Decay data and modelling of beta decays

X. Mougeot, CEA-LNHB

NACRE Workshop 2024

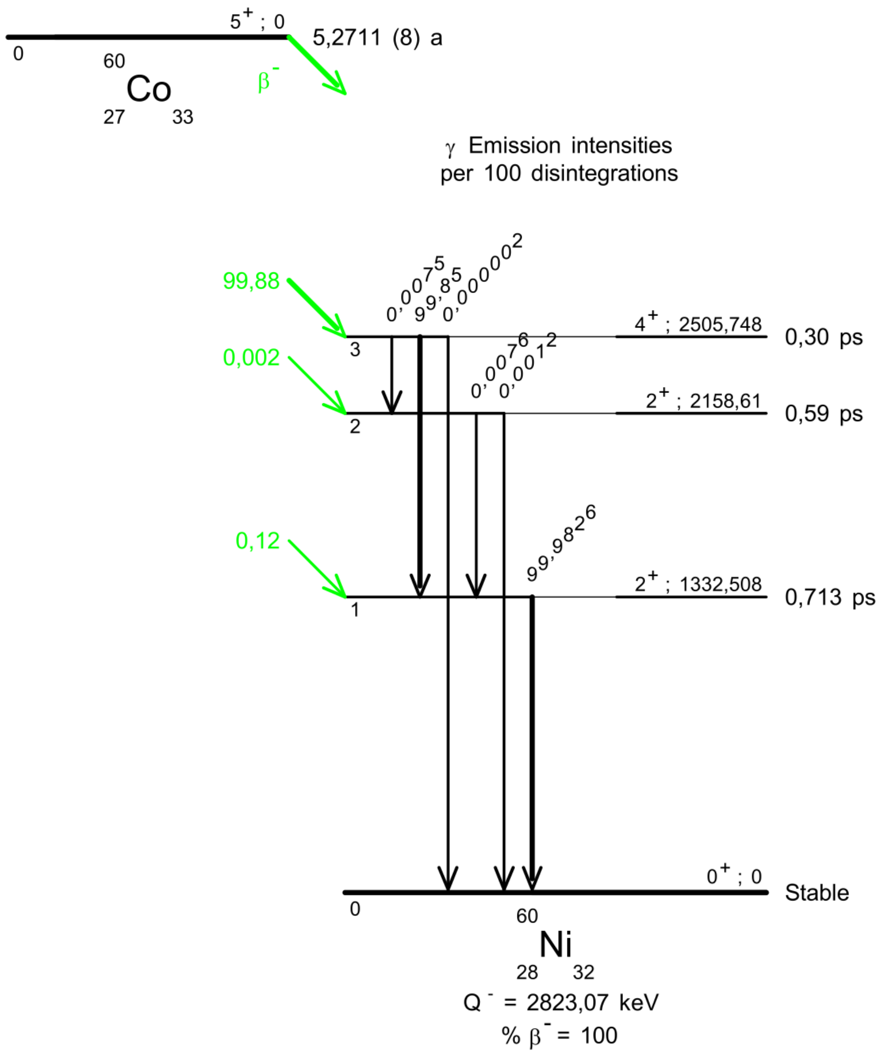
Decay data

DDEP

DDEP – Missions

- **Provide recommended decay data to non-specialists**
  - ✓ Metrology
  - ✓ Fundamental physics (detector calibration)
  - ✓ Nuclear medicine
  - ✓ Nuclear industry

- **Main information of interest**
  - ✓ Half-life, Q-value
  - ✓ Decay scheme
  - ✓ Intensity and energies
    - Alpha / beta / electron capture
    - Gamma and internal conversion
    - X-rays & Auger electrons



DDEP – Members

→ None of the members are full-time-equivalent, far from it.

- **DDEP Coordination**: Xavier Mougeot

- **LNHB Local team** (evaluation, review, edition, publication)
  - Sylvain Leblond
  - Xavier Mougeot
  - Mark A. Kellett (Special advisor)
  - Christophe Dulieu (IT support)

- **Decay data evaluators**
  - Alan L. Nichols* (Surrey University, UK)
  - Aurelian Luca (IFIN, Romania)
  - Brian E. Zimmerman (NIST, USA)
  - Rob Shearman (NPL, UK)
  - Xialong Huang (CIAE, China)
  - Nikolai Kuzmenko (KRI, Russia)

- **Additional support**
  - Tibor Kibédi* (BrIcc and BrIccMixing codes)
  - Balraj Singh*† (ENSDF collaboration)

* Retired.
† Deceased.

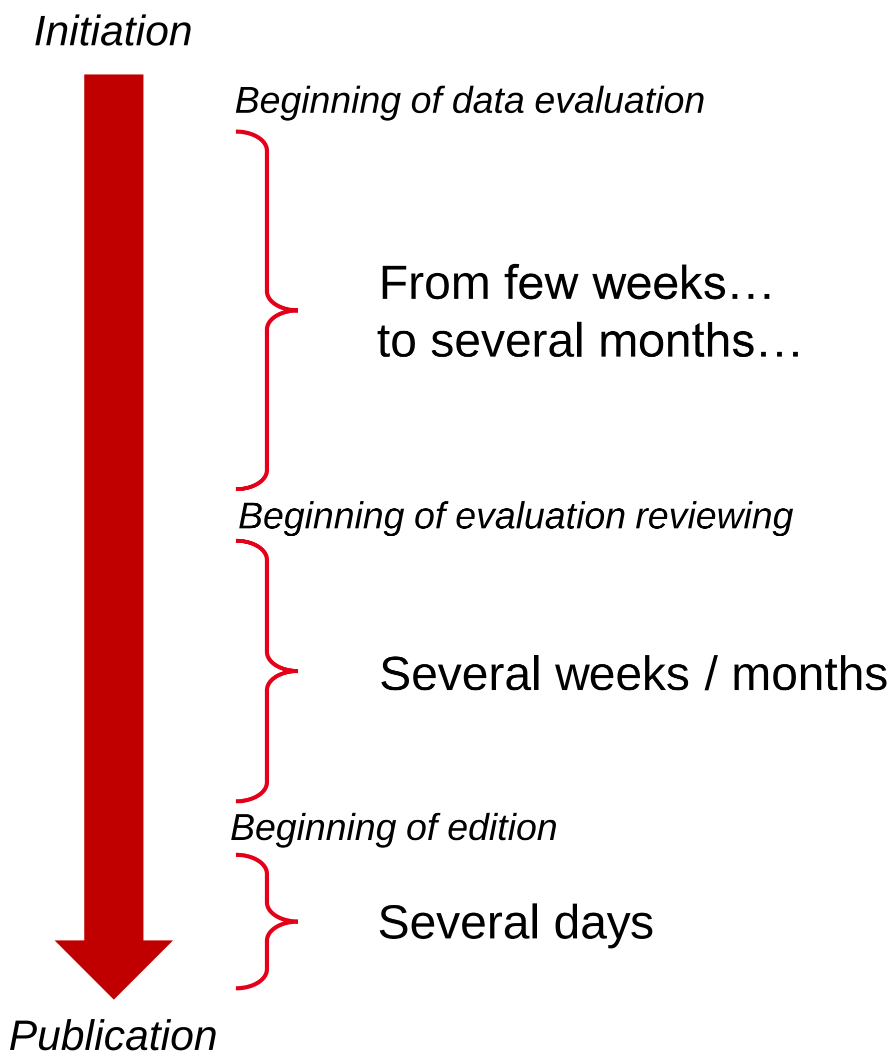
DDEP – Evaluation pipeline

1. Initiation of an evaluation
   - Need from a project / collaboration
   - Following a user request
   - Evaluator initiative

2. Data evaluation
   - Performed independently by 1 or 2 evaluators
   - Using DDEP guidelines and tools

3. Reviewing process
   - One DDEP reviewer is assigned
   - Complete verification of the evaluation
   - Discussion with evaluator until agreement

4. Edition and publication



DDEP – Various collaborations

- IAEA Coordinated Research Projects (CRP)
  - 2019: *Nuclear Data for Charged-particle Monitor Reactions and Medical Isotope Production*
  - 2013: *Library of Recommended Actinide Decay Data*
  - 2007: *Update of X Ray and Gamma Ray Decay Data Standards for Detector Calibration and Other Applications*
- Evaluations for Comprehensive Nuclear-Test-Ban Treaty Organisation (Mónica Galán, 2017 – 2019: Xe and I isotopes)
- Joint Evaluated Fission and Fusion file (JEFF) European library
- European Research Projects (EMPIR Euramet)
- CEA INSNU project (Reactor dosimetry and safety)

→ Funded projects always have the highest priority.

JEFF-3.3

The Joint Evaluated Fission and Fusion File (JEFF) is an evaluated library produced via an international collaboration of NEA Data Bank participating countries.

