"TAR: Impact of Taking into Account Correlations"

G. Palmiotti

Idaho National Laboratory USA

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Idaho National Laboratory

Introduction

- As new high fidelity covariance data become available they can be used to assess nuclear data target accuracies for future innovative nuclear systems. The new covariance data produced at BNL (with the support of LANL and ORNL) and called AFCI 1.2, have been used to update the findings of the NEA/WPEC Subgroup 26.
- The difference with the respect to the previous study of the Subgroup 26 (where the BOLNA covariance matrix was used) has been found in some cases be significant.
- However, the work I am presenting is devoted to target accuracy studies. In particular, one major (theoretical) issue has been investigated. This issue is related to the fact that in previous studies correlation terms have been neglected in target accuracy assessments.
- We will first illustrate the theory behind the target accuracy assessment, then provide results for applications to the advanced fast reactor systems considered in the NEA/WPEC Subgroup 26 study, and finally provide some indications on how to proceed for future studies.

THEORY

- When covariance data matrix (i. e. standard deviations on diagonal, and correlations on off-diagonal term) ***D*** and sensitivity coefficient arrays S_R for an integral parameter ***R***, one can calculate the uncertainty ΔR^2 on the integral parameter using the sandwich formula:

$$\Delta R^2 = S_R^+ D S_R$$

- A successive step is the assessment of target accuracy requirements Target accuracy assessments are the inverse problem of the uncertainty evaluation. To establish priorities and target accuracies on data uncertainty reduction, a formal approach can be adopted by defining target accuracy on design parameter and finding out required accuracy on data.
- In fact, the unknown uncertainty data requirements can be obtained by solving a minimization problem where the sensitivity coefficients in conjunction with the existing constraints provide the needed quantities to find the solutions

THEORY

- The unknown uncertainty data requirements d_i can be obtained (e.g., for variables i not correlated among themselves), by solving the following minimization problem for the functional Q:

$$Q = \sum_i \lambda_i / d_i^2 = min \quad i = 1 \ldots I$$

with the following constraints:

$$\sum_i S_{ni}^2 d_i^2 \le \left(R_n^T\right)^2 \qquad n = 1 \ldots N$$

where N is the total number of integral design parameters, S_{ni} are the sensitivity coefficients for the integral parameter R_n and R_n^T are the target accuracies on the N integral parameters; λ_i are "cost" parameters related to each σ_i and should give a relative figure of merit of the difficulty of improving that parameter (e.g., reducing uncertainties with an appropriate experiment).

THEORY

- In practical cases, in order to limit the number of variables (we remind that the unknown d_i variables are the standard deviations of the cross-sections for which target accuracies are required) and make the problem feasible, the number I is obtained by selecting the variables based on their contribution to the uncertainties; for instance, by selecting only those which globally account at least for a fixed quantity (e. g. 98%).
- When taking into account correlations the constraints become:

$$\sum_i G_i^n + \sum_{ii'} C_{ii'}^n + \sum_i F_i^n + P_n \le \left(R_n^T\right)^2 \qquad n = 1 \ldots N$$

$$G_i^n = S_{ni}^2 d_i^2 \qquad C_{ii'}^n = S_{ni} d_i Corr_{ii'} d_{i'} S_{ni'}^+$$

$$F_i^n = S_{ni} d_i Corr_{ij} d_j S_{nj} \qquad j = 1 \ldots . K$$

P_n represent the constant residual uncertainty for integral parameter R_n due to the unselected variables and K is the total number of constant terms that are correlated to variable i.

THEORY

- In order to solve the nonlinear minimization problem with nonlinear constraints we have used the SNOPT code. SNOPT uses a sequential quadratic programming (SQP) algorithm that obtains search directions from a sequence of quadratic programming subproblems. Each QP subproblem minimizes a quadratic model of a certain Lagrangian function subject to a linearization of the constraints. An augmented Lagrangian merit function is reduced along each search direction to ensure convergence from any starting point.
- As many other optimization codes SNOPT needs the problem Jacobian. The code can calculate derivatives in a numerical manner, but our experience is that it better performs both in execution time and accuracy when derivatives are directly provided by the user. Derivatives with respect to variable $\boldsymbol{d_i}$ can be analytically calculated so their corresponding analytical formulation was implemented in the user function subroutines that were provided to SNOPT.

TARGET ACCURACY ASSESSMENT FOR ADVANCED FAST REACTOR SYSTEM

- For the practical application we have chosen as reactor design those of fast reactor system that were used in the Subgroup 26 study: EFR (Na-cooled European Fast Reactor), GCFR (Gas Cooled Fast Reactor), SFR (Sodium Fast Reactor), LFR (Lead Fast Reactor), ADMAB (Accelerator Driven Minor Actinide Burner).
- We have used the new available AFCI 1.2 covariance data. One major difference of this matrix with respect to the BOLNA one used in the the NEA/WPEC Subgroup 26 study, is the energy group structure adopted that consists in 33 energy groups mostly intended for fast reactor applications.
- For integral parameter we have used only the multiplication factor K_{eff} in order to simplify calculations and better understand the obtained results.
- For the target value on the integral parameter the value of 300 pcm has been adopted for all fast systems.

EFR

Target accuracy assessment for EFR (pcm). 146 parameters selected

		G	***C***	***F***	***V***	***P***	Total
No corr.	Initial	**631**	**-**	**-**	**631**	**-**	**631**
	Final	**300**	**-**	**-**	**300**	**-**	**300**
With corr.	Initial.	**631**	**1044**	**164**	**1231**	**248**	**1256**
	Final	**93**	**122**	**71**	**169**	**248**	**300**

EFR target accuracy requirements on 5 most important variables. Standard deviations (%).

