

Advancing the Theory of Nuclear Data Evaluations

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Nuclear Data Group

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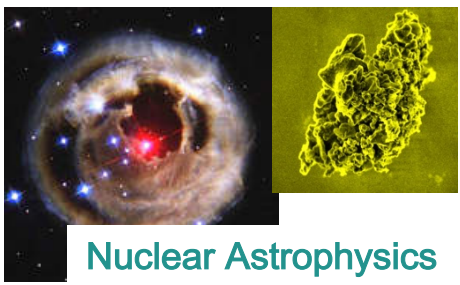
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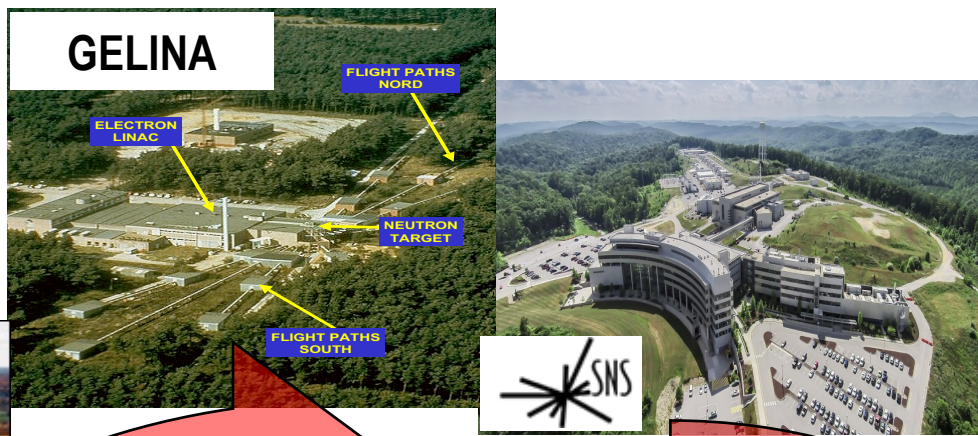
WONDER-2023

International Workshop On Nuclear Data Evaluation for Reactor Applications

Aix-en-Provence, France, June 5-9, 2023.



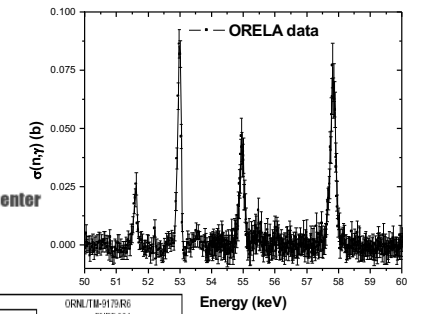
Nuclear Astrophysics



GELINA



Basic Science



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ORNL/TM-9179/R6
ENDF-364

SAMMY: MULTILEVEL R-MATRIX FITS TO NEUTRON DATA USING BAYES' EQUATIONS

SAMMY

Cross-Section Evaluations



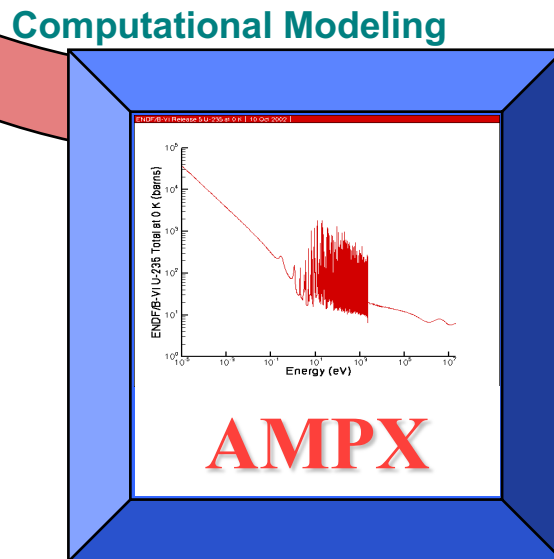
Applications

ORNL Data Support for Nuclear Applications

Computational Modeling

<http://www.ornl.gov/SCALE>

SCALE



Evaluated Nuclear Data Files (ENDF/B)

NNDC

Nuclear Criticality Safety Program (NCSP) Motivation:

- NCSP Mission & Vision, 5-year plans:
 - https://ncsp.llnl.gov/sites/ncsp/files/2021-04/ncsp_mission_vision.pdf
 - <https://ncsp.llnl.gov/program-management/ncsp-five-year-execution-plan>
- I. Uncertainty Quantification
 - Differential Nuclear Data (resolved resonance region (RRR) by SAMMY)
 - Integral Benchmark Experiments
- II. SAMMY Modernization
 - R-matrix formalism

Part I. Theory of evaluated nuclear data (ND) uncertainties

Common *assumptions* used in Bayesian ND evaluations:

1. **Linearity:**

- all models are linear

2. **Normality:**

- all probability distribution functions are normal, i.e., Gaussian

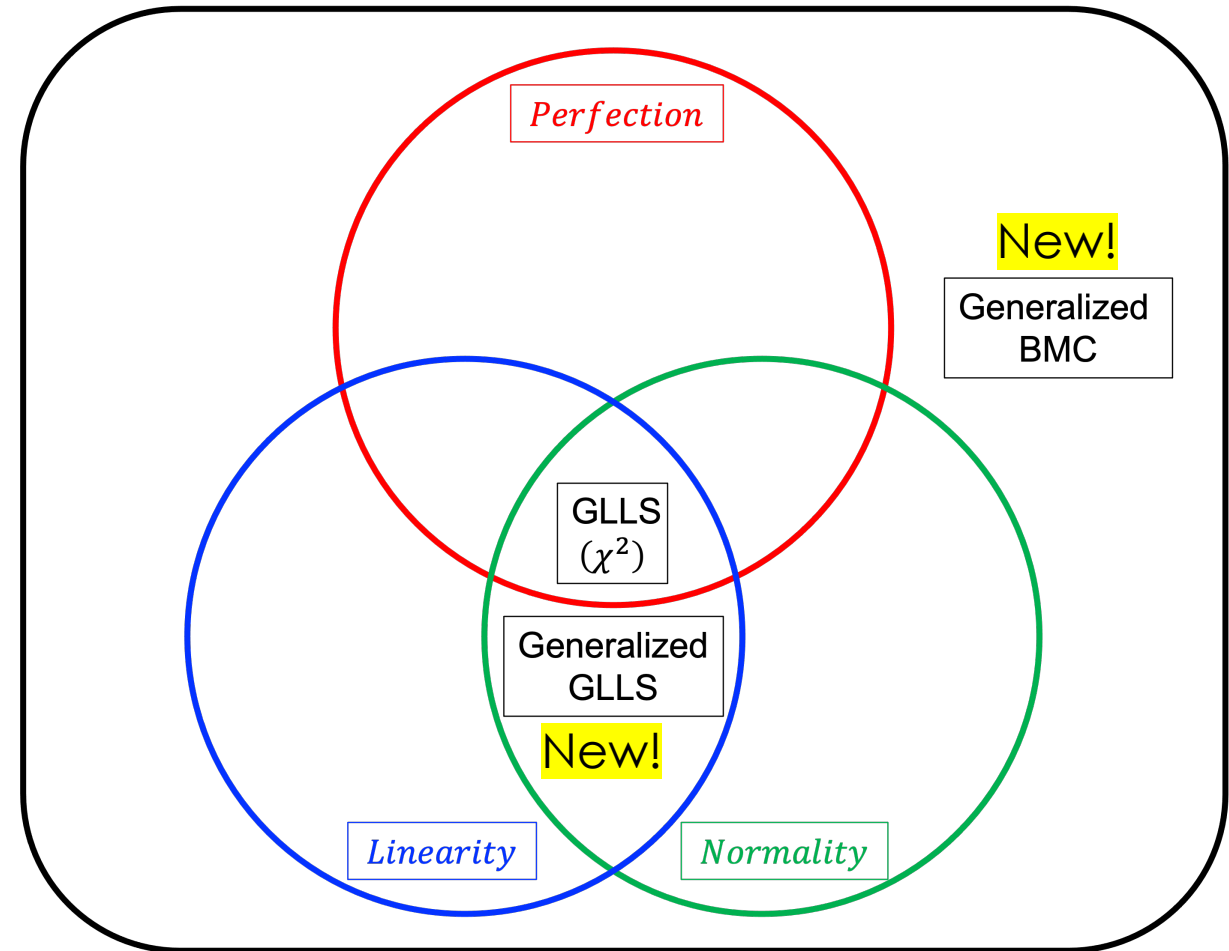
3. **Perfection:**

- a) The model provides a perfect description of the measured data
- b) The data are perfect and complete (*including* the covariances)

These assumptions can now be selectively removed or enforced

- **Linearity** and **Normality**:
 - Removed by, e.g., Metropolis Hastings Monte Carlo (MHMC); known as Bayesian Monte Carlo (BMC)
- **Perfection**:
 - Evaluator can remove this assumption by specifying posterior expectation values and covariance of *deviations* between the model and data

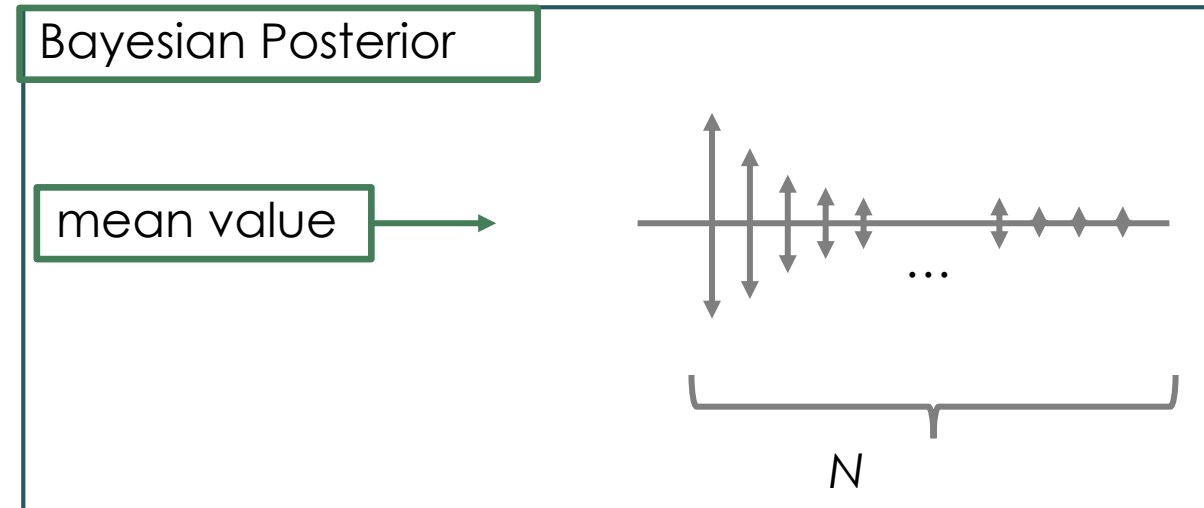
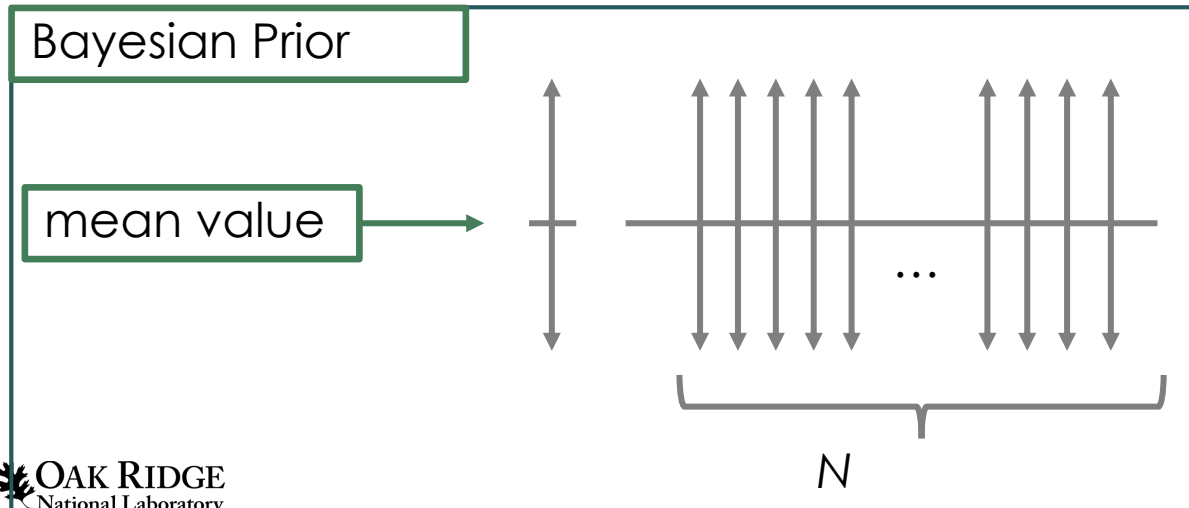
GLLS = Generalized Linear Least Squares
BMC = Bayesian Monte Carlo



