Oak Ridge National Laboratory

Reproducibility and Optimization Techniques for Evaluated Data in the Resolved Resonance Region: Set of Dysprosium Isotopes

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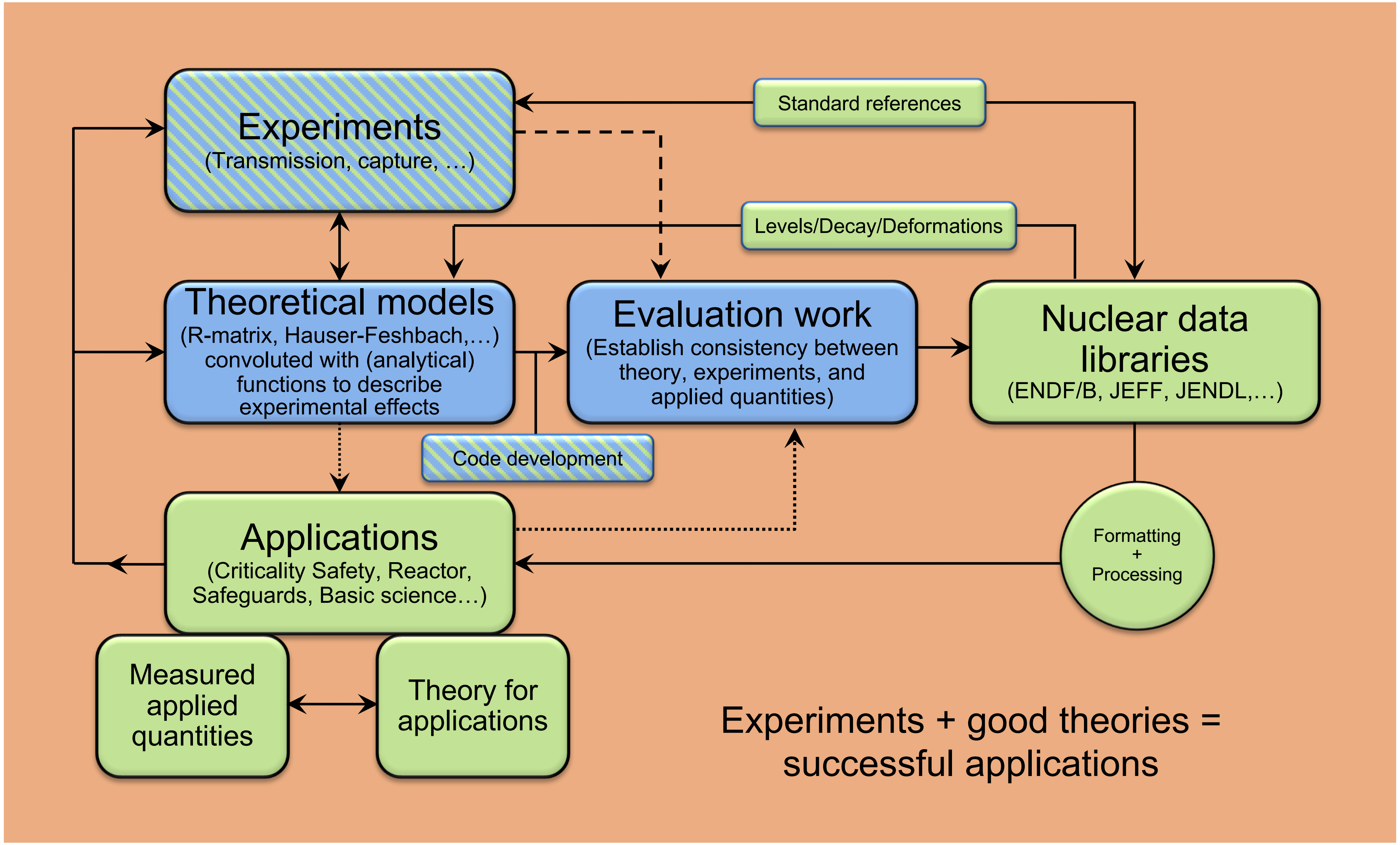
OUTLINE

- **Evaluation Workflow Scheme (Reminder)**
- **Why Dy Isotopes?**
- **Experimental Effects**
- **Covariance Generation**
- **Repository Structure**
- **Conclusions**
- **Appendix (Key Points of Previous Presentation)**

