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Subject: Report on Foreign Travel to Paris (virtual meeting)

Date: 07/01/2021

To: Dr. Angela Chambers, Nuclear Criticality Safety Program Manager, National Nuclear Security Administration / NA-511

From: Marco T. Pigni

Meeting Title: Working Party on International Nuclear Data Evaluation Co-operation (WPEC) sbgr 49 Reproducibility in Nuclear Data Evaluation

Meeting Location: Paris (virtually)

Meeting Date: 11 May 2021

Attendees on behalf of NCSP:

Meeting Purpose:
To present key ingredients to reproduce and generate nuclear data evaluation in the resolved resonance region.

Meeting Benefits to the NCSP:
Automated reproducibility aligns with the goal of generating nuclear evaluated data certified within a specific metric and physical constraints. This also to improve quality and reduce time to generate evaluations.

Purpose of Travel:

Invited talks were given at two WPEC49 meetings (November 2020 and May 2021) describing the coupling between theoretical models and experimental corrections and its fundamental importance for reproducibility purposes

Persons Contacted at Meeting:

Presentations, Chair Responsibilities, Etc.

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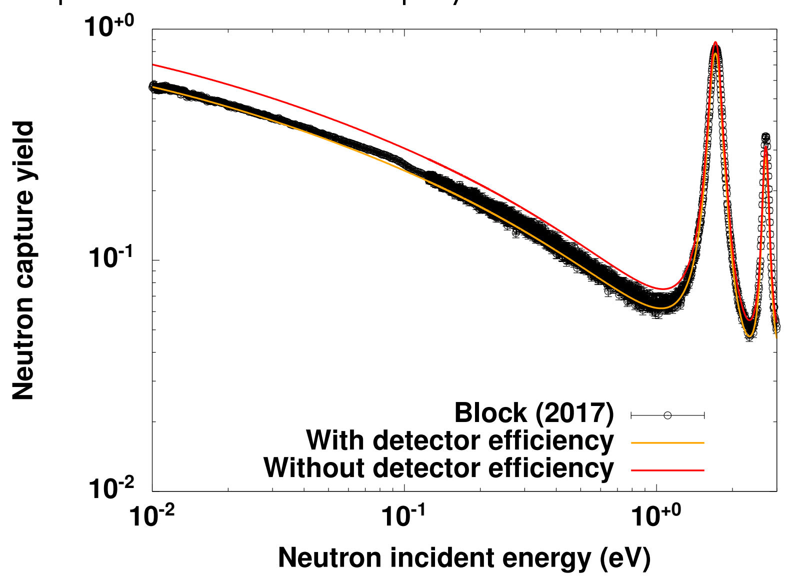
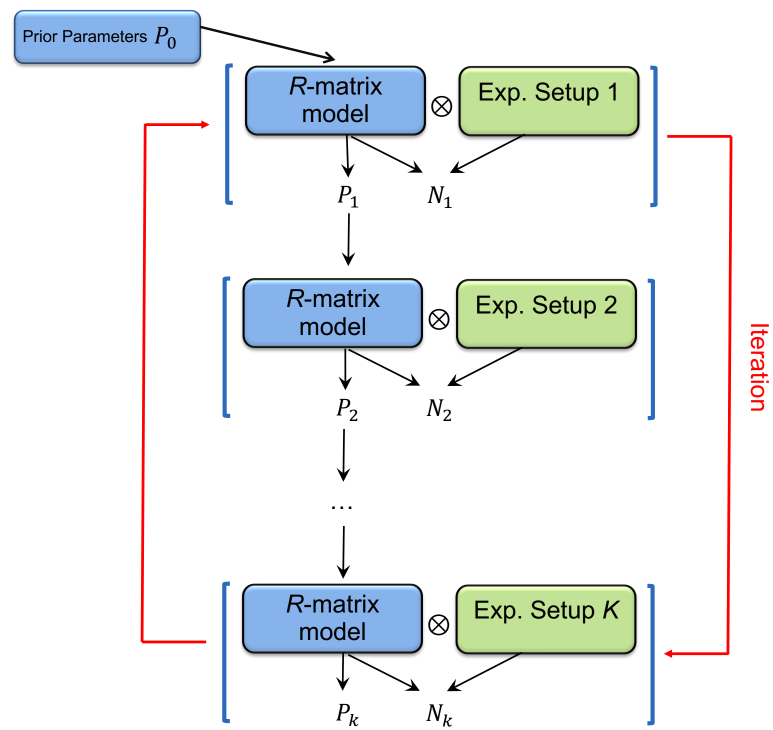
Reproducibility and Optimization Techniques for Evaluated Data in the Resolved Resonance Region: Set of Dysprosium Isotopes

