BetaShape status
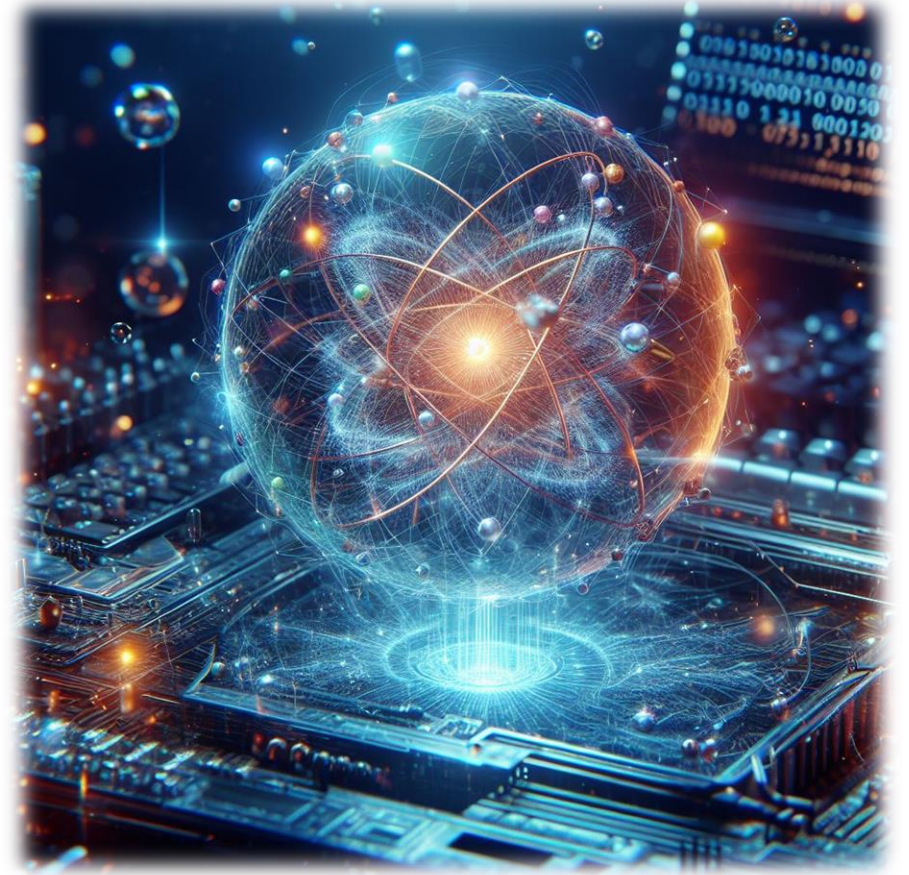
X. Mougeot, CEA-LNHB

Adoption by the NSDD network

Member of the US Nuclear Data Program

Adoption of the BETASHAPE code

T. Kibédi (ANU), F.G. Kondev (ANL), A. Nichols (U Surrey),
B. Singh (McMaster U) & X. Mougeot (CEA-LNHB)

NSDD Meeting, October 24-28, 2022, Canberra, Australia

✓ 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 improve the reliability of the results.

✓ Version 2.3 (September 2023), was released with all requests implemented. Version 2.3.1 in December 2023. Version 2.3.2 ready for release but things to be discussed.

✓ A manual is also provided, based on exercises given at the ICTP 2022 NSDD workshop. Full description of options and generated output files.

Developments for version 2.3

Technical

- ✓ Rounding limit can be changed via a simple option, from 1 to 99.