EVALUATION WORKFLOW SCHEME



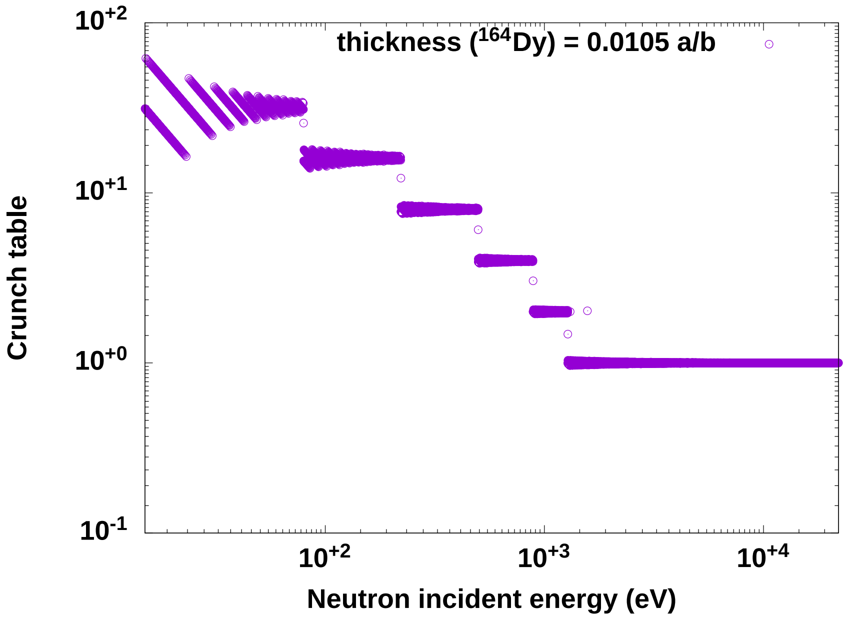
WHY DY ISOTOPES?

- Multi-isotope, multi-channel R-matrix analysis
  - seven stable isotopes, $^{156,158,160\text{-}164}$Dy, and three reaction channels (total, elastic, capture)
- Experimental configuration for natural and enriched sample measured data
  - Resolution and Doppler broadening
  - Multi scattering corrections
  - Detector efficiency[1] : the capture rate in ToF measurements may be determined by detecting γ-ray cascades emitted as the compound nucleus decays. Detecting efficiency of many detecting system increases nearly linearly with γ-ray energy implying independence from the γ-ray cascade emitted, and linear variation with the binding energy of a neutron in the compound nucleus being studied
- SAMMY is equipped with a spin-group-dependent detector efficiency (multiplicative factor), which can be used to model this effect
- Resonance parameter covariance generation for a single isotope from multi-isotope analysis

[1] M. C. Moxon and E. R. Rae, "A gamma-ray detector for neutron capture cross-section measurements," *Nucl. Instr. Meth.*, **24**, 445 (1963).

EXPERIMENTAL EFFECTS FOR DY ISOTOPES

- Major experimental campaigns: spectroscopy measurements by Liou (1975) [2] and Block (2017) [3]
- Liou's data reported in EXFOR as total cross section instead of transmission data for several sample thickness. Impact of detector efficiencies on Block's data.



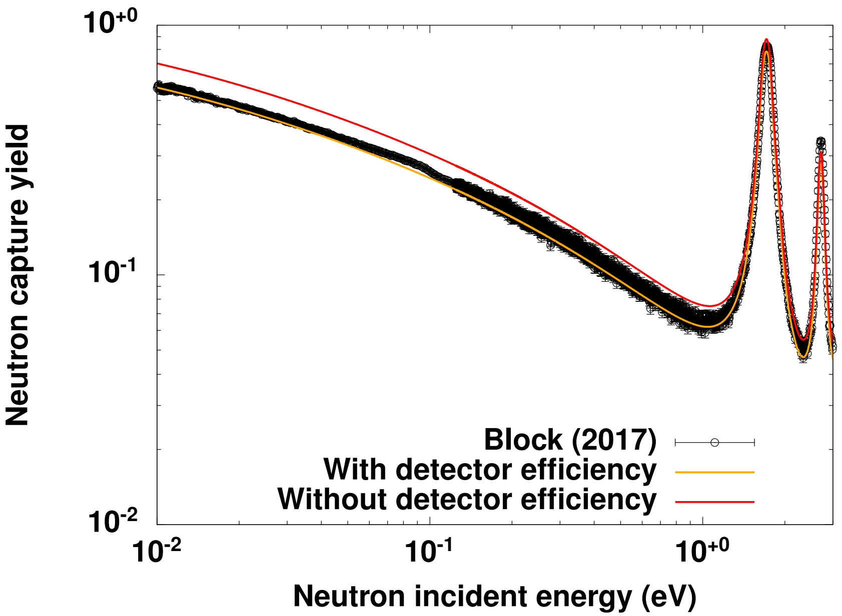
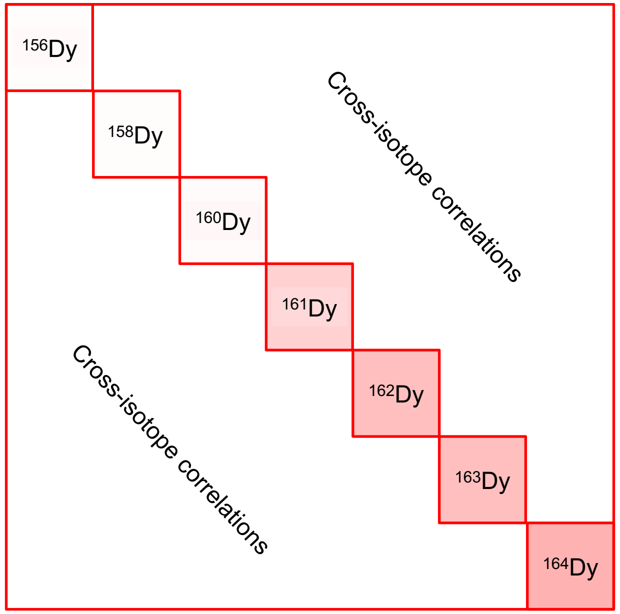