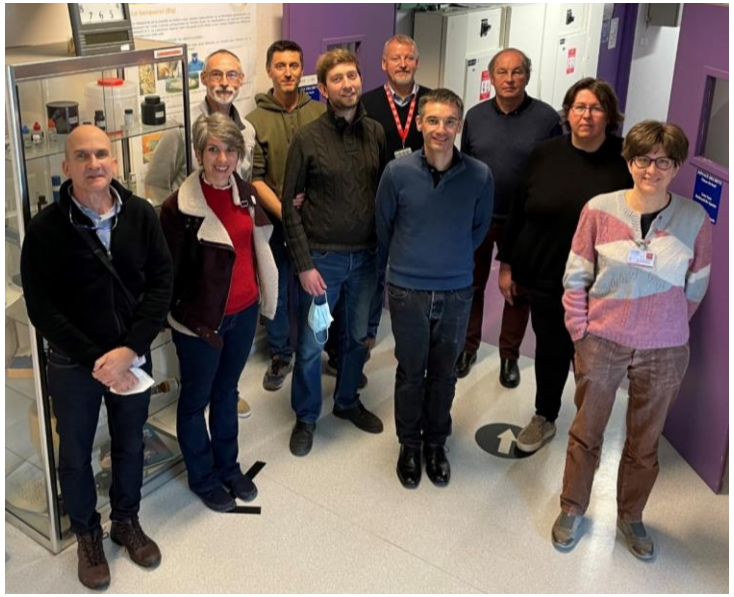
DDEP – Attempts to increase the workforce

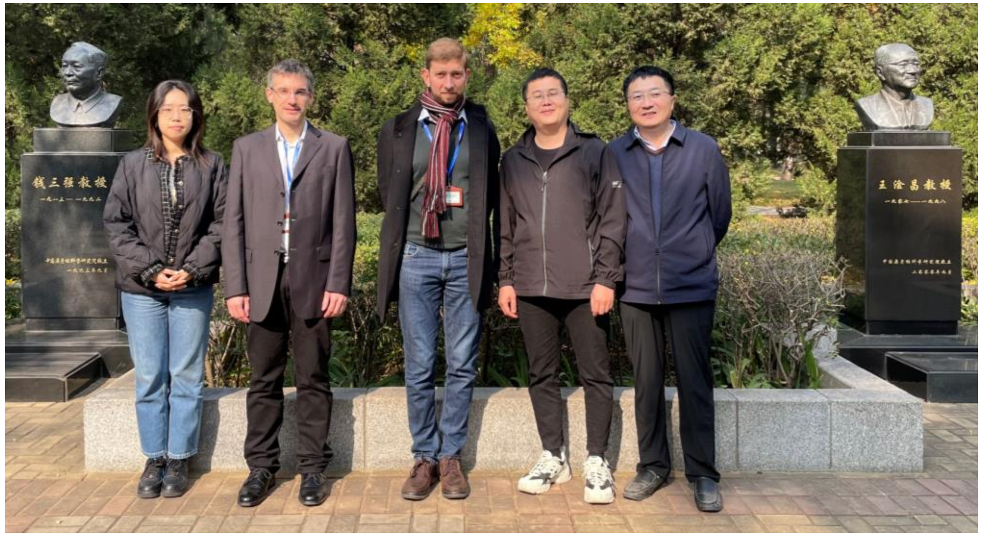
DDEP workforce remains limited. Actions engaged:

- 7th to 9th of March 2022: Organisation of a DDEP workshop dedicated to evaluator training.
- 21st to 28th of October 2023: Visit of China Nuclear Data Centre (Beijing, China).
- We plan to organize a training workshop around October 2024, inviting our colleagues from China.

→ Efforts which require additional work and time, taken on availability dedicated to DDEP.

→ Ratio investment / benefit must be considered.





DDEP – Evaluations

- ✓ Since JEFF 3.3 release, 11 DDEP evaluations published (2021-2023).
- ➢ By June 2024, 2 to 4 more are expected.

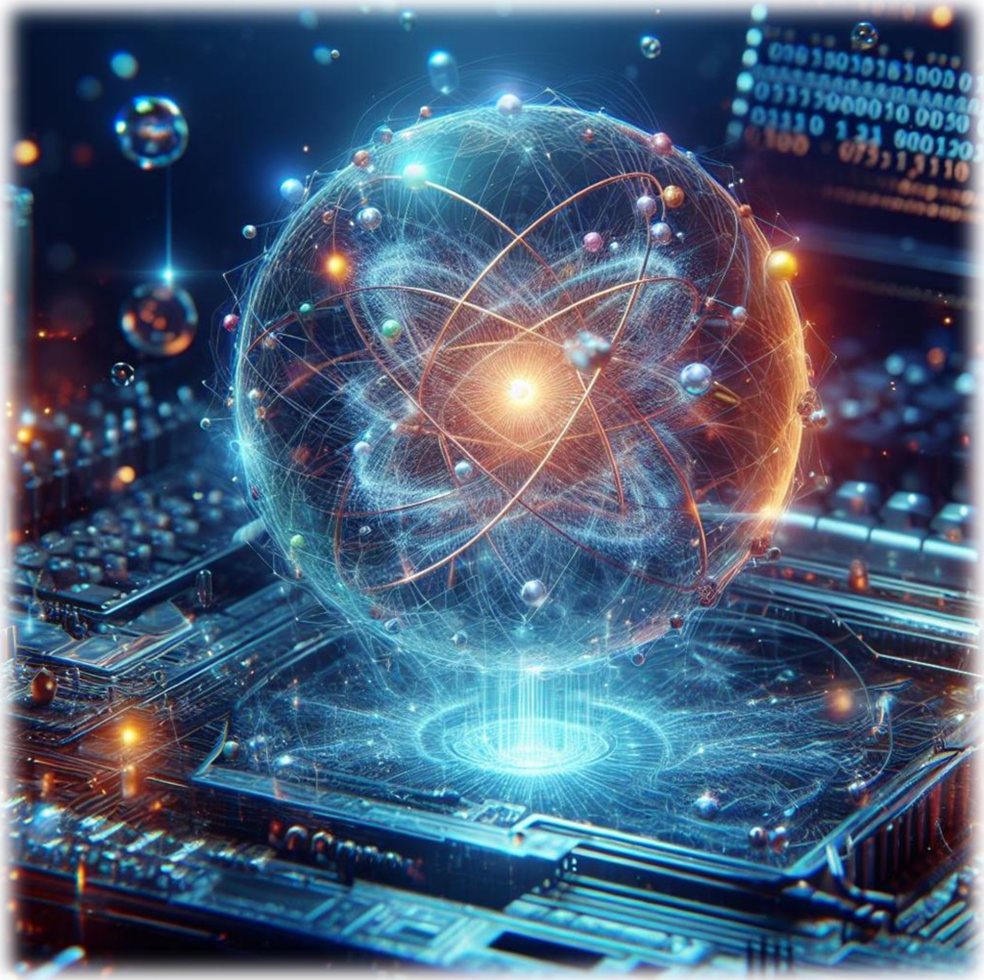
For JEFF 4:

- ➢ These evaluations can be included.
- ➢ We can benefit from the recent review of TAGS measurements and assessment of future needs.

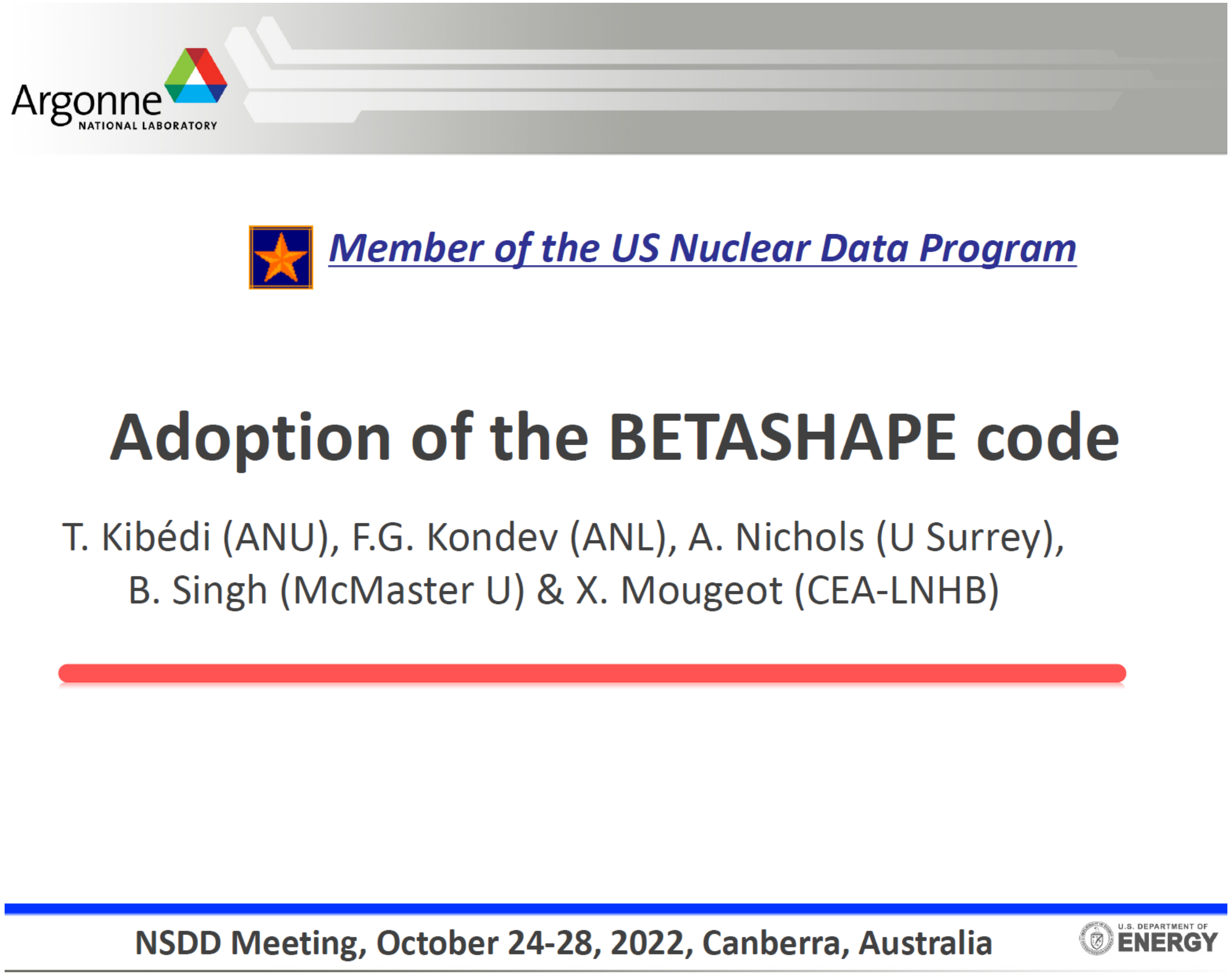
  A.L. Nichols et al., Eur. Phys. J. A (2023) 59:78
- ➢ We can also benefit from the recent review of log-ft values (see later).

