPACT-II

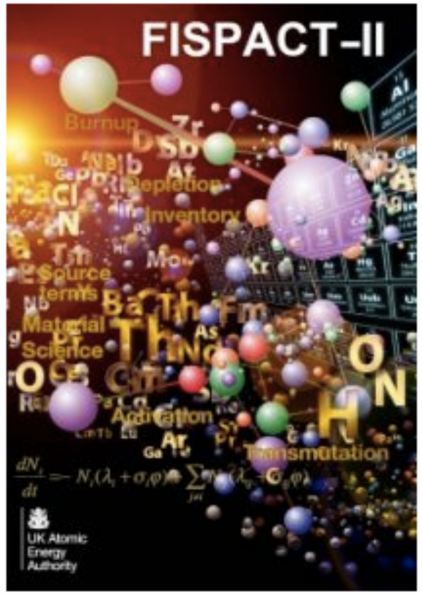
Overview | Methods » | Documentation » | Validation » | Nuclear data » | Links » | Contact | English »

Overview

FISPACT-II is an enhanced multiphysics, inventory and source-term code system providing a wide variety of advanced, predictive, spectral and temporal simulation methods employing the most up-to-date and complete nuclear data forms for both neutron and charged-particle interactions.

FISPACT-II has been developed and is maintained by the United Kingdom Atomic Energy Authority at Culham. As a comprehensive, modern object-oriented Fortran code, FISPACT-II fully processes all ENDF-6 nuclear data including the complete TENDL data with full covariances files. This extends the physics up to GeV energy with all channels and incident/emitted particles. Code features include self-shielding factors, broad temperature dependence, thin/thick target yields, robust pathway analysis, Monte-Carlo sensitivity and uncertainty quantification and propagation using full covariance data.

The latest generation of processing codes PREPRO, NJOY and CALENDF are used to provide the user with the most sophisticated incident-particle nuclear data from the TENDL-2015, ENDF/B.VII.1, JENDL-4.0, CENDL-3.1 and JEFF-3.2 international libraries, which are complemented with the latest decay and fission yield data, including the most recent GEFY-5.2 libraries. The maturity of modern, technological nuclear data including TENDL and GEF provides truly comprehensive data for all simulation requirements. The result is a multiphysics platform that can accommodate the needs of all nuclear applications including: activation, transmutation, depletion, burn-up, decays, source definition, full inventories, dpa, kerma, primary damage (PKA) spectra, gas/radionuclide production and more.



FISPACT-II web site

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FISPACT-II

Overview | Methods » | Documentation » | Validation » | Nuclear data » | Links » | Contact | English »

Documentation

The primary references for the FISPACT-II code are the user manual and the 2017 Nuclear Data Sheets paper:

The FISPACT-II User Manual UKAEA-R(11)11 Issue 8 December 2016

FISPACT-II: An Advanced Simulation System for Activation, Transmutation and Material Modelling *Nuclear Data Sheets* 139 (2017) 77-137

Other publications are divided into the following sections with their own sub-pages:

Reports

These include the official verification and validation reports for FISPACT-II and the nuclear data libraries it employs. Special attention is given to the general-purpose TENDL libraries. The materials handbooks for a variety of systems are included with their supplemental reports including PKA spectra and other materials simulation input data.

Articles

A wide range of articles related to and including FISPACT-II are listed, which range from *Nuclear Data Sheets* to *Fusion Engineering and Design* and *Nuclear Science and Engineering*. These include the various methods papers, studies produced using FISPACT-II and other research into nuclear observables, materials and nuclear data.