- ✓ 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.
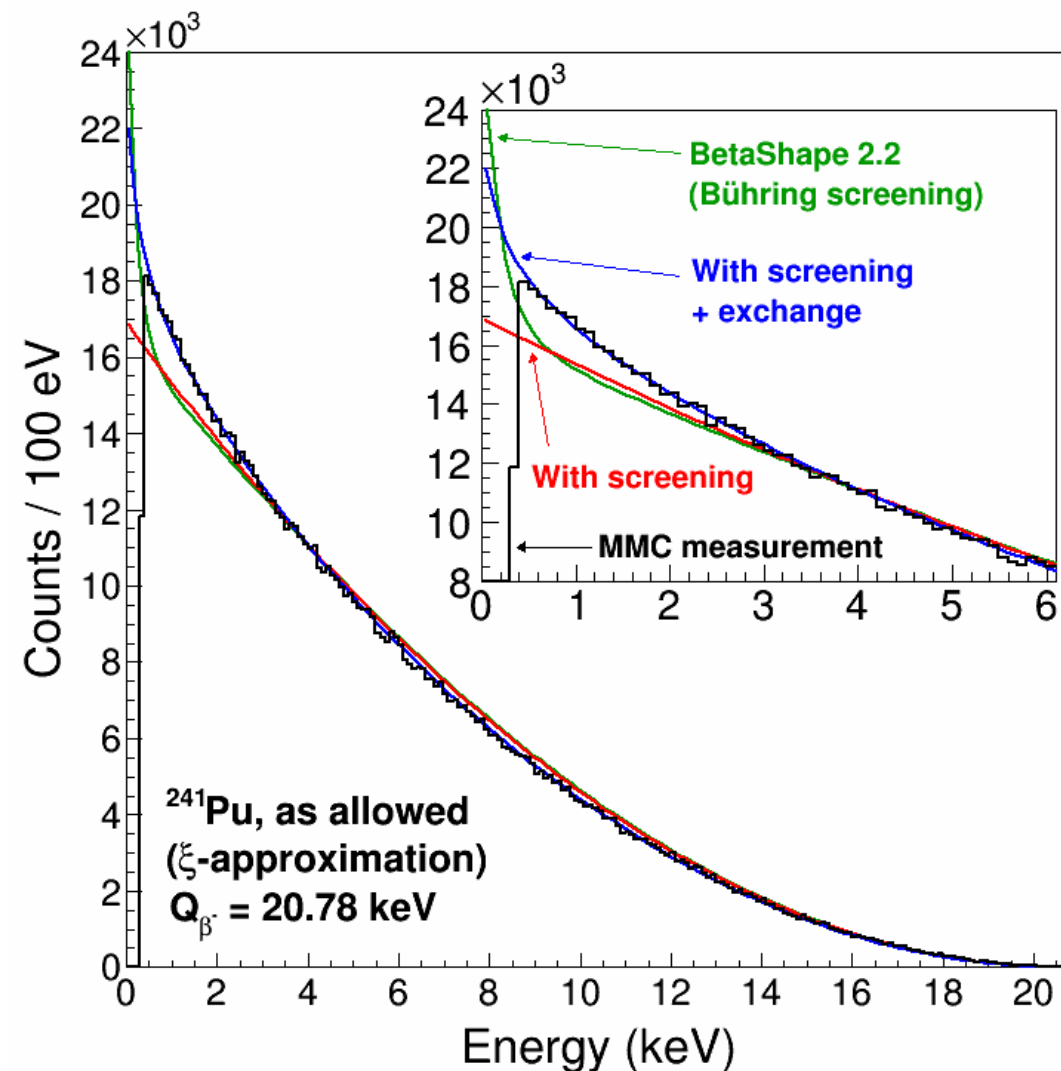