Nuclide		Z	Vol. (?)	UpDate
Ac-225	^{225}Ac	89	9	20/12/2023
Cs-137	^{137}Cs	55	9	07/09/2023
Ba-137m	^{137m}Ba	56	9	07/09/2023
Sm-151	^{151}Sm	62	9	07/09/2023
He-6	^{6}He	2	9	10/11/2022
Al-26	^{26}Al	13	9	10/11/2022
Rb-87	^{87}Rb	37	9	24/05/2022
Cs-131	^{131}Cs	55	9	21/09/2021
I-124	^{124}I	53	9	20/07/2021
Mn-52	^{52}Mn	25	9	09/02/2021
Mn-52m	^{52m}Mn	25	9	09/02/2021

Modelling of beta decays



Adoption by the NSDD network



- ✓ The DDEP community has already adopted BetaShape for many years for the calculation of beta and electron capture decay properties.
- ➢ The forthcoming version 2.3 of BetaShape was adopted by the NSDD network in October 2022.
- ➢ Specific requests have been formulated since then to match ENSDF policies and improved the reliability of the results.
- ✓ Version 2.3 (September 2023), followed by version 2.3.1 (December 2023), have been released with all requests implemented.
- ✓ A manual is also provided.

Developments for version 2.3

Technical

- ✓ Rounding limit can be changed via a simple option.
- ✓ Provision of *f*-values and average energy of emitted neutrinos (B and EC).
- ✓ Handling of branching ratios (BR and NB from N and PN records) and propagation of their uncertainties.
- ✓ Modification of forbiddenness assignment when J^{π} are ambiguous.
- ✓ Negative Q-values are now accepted: decay of isomeric state with stable ground state.

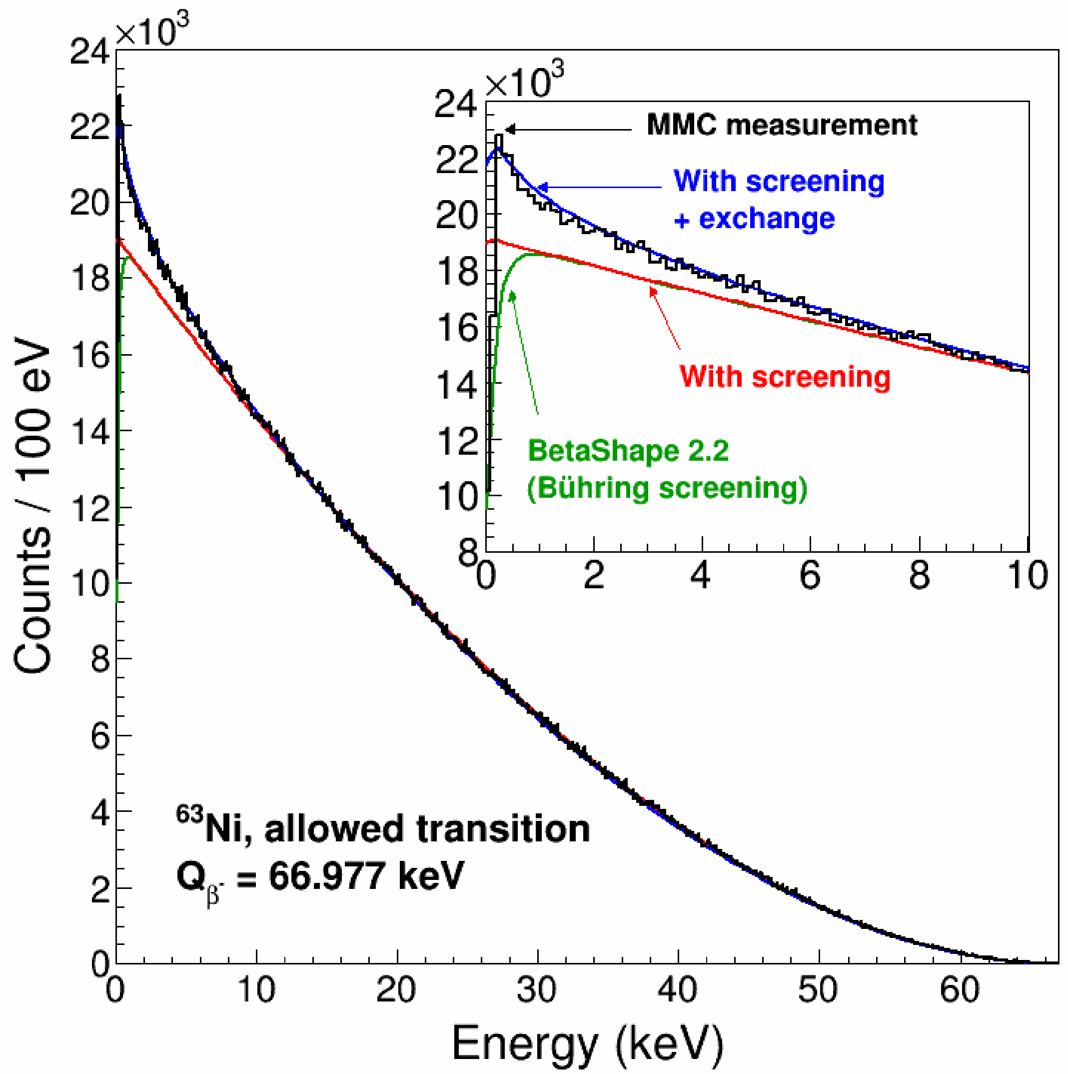
Physical model

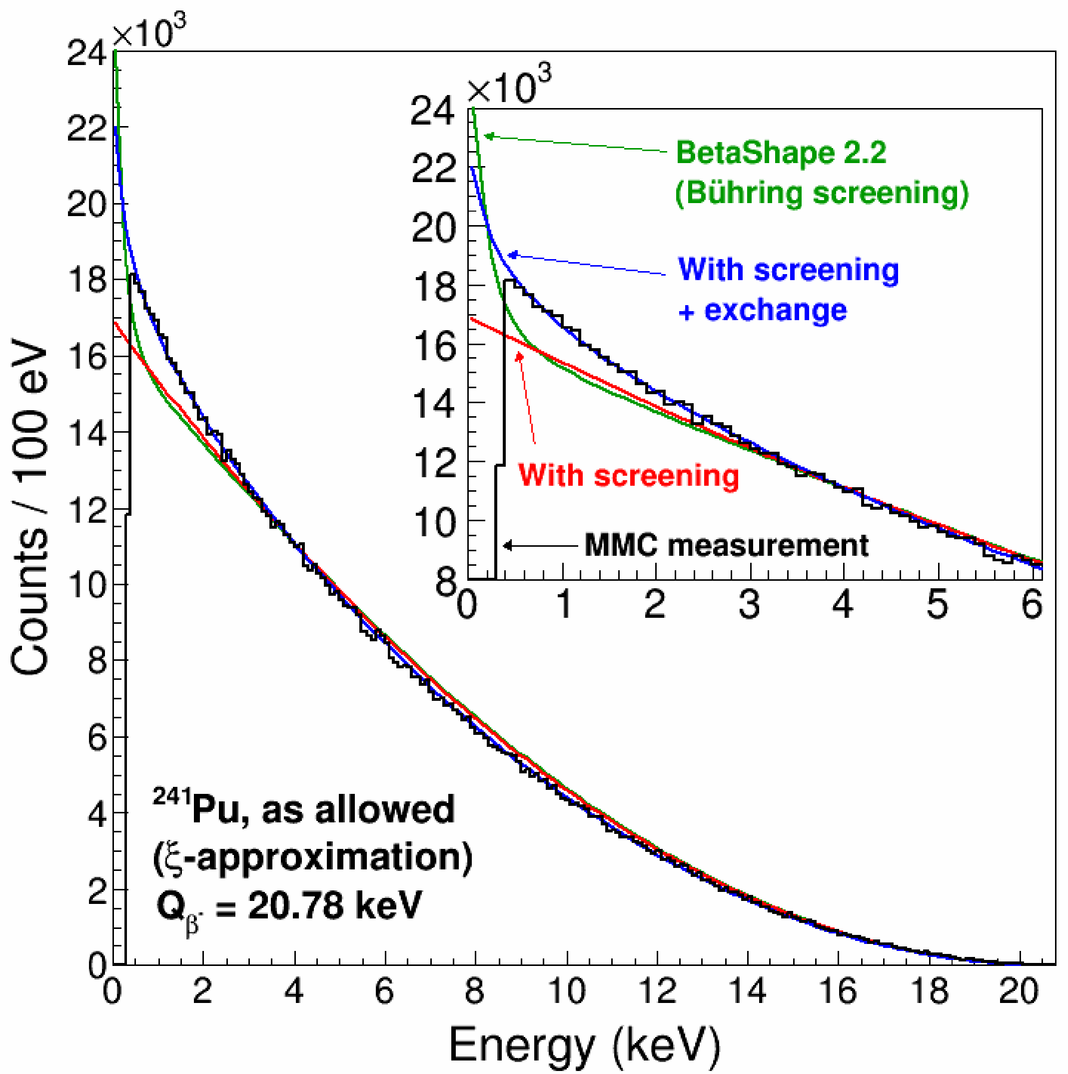
- ✓ Tabulation of atomic screening and exchange effects from full numerical calculations.
- ✓ Inclusion of the atomic overlap correction in beta decays. Negligible influence except close to the end-point energy, which can appear lower by hundreds of eV.