Note: everything else being the same, consistency with Bayes' theorem in this framework improves the likelihood of success. Reliability of a given evaluation still depends on evaluator's skill/expertise.

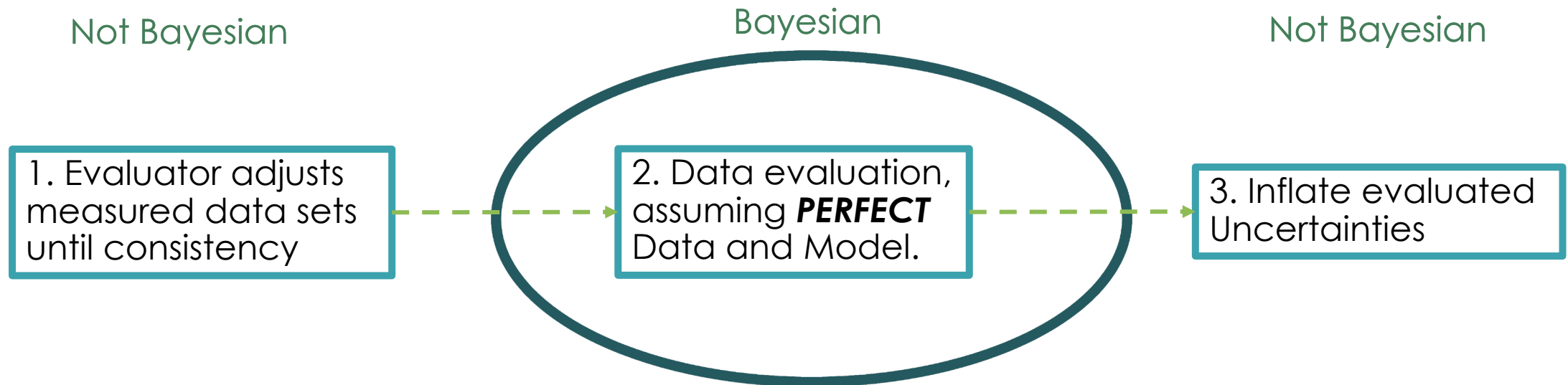
Illustrating a mechanism behind **small** evaluated uncertainties

- Example: suppose a large number (“ N ”) of identical measurements
 - Suppose measurements are identical in value as well as uncertainty
 - This enables focus on evaluated covariance/uncertainty since the mean values are unaffected
 - Suppose that the correlation among measurements is set to 0
 - Bayes’ theorem then yields uncertainty $\rightarrow 0$ as $N \rightarrow$ infinity (illustrated below)
 - Unrealistically small evaluated uncertainties are rectified by inflating them until reasonable
 - The uncertainties are underestimated less apparently for any value of N
- Our Bayesian framework provides tools to address this problem.



Conventional evaluation workflow is not completely Bayesian:

1. Evaluator uses expert judgment to align measured data sets before the evaluation
2. Bayesian evaluation is performed (implicitly) assuming **perfect** data and model
3. Unrealistically small uncertainties are inflated manually afterwards



New framework enables completely Bayesian evaluations:

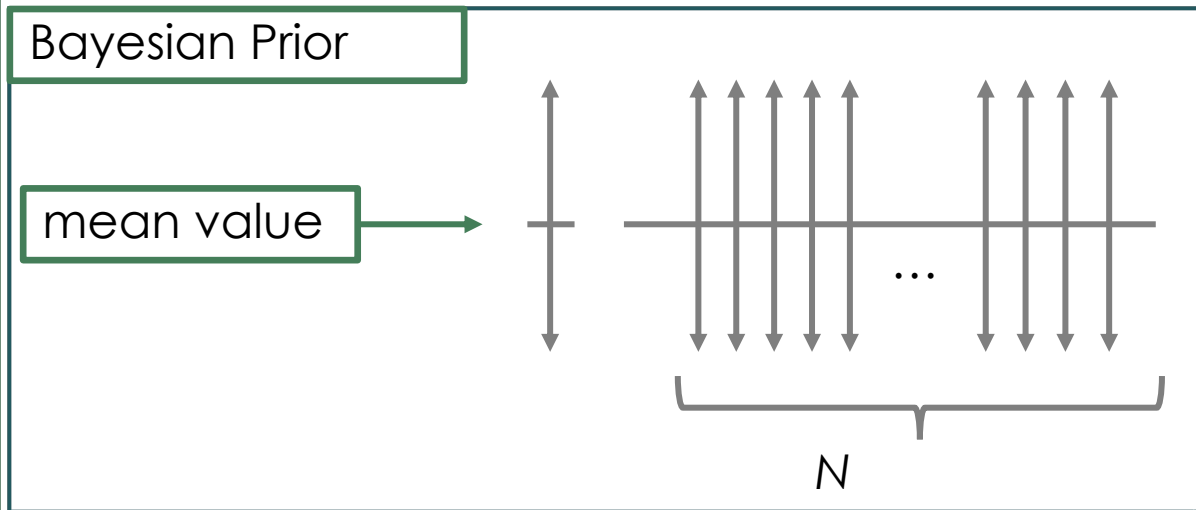
1. Evaluator **estimates** the effect of **imperfections** by **setting** Bayesian **posterior** expectation values of **deviations** as well as their **covariances**
 - **Deviation** is defined as a **difference** between the evaluated data and model
 - Evaluators' **expert judgment** (or **intuition**) now **formally recognized** within Bayes' theorem!
2. Bayesian evaluation is now determined by the **deviations** defined in 1.
 - No need to manually inflate evaluated uncertainties as in Step 3. previously

Bayesian

1. Evaluator assesses imperfections by setting posterior expectation values of deviations

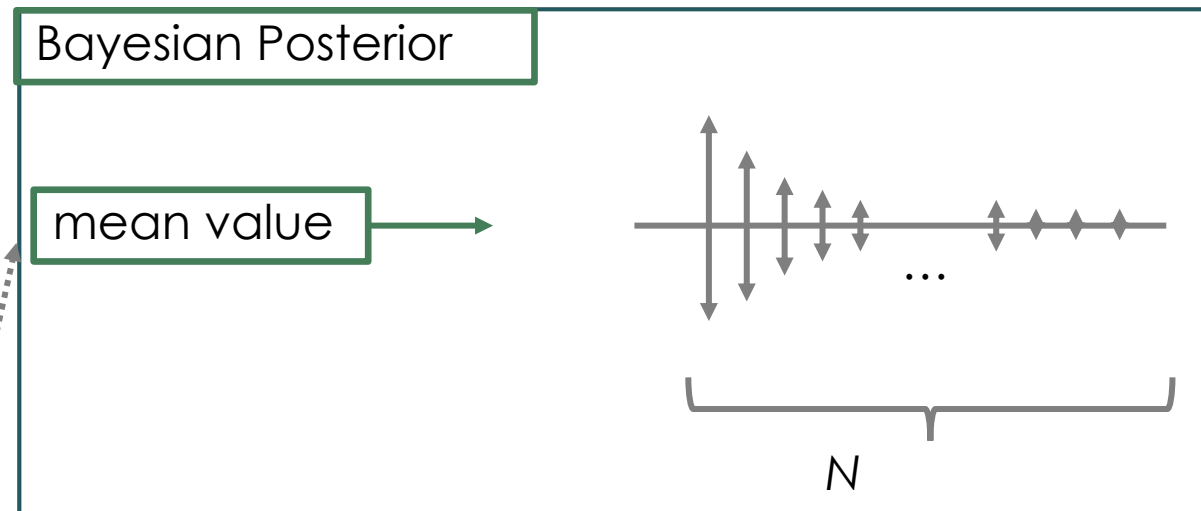
2. Data evaluation, assuming **IMPERFECT** Data and Model.

Illustration cont'd.:

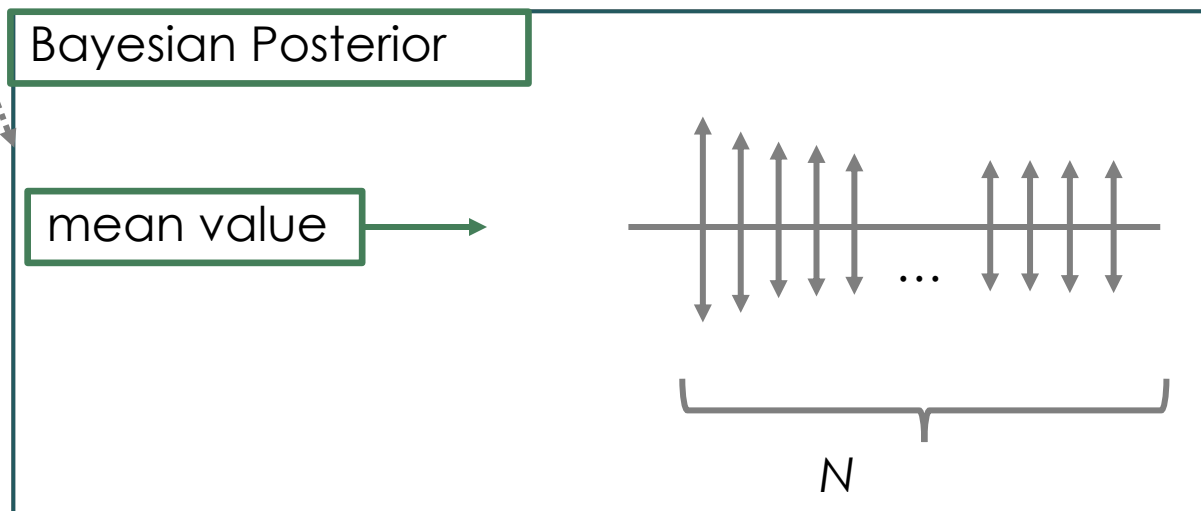


By virtue of setting **NON-zero** constraints on the posterior covariance matrix of deviations between the model and data

Before:



After:



Assumptions or approximations used with Bayes' Theorem

1. The *model and* the prior PDF of *data* are assumed to be perfect
2. The model is approximated by its 1st order (linear) expansion
3. Prior and posterior PDFs are approximated by normal PDFs.

