USER'S GUIDE TO SAMINT: A CODE FOR NUCLEAR DATA ADJUSTMENT WITH SAMMY BASED ON INTEGRAL EXPERIMENTS

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Reactor and Nuclear Systems Division

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FOREWORD

The code SAMINT is supplementary to the code SAMMY. Consequently, this user's manual assumes that the reader is intimately familiar with SAMMY. In particular, this user's manual uses some of the nomenclature used in the SAMMY user's manual, such as the alphanumeric commands given in the SAMMY input files. Following the SAMMY user's manual format, the necessary commands to be included in the SAMMY input files will be presented like so,

CROSS SECTION COVARIance matrix is wanted

where the mixed case of the letters indicates only the absolutely required text.

ACRONYMS

C/E	Computed k-eigenvalue divided by the Experimental k-egienvalue
CE	Continuous-energy
GLLS	Generalized Linear Least Squares
ICSBEP	International Criticality Safety Benchmark Experiments Project

ACKNOWLEDGMENTS

1 INTRODUCTION

The purpose of this project is to couple differential and integral data evaluation in a continuous-energy framework. More specifically, the goal is to use the Generalized Linear Least Squares (GLLS) methodology employed in TSURFER to update the parameters of a resolved resonance region evaluation directly. Recognizing that the GLLS methodology in TSURFER is identical to the mathematical description of the simple Bayesian updating carried out in SAMMY [Larson 2008], the computer code SAMINT was created to help use the mathematical machinery of SAMMY to update resolved resonance parameters based on integral data. Minimal modifications of SAMMY are required when used with SAMINT to make resonance parameter updates based on integral experimental data.

The code SAMINT is intended to be executed in the middle of a sequence of SAMMY runs. This is described in detail in Sect. 3. Code input instructions can be found in Sect. 4. Section 5 gives some miscellaneous details about the coding of SAMINT. Finally, Sect. 6 documents an existing test case, a use of the code to improve the resolved resonance region evaluation of ^{56}Fe.

2 METHODS

The CE TSUNAMI-3D module of the SCALE code package is able to produce binned sensitivity coefficients of the integral system eigenvalue to the different reaction cross sections based on continuous-energy physics. We define the relative sensitivity coefficient S_{ijn} of the eigenvalue k_i of system i with respect to partial cross section $\sigma_j(E)$ for reaction j in energy bin n as,

$$S_{ijn} = \frac{\left\langle \sigma_j(E) \right\rangle_n}{k_i} \frac{\partial k_i}{\partial \left\langle \sigma_j(E) \right\rangle_n} \ . \tag{1}$$

In the SAMMY Bayesian updating process, the derivative of the continuous-energy reaction cross section $\sigma_j(E)$ with respect to resonance parameter P_t is needed and therefore calculated by SAMMY. We define this derivative as,

$$G_{jt}(E) = \frac{\partial \sigma_j(E)}{\partial P_t} \ . \tag{2}$$

A very fine energy mesh is used for the calculations, allowing the following two approximations:

$$\sigma_j(E_n) \quad \approx \quad \left\langle \sigma_j(E) \right\rangle_n \ ; \tag{3}$$

$$G_{jt}(E_n) = \frac{\partial \sigma_j(E_n)}{\partial P_t} \quad \approx \quad \frac{\partial \left\langle \sigma_j(E) \right\rangle_n}{\partial P_t} \ , \tag{4}$$

where the variable E_n corresponds to the average energy of the energy bin n. Generation of the energy grid used to make the approximations in Equations 3 and 4 will be discussed in Sect. 3. The sensitivity of the integral system eigenvalue k_i to the resonance parameter P_t is then

$$\frac{\partial k_i}{\partial P_t} = \sum_j \sum_n \frac{k_i}{\sigma_j(E_n)} S_{ijn} G_{jt}(E_n) \ . \tag{5}$$

We have already pointed out in Sect. 1 that TSURFER and SAMMY use the same mathematical model, the GLLS methodology, to make their updates. The GLLS methodology is independent of the physics of the problem. All one needs is a set of a priori parameters, an optional a priori covariance matrix, a vector of derivatives of the *theory* with respect to the parameters and a set of experimental data and optionally, an associated covariance matrix.

We will use the SAMMY nomenclature to introduce the mathematical GLLS equations, and then we will describe what each of the mathematical variables corresponds to for SAMMY and TSURFER. Finally, we will present the basic linear algebra that went into SAMINT to use the SAMMY mathematical machinery to update resonance parameters based on integral data without any changes to the underlying SAMMY machinery.

The GLLS equations in SAMMY are written and calculated as follows,

$$
\begin{aligned}
M' &= (M^{-1} + W)^{-1} \ ; \tag{6} \\
W &= G^t V^{-1} G \ ; \tag{7} \\
P' &= P + M' Y \ ; \tag{8} \\
Y &= G^t V^{-1} (D - T) \ , \tag{9}
\end{aligned}
$$

where the variables are defined in the mathematical context as follows and primes indicate posterior values (the size of each variable is indicated in parenthesies):

P = parameters (1 × number of parameters);

D = data (1 × number of energy points);

T = *theory* (1 × number of energy points);

G = derivative of the *theory*, T, with respect to the parameters, P (number of parameters × number of energy points);

M = parameter covariance matrix (number of parameters × number of parameters); and

V = the data covariance matrix (number of energy points by number of energy points).

The variables W and Y are simply intermediate values in the GLLS equations. Note that this is not the only possible representation of the GLLS equations. It is only one of three variants presented in SAMMY. This particular version is referred to at the "M+W" version in SAMMY. TSURFER presents the GLLS equations in its own nomenclature. However, all of the variants can be analytically shown to give the same results.

TSURFER, in its current state, operates in the multi-group formalism and applies changes to multi-group reaction cross sections. Let us imagine that we had a continuous-energy TSURFER code (let's call it *CE TSURFER* in italicized font to remind ourselves that it is only a hypothetical code) that changed resonance parameters instead of multi-group cross sections. The variable P above would then be the resonance parameters, and the variable M would be the resonance parameter covariance matrix. This is the same as SAMMY. Therefore, only three differences between the SAMMY and *CE TSURFER* definitions for the above variables would remain.

Table 1. Differences between SAMMY and *CE TSURFER* in the definition of the GLLS variables

GLLS	SAMMY	*CE TSURFER*
G	G_{jt}	$\frac{\partial k_i}{\partial P_t}$
V	Differential data covariance matrix	Integral data covariance matrix
$(D - T)$	Disagreement in partial cross sections	Disagreement in eigenvalues

Notice that redefining the three variables described in Table 1 only affects the calculation of the intermediate variables W and Y from the GLLS equations. The code SAMMY has an option to read in previously generated W and Y matrices and perform the resonance parameter update based on Equations 6 and 9. Therefore, the whole idea of SAMINT is to read in G_{jt} and $\sigma_j(E)$ from SAMMY, combine it with S_{ijn} and k_i from CE TSUNAMI-3D and combine them as described above to calculate $\partial k_i/\partial P_t$. Further, SAMINT reads $k_e \pm \delta k_e$ and an integral data correlation matrix and calculates the W and Y matrices.