Figure 1: Crunch table derived from Liou's data (left). Impact of detector efficiencies on Block's dat (right).

[2] Liou et al.,"Neutron resonance spectroscopy: The separated isotopes of Dy", *Phys. Rev.*C, **11**, 462 (1975).
[3] R. C. Block et al.,"Neutron transmission and capture measurements and analysis of Dy from 0.01 to 550 eV," *Progr. Nuc. Energy*, **94**, 126 (2017).

COVARIANCE GENERATION

- Particularly, when natural data are used in the fitting for a multi-isotope case, the optimization procedure can generate cross-isotope correlations



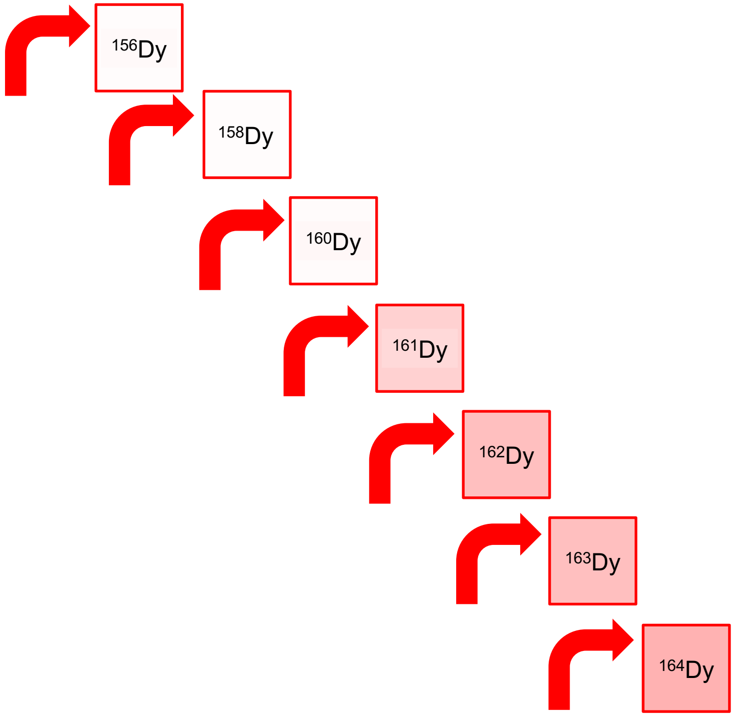


Figure 2: Resonance parameter covariance matrix as derived in the optimization procedure (left). Loss of cross-isotope correlations when single isotope is extracted and reported (right).

REPOSITORY STRUCTURE (IN PROGRESS)

docs dy(156,158,160–164) dynat endf exfor fit geraspin inputs ndf nndc parameter README **runs thermal**

- **exfor**: EXFOR data files (*.exf) used to generate the input data files (*.twenty) for SAMMY
- **inputs**: SAMMY inputs (*.inp) or “input decks” for each experiment containing the set of related exeprimental corrections
- **geraspin**: generation of quantum number information
- **ndf**: generation of endf file restricted to the RRR (+URR) to test the processing procedure with AMPX, NJOY, …
- **parameter**: set of parameter files (*.par or *.red)
- **runs**: scripts to generate theoretical data for each experiment calculated from a resonance parameter file (endf, v1, v2, …)
- **fit**: as **runs** but for the fitting procedure
- **thermal**: inputs and data files for the thermal values
- **dy(156,158,160–164) dynat**: SAMMY output files for each run
- **nndc**: final complete endf files submitted to ENDF repository
- **docs**: relevant published documentation (some of the papers might not be shareable)