Uncertainties

- ✓ Treatment of non-numeric uncertainties (AP, SY, GT, etc.). Up to version 2.2, treated as null.
- ✓ Treatment of asymmetric uncertainties. Important for large uncertainties on intensities and transition energies.

Tabulation of atomic screening and exchange effects

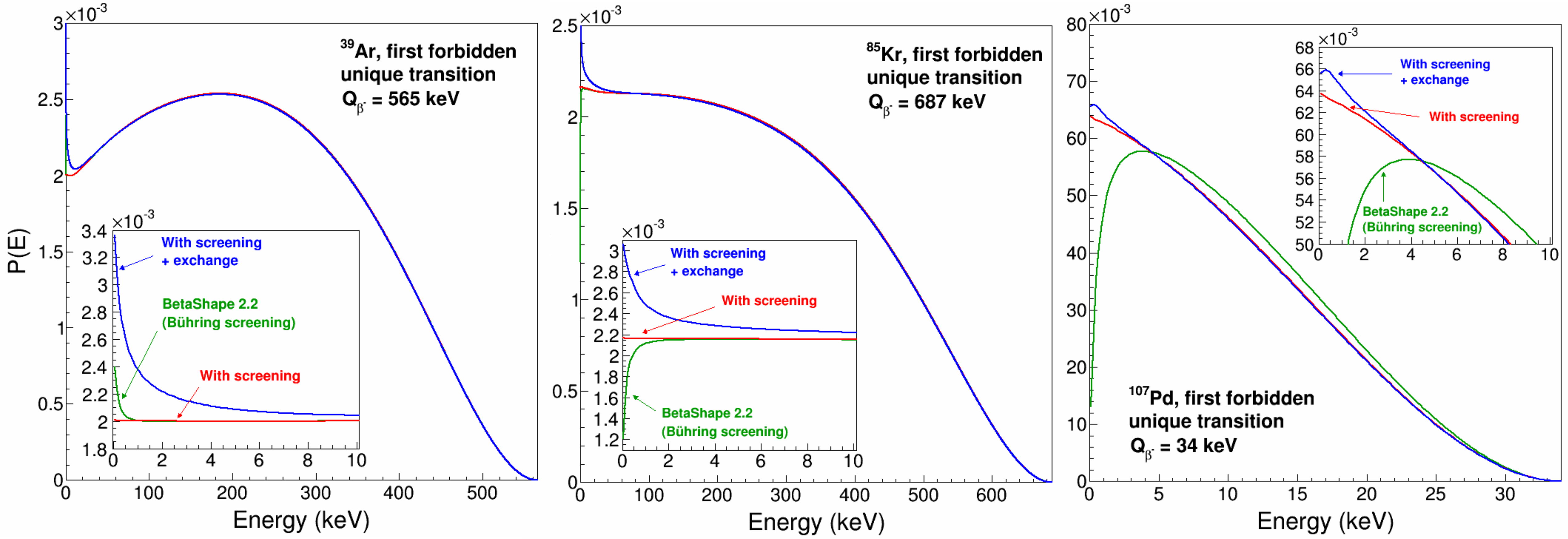




Extension of atomic exchange effect to forbidden unique transitions

→ **Contribution of additional atomic orbitals**

✓ *X. Mougeot, Appl. Radiat. Isot. 201, 111018 (2023)*



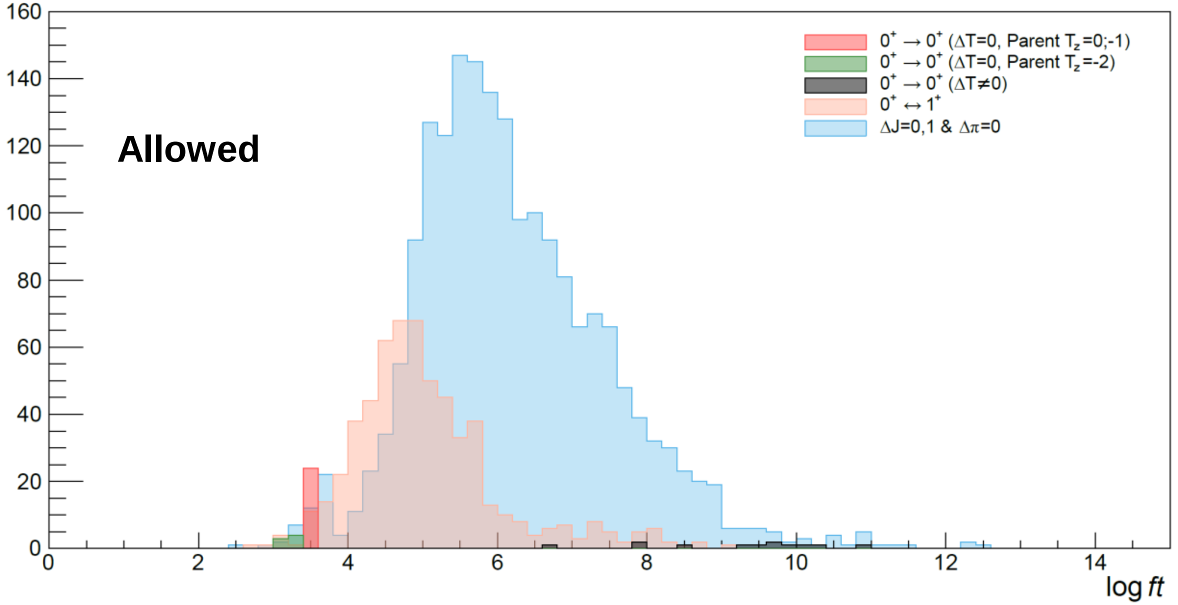
New review of log-*ft* values

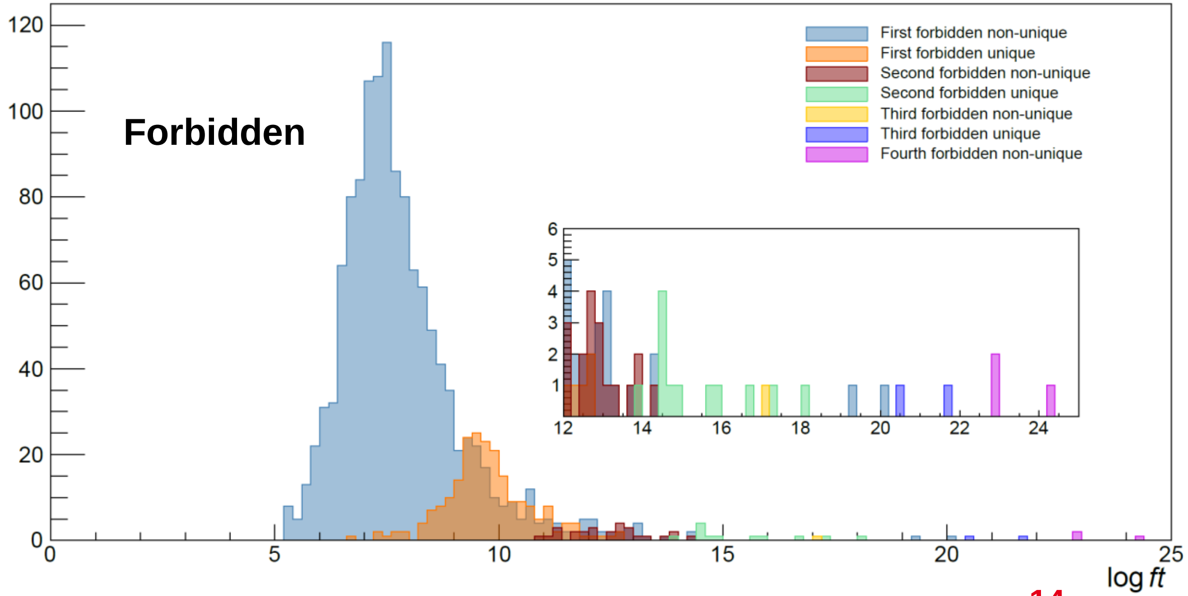
Former review of log-*ft* values, calculated with the LogFT code: *B. Singh et al., Nuclear Data Sheets 84, 487 (1998)*

These values are used in nuclear structure studies, e.g. to assign spin and parity to a level.

Collaborative work: B. Singh (McMaster University), S. Turkat and K. Zuber (TU Dresden), X. Mougeot (CEA-LNHB)

- ✓ Update of Β and EC decays present in ENSDF database (as of mid-April 2023).
- ✓ Use of BetaShape to calculate the log-*ft* values (including new developments since version 2.2).
- ✓ In total, 26 318 transitions calculated. Selection of well-defined transitions. Possible pandemonium nuclei flagged.
- ✓ 4 038 transitions survived this filtering. All distributions re-established. Specific transitions are discussed.
- ✓ *S. Turkat et al., Atomic Data and Nuclear Data Tables 152, 101584 (2023)*





Where to get BetaShape 2.3

LNHB website

http://www.lnhb.fr/rd-activities/spectrum-processing-software/

Presentation · Services · R&D activities · Nuclear data

Software and tools developed by the LNHB

BETASHAPE – BETA SPECTRA COMPUTING

The BetaShape program has been developed to improve nuclear data related to beta emission and electron capture properties. Use of the code, with options, and improvements over the previous versions are briefly described in the README.txt file.