The linear algebra behind SAMINT is,

$$W \;=\; \left(\frac{\partial k_i}{\partial P_t}\right)^{\dagger} (\delta k_e C_{kk} \delta k_e)^{-1} \left(\frac{\partial k_i}{\partial P_t}\right) \; ; \tag{10}$$

$$Y \;=\; \left(\frac{\partial k_i}{\partial P_t}\right)^{\dagger} (\delta k_e C_{kk} \delta k_e)^{-1} (k_e - k_c) \, , \tag{11}$$

where C_{kk} is the integral experiment correlation matrix, k_e is the experimentally measured eigenvalue and k_c are the calculated eigenvalues.

2.1 UPDATING η

The reactor physics parameter η is defined as,

$$\eta = \frac{\bar{\nu}\sigma_f}{\sigma_f + \sigma_\gamma} \, , \tag{12}$$

where $\bar{\nu}$ is the multiplicity for fission. In practice, η is usually used to update $\bar{\nu}$ based on integral experimental data.

As previously discussed, the GLLS methodology (or Bayesian updating) does not depend on the physical interpretation of the mathematical variables. Using the GLLS methodology, SAMINT is able to calculate the reactor physics parameter, η, for a given isotope such that it will satisfy the integral benchmark experiments in the least-squares way. The mathematical concepts behind updating η and updating the resonance parameters to better fit the integral benchmarks are exactly the same. However, the implementation in SAMINT is slightly different. The main difference is that to update η, SAMINT carries all of the computational burden rather than handing off some of it to SAMMY. The details of this discussion are given in Sect. 3.

To interpret Eqs. $6 - 9$ in the scope of η, we define each of the variables as follows,

$\text{P} = \eta(E_i),$

$\text{D} = k_e,$

$\text{T} = k_c,$

$\text{G} = \partial k / \partial \eta,$

$\text{M} = C_{\eta\eta},$

$\text{V} = C_{kk},$

where $C_{\eta\eta}$ is the η covariance matrix relating $\eta(E_i)$ to $\eta(E_j)$; it can be generated by SAMMY based on the resonance parameter covariance matrix.

The above definitions make it clear that computing an updated value of η is not difficult if we have $\partial k / \partial \eta$. Unfortunately, $\partial k / \partial \eta$ does not come easy. It must be derived from the sensitivity coefficients available from the sensitivity analysis codes and the continuous-energy cross sections that we calculate with SAMMY.

We can write,

$$\frac{\partial k}{\partial \eta} = \frac{\partial k}{\partial \sigma_\gamma}\frac{\partial \sigma_\gamma}{\partial \eta} + \frac{\partial k}{\partial \sigma_f}\frac{\partial \sigma_f}{\partial \eta} + \frac{\partial k}{\partial \bar{\nu}}\frac{\partial \bar{\nu}}{\partial \eta} \, . \tag{13}$$

We calculate the analytic partial derivatives,

$$\frac{\partial \sigma_\gamma}{\partial \eta} = \frac{-\bar{\nu}\sigma_f}{\eta^2} \ ; \tag{14}$$

$$\frac{\partial \sigma_f}{\partial \eta} = \frac{\bar{\nu}\sigma_\gamma}{(\bar{\nu} - \eta)^2} \ ; \tag{15}$$

$$\frac{\partial \bar{\nu}}{\partial \eta} = \frac{\sigma_\gamma + \sigma_f}{\sigma_f} \ . \tag{16}$$

Remembering that the relative sensitivity coefficient is defined as,

$$S_{\sigma_x} = \frac{\langle \sigma_x \rangle}{k} \frac{\partial k}{\partial \langle \sigma_x \rangle} \ . \tag{17}$$

it can be shown that,

$$\frac{\partial k}{\partial \eta} = \frac{k}{\eta} \left[\left(\frac{\sigma_f + \sigma_\gamma}{\sigma_\gamma} \right) (S_f - S_\gamma) + S_{\bar{\nu}} \right] \ . \tag{18}$$

2.2   ITERATIVE PROCEDURE

The GLLS procedure involves a linearity assumption which greatly restricts it area of application. In other words, if the initial guess is not *close* to the correct answer, the GLLS procedure may diverge. In SAMMY, an iterative procedure is described to help alleviate some of the restrictiveness of the linearity assumption. This is very necessary as, in our problem, we are faced with two non-linearities:

- The cross sections are not linearly dependent on the resonance parameters.

- The calculated eigenvalues are generally not strictly linearly dependent on the cross sections.

In this subsection, we reformulate the iterative procedure described in Sect. IV.A.3 of the SAMMY user's manual in terms of our choice of variables. Further sections in this manual will describe how to use the iterative updating methodology with SAMMY and SAMINT when fitting integral experimental data. Finally, note that this iterative capability takes SAMMY and SAMINT beyond the mathematical realm of TSURFER. TSURFER only implements the non-iterative form of the GLLS equations that have the previously described convergence problems.

Equation IV A3.3 from the SAMMY manual states,

$$M^{(n+1)} = (M^{(0)-1} + W^{(n)})^{-1} \ ; \tag{19}$$

$$W^{(n)} = G^{(n)\dagger} V^{-1} G^{(n)} \ ; \tag{20}$$

$$P^{(n+1)} = P^{(0)} + M^{(n+1)} Y^{(n)} \ ; \tag{21}$$

$$Y^{(n)} = G^{(n)\dagger} V^{-1} [D - T^{(n)} - G^{(n)}(P^{(0)} - P^{(n)})] \ , \tag{22}$$

where the superscript in parentheses indicates the iteration index. Now in the notation to update resonance parameters based on integral experiments,

6

$$M^{(n+1)} = (M^{(0)-1} + W^{(n)})^{-1} \ ; \tag{23}$$

$$W^{(n)} = \left(\frac{\partial k}{\partial P^{(n)}}\right)^{\dagger} (\delta k_e C_{kk} \delta k_e)^{-1} \left(\frac{\partial k}{\partial P^{(n)}}\right) \ ; \tag{24}$$

$$P^{(n+1)} = P^{(0)} + M^{(n+1)} Y^{(n)} \ ; \tag{25}$$

$$Y^{(n)} = \left(\frac{\partial k}{\partial P^{(n)}}\right)^{\dagger} (\delta k_e C_{kk} \delta k_e)^{-1} \left[k_e - k_c^{(n)} - \left(\frac{\partial k}{\partial P^{(n)}}\right)(P^{(0)} - P^{(n)})\right] \ . \tag{26}$$

Therefore, in order to iterate, we need to perform the following changes:

1. Evaluate the derivative of the eigenvalue of each integral experiment at the intermediate resonance parameter values, $P^{(n)}$.

2. Include the additional term in the last equation in the square braces.

3. Remember to provide the initial resonance parameters and covariance matrix even though the derivatives are evaluated at the intermediate resonance parameter values.

