

DDEP and BetaShape Status

X. Mougeot, CEA-LNHB (France)

USNDP meeting 2024





DDEP Status

DDEP – Missions

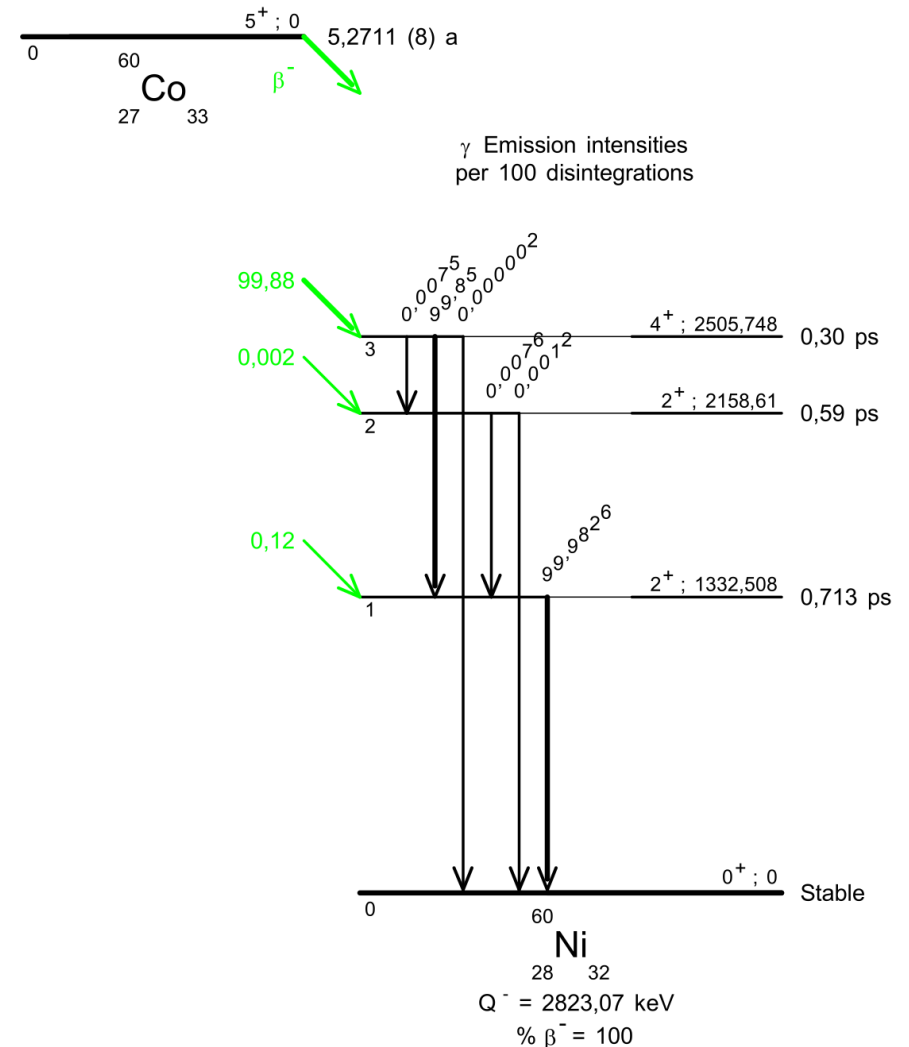
➤ Provide recommended decay data to non-specialists

- ✓ Metrology
- ✓ Fundamental physics (detector calibration)
- ✓ Nuclear medicine
- ✓ Nuclear industry

➤ Main information of interest

- ✓ Half-life, Q-value
- ✓ Decay scheme
- ✓ Intensity and energies (transitions, emissions)
 - Alpha / beta / electron capture
 - Gamma and internal conversion
 - X-rays & Auger electrons

Symmetric uncertainties only



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* (Brlcc and BrlccMixing codes)
- Balraj Singh*† (ENSDF collaboration)



* Retired.

† Deceased.