Variable	Initial	No Correl.	With Correl.
U8 σ^{inel} Gr. 5	**20.6**	**3.8**	**0.5**
U8 σ^{inel} Gr. 4	**19.4**	**3.2**	**0.5**
U8 σ^{inel} Gr. 6	**16.9**	**4.4**	**0.6**
U8 σ^{inel} Gr. 3	**20.1**	**5.5**	**0.7**
Pu1 σ^{fis} Gr. 10	**20.0**	**6.4**	**0.9**

GCFR

Target accuracy assessment for GCFR (pcm). 173 parameters selected

		G	***C***	***F***	***V***	***P***	Total
No corr.	Initial	**982**	**-**	**-**	**982**	**-**	**982**
	Final	**300**	**-**	**-**	**300**	**-**	**300**
With corr.	Initial.	**982**	**1640**	**174**	**1919**	**278**	**1939**
	Final	**52**	**81**	**59**	**113**	**278**	**300**

GCFR target accuracy requirements on 5 most important variables. Standard deviations (%).

Variable	Initial	No Correl.	With Correl.
U8 σ^{inel} Gr. 5	**20.6**	**2.1**	**0.3**
U8 σ^{inel} Gr. 4	**19.4**	**2.3**	**0.3**
U8 σ^{inel} Gr. 3	**20.1**	**3.1**	**0.4**
U8 σ^{inel} Gr. 6	**16.9**	**3.1**	**0.4**
Pu1 σ^{fis} Gr. 10	**20.0**	**4.2**	**0.5**

SFR

Target accuracy assessment for SFR (pcm). 201 parameters selected

		G	***C***	***F***	***V***	***P***	Total
No corr.	Initial	**903**	**-**	**-**	**903**	**-**	**903**
	Final	**300**	**-**	**-**	**300**	**-**	**300**
With corr.	Initial.	**903**	**1858**	**186**	**2074**	**251**	**2090**
	Final	**80**	**121**	**76**	**164**	**251**	**300**

SFR target accuracy requirements on 5 most important variables. Standard deviations (%).

Variable	Initial	No Correl.	With Correl.
Pu8 σ^{fis} Gr. 7	**50.0**	**4.7**	**0.9**
Pu8 σ^{fis} Gr. 8	**50.0**	**4.8**	**0.9**
Pu8 σ^{fis} Gr. 6	**50.0**	**5.1**	**1.0**
Pu1 σ^{fis} Gr. 10	**20.0**	**3.6**	**0.7**
Pu8 σ^{fis} Gr. 9	**50.0**	**6.2**	**1.1**

ADMAB

Target accuracy assessment for ADMAB (pcm). 270 parameters selected

		G	***C***	***F***	***V***	***P***	Total
No corr.	Initial	**1124**	**-**	**-**	**1124**	**-**	**1124**
	Final	**300**	**-**	**-**	**300**	**-**	**300**
With corr.	Initial.	**1124**	**2125**	**194**	**2411**	**257**	**2425**
	Final	**72**	**119**	**68**	**155**	**257**	**300**

ADMAB target accuracy requirements on 5 most important variables. Standard deviations (%).

Variable	Initial	No Correl.	With Correl.
Am1 σ^{fis} Gr. 6	**10.0**	**1.6**	**0.4**
Am1 σ^{fis} Gr. 5	**10.0**	**1.7**	**0.4**
Pu1 σ^{fis} Gr. 10	**20.0**	**2.8**	**0.5**
Pu1 σ^{fis} Gr. 9	**18.9**	**2.8**	**0.5**
Cm5 σ^{fis} Gr. 10	**50.0**	**4.8**	**0.9**

Conclusions

- We have performed a target accuracy assessment using new available covariance data, the AFCI 1.2 covariance data matrix, and looking at the issue of taking into account correlation terms. The major conclusions and recommendations obtained by this study are:
  - The impact of correlation terms is very significant in target accuracy assessment evaluation and produces very stringent requirements on nuclear data
  - For this type of study a broader energy group structure should be used, in order to smooth out requirements and provide better information to evaluators and cross section measurement experts
  - The main difference in results between using BOLNA or AFCI 1.2 covariance data are related to minor actinides, minor Pu isotopes, structural materials (in particular Fe56), and coolant isotopes (Na23)

Conclusions

- For future target accuracy requirements study a possible broader energy structure that we propose contains 7 energy groups. This structure covers the entire spectrum and could be used for studies of fast, epithermal, and thermal reactors.

Group	Upper Energy	Group	Upper Energy
1	$1.96403\ 10^{7}$	5	$2.03468\ 10^{3}$
2	$2.23130\ 10^{6}$	6	$2.26033\ 10^{1}$
3	$4.97871\ 10^{5}$	7	$5.40000\ 10^{-1}$
4	$6.73795\ 10^{4}$		

- The energy limits are based on physical consideration with bands that cover the region above the threshold of fertile isotope fission cross-sections, and of many inelastic cross-sections, the region of the continuum down to the upper unresolved resonance energy limit, the unresolved resonance energy region, the resolved resonance region, the epithermal range, and thermal range.
- The goal of this structure is to reduce the number of variables of the minimization problem, and smooth out the resulting target accuracy requirements.