- **Background:** The goal of the Working Part on International Data Evaluation (WPEC) Subgroup 49 at the Nuclear Energy Agency (NEA) is to facilitate the evaluation process. In doing this, the first step focuses on the reproducibility and preservation of existing and future evaluations. Subgroup 49 is centered on the features of the R-matrix codes applied to the evaluation procedures related to light and (fissile) heavy nuclei
- **Purpose:** Invited talks* were given at two WPEC 49 meetings (November 2020 and May 2021) describing the coupling between theoretical models and experimental corrections and its fundamental importance for reproducibility purposes.
- **Impact:** Automated reproducibility aligns with the goal of generating nuclear evaluated data certified within a specific metric and physical constraints





* RESolution PUB IDs **149318** and **157339**

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Sponsor: Nuclear Criticality Safety Program

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

Marco T. Pigni
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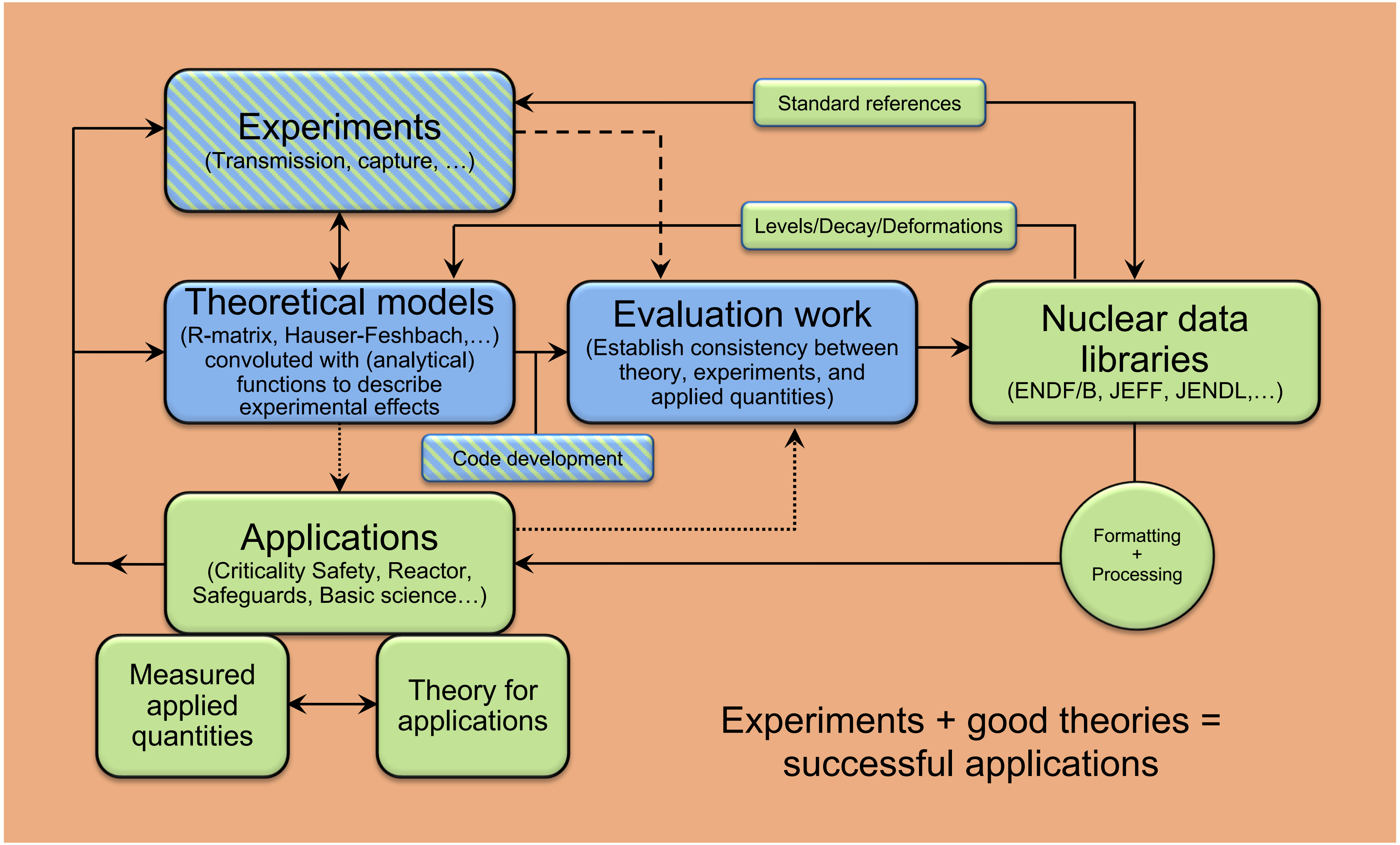
Nuclear Energy Agency, Working Party on International Data Evaluation, Subgroup 49
Paris, France, May 2021