To be absolutely correct, one must regenerate the cross-section libraries and all of the sensitivity data files for each iteration of the resonance parameters, such that the term $(\partial k/\partial P^{(n)})$ is properly represented. This is indeed the only safe way! However, generating sensitivity data files is currently quite computationally costly for real-world problems. Therefore, we suggest that the user consider whether the sensitivity data file will change significantly with the new updated cross sections. If the user feels that the sensitivity data file generated based on the original cross sections will not change much if the new cross sections are used, he or she may elect to keep the old sensitivity data files and only update the partial derivative of the cross sections with respect to the resonance parameters. The sensitivity data files are all in relative format. So the user may ask the question of how good is the following approximation,

$$\frac{\sigma^{old}}{k} \frac{\partial k}{\partial \sigma^{old}} \approx \frac{\sigma^{new}}{k} \frac{\partial k}{\partial \sigma^{new}} \ . \tag{27}$$

Should the user consider this approximation to be good enough for his or her purposes and use the old sensitivity file with SAMINT, he or she will be making the following approximation,

$$\frac{\partial k}{\partial \sigma^{old}} \frac{\sigma^{old}}{\sigma^{new}} \approx \frac{\partial k}{\partial \sigma^{new}} \ . \tag{28}$$

Note that this is different from stating,

$$\frac{\partial k}{\partial \sigma^{old}} \approx \frac{\partial k}{\partial \sigma^{new}} \ . \tag{29}$$

Regardless of which sensitivity data file is used, original or updated, the effect of the non-linearity in the cross section with respect to the resonance parameter should be reduced by the use of this iterative procedure.

The authors would simply like the user to be aware of this fact. However, the authors state that it is up to the user to judge how accurate the approximation is in Eq. 28 and avoid it by re-evaluating the sensitivity files whenever possible.

2.3 PREDICTED POSTERIOR EIGENVALUE

It is possible to predict the posterior eigenvalue if the behavior of the integral benchmarks was exactly linear with respect to the affected resonance parameters. As we have discussed above, the linearity assumption is only valid for small changes in resonance parameters. If any significant changes occur, the linearity assumption will most likely be violated and the subsequent neutronics calculations will not reproduce the predicted posterior eigenvalue. For this reason, we term the posterior eigenvalue as the *predicted* eigenvalue. The predicted eigenvalue, $k_p^{(0)}$, for the non-iterative case is given by,

$$k_p = k_c + \left(\frac{\partial k}{\partial P}\right)(P' - P) . \tag{30}$$

By visual inspection, we see that the same equation is true for the $k_p^{(n+1)}$ eigenvalue from the iterative case with the exception that we must add a correction to k_c,

$$k_p^{(n+1)} = \left[k_c^{(n)} + \left(\frac{\partial k}{\partial P^{(n)}}\right)(P^{(0)} - P^{(n)})\right] + \left(\frac{\partial k}{\partial P^{(n)}}\right)(P^{(n+1)} - P^{(0)}) . \tag{31}$$

While it is true that Eq. 31 can be simplified to,

$$k_p^{(n+1)} = k_c^{(n)} + \left(\frac{\partial k}{\partial P^{(n)}}\right)(P^{(n+1)} - P^{(n)}) . \tag{32}$$

For computational reasons, we prefer to keep it in the following general form, which collapses to Eq. 30 for the $n = 0$,

$$k_p^{(n+1)} = k_c^{(n)} - \left(\frac{\partial k}{\partial P^{(n)}}\right)(P^{(n)} - P^{(0)}) + \left(\frac{\partial k}{\partial P^{(n)}}\right)(P^{(n+1)} - P^{(0)}) . \tag{33}$$

3   USING SAMINT WITH SAMMY

This section covers how to integrate the use of the program SAMINT into a sequence of SAMMY runs. This section treats SAMINT as a black box. Section 4 describes how to operate SAMINT.

The following can be used as a recipe for including an adjustment of resonance parameters based on integral data in a series of sequential SAMMY updates. Before starting, identify a single suitable energy grid that describes, in enough detail, your partial cross sections. A suggested method of obtaining a seemingly adequate grid is to use the one of the two methods described in Sect. V.A of the SAMMY user's manual. The user should check, using SAMMY, that the automatically generated energy grid describes the partial derivatives of the cross section with respect to the resonance parameters in sufficient detail as a function of energy. Should the default energy grid from SAMMY be found to be inadequate, there are methods described in Sect. V.A of the SAMMY user's manual for refining the automatically generated energy grid. If the user fails to generate an appropriate energy grid, there will be a loss off accuracy of the methodology implemented in SAMINT.

After an appropriate energy grid is selected and before any SAMMY calculations are made, the CE TSUNAMI-3D or MCNP runs can be set up and launched. These integral calculations should be made using cross-section libraries generated from the latest resonance parameters using the AMPX or NJOY code as appropriate. SAMINT is fully capable of operating with either or both CE TSUNAMI-3D and MCNP eigenvalue sensitivity capabilities. The energies from the determined energy grid should be used as the mid-points for the sensitivity energy bins. A special feature of SAMINT can be used to convert the SAMMY energy grid to a suitable sensitivity energy structure. The appropriate way to access this special feature is to pass the seven-character keyword, *mid2bin*, as the first argument following the SAMINT executable in the command line. The SAMMY.LST file containing the desired energy grid is the second command line argument after the name of the executable. An example is

samint mid2bin SAMMY.LST.

With the keyword *mid2bin*, SAMINT will write a file called *energy.dat* containing the corresponding energy grid that must be inserted into the CE TSUNAMI-3D input files. The CE TSUNAMI-3D energy grid is the default. To produce an energy grid compatible with MCNP input, put a third command line argument *MCNP* (all upper-case) after the path to the SAMMY.LST file:

samint mid2bin SAMMY.LST MCNP.

Note that when consequently executing SAMINT, it expects a similar energy structure as output by the use of the *mid2bin* feature. If you chose to write your own version of *mid2bin*, you must keep in mind that SAMINT will ignore the sensitivities of the first and last energy bins from the *.SDF file produced by TSUNAMI. That is, SAMINT expects to find the a number of energy bins corresponding to the number of energy points in the SAMMY.LST files plus an additional two energy bins, one at the lower energy end and one at the higher end. This is done because CE TSUNAMI-3D requires the lower bound of the first energy bin to go to zero and the upper bound of the last energy bin to go to 20 MeV. This fact is rather inconvenient when trying to calculate the summation of Eq. 5. Therefore, the *mid2bin* feature will assume the same bin width for the first energy bin as for the second energy bin and the same bin width for the last energy bin as for the second-to-last energy bin. SAMINT, knowing this, will ignore the two outermost sensitivity coefficients. MCNP is not as particular about the required energy bin structure as CE TSUNAMI-3D; none the less, the *mid2bin* feature will output the same energy structure for MCNP input, and SAMINT will similarly ignore the first and last sensitivity coefficients from the MCNP output.

To begin, follow the procedure outlined in Sect. IV of the SAMMY user's manual for doing sequential data adjustment, saving the posterior resonance parameters and associated covariance data. When the user would like to include an adjustment based on integral data, the instructions below should be followed:

1. For each of the partial reactions (such that the sum is equal to the total cross section), perform a SAMMY run to generate Y and W matrices using the same set of input resonance parameters. The point of these runs is to generate the partial derivatives of the theoretical cross section with respect to the resonance parameters and the theoretical cross sections corresponding to those used in the integral experiment calculations. To accomplish this, do not use any experimental data corrections other than temperature broadening, and include the following two lines in card set 3 of your INPut files:

   GENERATE Y AND W MATrices
   SAMINT

   In the updated version of SAMMY, the alphanumeric command *SAMINT* will cause SAMMY to create a binary output file called *SAMMY.INT* that contains the partial derivatives and theoretical cross sections. Save this file under a unique name for each partial reaction. For these runs, use the energy grid identified before starting the SAMMY calculations. You should discard the SAMMY.YWY file that comes out of these runs. In the next step, SAMINT will provide the appropriate SAMMY.YWY file for all of the integral data.