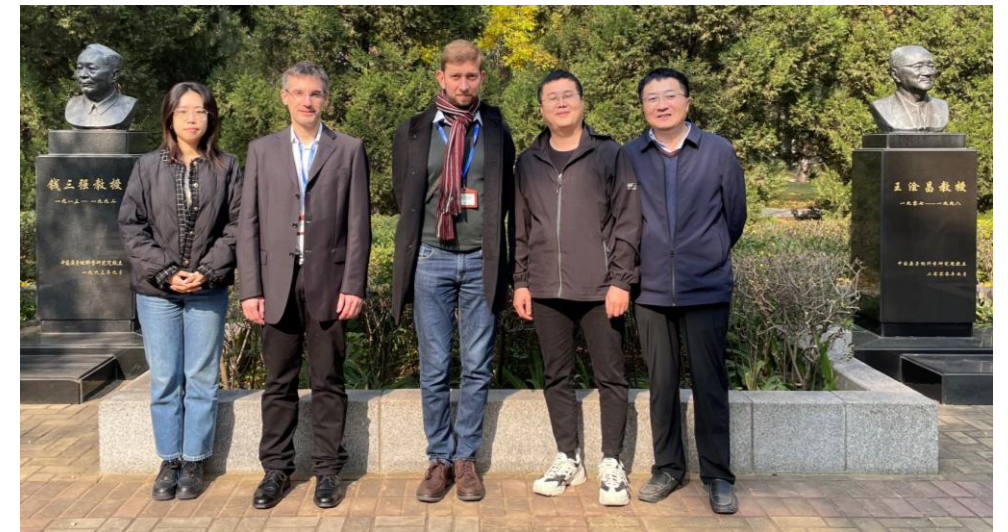
DDEP – Attempts to increase the workforce

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).
- 7th to 11th of October 2024: Visit of China Nuclear Data Centre (Beijing, China).
- 21st to 25th of October 2024: Organisation of a DDEP workshop dedicated to evaluator training.

8 participants from the US, China and Europe + local (LNHB) participants.

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



DDEP – Evaluations



- ✓ Since 2021 (change of coordination), 17 evaluations published.
- ✓ Since latest BIPM vol. 8 monography (2016), 21 evaluations published.
- By end of 2024, ^{45}Ti and ^{56}Co are also expected.

| Nuclide | Z | Vol. (?) | UpDate | |
|---------|---------------------------|----------|--------|------------|
| Co-55 | ^{55}Co | 27 | 9 | 04/09/2024 |
| Rh-103m | $^{103\text{m}}\text{Rh}$ | 45 | 9 | 29/08/2024 |
| Pd-103 | ^{103}Pd | 46 | 9 | 29/08/2024 |
| Ho-166 | ^{166}Ho | 67 | 9 | 24/06/2024 |
| Fe-55 | ^{55}Fe | 26 | 9 | 19/03/2024 |
| Sn-129m | $^{129\text{m}}\text{Sn}$ | 50 | 9 | 13/03/2024 |
| Ac-225 | ^{225}Ac | 89 | 9 | 20/12/2023 |
| Cs-137 | ^{137}Cs | 55 | 9 | 07/09/2023 |

| Nuclide | Z | Vol. (?) | UpDate | |
|---------|---------------------------|----------|--------|------------|
| Ba-137m | $^{137\text{m}}\text{Ba}$ | 56 | 9 | 07/09/2023 |
| Sm-151 | ^{151}Sm | 62 | 9 | 07/09/2023 |
| He-6 | ^6He | 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 | $^{52\text{m}}\text{Mn}$ | 25 | 9 | 09/02/2021 |