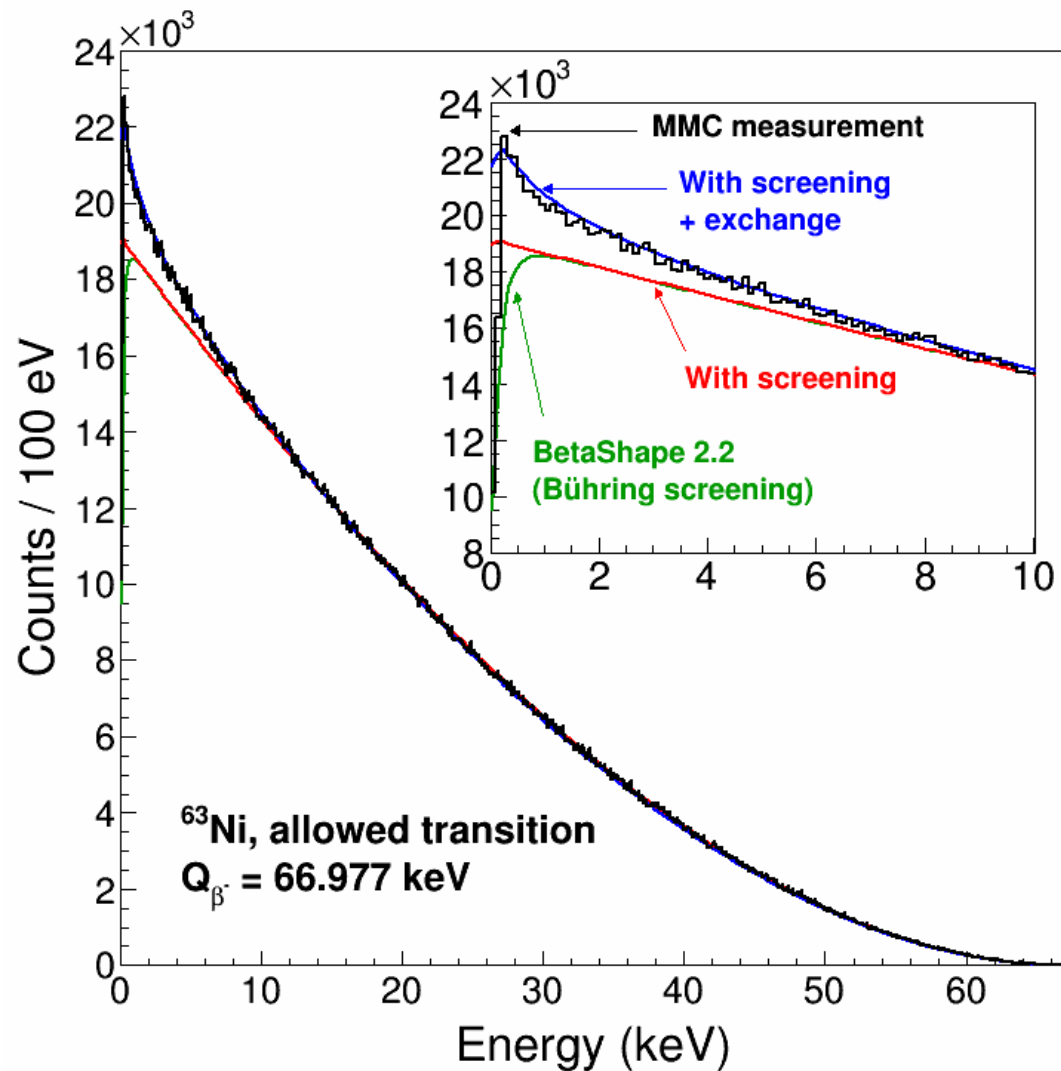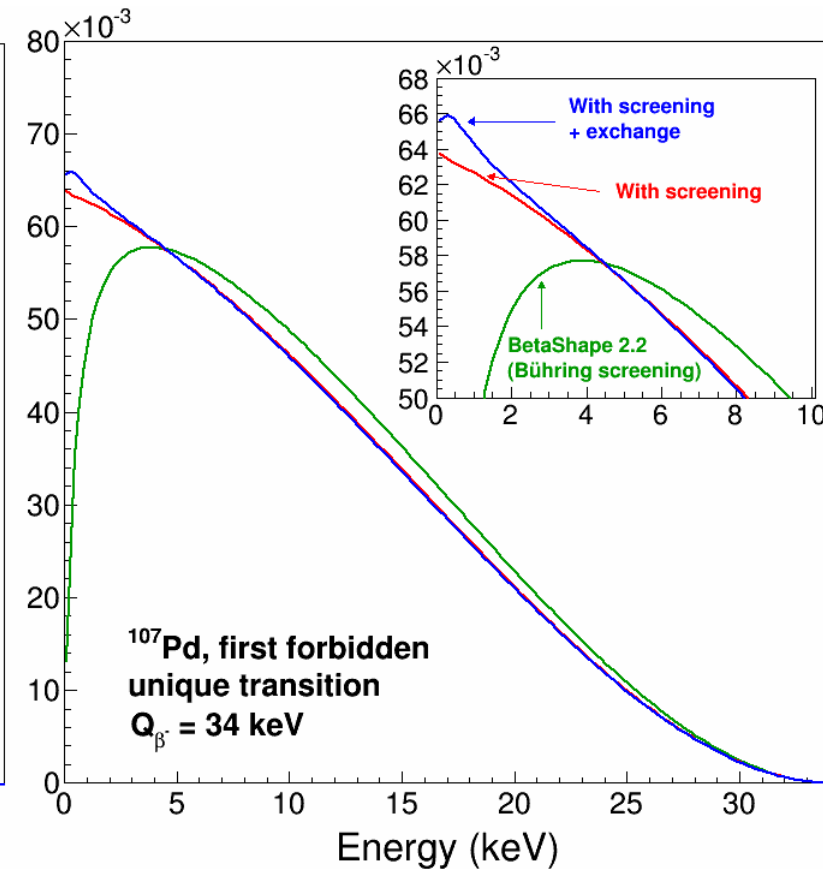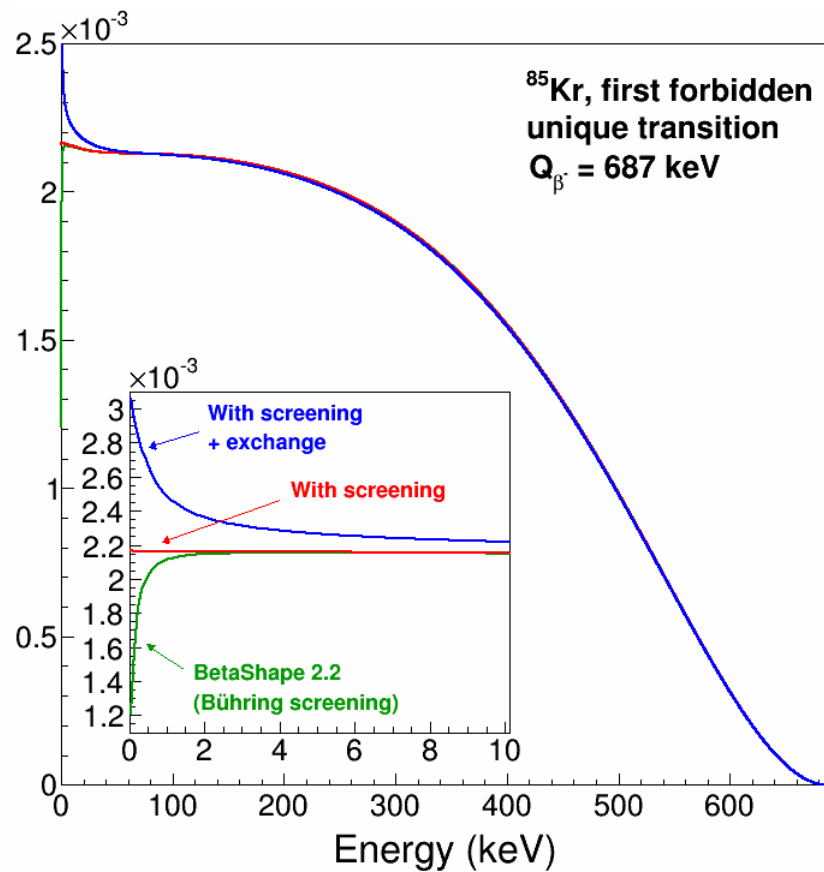