IAEA 60 Years
Atoms for Peace and Development

FISPACT-II web site

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FISPACT-II

Overview | Methods » | Documentation » | Validation » | Nuclear data » | Links » | Contact | English »

Reports

Verification and Validation Reports

Validation of FISPACT-II decay heat and inventory predictions for fission events CCFE-R(15)28

Probing experimental and systematic trends of the neutron-induced TENDL-2014 nuclear data library UKAEA-R(15)30

Maxwellian-averaged neutron-induced cross sections for kT=1 keV to 100 keV, KADoNiS, TENDL-2014, ENDF/B-VII.1 and JENDL-4.0u nuclear data libraries UKAEA-R(15)29

Integro-differential verification and validation, FISPACT-II & TENDL-2014 nuclear data libraries CCFE-R(15)27

Decay heat validation, FISPACT-II & TENDL-2014, JEFF-3.2, ENDF/B-VII.1 and JENDL-4.0 nuclear data libraries CCFE-R(15)25

Decay heat validation, FISPACT-II & TENDL-2013,-2012 and EAF-2010 nuclear data libraries CCFE-R(14)21

FISPACT-II web site

FISPACT-II material handbooks

Handbook of activation, transmutation and radiation damage properties of the elements and of ITER materials simulated using FISPACT-II & TENDL-2015; ITER FW armour focus CCFE-R(16)37

Handbook of activation, transmutation and radiation damage properties of the elements simulated using FISPACT-II & TENDL-2015; Magnetic Fusion Plants CCFE-R(16)36

Handbook of activation, transmutation and radiation damage properties of the elements simulated using FISPACT-II & TENDL-2014; Magnetic Fusion Plants CCFE-R(15)26

Handbook of activation, transmutation and radiation damage properties of the elements simulated using FISPACT-II & TENDL-2014; Nuclear Fission Plants **(PWR focus)** UKAEA-R(15)31

Handbook of activation, transmutation and radiation damage properties of the elements simulated using FISPACT-II & TENDL-2014; Nuclear Fission Plants **(HFR focus)** UKAEA-R(15)32

Handbook of activation, transmutation and radiation damage properties of the elements simulated using FISPACT-II & TENDL-2014; Nuclear Fission Plants **(FBR focus)** UKAEA-R(15)33

Supplements

Decay datacomparisons for decay heat and inventory simulations of fission events CCFE-R(15)28_S1

Fission yield comparisons for decay heat and inventory simulations of fission events CCFE-R(15)28_S2

PKA distributions of the elements simulated using TENDL-2015; Magnetic Fusion Plants CCFE-R(16)36-supplement

PKA distributions of the elements simulated using TENDL-2014; PWR Nuclear Fission plants UKAEA-R(15)31-supplement

PKA distributions of the elements simulated using TENDL-2014; HFR Nuclear Fission plants UKAEA-R(15)32-supplement

PKA distributions of the elements simulated using TENDL-2014; FBR Nuclear Fission plants UKAEA-R(15)33-supplement

FISPACT-II web site

ICTP Trieste Nuclear Data Workshop Oct 2-13 2017

The Joint ICTP-IAEA Workshop on the Evaluation of Nuclear Reaction Data for Applications will be held in Trieste, October 2-13 2017. There is no registration fee. The deadline for applications ...