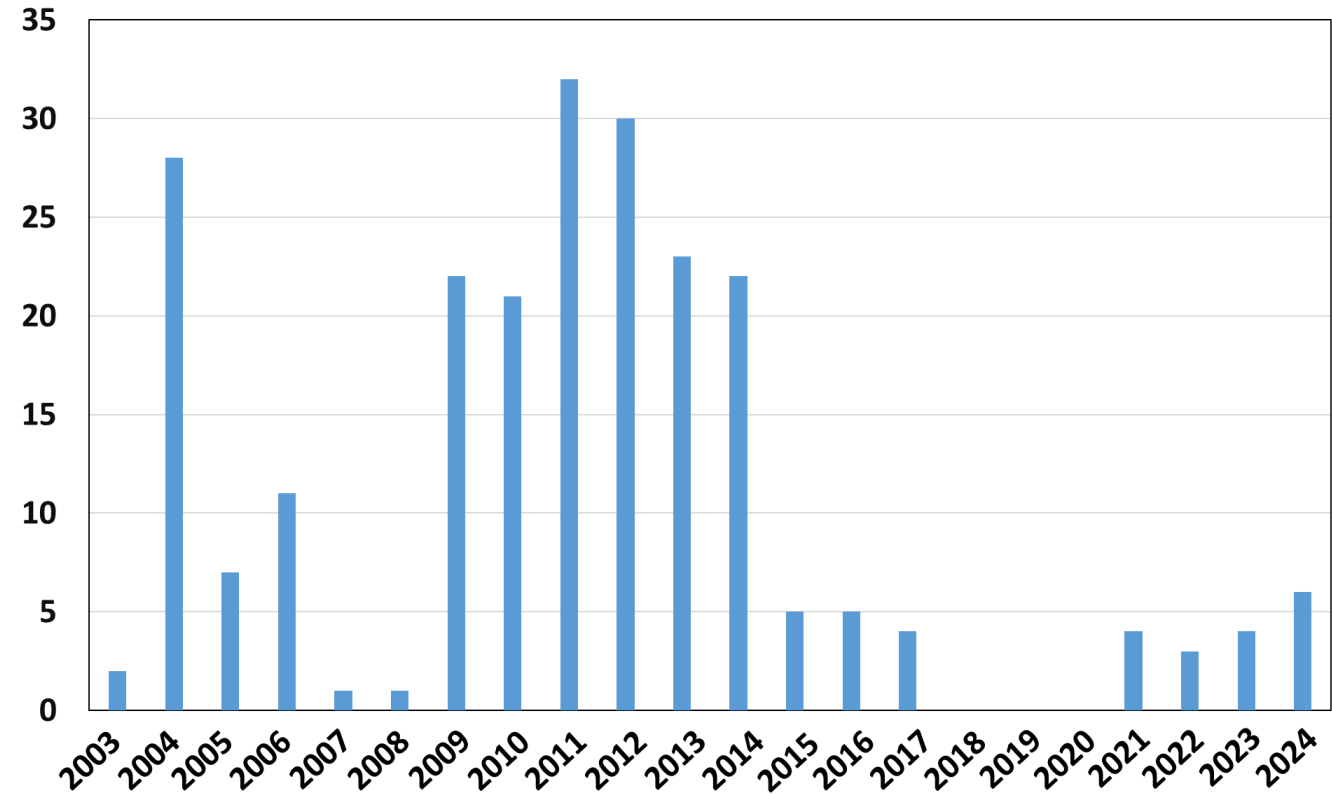
Conclusion

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.

