Oak Ridge National Laboratory

Reproducibility and Optimization Techniques for Evaluated Data in the Resolved Resonance Region

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OUTLINE

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- Observables Definition
- Typical Cases of Explicit Experimental Effects
- Basic Quantities for Reproducibility
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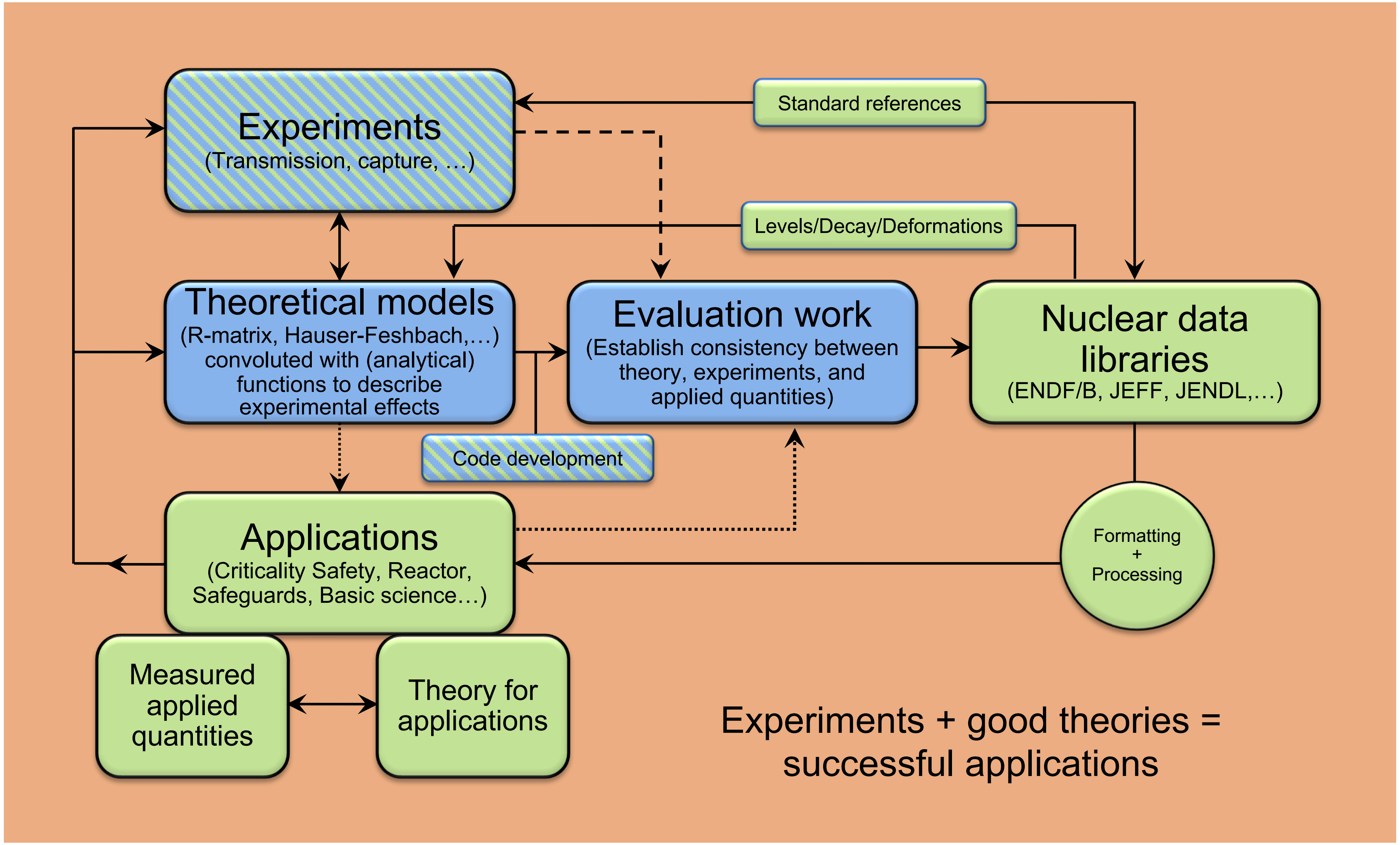
- Conclusions

EVALUATION WORKFLOW SCHEME



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

TYPICAL CASES OF EXPLICIT EXPERIMENTAL EFFECTS[1]

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

$$\tilde{\sigma}(E) = \int_t I(t(E) - t')\,\sigma(E(t');\mathbf{p})dt'$$

$$I(t-t') = \int I_1(t-t_1)dt_1 \left(\prod_{k=1}^{N} \int I_{k+1}(t_k - t_{k+1})dt_{k+1} \right) I_{N+1}(t_{N+1} - t')$$

  $I_k(t)$ 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[23]
- **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

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[1]As implemented in the SAMMY code.

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

[3]**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.