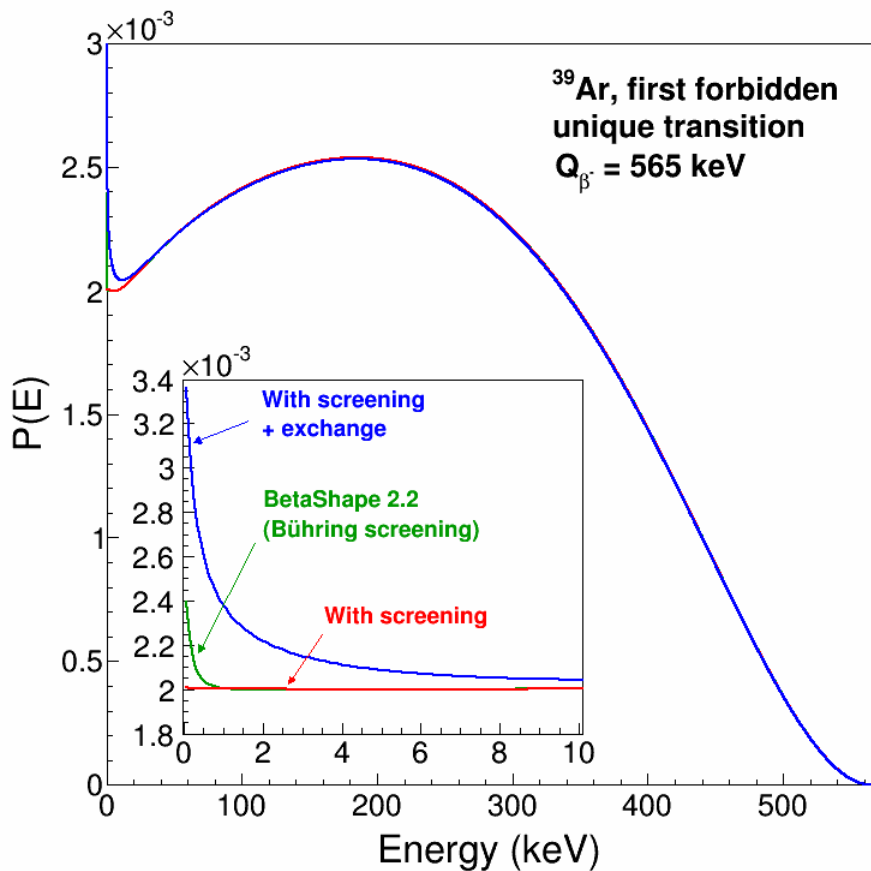
Tabulation of atomic screening and exchange effects