- We recognize that 1. is equivalent to constraining the *posterior* expectation values of δ , and of its covariance matrix, to 0:

$$\langle \delta \rangle' = 0 \quad \Delta' \equiv \langle (\delta - \langle \delta \rangle') (\delta - \langle \delta \rangle')^T \rangle' = \mathbb{0} \quad \delta \equiv \delta(z, T(P)) \equiv T(P) - D \quad z \equiv \begin{pmatrix} P \\ D \end{pmatrix}$$

- We remove 1. by letting evaluator choose values of $\langle \delta \rangle'$ and Δ'
- 2. and 3. can be removed by Metropolis-Hastings Monte Carlo

Overview of approximations used by ORNL codes

Algorithm / Code	$\langle \delta \rangle'$	Δ'	Prior/Post PDF	Cost Function	Minimization
GLLS / SAMMY	0	0	Normal/Normal	Chi ²	Linear (iterative)
GLLS /TSURFER	0	0	Normal/Normal	Chi ²	Linear (single step)
Generalized GLLS	Any	Any	Normal/Normal	Generalized Chi ²	Linear
BMC	Any	Any	Any/any	Posterior PDF	MHMC

- Bayes' theorem with arbitrary constraints:

$$p'(z|\beta\gamma) = p'(z|\gamma\beta) = N' \mathcal{L}(\beta|z\gamma) \times p(z|\gamma)$$

$$\mathcal{L}(\beta|z, \gamma) \leftarrow \mathcal{L}(\langle \delta \rangle', \Delta'|z, \gamma) = e^{-\frac{1}{2}(\delta - \lambda)^\top \mathbf{\Lambda}^{-1}(\delta - \lambda)}$$

- $\beta \leftarrow \{\text{any constraints on posteriors imposed by evaluator}\},$
- $\gamma \leftarrow \{\text{any parameters needed to define the prior PDF, } p(z|\gamma)\}$

Generalized GLLS Framework in TSURFER notation

Using TSURFER-like notation:

$$z \equiv \begin{pmatrix} \alpha \\ m \end{pmatrix}$$

$$\tilde{C}_{zz} = \begin{pmatrix} \tilde{C}_{\alpha\alpha} & \tilde{C}_{\alpha m} \\ \tilde{C}_{m\alpha} & \tilde{C}_{mm} \end{pmatrix}$$

$$\begin{aligned} \tilde{S} &\equiv \nabla_z \tilde{d}^T = \begin{pmatrix} \nabla_\alpha \\ \nabla_m \end{pmatrix} (k(\alpha) - m)^T \\ &= \begin{pmatrix} \nabla_\alpha k(\alpha)^T \\ -\nabla_m m^T \end{pmatrix} = \begin{pmatrix} \tilde{S}_{k\alpha}^T \\ -\mathbb{I} \end{pmatrix}, \quad (\mathbb{I} = \text{identity matrix}) \end{aligned}$$

$$\tilde{C}_{dd} = \tilde{S} \tilde{C}_{zz} \tilde{S}^T$$

α = nuclear data
 m = measured response
 $d = k(\alpha) - m$

■ = implicitly assumed 0 in TSURFER

$$\tilde{C}_{z'z'}^{-1} = \tilde{S} [\tilde{C}_{d'd'}^{-1} - \tilde{C}_{dd}^{-1}] \tilde{S}^T + \tilde{C}_{zz}^{-1}$$

$$z' = z + \tilde{C}_{zz} \tilde{S} \tilde{C}_{dd}^{-1} (\tilde{d}' - \tilde{d})$$

Note: SAMMY uses the GLLS *iteratively*, by re-computing sensitivities in each iteration, as a way to approximately account for non-linearity of the R-matrix formalism.

Benefits of a generalized form of the Bayes' Theorem (BT):

- It could improve evaluations of any data, separately or jointly
 - differential cross sections (SAMMY),
 - integral benchmarks (TSURFER/SAMPLER), ...
- Enables Bayesian Monte Carlo evaluation of large data sets
 - Useful for, e.g., TSL evaluations of SNS data, RRR, ...
- Enables Bayesian evaluation of:
 - inconsistent data sets, and/or
 - defective model
- Conventional BT is recovered when imperfections made to vanish
 - A seamless connection to the BT in SAMMY/TSURFER/SAMPLER
- API implementation in the SCALE code system

For more information on uncertainty evaluation consider:

- ORNL/TM-2022/2448 Technical Report
 - Brown, Jesse M., Arbanas, Goran, Wiarda, Dorothea, and Holcomb, Andrew, “Bayesian Optimization Framework for Imperfect Data or Models”. United States: 2022. <https://doi.org/10.2172/1874643>.
- ANS Winter Meeting 2022:
 - Jesse M. Brown, Goran Arbanas, Hany Abdel-Khalik, Ugur Mertuyurek, William B. Marshall, William A. Wieselquist, “Generalized Bayesian Framework for Evaluation of Integral Benchmark Experiments”, Transactions, Volume 125, Number 1, December 2021, Pages 691-694.
- ND 2022:
 - Jesse M. Brown, Goran Arbanas, Andrew Holcomb, Dorothea Wiarda, “Bayesian Evaluation Framework for Imperfect ^{233}U Data and Models”, Proceedings of the 15. Int.'l Conference on Nuclear Data for Science and Technology (ND2022), Sacramento, California, 21-29 Jul 2022.