2. Run SAMINT following the directions in Sect. 4. You will provide the path to the reaction SAMMY.INT file for each of the partial reactions that you saved in the previous step and the paths to the integral experiment *.SDF files for each of the integral experiments you wish to include as input. You will receive a single SAMMY.YWY binary file that you will use in the next step as output.

3. Make a SAMMY run with the following line in card set 3 of your INPut file.

   READ Y AND W MATRICEs

   and provide the SAMMY.YWY file that SAMINT created. SAMMY also produces a temporary file called SAM46.DAT, which is typically deleted. However, if you would like to know the experimental eigenvalues expected using the updated nuclear data, save this file under a unique name. You are then able to insert it as a second command line argument with SAMINT to calculate the expected experimental eigenvalues based on the assumption that your experiments behave linearly with respect to the nuclear data. You must use the input file style input, as described in Sect. 4, and give the name of the SAM46.DAT file as the second command line argument:

   samint input SAM46.DAT

   Giving SAMINT a second command line argument will cause it to produce a *NewK.txt* file, so named because it will contain the *new k_c* values for each of the integral experiments in the input file.

That is all. The resonance parameters and associated covariance matrix should now be updated based on the integral data information. You can continue with your sequential data adjustment and analyze further differential experimental data.

The above procedure up to point 2 has the sole purpose of generating a SAMMY.YWY file. The users may then use that SAMMY.YWY file from SAMINT as any ordinary SAMMY.YWY file in updating resonance parameters simultaneously based on different experimental data set.

See the flow diagrams in Figs. 1 and 2 for a visual guide.

3.1 USING SAMINT TO UPDATE $\bar{v}$

The procedure described above can be used in combination with SAMMY's ability to fit η to adjust $\bar{v}$ based on integral experimental data. The reactor physics parameter η is defined in Eq. 12. The mathematical arguments presented below show that nothing needs to change in the SAMINT operation to facilitate the adjustment of $\bar{v}$.

We consider that Eqs. 10 and 11 are still valid if P_t is replaced by $\bar{v}$ provided we can find $\partial k/\partial \bar{v}$. CE TSUNAMI-3D provides the sensitivity to $\bar{v}$ in the relative format. That is,

$$S = \frac{\bar{v}}{k}\frac{\partial k}{\partial \bar{v}} \ . \tag{34}$$

When SAMMY fits η, the derivative, G, is defined as

$$G = \frac{\partial \eta}{\partial v} \ . \tag{35}$$

The last piece of the puzzle is to observe that,

$$\frac{\partial \eta}{\partial \bar{v}} = \frac{\eta}{\bar{v}} \ . \tag{36}$$

Therefore, when we do as we did before and multiply to convert S to absolute format and then multiply by G, we still get exactly what we are looking for. Notice, that here we maintain the algorithm laid out in Sect. 3 and use the *theoretical* value that comes from the SAMMY.LST file to convert S. In this case, that value is η.

$$\frac{k}{\eta}S = \frac{k}{\eta}\frac{\bar{v}}{k}\frac{\partial k}{\partial \bar{v}} \ ; \tag{37}$$

$$\frac{k}{\eta}S = \frac{\partial k}{\partial \bar{v}}\frac{\partial \bar{v}}{\partial \eta} \ ; \tag{38}$$

$$\frac{k}{\eta}S = \frac{\partial k}{\partial \eta} \ ; \tag{39}$$

$$\frac{k}{\eta}SG = \frac{\partial k}{\partial \eta}\frac{\partial \eta}{\partial \bar{v}} \ ; \tag{40}$$

$$\frac{k}{\eta}SG = \frac{\partial k}{\partial \bar{v}} \ . \tag{41}$$

We see that using the same mechanism as before, we obtain our desired result, $\partial k/\partial \bar{v}$. When the SAMINT command is used in SAMMY and the data type being fit is ETA, the SAMINT command results in all resonance parameter derivatives being set to zero. This is done so that the above equations can be used without changes.

SAMMY:
No fitting
Generate energy mesh

SAMMY:
Differential
Experimental Data

SAMMY.LST:
Use for energy mesh

SAMMY.PAR

SAMMY.COV

MID2BIN

SAMMY:
YW, SAMINT
No exp. corrections
Doppler broadening

For each reaction

energy.dat
Energy mesh for
TSUNAMI input

SAMMY.INT

For each integral
experiment

TSUNAMI
or MCNP

Create cross-section library

SDF files
or MCNP output

SAMINT

SAMMY.YWY

SAMMY:
Read y and w matrices

SAMMY.PAR
SAMMY.COV

SAMMY:
Bayes

Legend

CODE

File

Fig. 1. Sequential work flow diagram.