→ **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 B 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)*
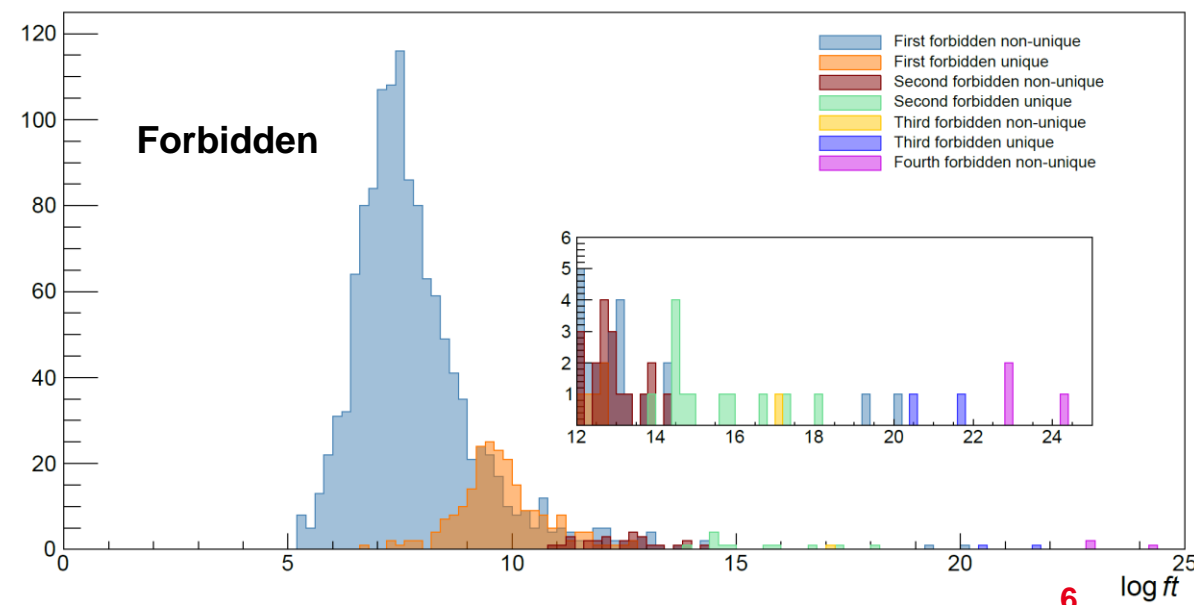