Beta Transitions
Mean energies, log (ft) values, beta and neutrino spectra for single and multiple transitions are provided. A database of experimental shape factors is included and has been updated. The uncertainties provided by the input parameters are taken into account and propagated.

Electron captures
Capture probabilities and capture-to-beta-plus ratios are provided for each atomic subshell. The log(ft) value of each transition is calculated. For a given branch, the splitting between capture and beta plus transitions is also determined.

The spectra and capture probabilities pre-calculated with BetaShape are available on the atomic and nuclear data page, in the column 'ASCII files', by clicking on the 'B' button for the desired nuclide.

REFERENCES:
– X. Mougeot, Applied Radiation and Isotopes 201 (2023) 111018
DOI : https://doi.org/10.1016/j.apradiso.2023.111018
– X. Mougeot, Applied Radiation and Isotopes 154 (2019) 108884
DOI: https://doi.org/10.1016/j.apradiso.2019.108884

Download BetaShape – Stable version: 2.3 (9/30/2023):

BetaShape – V2.3 – Windows 10 (Zip file, 24.9 MB)
BetaShape – V2.3 – Scientific Linux 6.4 (Zip file, 11.1 MB)
BetaShape – V2.3 – Linux Ubuntu 20.04 (Zip file, 22.7 MB)
BetaShape – V2.3 – Linux CentOS 8 (Zip file, 21.6 MB)
BetaShape – V2.3 – macOS Monterey (M1) (Zip file, 7.57 MB)
BetaShape – V2.3 – macOS Monterey (Intel) (Zip file, 7.65 MB)
BetaShape – ReadMe (Txt file)
BetaShape – Manual (Pdf file)
Warning: For Linux/macOS users, please read first the README file about the environment variable PATH.

IAEA GitHub Repository

https://github.com/IAEA-NSDDNetwork

IAEA-NSDDNetwork / BetaShape Public

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main · 1 branch · 0 tags · Go to file · Code

xavier-mougeot Update README.md · 630c305 2 weeks ago · 46 commits

packages	Add files via upload	2 weeks ago
BetaShape_Manual.pdf	Add files via upload	2 weeks ago
LICENSE	Initial commit	2 weeks ago
README.md	Update README.md	2 weeks ago

About

Calculation of beta and electron capture decays

www.lnhb.fr/rd-activities/spectrum-proc...

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Releases
No releases published

Packages
No packages published

README.md

BetaShape

The BetaShape program calculates **beta and electron capture decays**, and provides for each transition:

- Energy spectra of the emitted β and ν particles.
- Capture probabilities and capture-to-positron ratios for all subshells.
- Average β and ν energies.
- log-*ft* values.
- In case of multiple branches, total decay spectra are also generated for each type of particles.

All results are provided as formatted text files, including updated ENSDF files and CSV files.

BetaShape is part of the ENSDF Analysis and Utility Programs. It is also made available on LNHB website as part of the Utility Programs of the Decay Data Evaluation Project (DDEP). Any question can be addressed to Xavier Mougeot: xavier.mougeot@cea.fr

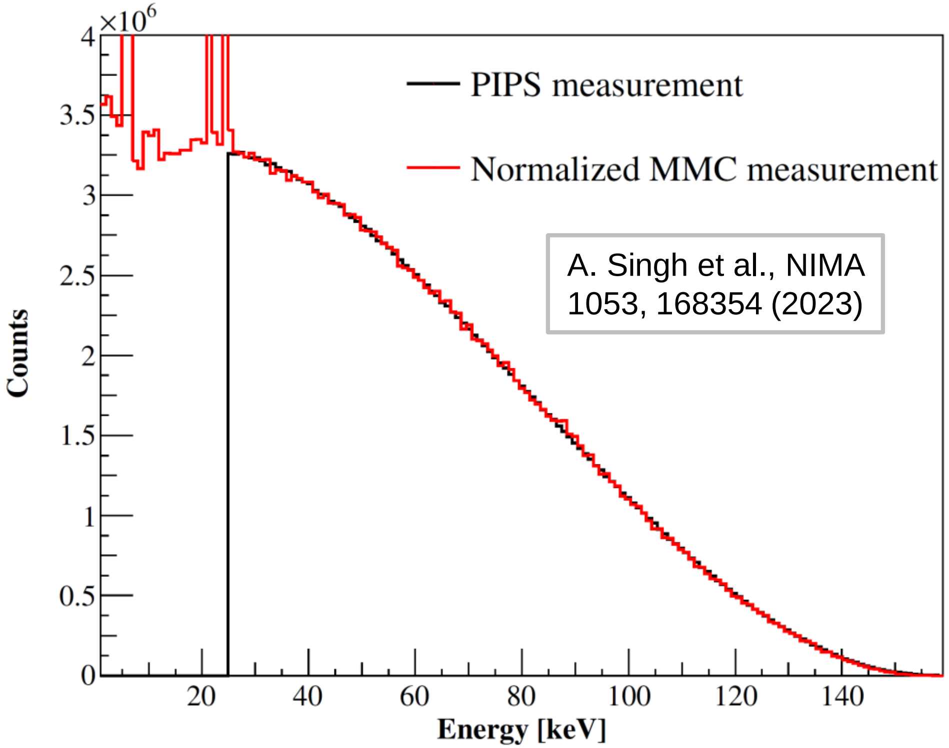
Downloads

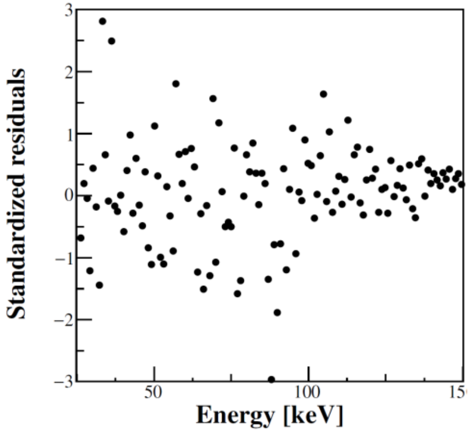
The **packages** directory contains the executables for Windows (10), macOS (Monterey M1 and Intel) and Linux (CentOS 8, Ubuntu 20.04.2 LTS, Scientific Linux 6.4).

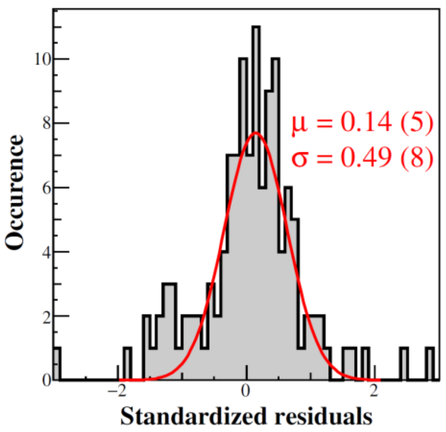
Quick start

The program takes as input a formatted ENSDF file, for example Ni63.txt for ^{63}Ni decay. With default options

^{14}C decay



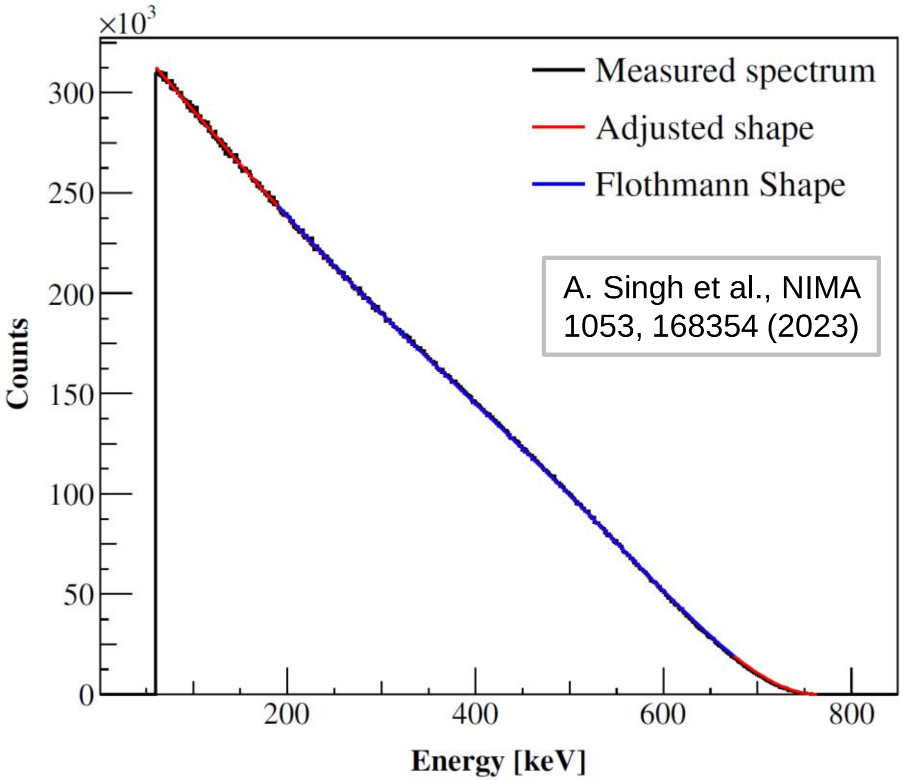


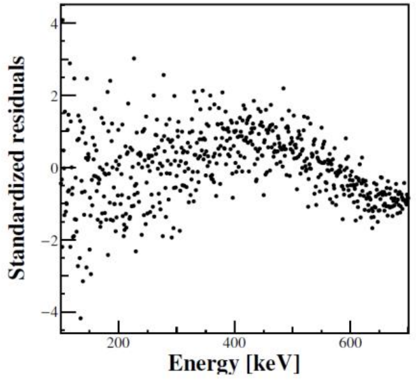


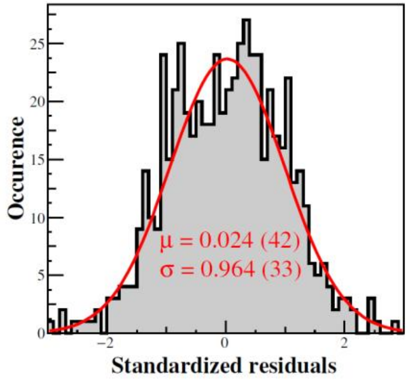
- ➢ Distortion remains in the measured spectrum: particle escape, dead layers, source.
  - → Unfolding process based on precise mono-energetic Monte Carlo simulations.
- ➢ Comparison with a high-precision measurement with a Metallic Magnetic Calorimeter (MMC) is possible.
- ✓ Excellent agreement of the spectra in the common energy range.
- ✓ Extracted Q-value = 156.49 (49) keV fully consistent with AME2020 value of 156.476 (4) keV.
- ✓ Controversy on the spectrum shape: weak magnetism term confirmed.