231 DDEP evaluations



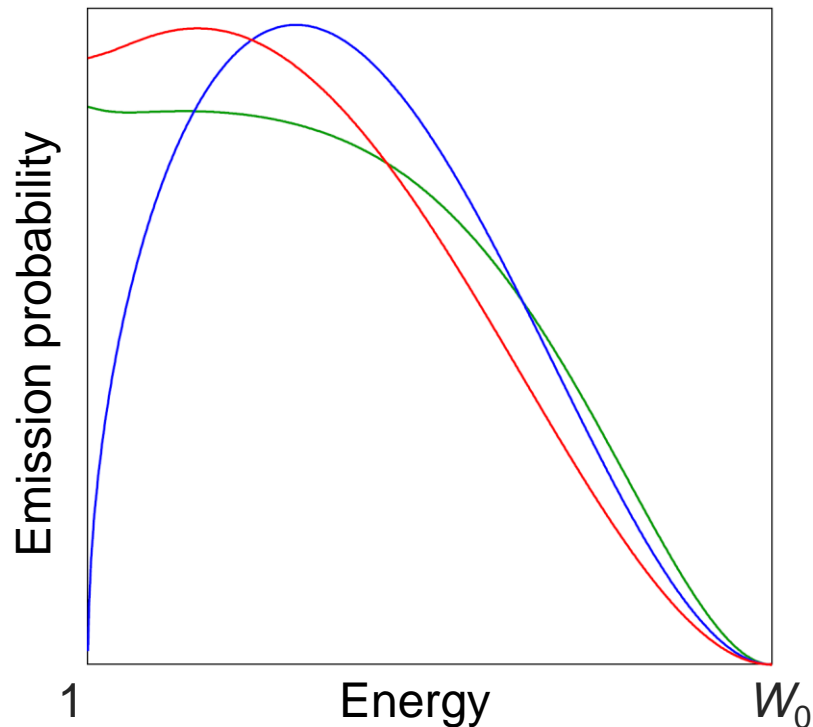


BetaShape Status

Beta spectrum shape

Phase space Fermi function Shape factor

$$\frac{dP}{dW} \propto pWq^2 \cdot F(Z, W) \cdot C(W)$$



W electron energy, W_0 transition energy

p electron momentum, q neutrino momentum

Allowed

$$C(W) = 1$$

First forbidden unique

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

Second forbidden unique

$$C(W) = q^4 + \lambda_2 q^2 p^2 + \lambda_3 p^4$$

Third forbidden unique

$$C(W) = q^6 + \lambda_2 q^4 p^2 + \lambda_3 q^2 p^4 + \lambda_4 p^6$$

Etc.

- ✓ The BetaShape program (version 2.4) now replaces the LogFT code for the new ENSDF evaluations. Electron captures also treated.
→ Available on IAEA-NSDD GitHub: <https://github.com/IAEA-NSDDNetwork>
- ✓ $F(Z, W)$ and λ_k parameters determined from the relativistic electron wave functions, obtained by numerical solving of the Dirac equation.
- ✓ Included: extended nucleus; atomic exchange, overlap and screening; radiative corrections; database of experimental shape factors.

For forbidden non-unique transitions, coupling with nuclear structure is necessary.

→ ξ -approximation possible but accuracy is questionable.

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.

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.

Summary on the recent versions

- ✓ Version 2.3 (September 2023), was released with all requests implemented.
- Feedbacks at 2023 USNDP meeting
- ✓ Version 2.3.1 in December 2023.
 - A few bugs fixed in generated CSV files.
 - Insertion of a comment line with the code version in updated ENSDF files.
 - Description of CSV format in a separate Microsoft Office Excel file.
- Feedbacks at 2024 NSSD meeting
- ✓ Version 2.4 in June 2024.
 - Acceleration of electron capture calculations by a factor of 50. Could take several minutes per transition before. Extensive tabulation of wave function overlaps.
 - An environment variable (**BSINSTALL**) can be defined to run the code from any directory.
 - Validation of the code on the entire ENSDF database, archived version of January 2024.
- **Feel free to send me any bug report or suggestion of improvements. I already have some from Jun Chen.**

Where to get BetaShape

LNHB website

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



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

<> Code Issues Pull requests Actions Projects Security Insights

main 1 branch 0 tags

Go to file Code

| File | Commit | Time |
|---------------------------------|----------------------|------------------------|
| 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 |

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

Effective coupling constants

- Free-nucleon value $g_V = 1$ according to CVC
- Free-nucleon value $g_A = 1.2754(13)$ [PDG 2020]

Review of J. Suhonen in Front. Phys. 5, 55 (2017)

→ Coupling constants g_V and g_A of the weak interaction can be affected by:

- Nuclear medium effects

The nucleon decays within a finite nucleus. Beyond the impulse approximation.