Read More

5th July 2017 / Michael Fleming / Nuclear Data, Training, Workshops

Workshop on TALYS/TENDL developments, 13-15 November 2017, Prague

FISPACT-II 3-20 available through OECD-NEA Data Bank

FISPACT-II 3-20-00 code release

FISPACT-II 3-00-00 available through ORNL RSICC

UK Atomic Energy Authority

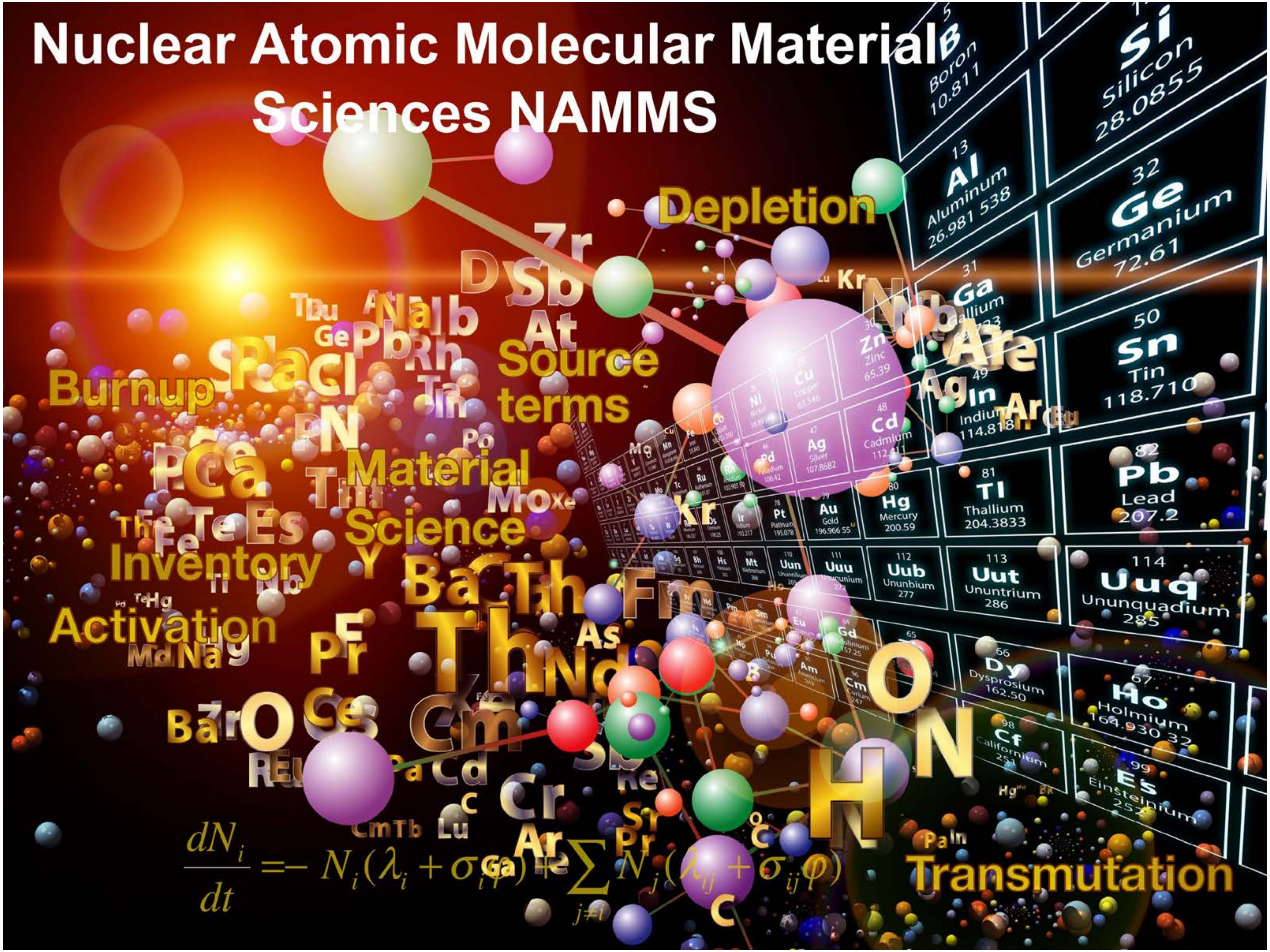
CCFE

Forum

PDF Adobe

Remarks and conclusions

- All FISPACT-II V&V suites will be deployed again on the forthcoming TENDL-2017, ENDF/B-VIII.0 and JEFF-3.3
- All integral relevant/pertinent information will also be embedded, systematically mirrored (when applicable) in the next generation of the T's codes
- Angular data, recoils, emitted particle spectra pose now the next challenges
- Multi-faceted, multi-scale validation processes are also needed


Nuclear Atomic Molecular Material Sciences NAMMS
Depletion
Source terms
Burnup
Material Science
Inventory
Activation
Transmutation
$\frac{dN_i}{dt} = -N_i(\lambda_i + \sigma_i\varphi) + \sum_{j \neq i} N_j(\lambda_{ij} + \sigma_{ij}\varphi)$