Study	a in MeV^{-1}	Comment
[44]	−0.386	CVC from exp. not certain
[45]	−0.37 (4)	SM, ×2 difference with CVC
[36]	−0.43	SM, consistent with CVC
[41]	−0.45 (4)	^{14}C-doped Ge detector
[8]	−1.038 (28)	Wall-less prop. counter
This work	−0.430 (37)	Si detector, with $F_0 L_0$

^{204}Tl decay







- ➢ Distortion remains in the measured spectrum: particle escape, dead layers, source.
  - → Unfolding process based on precise mono-energetic Monte Carlo simulations.
- ➢ Comparison with the reference spectrum in the literature from Flothmann et al., Z. Phys. A 225, 164 (1969).
- ✓ Excellent agreement of the spectra in the common energy range.

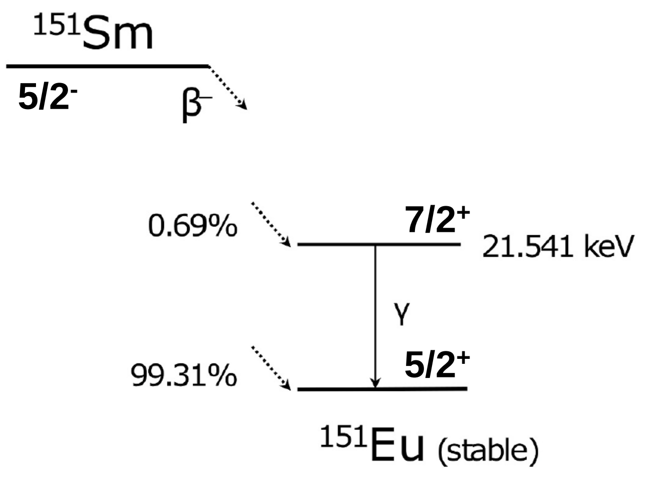
$$C(W) = dq^2 + \lambda_2 p^2$$

The shape parameter is identical if Fermi functions are too: Flothmann et al. d = 1.097 (8) vs d = 1.095 (13) here.

- ✓ Extracted Q-value = 763.7 (22) keV fully consistent with AME2020 value of 763.75 (18) keV.
- ✓ Extended knowledge of the spectrum from 60 keV to endpoint energy.

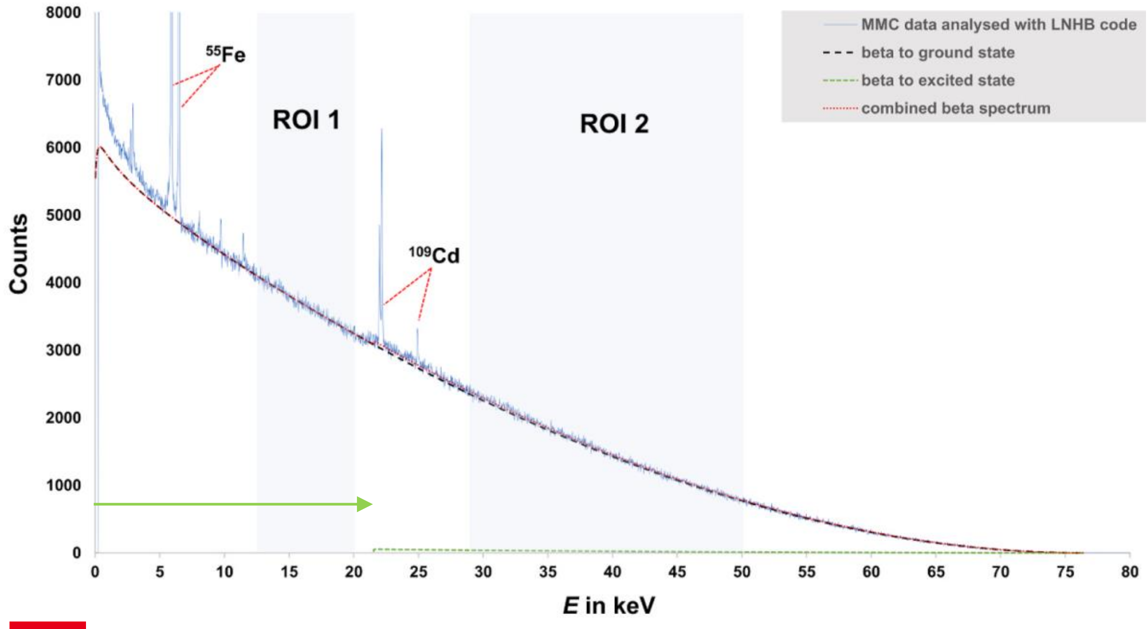
With numerical Fermi function, d = 1.075 (13).

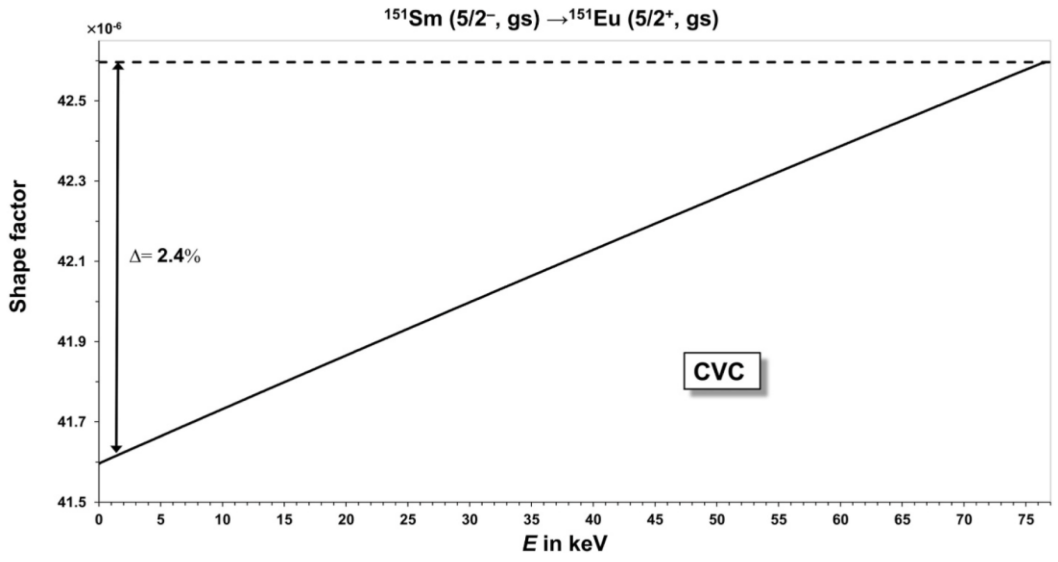
^{151}Sm decay



First forbidden non-unique transitions

- ✓ High-precision measurement of ^{151}Sm spectrum with Metallic Magnetic Calorimeters (MMC) at LNHB.
- ✓ **New Q-value = 76.430 (68) keV** more precise than AME2020 value of 76.5 (5) keV.
- ✓ New determination of branching ratios: 99.31 (11)% and 0.69 (11)%.
- ✓ Kossert et al., Appl. Radiat. Isot. 185, 110237 (2022)