OUTLINE

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

EVALUATION WORKFLOW SCHEME



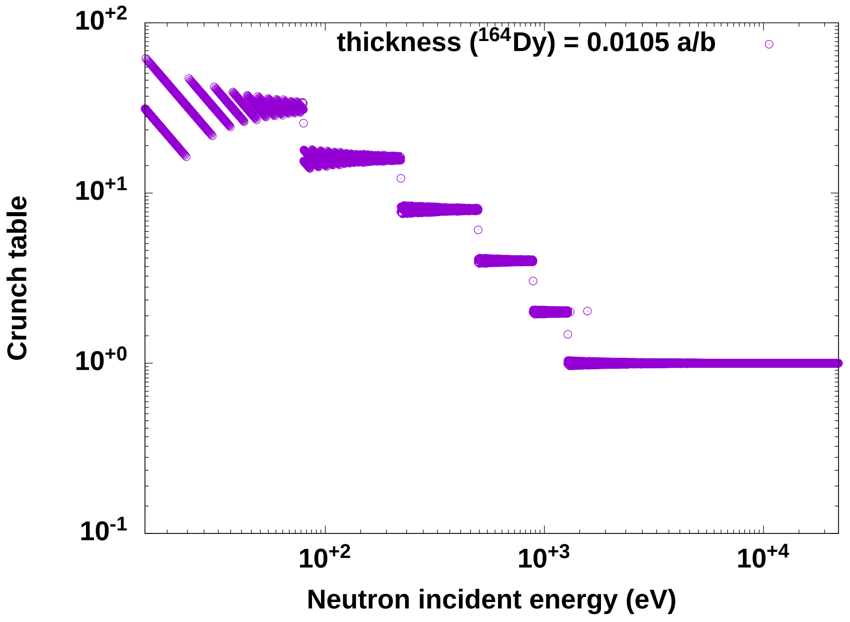
WHY DY ISOTOPES?

- 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.