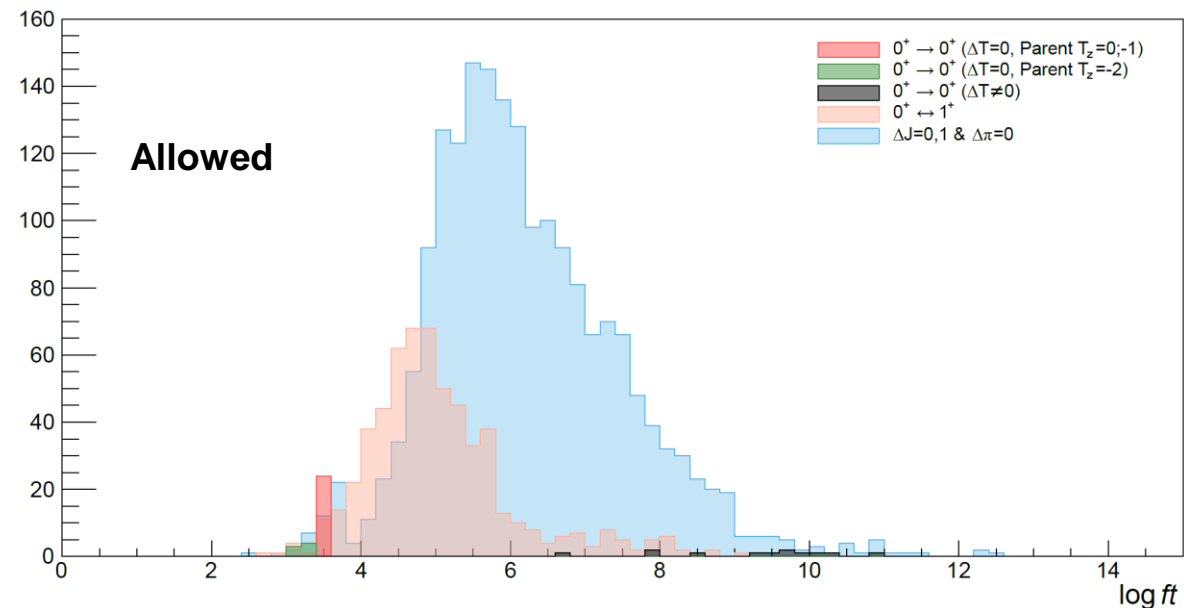
Overview distribution for Jπ assignment
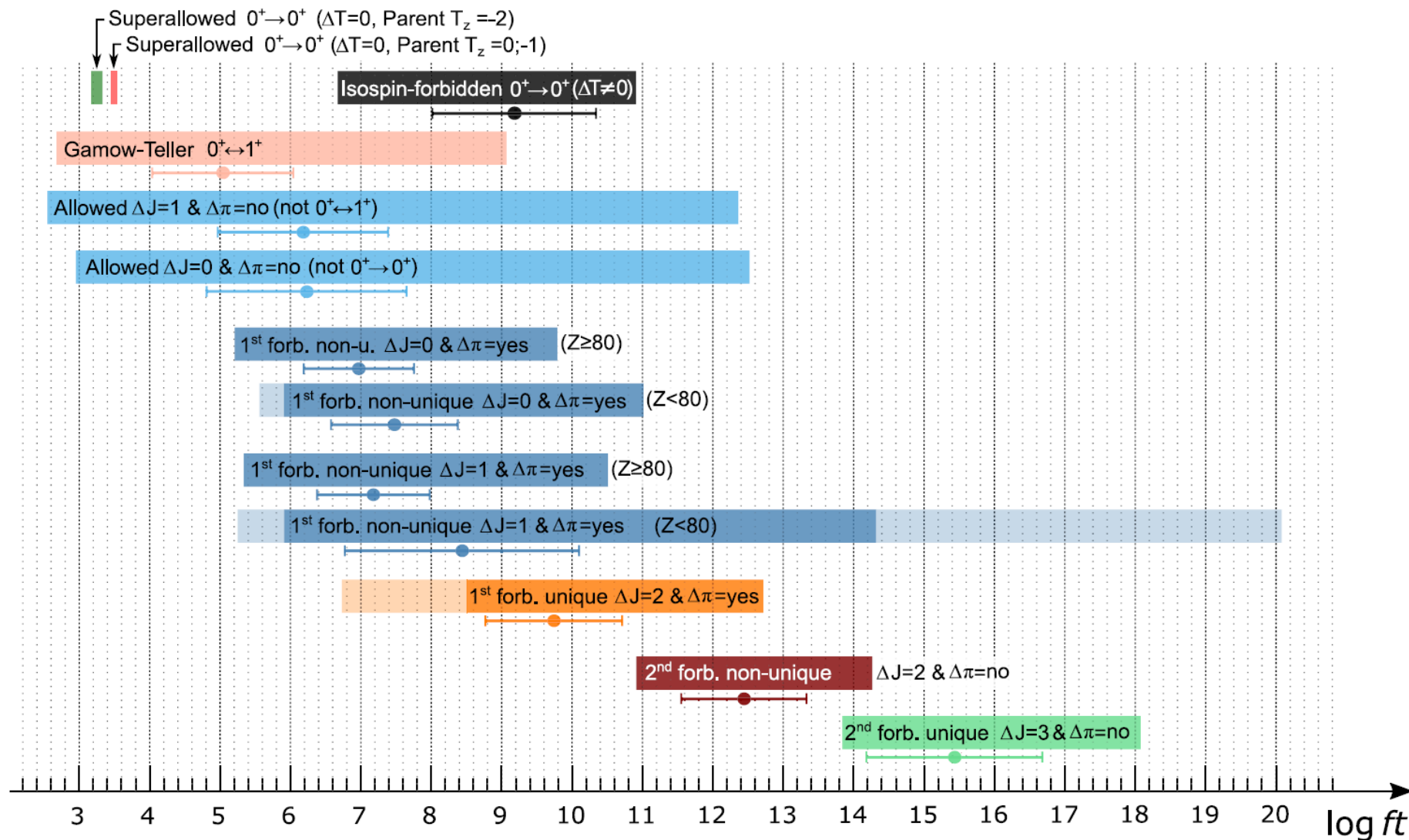
EURAMET Case Study