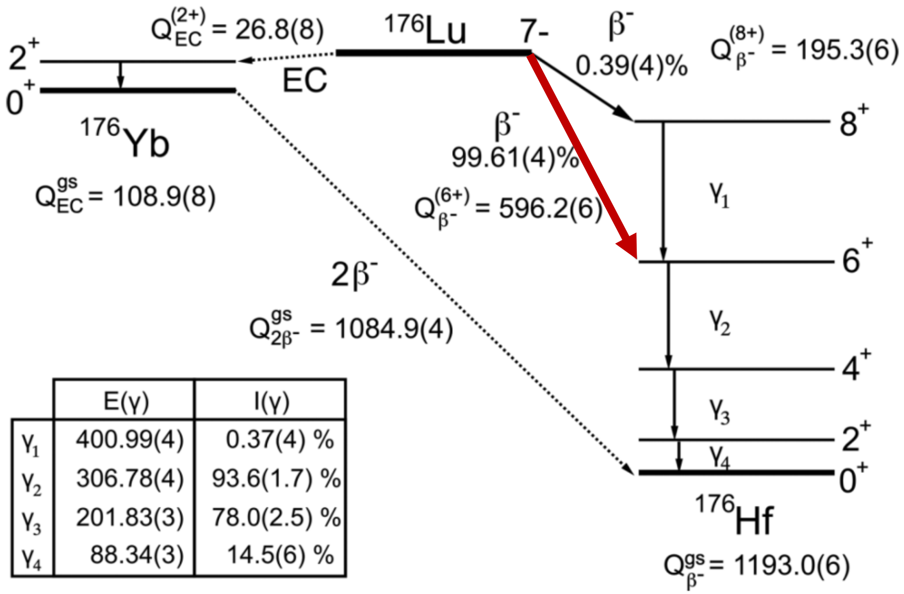




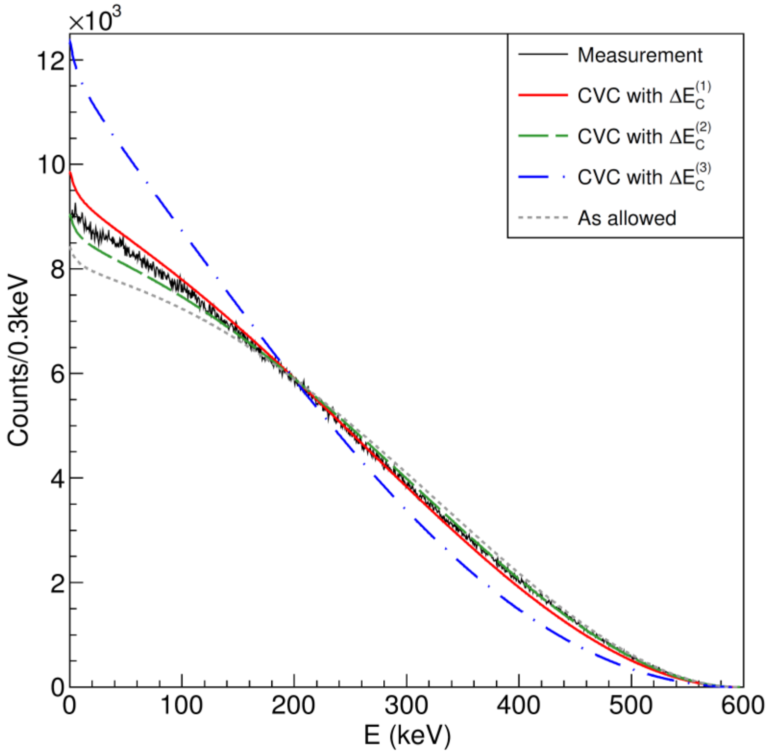
Detailed calculations with nuclear structure

→ Testing the accuracy of the ξ-approximation

^{176}Lu decay



	E(γ)	I(γ)
γ_1	400.99(4)	0.37(4) %
γ_2	306.78(4)	93.6(1.7) %
γ_3	201.83(3)	78.0(2.5) %
γ_4	88.34(3)	14.5(6) %

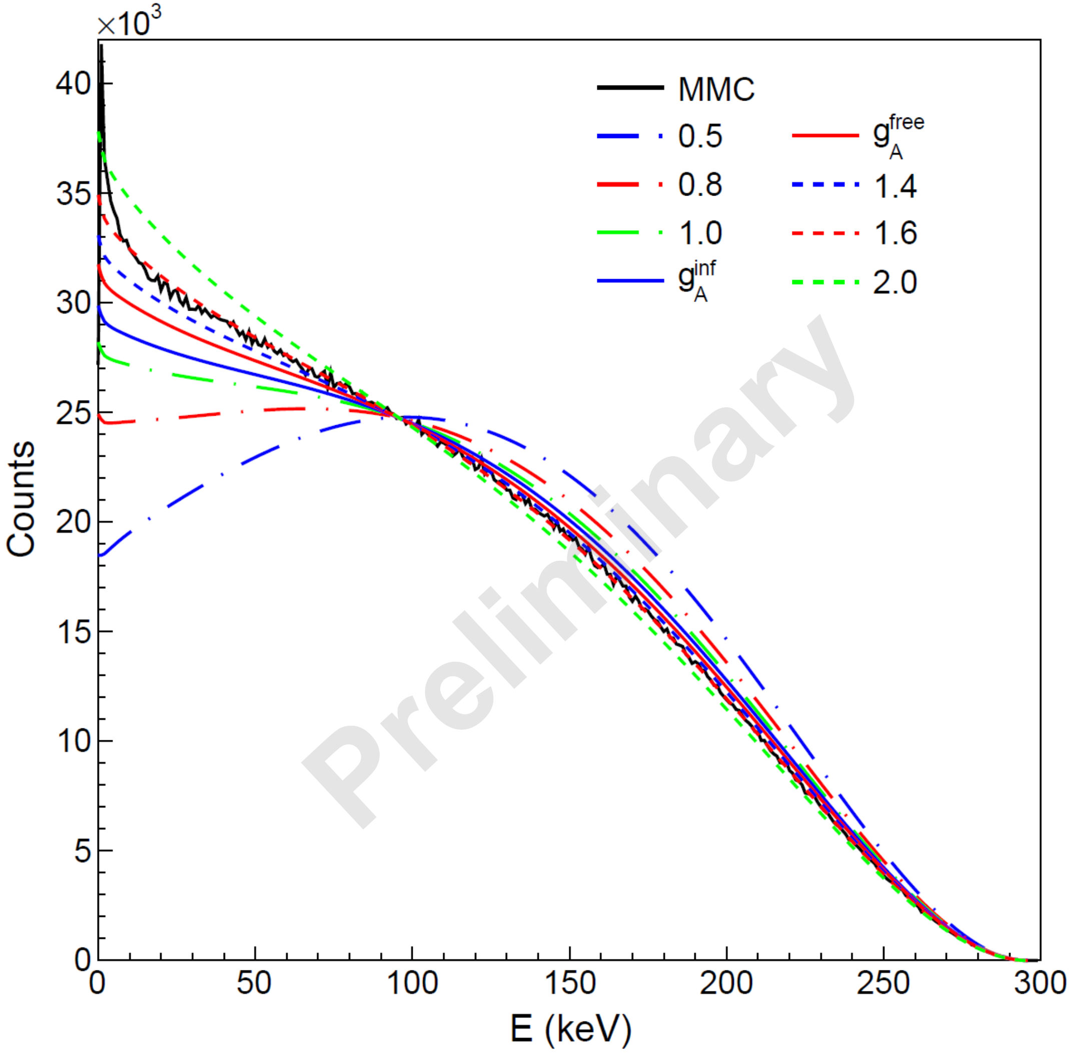


First forbidden non-unique transition

- ✓ First high-precision spectrum measurement from self-scintillation of a LuAG:Pr crystal at TU Delft.
- ✓ New Q-values: Q_β = 1193.0 (6) keV and Q_ε = 108.9 (8) keV. From AME2020: Q_β = 1194.1 (9) keV and Q_ε = 109.0 (12) keV.
- ✓ Spectrum shape retrieved adjusting the Coulomb displacement energy ΔE_C or the axial-vector coupling constant g_A.
- × Calculated half-life shorter by 13 orders of magnitude!

  → **Detailed analysis would require accurate modelling with nuclear deformation: hindered transition ($\Delta K = 7$).**
- ✓ F.G.A. Quarati et al., Phys. Rev. C 107, 024313 (2023).