Part II. *R*-matrix formalism: Background and Outline

- Classes of nuclear reaction processes, by increasing complexity:
 1. **Direct:** direct channel coupling, direct capture, ...
 2. **Doorway:** Giant Dipole Resonance, Isobar Analogue Resonance, 2p1h, ...
 3. **Compound:** narrow resonances of the Resolved Resonance Region
- Only the *compound* kind parameterized in the extant *R*-matrix
- New *R*-matrix parameterization of direct and doorway processes
 - **Direct:** parameterized exactly, using an idea suggested by Wigner [8]
 - **Doorway:** parameterized analogously to a corresponding *K*-matrix way [1]
- *R*-matrix formalism for evaluations *redagonalizes* parameterization of any many body Hamiltonian, obviating the need for doorways:
 - Elimination of capture channels yields *complex* resonance energies, widths

Non-resonant (or external) direct reactions in R -matrix

- Direct channel coupling is introduced by mixing among channels of the incoming, \mathbf{I} , and the outgoing, \mathbf{O} , formerly diagonal matrices of wave functions: $\Psi = \mathbf{I}\mathbf{y} + \mathbf{O}\mathbf{x}$

$$\mathbf{x} = -\mathbf{U}\mathbf{y}$$

$$\mathbf{y} \leftarrow \mathcal{M}\mathbf{y} \quad \mathbf{x} \leftarrow \mathcal{M}^*\mathbf{x}$$

where \mathcal{M} is a unitary matrix parameterizing direct reactions.

A corresponding scattering matrix \mathbf{U} is then found to be:

$$\mathbf{U}_{\mathcal{M}} = \mathcal{M}^{\top}\mathbf{U}\mathcal{M},$$

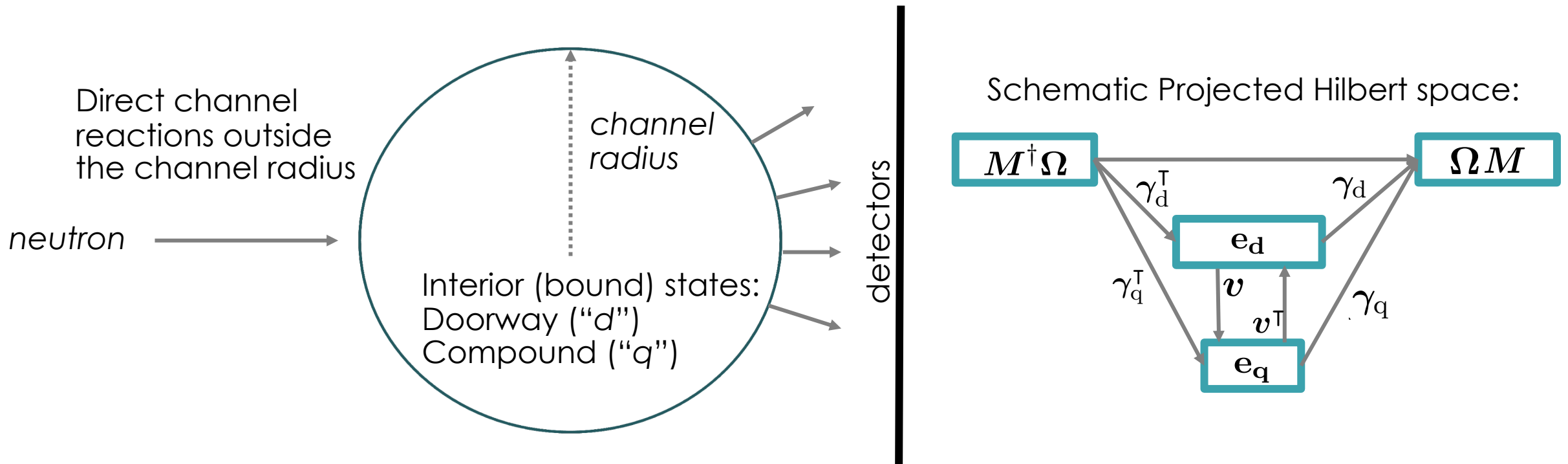
$$\mathcal{M}^{-1} = \mathcal{M}^{\dagger} \equiv (\mathcal{M}^*)^{\top}$$

Suggested by Wigner in a paper on generalized Euler angles [8].

- Its analogue in the T -matrix by H. Feshbach in Eq. (III.2.26) of [7] is an example of similarities among R -, T -, K -matrix formalisms.

Introducing doorway states into R -matrix formalism

- Generalized R -matrix parameterization of doorway states (“ d ”):
 - Comparison of formal expressions for doorway state K -matrix (derived by Feshbach’s projection operator formalism [1,2]) to the Brune’s alternative R -matrix [9] has helped uncover an analogous R -matrix parameterization (using a simple derivation shown on the next slide):



(This is another example of leveraging similarities among the R -, T -, K -matrix formalisms.)

Doorway state parameterization in conventional R-matrix [3]

$$\begin{aligned} \mathbf{R} &= \boldsymbol{\gamma}^\top \mathbf{Q} \boldsymbol{\gamma}, & \text{where:} & & \boldsymbol{\gamma} &= \langle \lambda | c \rangle, & \text{Projection:} & & \langle \lambda | \leftarrow \begin{pmatrix} \langle d | \\ \langle q | \end{pmatrix}, \\ \mathbf{Q}^{-1} &= \mathbf{e} - E\mathbf{1}, & & & \mathbf{e} &= \langle \lambda | \mathbf{H}_0 | \lambda \rangle, & & & \end{aligned}$$

$$\begin{aligned} \text{yields:} & & \boldsymbol{\gamma} \leftarrow \begin{pmatrix} \gamma_d \\ \gamma_q \end{pmatrix}, & \text{where} & & \mathbf{e} \leftarrow \begin{pmatrix} \mathbf{e}_d & \mathbf{v} \\ \mathbf{v}^\top & \mathbf{e}_q \end{pmatrix}, & \text{where} & & \\ & & \gamma_d \equiv \langle d | c \rangle & \text{and} & \gamma_q \equiv \langle q | c \rangle & \mathbf{v} \equiv \langle d | \mathbf{H} | q \rangle, & \mathbf{e}_d \equiv \langle d | \mathbf{H} | d \rangle, & \mathbf{e}_q \equiv \langle q | \mathbf{H} | q \rangle \end{aligned}$$

- \mathbf{Q}^{-1} : a 2x2 block matrix of *expectation values of projected $\mathbf{H} - E\mathbf{1}$*
 - The projected R-matrix is simpler than the projected T-,K-matrix in [1, 2]
- $\mathbf{v} \equiv \langle d | \mathbf{H} | q \rangle$ is a doorway-compound coupling parameter matrix
- Doorway states are far *fewer* and *wider* than compound states
 - The new doorway R-matrix parameters are: \mathbf{e}_d , γ_d , and \mathbf{v}
 - Extensible to multistep reactions by adding new subspaces into $\langle \lambda |$
 - Single-particle resonances for direct processes, 3p2h for "hallway" states, ..., CN.