SAMMY:
No fitting
Generate energy mesh

SAMMY.LST:
Use for energy mesh

MID2BIN

SAMMY:
YW, SAMINT
No exp. corrections
Doppler broadening

For each reaction

energy.dat
Energy mesh for
TSUNAMI input

SAMMY.INT

TSUNAMI
or MCNP

For each integral
experiment

Cross-section library

SDF files
or MCNP output

SAMINT

SAMMY:
Differential
Experimental Data

SAMMY.YWY

SAMMY.YWY

SAMMY:
Read y and w matrices

SAMMY.PAR
SAMMY.COV

SAMMY:
Bayes

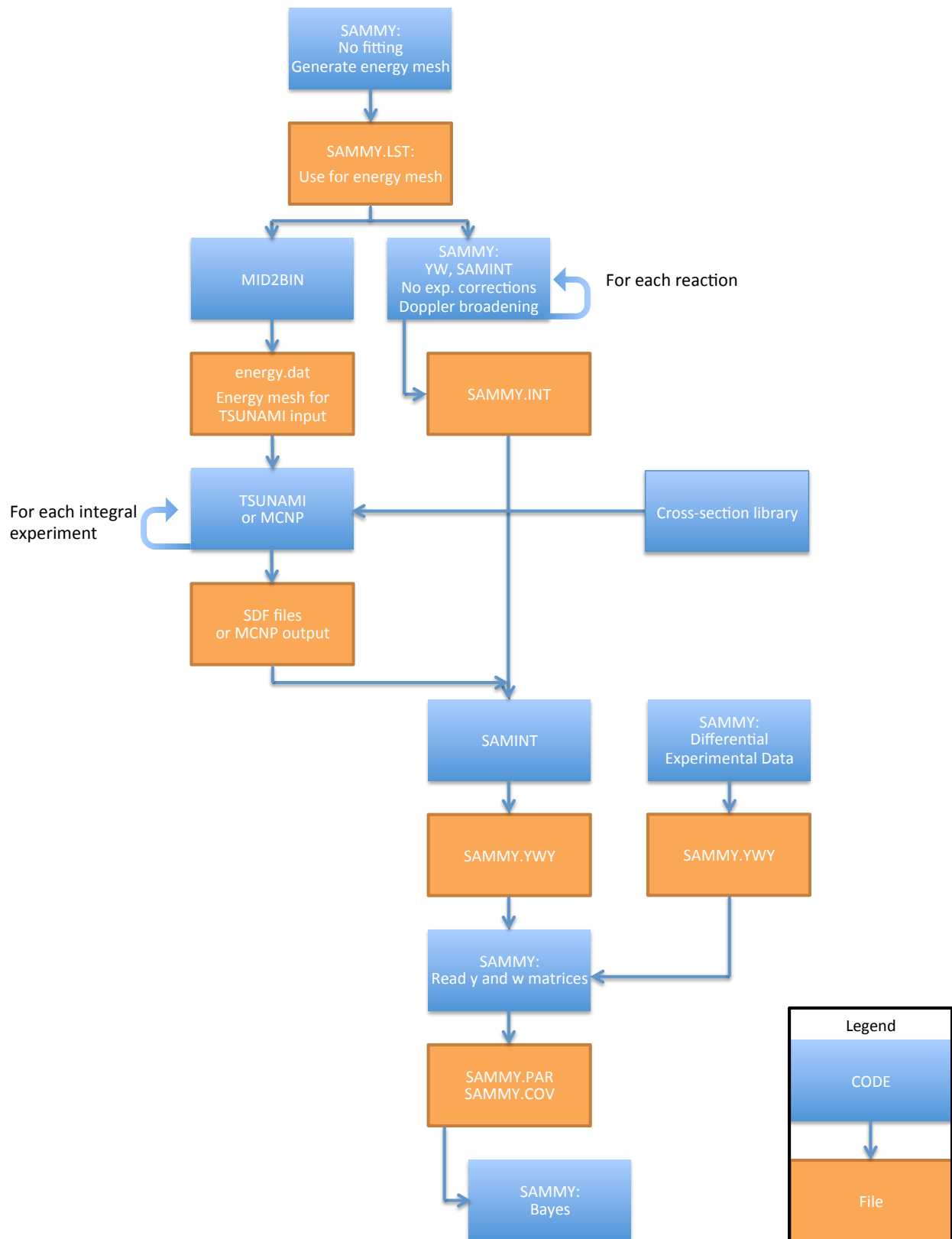Legend

CODE

File

Fig. 2. Simultaneous work flow diagram.

3.2 USING SAMINT TO UPDATE η

It is possible to produce updated values for η as a function of energy that will satisfy the integral benchmarks in the least squares way. To do so, the user should follow the procedure described from the beginning of Sect. 3 all the way through Step 1. For Step 1, he or she should generate SAMMY.INT files only for η, σ_f and σ_γ. Additionally, the user must provide SAMINT uncertainty information for η as a function of energy in one of two ways described below. To do so, the user should make a *no Bayes* run with SAMMY and include the following command in card set 3 of the INPut file:

SAMINT

and one of the following two commands:

1. CROSS SECTION COVARIance matrix is wanted

2. INCLUDE THEORETICAL uncertainties in plot file

The first choice will cause SAMMY to produce a binary file called SAMCOV.BIN, which is a binary version of the ordinary SAMMY file SAMCOV.PUB. SAMCOV.BIN will be used to provide SAMINT with the prior covariance matrix, $C_{\eta\eta}$. The alternate choice will simply put the variance of the theoretical calculations into the sixth column of the SAMMY.LST file, which will later be passed to SAMINT. **It is important to note that SAMMY will generate the η covariance matrix based only on the resonance parameter covariance matrix of the flagged resonance parameters. Therefore, it is crucial to flag all relevant resonance parameters (and $\bar{\nu}$ values) to the energy of interest in the parameter file used in the *no Bayes* run to generate the η covariance data.** On the other hand, it is irrelevant which resonance parameters are flagged when generating the SAMMY.INT files in Step 1 as long as SAMMY finds at least one flagged parameter.

From here, SAMINT is executed utilizing the *DATA block* of the input stream. See Sect. 4 for the details of how to evoke η updating with SAMINT.

SAMINT will update η and generate three files with the following information and interpretation:

- SAMMY.DAT — A file with three columns in TWENTY format. The first column contains the energies; the second, the updated η values; and the third, the uncertainty regarding the updated η values.

- SAMINT.COV — A file containing the posterior η covariance matrix in free format. This file can be fed into SAMMY as the data covariance matrix if it is desirable to fit the resonance parameters based on the updated η values. To do so, the user should insert the following command in card set 3 of the SAMMY INPut file:

  FREE FORMAT DATA COVariance

  with the file name in columns 31 to 40 of the same line.

- NewK.txt — A file containing the names of the integral benchmark files and the corresponding predicted posterior eigenvalue.

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3.3 USING SAMINT TO UPDATE CONTINUOUS-ENERGY CROSS SECTIONS

The reactor physics parameter η can be viewed as just a *complicated differential cross section* from the point of view of making adjustments to fit integral benchmarks. Therefore, similarly to adjusting η, it is possible to use SAMINT to adjust any other kind of partial cross section that is independent of any other partial cross section. For example, the user can calculate the adjusted fission cross section or the adjusted capture cross section, but not the adjusted absorption cross section. Should the need arise to adjust these *compound* cross sections, contact the author. The procedure for adjusting these *simple* partial cross sections follows the steps laid out above for η. Most of the required changes should be obvious:

- Generate the uncertainty information for the partial cross section of interest instead of for η.

- Generate only one SAMMY.INT file. That file should correspond to the partial cross section of interest.

Giving SAMINT a single SAMMY.INT file in the input (as opposed to three SAMMY.INT files as required for η) will make SAMINT understand that it is dealing with a *simple* partial cross section rather than η.

4   INPUT DESCRIPTION

There are two similar methods of providing SAMINT input information. The more streamlined method for the experienced user is to use the input file described in Sect. 4.2. For the beginning user or in case the user has forgotten the format of the input file, there is the option of using the command prompt interactive input. That option is described in the next subsection.

To evoke the interactive input, the user runs the SAMINT executable with no further command line arguments. Putting the path to the input file after the name of the SAMINT executable will evoke the input file option. For example,

samint samint.inp

will imply that the user has provided the properly formatted SAMINT input in the file samint.inp.

4.1   ITERATIVE INPUT

The interactive input option closely follows the structure of the input file but provides queues to the user to remind him/her what comes in what order. See Sect. 4.2 for a full description of the input file.

4.2   INPUT FILE

SAMINT has been designed to be able to accept input files in a format similar, but not identical, to the TSURFER input format. Minimal changes are needed to reuse existing TSURFER input files with SAMINT.

The input file has the following structure:

- The code will search the input file for the unique string *read response* in any combination of upper and lower case. Note, however, that unlike TSURFER, SAMINT does not accept *read experiments* or *read applications*. Other TSURFER input blocks such as *read parameter* can be left in the input file, and SAMINT will ignore them. After SAMINT has found the unique string *read response*, it will expect the following:

  - The first line following *read response* contains the path to the integral data correlation matrix. The integral data correlation matrix file provides the correlation matrix in free format. The first column of every line must be filled; the values may be space-, comma- or tab-delimited, and only the lower triangular part of the matrix is absolutely required. The ordering of the rows is defined by the order that the *.SDF files are provided in the input file. If no integral experiment correlations exist or none are desired to be reported, the first line should be left blank. In this case, the user should be careful to not leave even a space in this line as the code may pick that up as an entry. An identity matrix will be assumed if a correlation file is not given. This will save computation time as the code will bypass the inversion of the integral data covariance matrix.