European Metrology Programme for Innovation and Research

Delivering Impact

- ✓ Developments of the code partially funded by three successive European projects: MetroBeta, MetroMMC and PrimA-LTD.

- ✓ Impact recognized by EURAMET in publishing a dedicated Case Study:

  https://www.euramet.org/casestudies/casestudiesdetails/news/betashape-an-improved-code-for-calculating-beta-radiation-decay-spectra

BetaShape: An improved code for calculating beta radiation decay spectra

Improving knowledge of radiation physics

Credit: Xavier Mougeot

Where to get BetaShape 2.3.x

LNHB website

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

IAEA GitHub Repository

https://github.com/IAEA-NSDDNetwork

Version 2.3.1

➢ The new implemented features for version 2.3 have complicated a lot different parts of the code. Despite many tests, there can be some remaining bugs for specific combination of different options.

Feedbacks on version 2.3 (September 2023) at USNDP meeting in November 2023

✓ A few bugs fixed when generating CSV files

✓ A description of the CSV is now provided in a separate Excel file to avoid any confusion

✓ Insertion of a comment line that states the code version (first attempt!)

✓ Version 2.3.1 released on December 2023

Version 2.3.2

➢ Problems when using Windows ENSDF files in Unix based system (CR/LF end-of-line character).

✓ Corrected by re-writing the input ENSDF file (which is saved as e.g. your_cd115.ens), correcting also line lengths different from 80 columns.