Elimination of capture channels yields an *effective* R-matrix:

Eqs. (X.1.7-9a) of Lane and Thomas (LT) express a reduced R -matrix as

$$\mathcal{R} = \gamma_r^\top \mathbf{A}^{-1} \gamma_r \quad (1)$$

$$= \gamma_r^\top [\mathbf{e} - \boldsymbol{\xi} - E\mathbf{1}]^{-1} \gamma_r, \quad (2)$$

where¹

$$\boldsymbol{\xi} \equiv \gamma_e \mathbf{L}'_e \gamma_e^\top, \quad (3)$$

is a symmetric matrix, and where $\mathbf{L}'_e = \mathbf{L}_e^0 \equiv \mathbf{L}_e - \mathbf{B}_e$ for $\mathbf{R}_{ee}^0 = 0$, as in Section X.1 of LT. In order to show how an *effective* set of reduced R -matrix parameters may become complex-valued, a singular value decomposition (SVD) of a *symmetric*² matrix $\mathbf{e} - \boldsymbol{\xi}$ is assumed to exist, *i.e.*,

$$\mathbf{e} - \boldsymbol{\xi} = \mathbf{v} \boldsymbol{\epsilon} \mathbf{v}^\top, \quad (4)$$

where $\mathbf{v} \mathbf{v}^\top = \mathbf{1}$ and $\boldsymbol{\epsilon}$ is diagonal³. Utilizing this SVD in Eq. (2) yields an equivalent expression for the reduced R -matrix of LT,

$$\mathcal{R} = \gamma_r^\top [\mathbf{v} \boldsymbol{\epsilon} \mathbf{v}^\top - E\mathbf{1}]^{-1} \gamma_r \quad (5)$$

$$= \gamma_r^\top [\mathbf{v} (\boldsymbol{\epsilon} - E\mathbf{1}) \mathbf{v}^\top]^{-1} \gamma_r \quad (6)$$

$$= \gamma_r^\top (\mathbf{v}^\top)^{-1} [\boldsymbol{\epsilon} - E\mathbf{1}]^{-1} \mathbf{v}^{-1} \gamma_r \quad (7)$$

$$= (\gamma_r^\top \mathbf{v}) [\boldsymbol{\epsilon} - E\mathbf{1}]^{-1} (\mathbf{v}^\top \gamma_r) \quad (8)$$

$$= \mathbf{g}_r^\top [\boldsymbol{\epsilon} - E\mathbf{1}]^{-1} \mathbf{g}_r \quad (9)$$

where

$$\mathbf{g}_r \equiv \mathbf{v}^\top \gamma_r; \quad (10)$$

$(\boldsymbol{\epsilon}, \mathbf{g}_r)$ may be viewed as an *effective* reduced R -matrix parameter set which could be optimized independently of the formal reduced parameter set (\mathbf{e}, γ_r) ;

Taken from a draft of our WONDER 2023 proceedings.

Note: the form of the the R-matrix formalism remains the same; the effective parameters become complex-valued.

Unlike the conventional Reich-Moore approx. [5], the total capture cross section is exact, as in [6].

¹Labels r and e refer to “retained” and “eliminated” subset of channels, respectively.

²The same form of SVD holds for *complex*-valued symmetric matrix, for which \mathbf{v} and $\boldsymbol{\epsilon}$ may be complex-valued.

³Note that a symmetric matrix \mathbf{e} need not be diagonal.

Outlook:

- Other potential applications of this R -matrix parameterization:
 - Refining the assumptions of the Random Matrix Theory in nuclear physics by investigating the effect of direct and doorway states on statistical distributions of resonance widths (Porter-Thomas), energy spacing (Wigner)
 - A new way for modeling *multistep* (3p2h “hallway”, ...) nuclear reactions
- Look for other ways to exploit similarities among various formalisms
- To be implemented into SAMMY [4] after code modernization
 - See the presentation by Doro Wiarda (ORNL) on SAMMY modernization
 - https://ncsp.llnl.gov/sites/ncsp/files/2023-03/60_sammy_tpr_2023.pdf

SAMMY and all dependencies are freely available



SAMMY 

Project ID: 6231 

<https://code.ornl.gov/RNSD/SAMMY>



SCALE-Public

Project ID: 11984 

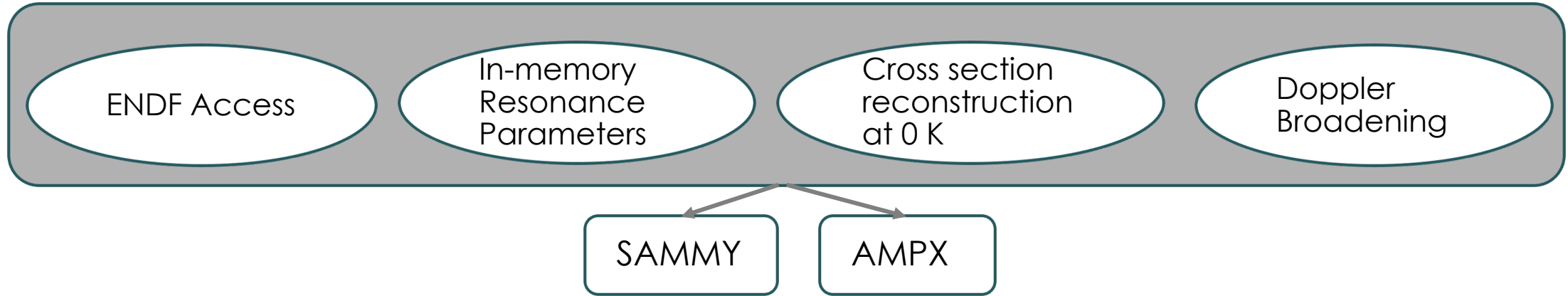
<https://code.ornl.gov/scale/code/scale-public>

- The build system has been updated to automatically retrieve and build all dependencies.
- The README has been updated.