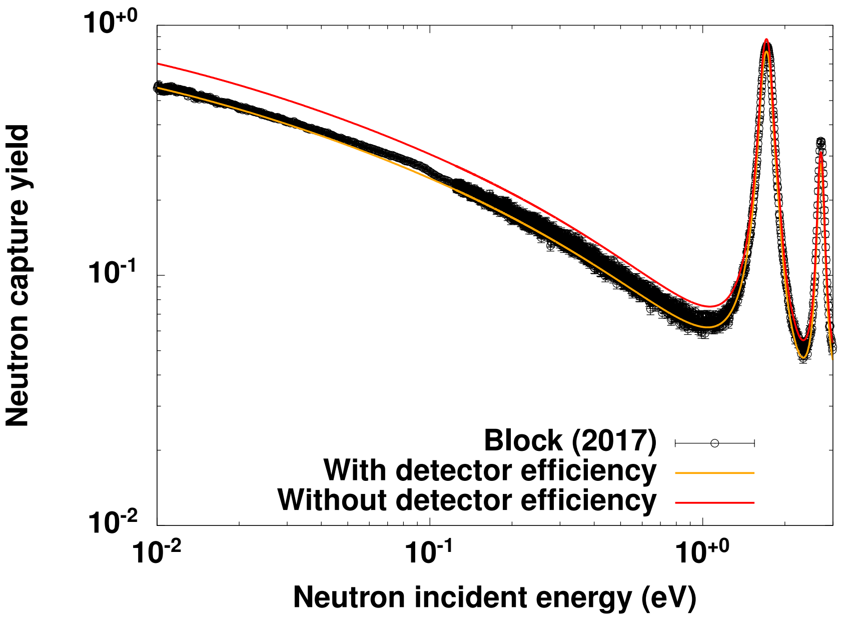


Figure 1: Crunch table derived from Liou's data (left). Impact of detector efficiencies on Block's dat (right).

[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

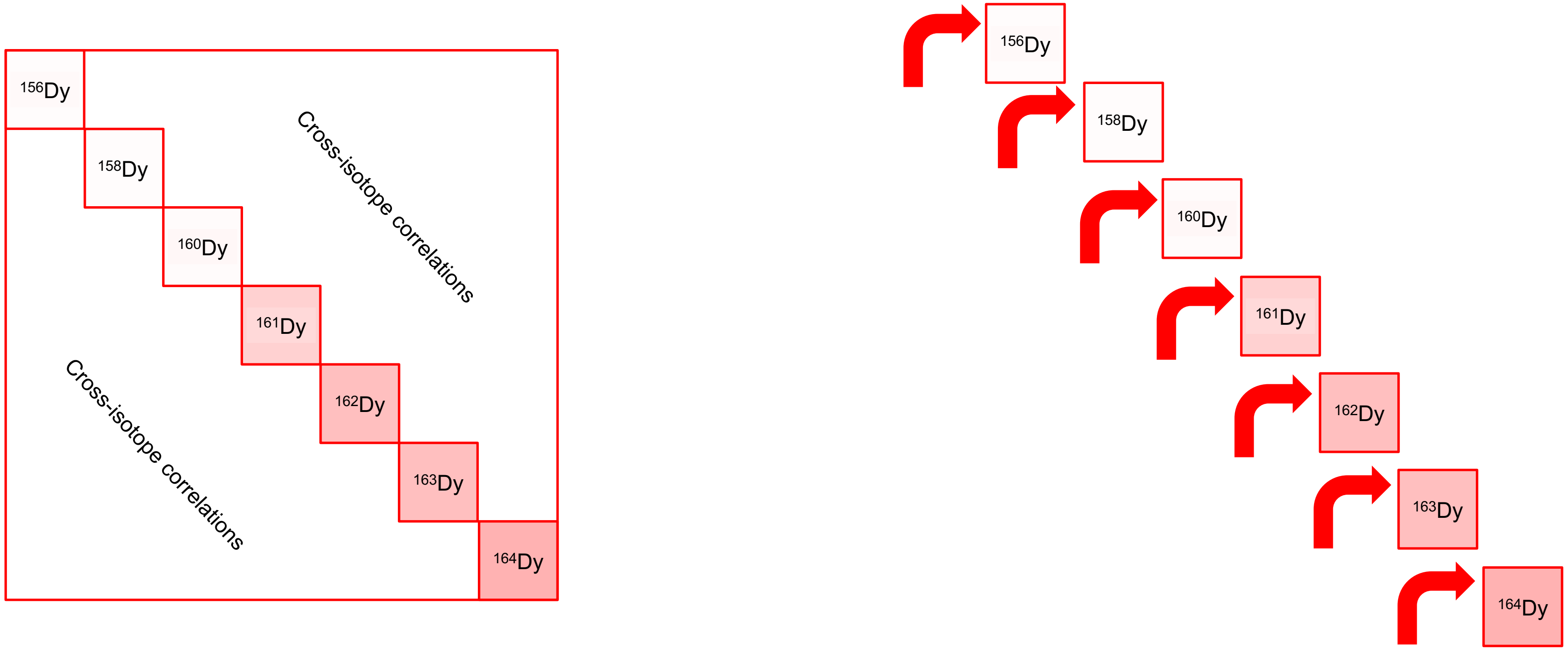


Figure 2: Resonance parameter covariance matrix as derived in the optimization procedure (left). Loss of cross-isotope correlations when single isotope is extracted and reported (right).