- Nuclear many-body effects

Simplification of the many-body problem: core excitation, nucleon correlations, etc.

Unfortunately, it is almost impossible to disentangle between these two categories of effects by analyzing beta decays.

Spectral shapes can help for a better quantification of the effective values → **the Spectrum Shape Method**.

→ **1st forbidden non-unique**

$$g_V^{\text{eff}} \sim 0.3 - 0.7 \text{ and } g_A^{\text{eff}} \sim 0.46 - 0.56$$

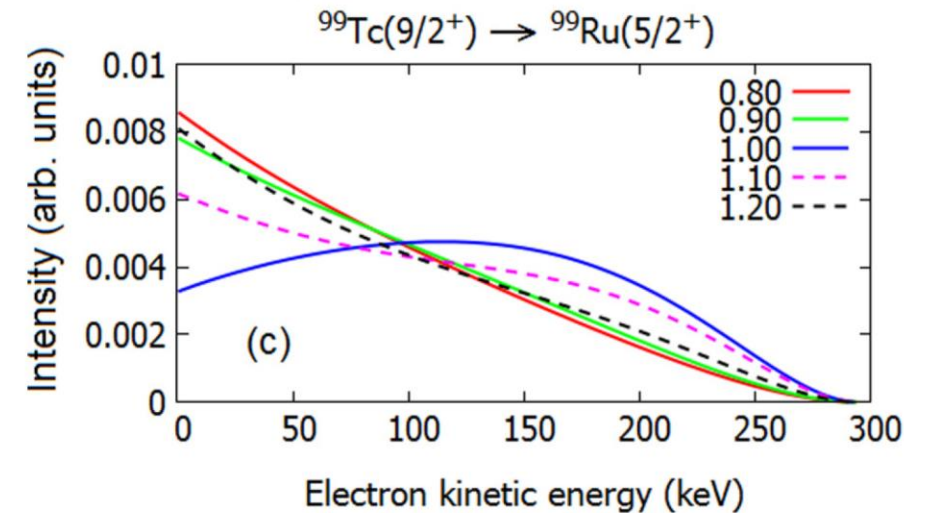
→ **Higher non-unique**

Lack of high-quality measurements

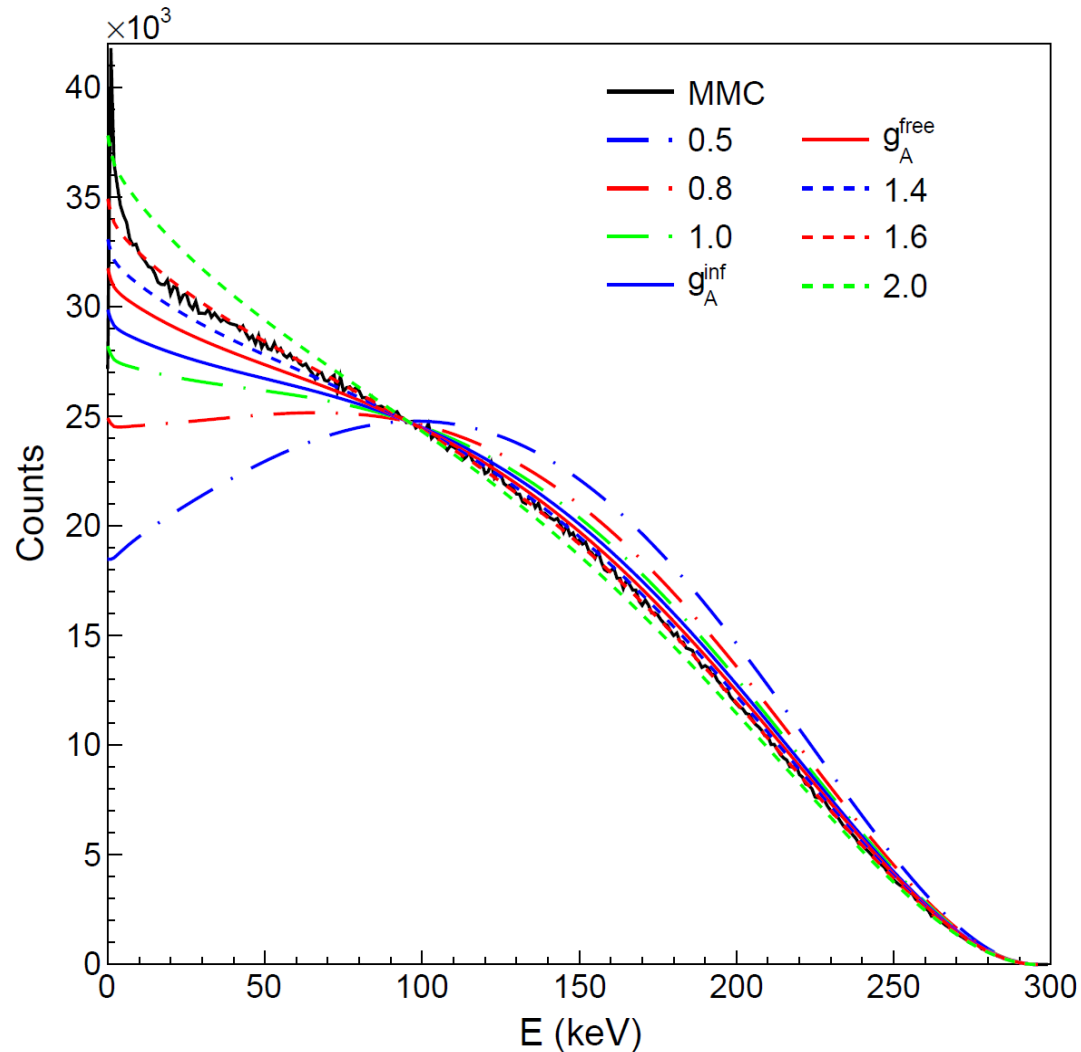
Suggests $g_V = 1$ and $g_A^{\text{eff}} \sim 0.4$

^{99}Tc beta spectrum, second forbidden non-unique, predicted to be very sensitive to g_A .