✓ Problem noted by Tibor Kibedi about input file name: improved, but character chains that define options for the code must be avoided (which is not really a big deal).

✓ Blank line of 80 columns at the end of the dataset: bug corrected, now should be fine. This rule is not followed in archive ENSDF files.

✓ Adding code reference, quantities and version, following format checking prescriptions from Jun Chen.

✓ **Mass chains**: tested over the whole database (archive version as of January 2024). A few bugs fixed: reading/writing files in specific cases with new options; totally blank B and EC records have never been expected before. **The code now works well when run over any mass chain.**

Executables

Environment variables

➢ Execution of the code from anywhere on the computer. Help from Tibor Kibedi this week.

macOS version

➢ Libby Ricard mentioned impossibility to run the code on previous or later version.

• CEA security has blocked macOS version to Monterey until March 2024. Compiled on Monterey until 2.3.1. New version compiled on Sonoma (macOS 14).

• Please check the version you need (Intel or M1 processor). I do not know what happens on M2 processors: **any feedback?**

• Please check rights on the executables, because they can be blocked to read-only when downloading. Make a 'chmod 777' on all executables to have full rights.

• Apparently, it is not possible to make a standalone version with gcc (static libraries not available). It is already done in version 2.3.1 for Windows and Ubuntu (version compiled on 20.04 LTS which works well on 18.04 LTS). **Any help?**

To be discussed for version 2.3.2

A remark from Filip Kondev and Tibor Kibedi:

Which uncertainty to recommend when no uncertainty on level energy, or any other quantity?

In BetaShape version 1, unc. = value / $\sqrt{3}$ (rectangular distribution from zero to value), whatever the quantity.

Good for small branching ratios but too large for level energies.

Balraj Singh suggested to remove such an approach, what has been done since version 2.

Example: ^{144}Tb decay with no uncertainty on Q-value (9074 keV SY) and $T_{1/2}$ (1 s AP).

Ground state to ground state transition: no uncertainty on log *ft* value.

But uncertainty on level energies: only a single component, uncertainty on log *ft* value very small.

Possible future developments

➢ **ENSDF standard options?** Would be defined in an external file, for instance:

Rounding limit (default is 50); Neutrino energies and spectra; Generating CSV files

Asymmetric uncertainties (if x=y in +x-y, automatically put in symmetric format)

Automatic update of Q-value (from AME2020)

Fixing EC and B+ intensities (instead of automatically calculate them)

Various other options…

➢ **Coupling with UncTools** from Tibor Kibedi

Monte Carlo propagation, important for asymmetric propagations

➢ **Reading input ENSDF files in JSON format**
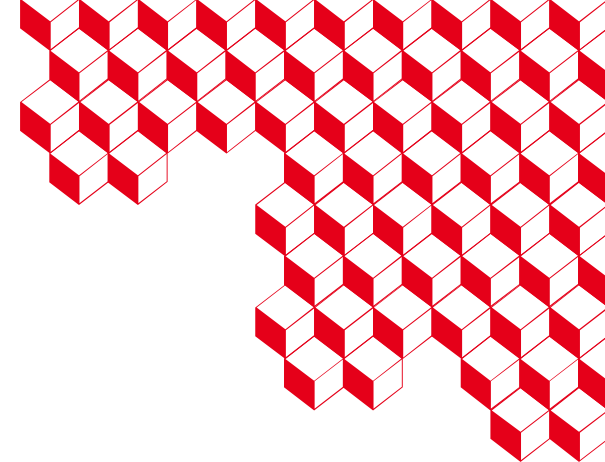
I would need guidance and help from NNDC

Conclusion

Main features of the BetaShape code

➢ More precise mean energies (beta and neutrinos), capture probabilities and log-ft values.

➢ Additional useful information: energy spectra, subshell capture probability, etc.

➢ Code, modelling and output continuously improved.

Your feedbacks are of the utmost importance to identify possible bugs and to improve the reliability of the code.

➢ Please send me any question, comment or feedback. If you have any problem, just send me an email with your input file.

➢ Do not forget to tell me if you have (strict) deadlines or constraints. I have too, it is important for managing the priorities.

Thank you for your attention