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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Collaborators: D. Wiarda, J. McDonnell, C. Chapman, A. Holcomb, J. Brown, G. Arbanas, K. Guber
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** : $B(t) = B_0 + B_1(t) + \ldots$
- **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)

[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.

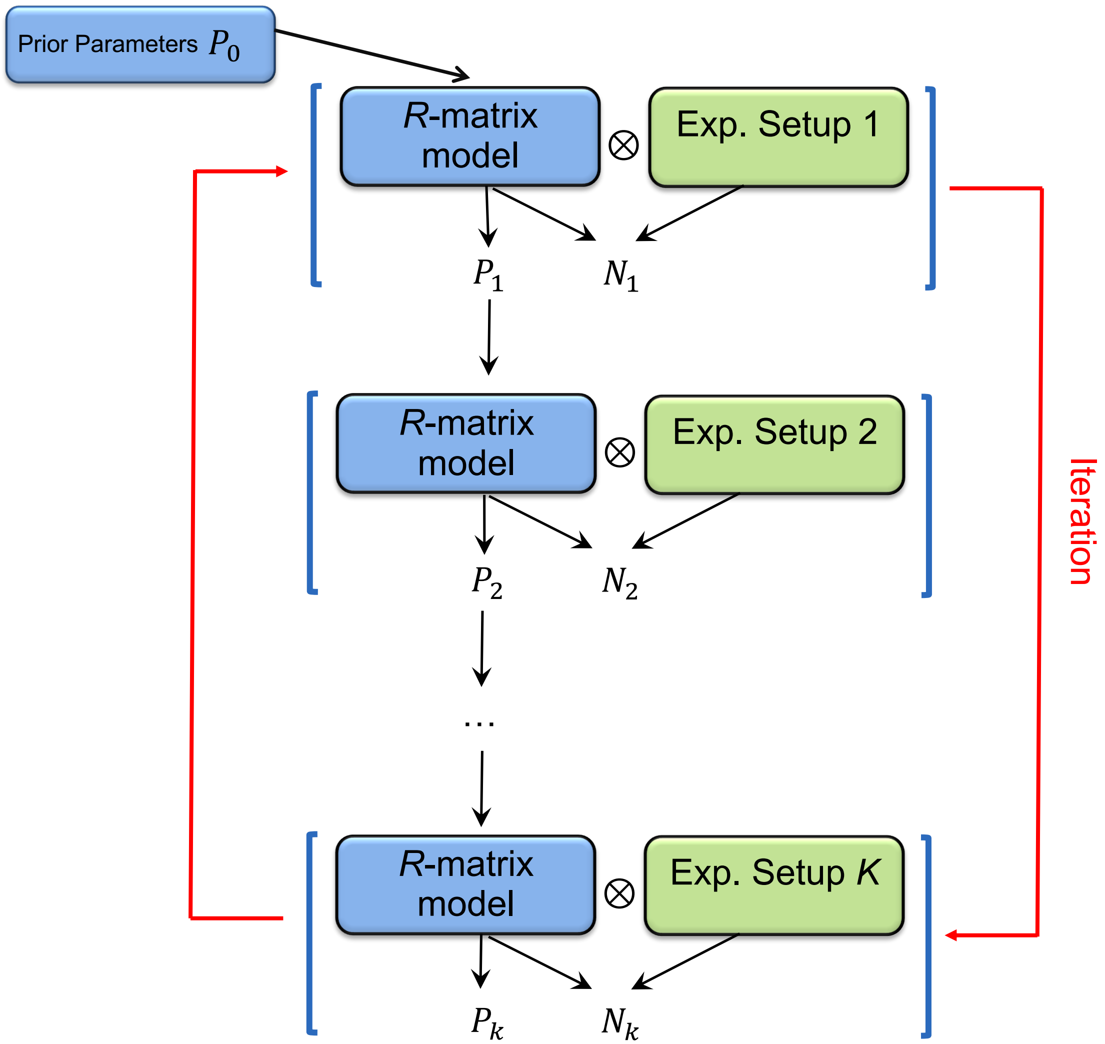
APPENDIX: BASIC QUANTITIES FOR REPRODUCIBILITY

- 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.

APPENDIX: BASIC QUANTITIES FOR REPRODUCIBILITY



- 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

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