J. Kostensalo, J. Suhonen, PRC 96, 024317 (2017)



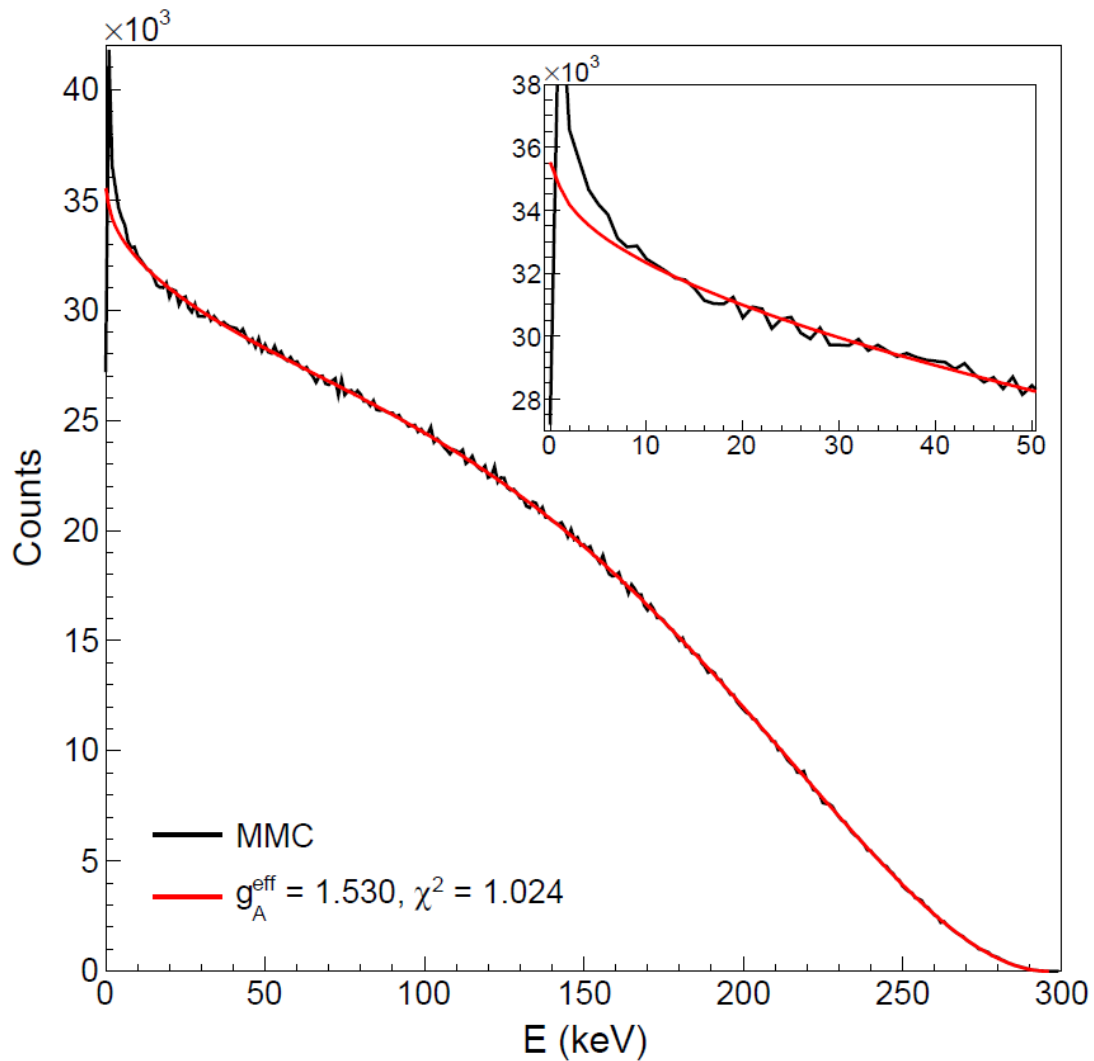
^{99}Tc 2nd forbidden non-unique decay



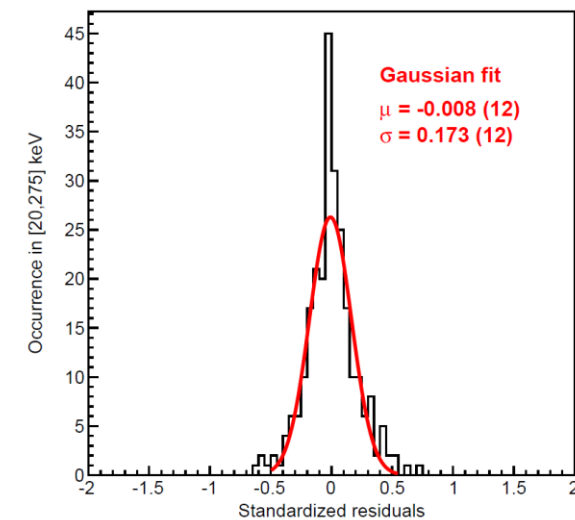
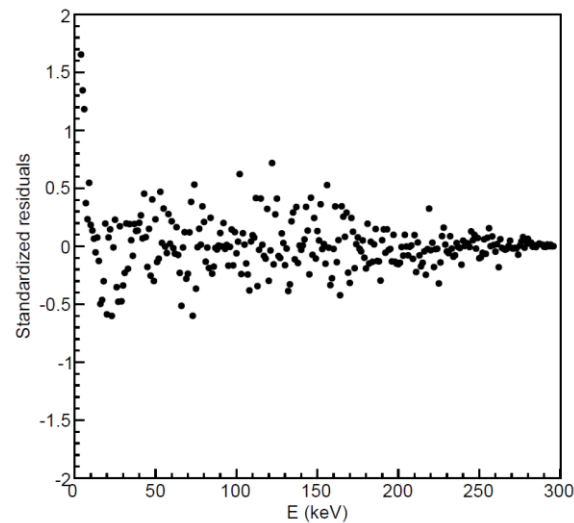
Within the European project PrimA-LTD