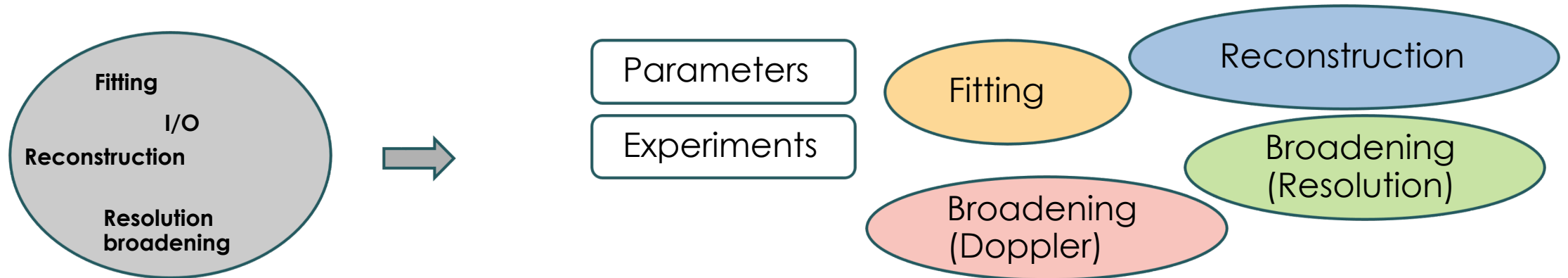
SAMMY Modernization and Maintenance goals

We plan to modernize as follows:

- Write code once and reuse

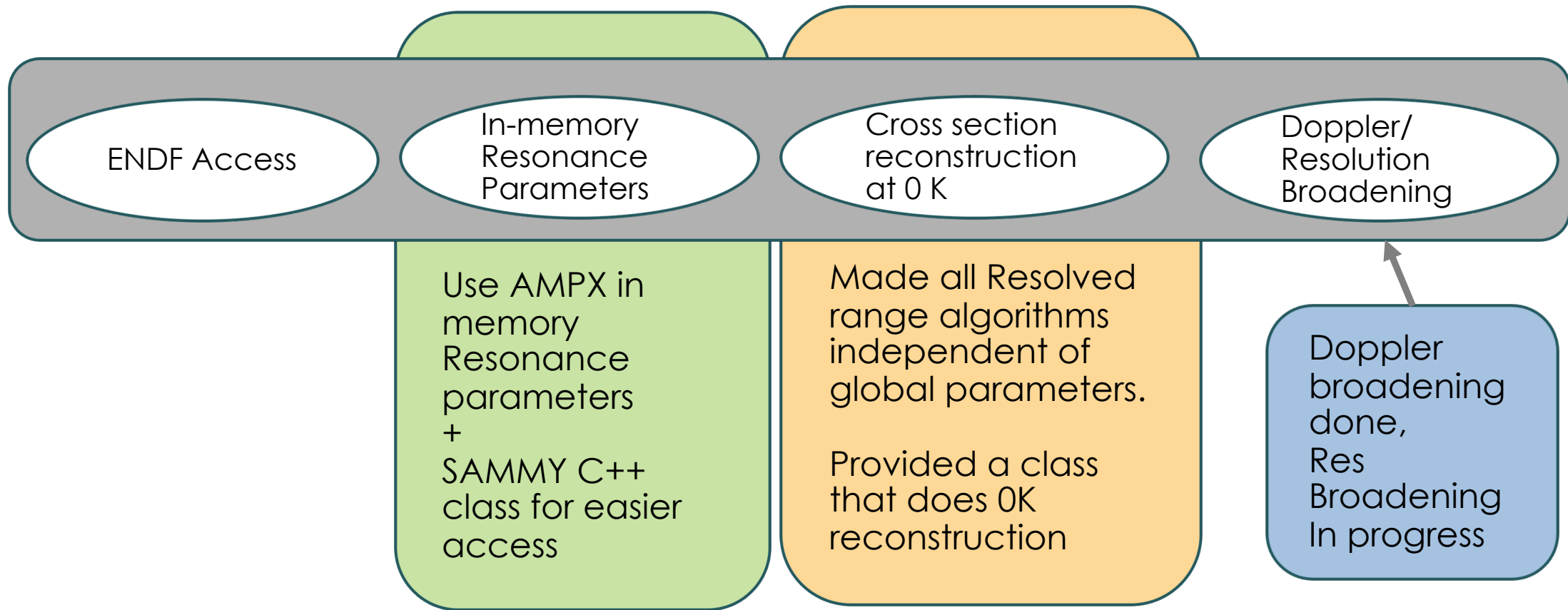


- Transform SAMMY into a modular code, with independent modules with clear interfaces.



- Add new features, which is now easier as only the desired module needs to be changed.

SAMMY Modernization Accomplishments



These modernizations will make adding new R-Matrix features easier as changes will be localized to the relevant part of the code as no global parameters are used. In addition, this will allow more parallelization of the code in the future.

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- Dr. Douglas Bowen (ORNL)

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