CONCLUSIONS

- Again, experimental setup input parameters are basic and fundamental quantities for reproducibility (see e.g. detector efficiency)
- Again, the goal is to increase quality of the evaluated data and decrease time needed for an evaluation. Some information can be lost for multi-isotope analyses in the current procedure when evaluated data
  - SAMMY.COV (multi-isotope) resonance parameter covariance matrix should be reported
- Preliminary repository scheme was generated

ACKNOWLEDGMENTS

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Questions?

APPENDIX: OBSERVABLES DEFINITION

- **Theoretical observable**: quantity (e.g. cross section) purely calculated from nuclear model parameters (e.g. resonance parameters) defined within a nuclear theoretical model (e.g. R-matrix theory)
- **Calculable observable**: quantity defined by the convolution of the theoretical observable and functions to quantify “explicit” experimental effects or corrections (see next slide)
- **Measured observable**: quantity reported in the experimental database and uncorrected for any explicit effect included in the calculable observable
  - Note: there are “implicit” experimental corrections not usually included in the evaluation procedure (e.g., the background subtraction of transmission data $T^{exp} = (C_{in} - B)/(C_{out} - B)$), neutron sensitivity, energy binning
- For reproducibility purposes, the implicit experimental corrections should be available and, for full consistency, included in the calculable observable definition: implicit$\rightarrow$explicit
- Generally, implicit+explicit effects are not negligible, therefore, theoretical and measured quantities can not be directly compared
- Generally, evaluated data reported in the nuclear data libraries are theoretical quantities

APPENDIX: EXPERIMENTAL EFFECTS[4]

- **Convoluted resolution broadening** $I(t)$: specific experimental facilities (or setups)

$$\tilde{\sigma}(E) = \int_t I(t(E)-t')\,\sigma(E(t');\mathbf{p})dt' \quad \text{with} \quad I(t-t') = \int I_1(t-t_1)dt_1 \left(\prod_{k=1}^{N} \int I_{k+1}(t_k - t_{k+1})dt_{k+1} \right) I_{N+1}(t_{N+1}-t')$$

  $I_k(t)$ are functions used to describe *electron burst*, *time-of-flight channel width*, *detector types*, *neutron sources*,...

- **Doppler broadening** : temperature
- **Normalization or background corrections** : $B(t) = B_0 + B_1(t) + \dots$
- **Self-shielding** : reduction in the measured capture counts due to interactions of incident neutrons with other nuclei
- **Multiple scattering corrections** : finite size sample[5][6]
- **Corrections for nuclide abundances** : relevant because highly enriched sample targets can be costly
- **Peak alignment** : the neutron energy in time-of-flight measurements depend on the flight-path length L and initial time t_0. These can be adjusted to have agreement among data measured sets
- **Detector efficiencies** : (see slide 4)

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[4] As implemented in the SAMMY code.

[5] A reasonable sized sample is needed to have enough counts.

[6] **Neutron sensitivity** is another experimental effect (not yet treated) for which not only γ-rays but also scattered neutrons reach the detector and create a “false” capture event.

APPENDIX: BASIC QUANTITIES FOR REPRODUCIBILITY

- Set of measured data including modifications or corrections: normalization (e.g. neutron capture yield[7]), lack of uncertainties and/or correlations, duplicate of incident energies, ...
- Inputs containing the experimental corrections (as specified on slide 5) for the set of analyzed measured data used in the fitting procedure
- Prior set of resonance parameters and number of parameters included in the fitting procedure
  - Assumption : spin assignment and experimental set up is determined
  - Note : R-matrix parameters and scaling factors are usually the varied parameters
- Number of iterations (it_{max}) to reach convergence for a given metric (e.g. χ^2)
- Energy ranges ($E^k_{\text{min/max}}$) for each fitted data set (k)
- ... and, of course, a repository and code release!

Note: ideally, “physical constraints” such as (in)coherent scattering lengths, statistics on the resonance parameters, compatibility between different resonance parameter basis[8], ..., should be included in the optimization procedure

[7] Neutron capture yield can be reported as normalized to the thickness sample. However, in some cases, this is not the correct choice.
[8] Conversion from R-matrix pole energies (or eigenvalues) to Brune basis and vice versa.