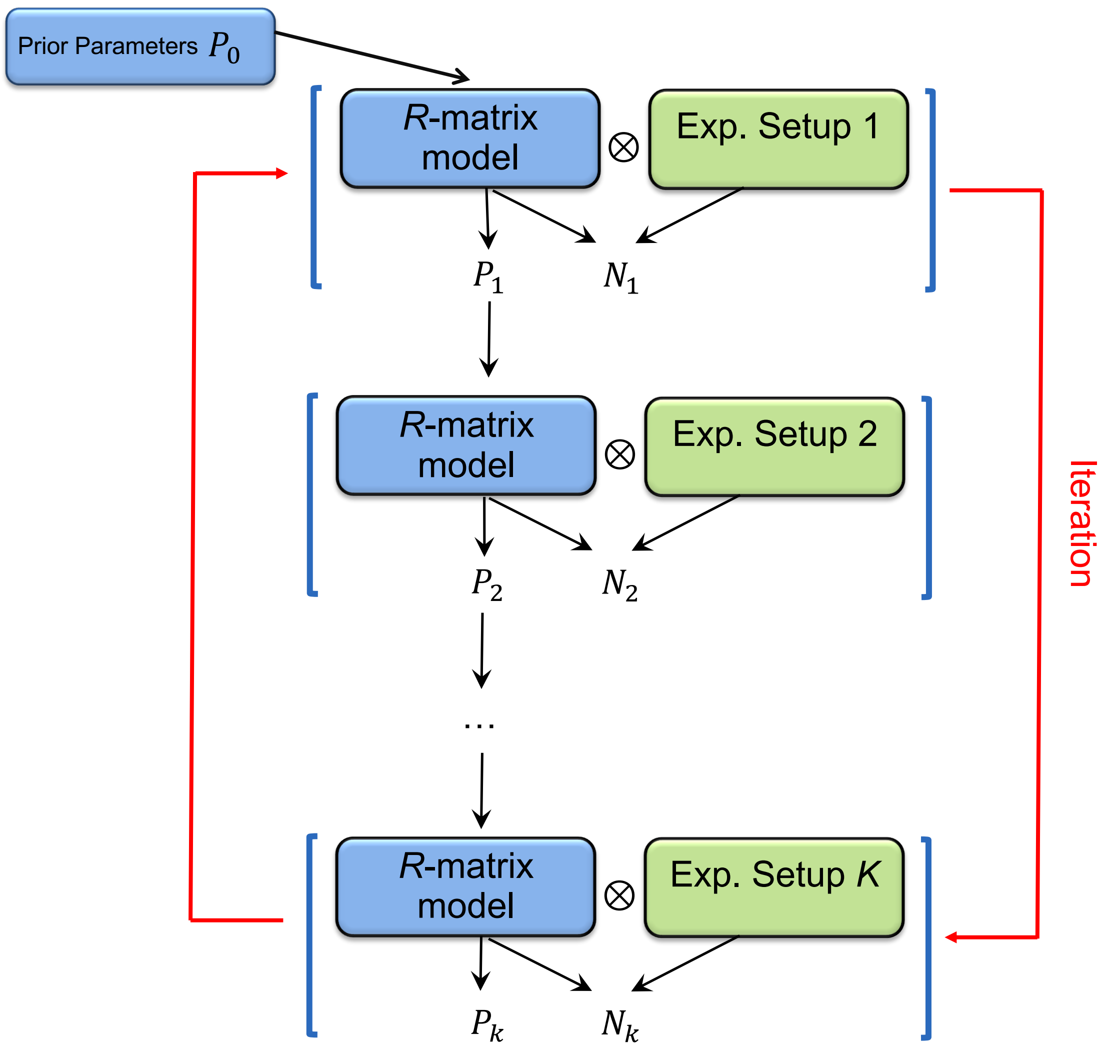
BASIC QUANTITIES FOR REPRODUCIBILITY

- Set of measured data including modifications or corrections: normalization (e.g. neutron capture yield[4]), 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!

Note: ideally, "physical constraints" such as (in)coherent scattering lengths, statistics on the resonance parameters, compatibility between different resonance parameter basis[5], ..., should be included in the optimization procedure

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

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

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

QUESTIONS ON REPRODUCIBILITY

Common problems on the way to reproducibility

Q: How is P_0 (prior set of parameters) generated?

A: Usually taken from existing library, P_0 is modified in the number of levels if the evaluation is extended and corrected in the spin assignment if needed. External function definition is also needed

A: For a fixed number of levels with assigned spin and given "direct" constraints[6], the choice of P_0 should not affect the optimized set of parameters if convergence is achieved and optimal multidimensional mapping is performed

P: Cumbersome/inefficient procedure to impose "indirect" constraints such as a chosen distribution of the resonance parameters

Q: What about the importance of the normalization factors?

A: From the optimization procedure, the correlations between measured data should be obtained. The scaling factors are important to establish consistency among measured data sets and, objectively, the only way to compare measured data

P: Cumbersome/inefficient and time consuming procedure to find convergence if the scaling factors can not be included in the optimization procedure

Q: Is the convergence of the fit fast to achieve?

...

[6]Measured data with uncertainty and correlations.

CONCLUSIONS

- Experimental setup input parameters are basic quantities for reproducibility
- The goal is to increase quality of the evaluated data and decrease time needed for an evaluation
  - Full reproducibility should be achieved efficiently by including any type of constraints in the optimization procedure
  - Improve computational time to reach convergence
- The goal of an automated reproducibility aligns to the goal of “certified” evaluated data, i.e., defined by a well defined metric

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Questions?