^{99}Tc decay

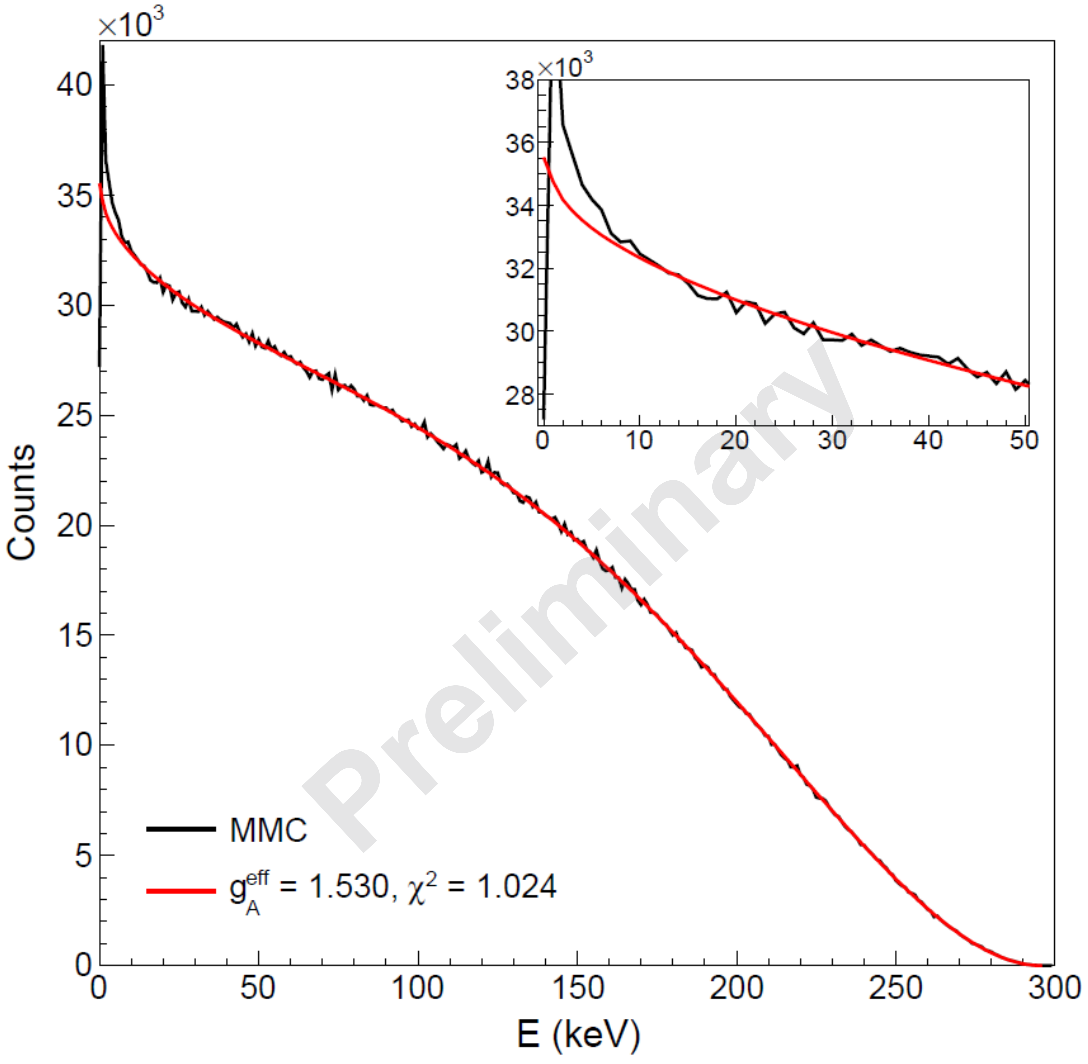


The value of g_A can be affected by several nuclear effects due to the necessary assumptions in nuclear models to deal with the many-body problem.

- ✓ High-precision measurements of ^{99}Tc spectrum with MMC at CEA-LNHB and PTB, and with Silicon detectors at CEA-LNHB.
- ✓ Excellent agreement of all the three spectra.
- ✓ **New Q-value = 295.82 (16) keV** not consistent with AME2020 value of 297.5 (9) keV.
- ✓ ^{99}Tc beta spectrum, second forbidden non-unique, has been predicted to be very sensitive to g_A. Free-nucleon value [PDG 2020] g_A^{free} = 1.2754 (13).

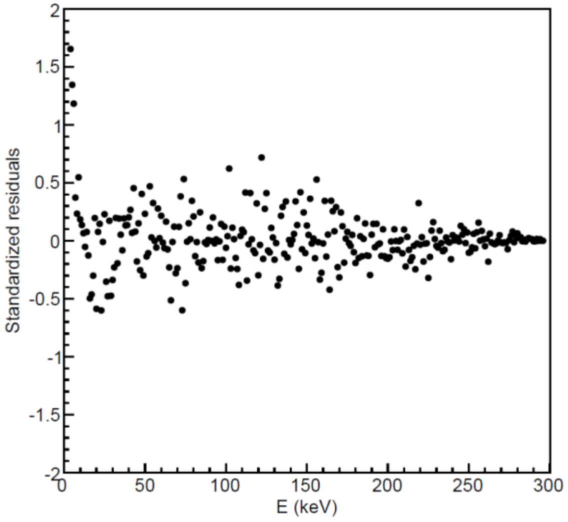
  → **Confirmed.**

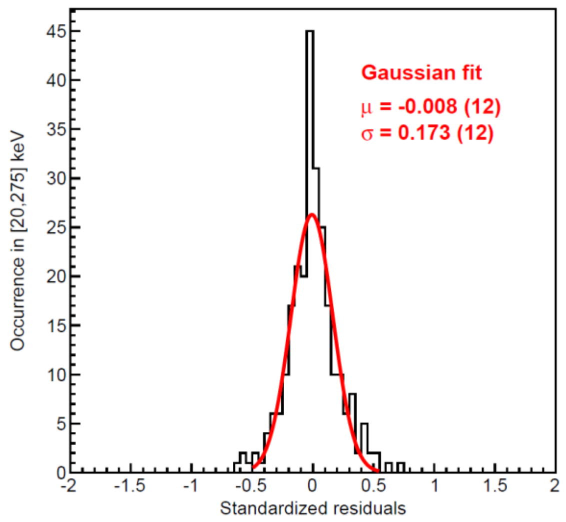
^{99}Tc decay



The value of g_A can be affected by several nuclear effects due to the necessary assumptions in nuclear models to deal with the many-body problem.

- ✓ Theoretical calculations with nuclear structure, CVC and complete lepton current.
- ✓ Best adjustment gives an effective axial-vector coupling constant g_A^{eff} = 1.53 (8).
- ✓ Excellent residuals, without any trend down to 6 keV.





^{99}Tc decay

Eur. Phys. J. Plus (2022) 137:665
https://doi.org/10.1140/epjp/s13360-022-02865-7

THE EUROPEAN PHYSICAL JOURNAL PLUS

Regular Article

Check for updates

Nuclear data evaluation for decay heat analysis of spent nuclear fuel over 1–100 k year timescale

Hannah R. Doran[1,2,a], **Alan J. Cresswell**[2], **David C. W. Sanderson**[2], **Gioia Falcone**[1]

[1] James Watt School of Engineering, University of Glasgow, Glasgow G12 8QQ, UK
[2] Scottish Universities Environmental Research Centre, East Kilbride G75 0QF, UK

Table 3 Mean beta energies from different evaluated libraries (keV)

Nuclide	Evaluated library					
	JEF2.2	JEFF3.1.1	JEFF3.3	ENDF/B-VIII.0	ENSDF	DDEP
99Tc	**85.0**	**85.4 ± 0.6**	**95.3 ± 0.4**	**55.2 ± 0.3**	**84.6 ± 0.5**	**94.6 ± 1.7**

→ E_{mean} = 98.45 (20) keV

JEFF 4

JEFF 4 release is an arduous constraint

- Update of decay data in JEFF database can only be limited.
- TAGS measurements can only be accounted for as done for JEFF 3.3.
- Unfortunately, expertise of Olivier Bersillon (CEA-DAM) has been lost. Significant effort is required to take it over, at least sufficiently to ensure data of good quality.
- Coupling BetaShape with sdf2ndf (Olivier Bersillon's code for generating JEFF decay data library) is necessary. Sdf2ndf is a fortran code based on Radlist of more than 35 000 lines.

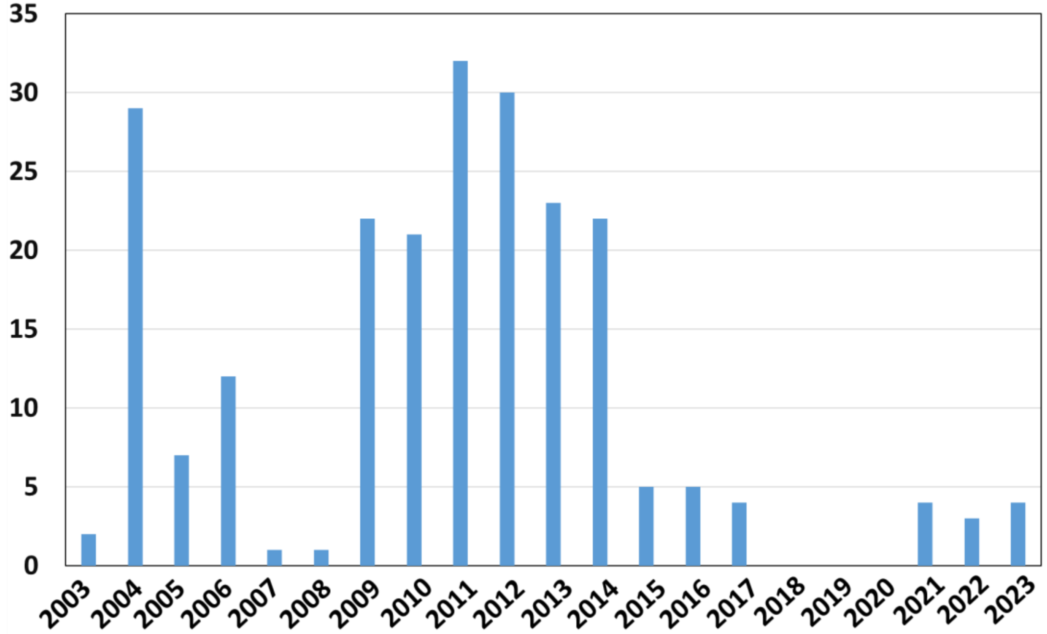
As of today, focus on beta minus transitions

- (Anti)neutrino particles allowed in ENDF format end of 2012, but sdf2ndf version is from 2010!
- Updates in sdf2ndf: names of elements up to 118; mass excesses from AME2020 (3558 nuclei), before from AME2003 (3179 nuclei); physical constant values from NIST.
- Specific implementation in BetaShape to generate a formatted file to be read by sdf2ndf.
- Specific function implemented in sdf2ndf to run automatically BetaShape from sdf2ndf.
- Average energies and spectra for beta and neutrino particles are then retrieved.
- Propagation of information has been revised because not adapted anymore. A few bugs fixed.

Conclusion

Conclusion

DDEP evaluations are back on track… But manpower still remains limited.



Lot of work to somehow maintain the situation

- Pending evaluations need to be finalized.
- New DDEP evaluators (and evaluations) needed.
- Updates of existing DDEP evaluations needed.
- Software and database need a complete refoundation.

In nuclear decay data evaluations, the BetaShape code now replaces the longstanding used LogFT code.

- More precise mean energies, capture probabilities and log-ft values.
- Additional useful information: energy spectra, subshell capture probability, etc.
- Living code: modelling and output continuously improved.
- Coupling with sdf2nfd for the production of JEFF Decay Library ongoing.

Thanks for welcoming us in Strasbourg!