  - The rest of the lines in this input block describe individual CE TSUNAMI-3D runs. For as many lines as necessary, the user should report the path to the sensitivity data file, the experimental eigenvalue and the absolute uncertainty on the eigenvalue. These may be space- or tab-delimited. However, the first column must be filled. Also, notice that unlike TSURFER, SAMINT is only expecting an absolute eigenvalue uncertainty. No option to give a relative

uncertainty exists. The name of the CE TSUNAMI-3D *.SDF file must end in a lower case *sdf*. Otherwise, SAMINT will assume that it is an MCNP output file containing the sensitivities. A sample input line may look like

exp1.sdf 1.001 0.010

This format should be repeated as many times as necessary. Do not leave blank lines, and conclude with an *end response* line.

- Then, somewhere below the *read response* block, possibly at the end of the original TSURFER input, the user should include a *SAMINT* block. Begin with *read SAMINT* in any case.

  - On the first line following *read SAMINT*, give the name of the isotope to be adjusted using the same string as in the *.SDF files.

  - The consequent lines are devoted to reaction information. The format is to state the path to the SAMMY.INT file corresponding to a particular reaction and then give the corresponding name of this reaction exactly as it appears in the *.SDF files. These may be space- or tab-delimited. An input line may look like

    fiss.int fission

    Repeat this format as many times as necessary. Do not leave blank lines, and conclude with an *end SAMINT* line.

A sample input is given below for an adjustment of the ^{235}U resonance parameters based on four integral experiments.

READ RESPONSE
integtral_experiment_correlation_file.corr
exp1.sdf 1.001 0.010
exp2.sdf 1.002 0.020
exp3.sdf 1.003 0.030
exp4.sdf 1.004 0.040
END RESPONSE
READ SAMINT
u-235
els.int elastic
fis.int fission
gam.int n,gamma
END SAMINT

4.3   USE WITH MCNP6

Should the user desire to use the eigenvalue sensitivity capability in MCNP6 instead of CE TSUNAMI-3D, the SAMINT code should provide a seamless transition. The following are reminders of things that must be changed in the operating procedure to accommodate the use of MCNP6 sensitivity capabilities. Most of this list should be logical based on an understanding of how SAMINT operates.

1. Provide the name of the MCNP output file with the sensitivity data in place of the *.SDF file, and make sure that the last three characters of the file name are not lower-case *sdf*.

2. In the READ SAMINT block of the input, provide the name of the isotope in *MCNP* format. For MCNP, that is usually the library name. For example, the input that was *u-235* for CE TSUNAMI-3D might be *92235.70c* for MCNP.

3. Similarly, remember to give the proper reaction names as they appear in the MCNP output file. The authors make no guarantees that these are the same for both codes.

The previously presented input file is given here in the context of what it might look like for use with MCNP.

```
READ RESPONSE
integtral_experiment_correlation_file.corr
exp1.out 1.001 0.010
exp2.out 1.002 0.020
exp3.out 1.003 0.030
exp4.out 1.004 0.040
END RESPONSE
READ SAMINT
92235.70c
els.intt elastic
fis.int fission
gam.int n,gamma
END SAMINT
```

4.4 DATA BLOCK

To evoke the updating of η as a function of energy rather than resonance parameters based on integral benchmarks, the user should either follow the command line instructions in the interactive input option or include a DATA block in the input file.

The DATA block consists of three lines. The first line is *read data*; the second line is the path to the SAMCOV.BIN file containing the η covariance data; and the third line reads *end data*. The DATA block may be inserted anywhere in the input file below the SAMINT block.

Also, in the SAMINT block, the user must give three and only three SAMMY.INT files and associated reaction keywords. These must be in strict order, corresponding to η first, *fission* second and *capture* third. A representative input file might look like

```
READ RESPONSE
integtral_experiment_correlation_file.corr
exp1.out 1.001 0.010
exp2.out 1.002 0.020
exp3.out 1.003 0.030
exp4.out 1.004 0.040
END RESPONSE
READ SAMINT
```

92235.70c
eta.intt prompt
fis.int fission
gam.int n,gamma
END SAMINT
READ DATA
SAMCOV.BIN
END DATA

4.5   INPUT FOR ITERATION

In order to evoke the linear algebra required for the iterative fitting procedure, the user must use the ITERATE block of the input structure. This block automatically comes up after the SAMINT block when using the interactive input option; it requires a new block in the input file if the input file option is used. This new block must appear anywhere after the RESPONSE block (that is, before or after the SAMINT block).

The block must begin with a *read iterate* line.

- On the first line after the *read iterate* line, enter the path to the first SAM46.DAT file. The meaning of the first and second SAM46.DAT files is explained below.

- On the second line after the *read iterate* line, enter the path to the second SAM46.DAT file or leave it blank.

- The following lines require the calculated eigenvalues based on the latest updated cross sections. These are entered in free format, one per line, and in the same order as the sensitivity data files were given in the *read response* block.

- The block is closed by an *end iterate* line

The easiest way to explain the interpretation of the *first* and *second* SAM46.DAT files is to speak in terms of Eq. 33. The first SAM46.DAT file will contain the change in resonance parameters corresponding to $(P^{(n)} - P^{(0)})$. The second SAM46.DAT file will contain the change in resonance parameters corresponding to $(P^{(n+1)} - P^{(0)})$. From the equations of Sect. 2, it is obvious that only the first file is needed to calculate the Y and W matrices, whereas both files are needed to calculate the predicted eigenvalues. This logic is mirrored in the behavior of the code: if only the first file is given (and the second line is left blank), a SAMMY.YWY file will be generated. If both files are given, a NewK.txt file will be generated.

In order to generate a SAMMY.YWY file for the second iteration, the following example block would need to be added to the above inputs,

READ ITERATE
SAM46.DAT
0.9932
0.9932
0.9932
0.9932
END ITERATE

where the SAM46.DAT file had been generated during the first iteration.

Assume that all four of the integral benchmark cases produced a 0.9932 eigenvalue using the updated cross sections. After SAMMY is executed with the

READ Y AND W MATRICEs

command, SAMINT can be rerun with the same input file as before, but this time the ITERATE block will look like

READ ITERATE
SAM46.DAT
SAM46.DAT
0.9932
0.9932
0.9932
0.9932
END ITERATE

where the SAM46.DAT file was just generated by the latest SAMMY run.

Finally, a explicit note is given here about passing the appropriate parameter and covariance files when using the iterative procedure. Remember that the SAMMY runs with the commands

GENERATE Y AND W MATrices
SAMINT

must be made with the latest intermediate resonance parameter files, whereas the SAMMY runs with the

READ Y AND W MATRICEs

must be made with the original resonance parameters and associated resonance parameter covariance matrices. This description is somewhat different from the iterative simultaneous fitting procedure described in Sect. IV.E.1 of the SAMMY user's manual due to the changes associated with the integral data; however, the mathematical equations are the same.