- ✓ 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.
- ✓ **High sensitivity to the effective value of g_A confirmed.**

^{99}Tc 2nd forbidden non-unique decay



- ✓ Three different model spaces used with NushellX (GL, GLEKPN, jj45pn) to quantify the influence of nuclear structure.
- ✓ Theoretical calculations with nuclear structure, CVC and complete lepton current.
- ✓ Best adjustment gives an effective axial-vector coupling constant $g_A^{\text{eff}} = 1.526 (92)$, far from $g_A^{\text{eff}} \sim 0.4$.
- ✓ Excellent residuals, without any trend down to 6 keV.



^{99}Tc 2nd forbidden non-unique decay



!! Effective g_A value is **enhanced** while should be **quenched**. What happens?

- Calculated half-life is about one order of magnitude too low.
- From DDEP: $T_{1/2} = 211.5 (11) \cdot 10^3 \text{ y}$
Evaluated value is mainly based on one publication, authors providing a *suggested* value.
- We can use it to renormalize the calculation and obtain a consistent picture: accurate shape, accurate half-life.

First possibility: renormalization of the OBTD

Example: GLEKPN

| Multipole | Transition | Original | Corrected |
|-----------|---------------------------------------|----------|-----------|
| K = 2 | n $1g_{7/2} \rightarrow$ p $1g_{9/2}$ | 0.00994 | 0.00362 |
| | n $2d_{5/2} \rightarrow$ p $1g_{9/2}$ | 0.47752 | 0.17383 |
| K = 3 | n $1g_{7/2} \rightarrow$ p $1g_{9/2}$ | -0.01709 | -0.00622 |
| | n $2d_{5/2} \rightarrow$ p $1g_{9/2}$ | -0.43403 | -0.15800 |
| | n $2d_{3/2} \rightarrow$ p $1g_{9/2}$ | 0.03143 | 0.01144 |

Second possibility: renormalization of g_V and g_A

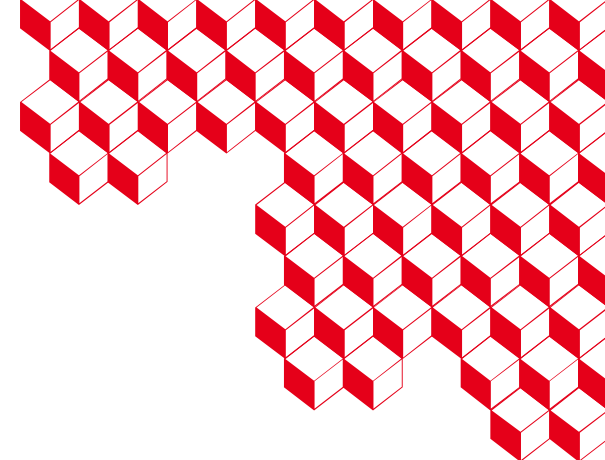
$$\rightarrow g_V^{\text{eff}} = 0.376 (5) \text{ and } g_A^{\text{eff}} = 0.574 (36)$$

Consistent with 1st forbidden non-unique results

$$g_V^{\text{eff}} \sim 0.3 - 0.7 \text{ and } g_A^{\text{eff}} \sim 0.46 - 0.56$$

→ **What about CVC hypothesis?**

- Eventually, one also deduces: $\log f = -0.47660 (22)$, $\log ft = 12.3478 (23)$, $\overline{E_\beta} = 98.51 (23) \text{ keV}$.



Thank you for attention