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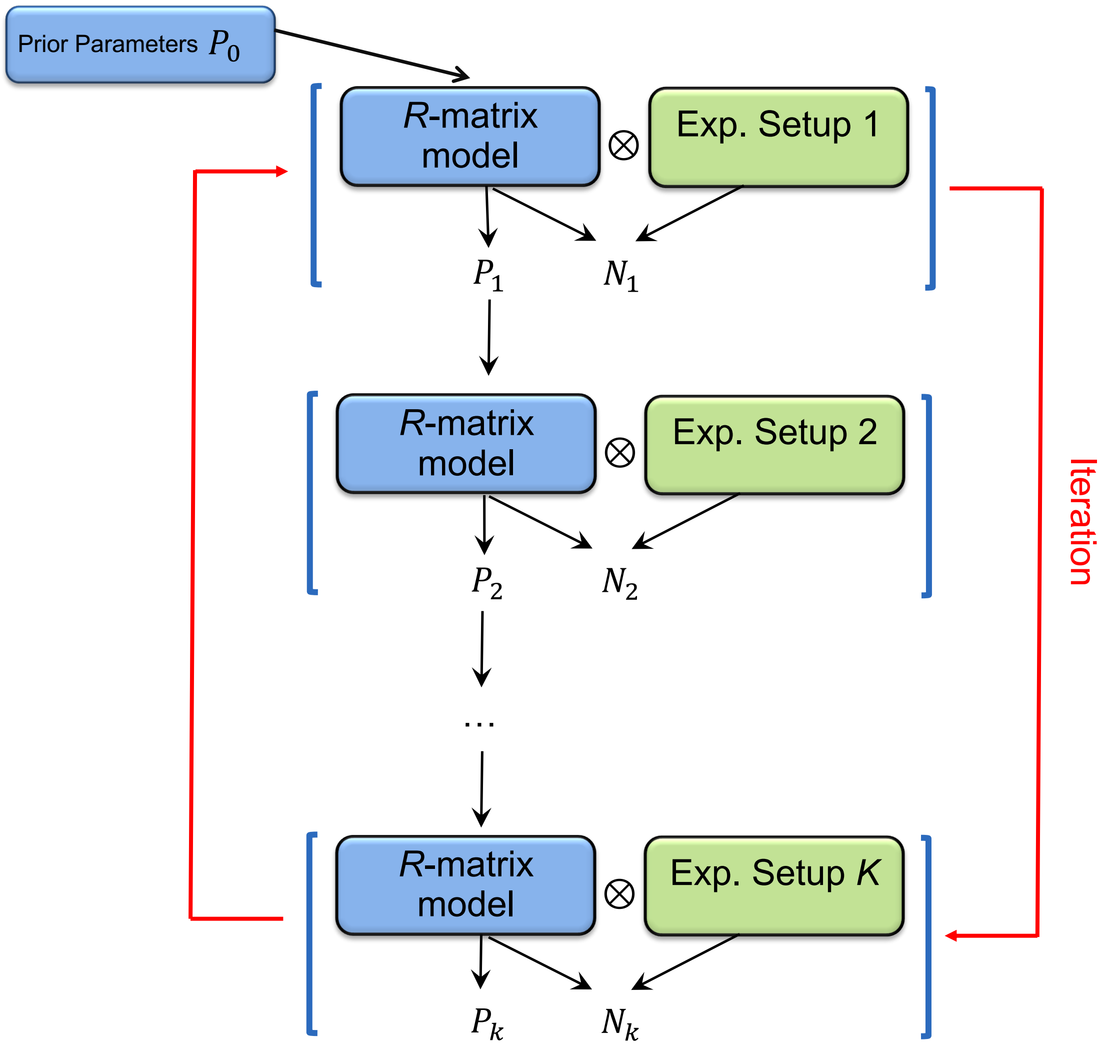

- Ideally, the optimization procedure should reveal inconsistent measured data when the scaling factor N is largely deviating from unity
- Parameters for the experimental setup could be optimized, however, they are very well known
- Note: computation time (t_{comp}) to reach convergence is different from case to case
-
  - Light nuclei have usually many channel spins (n_c) and a relatively small number of levels (n_{lev})
  - Heavy (fissile) nuclei have usually a few channel spins (e.g. 1 or 2) and a very large number of levels
  - Set of resonance parameters of minor nuclide abundances for experimental data (usually measured on natural or oxide sample) are needed

$$t_{\text{comp}} \propto (n_{\text{lev}} \times n_c)_{\text{iso}} \times n_{\text{iso}} \times n_{\text{it}} \times n_{\text{exp}} \times (n_{\text{data-point}})_{\text{exp}}$$