5 COMPUTER CODE

Under the hood, SAMINT uses the Eigen C++ library [Eigen 2014] to do the matrix inversion for C_{kk}. In fact, this matrix is never inverted; rather the system ($AX = B$) is solved for ($X = A^{-1}B$). The default solution algorithm is the LU decomposition of a matrix with complete pivoting which, according to the Eigen user manual, has proven reliability and accuracy. The trade-off is that it is a slow algorithm. Remember that this matrix has a rank equal to the number of integral experiments involved. For relatively small numbers of integral experiments, these default options are recommended as they are considered to be reliable. As the number of integral experiments increases and the user finds that an unacceptable amount of time is used up by SAMINT, the user may recompile the code with the *bFast* flag set to *true* in the SAMINT.cpp source code file. This will evoke the use of the Robust Cholesky decomposition of a matrix with pivoting for the inversion of C_{kk}. The method assumes that the integral data covariance matrix is positive semidefinite (as the case should be); it a very fast method. This method is known to have good, but not proven, algorithm accuracy and reliability. All of the solution algorithms were used in the testing of SAMINT. The authors did not find any difference in the accuracy or speed of the computations among the different algorithm options.

For updating η, the N+V version of the Bayes equations has been coded into SAMINT. This was done so that the size of the matrix being inverted scales with the number of integral experiments being simultaneously analyzed rather than with the number of energy points. The *bFast* boolean flag in the SAMINT code will evoke the Householder rank-revealing QR decomposition of a matrix with column-pivoting algorithm. This algorithm is considered to be fast and have good algorithm reliability and accuracy. The default is still the LU decomposition of a matrix with complete pivoting.

The code was written with easy debugging in mind rather than low memory usage. Therefore, memory usage scales linearly with the number of energy points and resonance parameters and quadratically with the number of integral experiments. If the user finds the there are practical cases where SAMINT runs out of memory, he or she should contact the author, and the code can be rewritten to have a smaller memory footprint. However, until such a need arises, the code will remain in its current, debug-friendly, structure.

6 TEST CASES

The necessity for testing of the computer code SAMINT, the new features added to SAMMY, as well as the integration of SAMINT with SAMMY, goes without saying. This section is devoted to testing some of the physics and mathematics behind the project. Several test cases have been created in the sprit of SAMMY test cases. Table 2 provides a summary of the test cases and some additional notes.

Table 2. Minimal description of the existing test cases for SAMINT

Case Name	Part of SAMINT Being Tested	Sensitivity Code	Notes
tr181	Non-iterative updating, η updating w/ correlations, η updating w/o correlations, integral experiment covariance matrix	CE TSUNAMI-3D (artificial data)	Non-physical numbers used, independently confirmed by MATLAB calculations
tr182	Non-iterative updating	CE TSUNAMI-3D	Basic infinite homogeneous integral problem, long runtime
tr184	Realistic case for ^{56}Fe, fitting with inelastic channel open	MCNP6	Complication comes from appearance of zero cross sections due to threshold reactions
tr185	Realistic case for ^{239}Pu, fitting resonance parameters and $\bar{\nu}$ simultaneously, independent η updating	MCNP6	

6.1 ^{56}Fe EVALUATION RESULTS

This section documents one of the earliest practical applications of SAMINT. The SAMINT code was used to improve the resolved resonance region evaluation of ^{56}Fe which had previously given discrepant results when used in integral benchmark calculations. Four integral experiments from the International Criticality Safety Benchmark Experiments Project (ICSBEP) [Briggs 2013] were selected for the task. Table 3 gives the descriptive name of the four experiments as well as their titles in the ICSBEP nomenclature.

Table 3. Four integral experiments used in the ^{56}Fe evaluation

ICSBEP Name	Experiment Title
HMF013	Sphere of highly enriched uranium reflected by steel
HMF021	Steel-reflected spherical assembly of ^{235}U(90%)
PMF025	Spherical assembly of ^{239}Pu(δ, 98%) with 1.55-cm steel reflector
PMF032	Steel-reflected spherical assembly of ^{239}Pu(α, 88%)

In the analysis based on the integral data, all of the gamma widths in the evaluated resolved resonance region of ^{56}Fe above 450 keV were varied. Also, both of the widths associated with the inelastic channels were varied. A total of 1,190 resonance widths were varied. These were the only resonance parameters that were deemed to be of importance by the evaluator. The entire evaluated resolved resonance region, 1e-5 eV

to 2 MeV, was considered, and an initial relative uncertainty of 0.1 was set for all varied resonance parameters.

Table 4 presents the computed k-eigenvalue divided by the experimental k-eigenvalue (C/E) before and after the resonance parameters were adjusted using SAMINT as well as the posterior k-eigenvalue predicted by SAMINT based on the linearity assumption. The desired k-eigenvalue for all four experiments was unity with 100 pcm uncertainty.

Table 4. C/E values for iron benchmarks before and after adjustment with SAMINT

ICSBEP Name	C/E Before Adjustment	C/E After Adjustment	C/E Predicted
HMF013	0.99850	1.00035	0.99933
HMF021	0.99633	1.00005	0.99950
PMF025	0.99892	1.00001	0.99994
PMF032	0.99792	1.00017	0.99968

The updating procedure has produced the desired results of satisfying the integral benchmark calculations while maintaining a good fit of the differential data. Figures 3 and 4 present the reconstructed cross section, before and after the adjustment, on top of the differential experimental data used to come up with the evaluation before the integral data adjustment. These figures show how the information from the integral experiments can be used to make minor adjustments in the continuous-energy cross section that are beyond the resolution of the differential experimental data. Figure 3 shows a segment of the inelastic cross section plotted on top of differential experimental data of Negret et al. [Negret 2011]. Figure 4 shows a different segment of the inelastic cross section plotted on top of differential experimental data of Perey et al. [Perey 1971]. Only these two energy segments are shown because these are the only energy regions where observable changes in the inelastic cross section had occurred. For all other energy regions, the posterior evaluation looks almost identical to the initial evaluation on a cross-section plot.

Judging by Figs. 3 and 4, it is difficult to argue whether the initial or posterior evaluation is a better fit of the experimental data. The least-squares chi-squared values for both differential experimental data sets evaluated over the entire energy region of validity are presented in Table 5. In this situation, the changes made based on the integral experimental data are on a finer scale than the differential experimental data. Using the integral experimental data to compliment the differential experimental data is much of the goal of the SAMINT project.

Table 5. Least-squares chi-squared value for differential experimental data

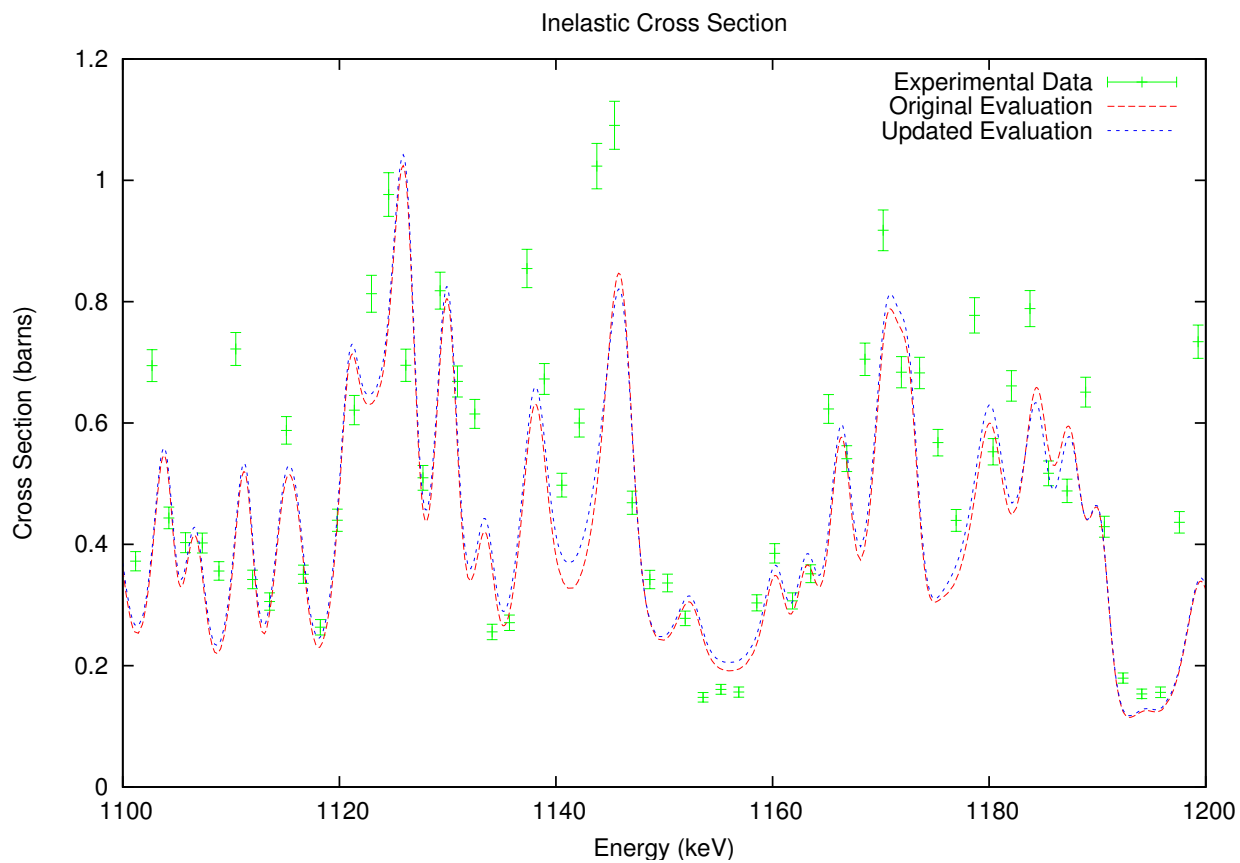| Experimental Data	χ^2 Before Adjustment	χ^2 After Adjustment
Plompen	73.3382	73.6877
Perey	23.6023	22.9036

Fig. 3. Inelastic cross section of ^{56}Fe before and after the adjustment based on integral experimental data plotted on top of differential experimental data of Plompen, presented with one standard deviation error bars.
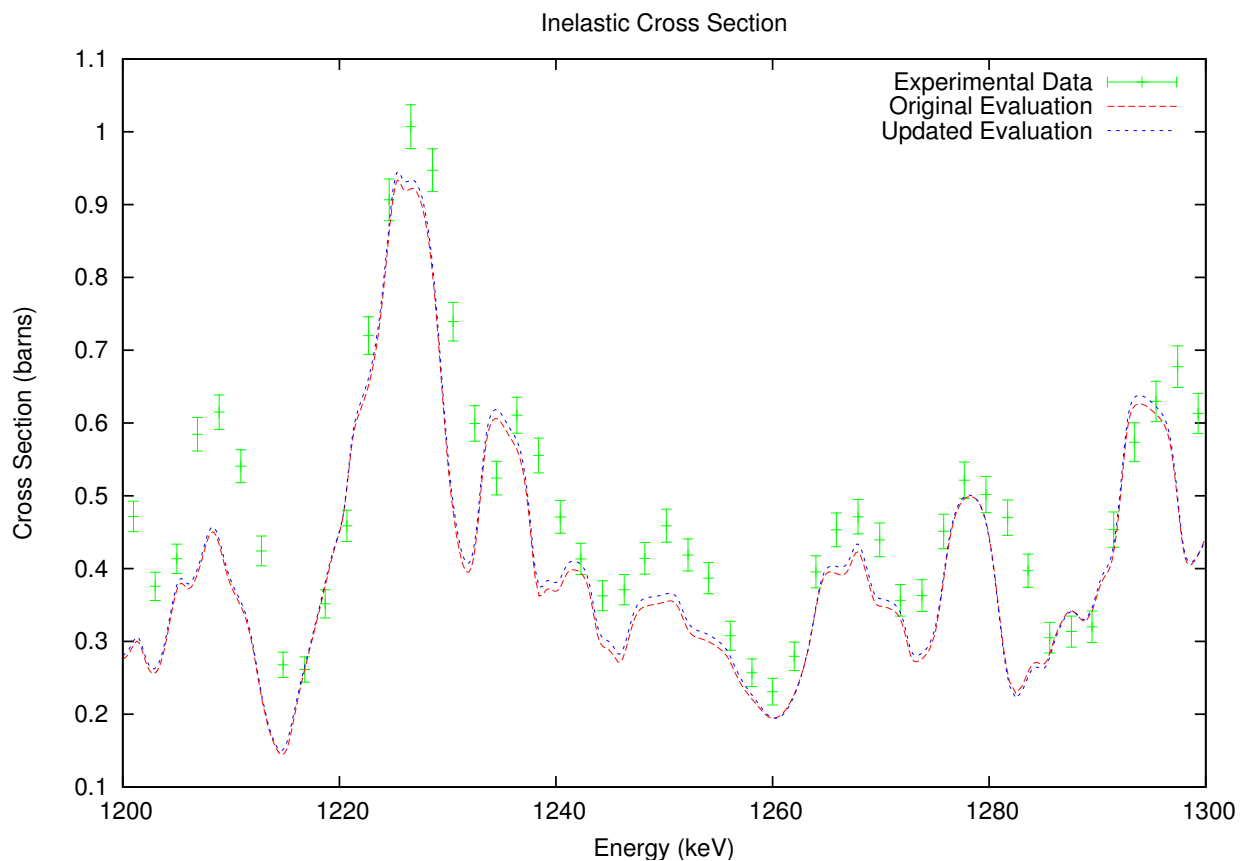
Fig. 4. Inelastic cross section of ^{56}Fe before and after the adjustment based on integral experimental data plotted on top of differential experimental data of Perey, presented with one standard deviation error bars.

7 REFERENCES

Briggs, J., et al., *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, Report
    NEA No. 7166 (2013).

Eigen, open-source project, URL: http://eigen.tuxfamily.org/index.php?title=Main_Page (2014).

Larson, N. M., "Updated users' guide for SAMMY." ORNL/TM-9179/R8 (2008).

Negret, A., C. Borcea, and A. J. M. Plompen, "Cross Section for Neutron Inelastic Scattering on ^{28}Si," Jo.
    Korean Phys. Soc., **59**, 2, 1765–1768 (2011).

Perey, F. G., W. E. Kinney, and R. L. Macklin, "High Resolution Inelastic Cross Section Measurements for
    Na, Si, and Fe," 3rd Conf. Neutron Cross Sections+Tech, 1, 191 (1971).

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