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Combining Total Monte Carlo and Unified Monte Carlo: Bayesian nuclear data uncertainty quantification from auto-generated experimental covariances

P. Helgesson [a, b, *], H. Sjöstrand [a], A.J. Koning [a, b], J. Rydén [c], D. Rochman [d], E. Alhassan [a], S. Pomp [a]

[a] Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden
[b] Nuclear Research and Consultancy Group NRG, Petten, The Netherlands
[c] Department of Mathematics, Uppsala University, Uppsala, Sweden
[d] Paul Scherrer Institute PSI, Villigen, Switzerland

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ABSTRACT

The Total Monte Carlo methodology (TMC) for nuclear data (ND) uncertainty propagation has been subject to some critique because the nuclear reaction parameters are sampled from distributions which have not been rigorously determined from experimental data. In this study, it is thoroughly explained how TMC and Unified Monte Carlo-B (UMC-B) are combined to include experimental data in TMC. Random ND files are weighted with likelihood function values computed by comparing the ND files to experimental data, using experimental covariance matrices generated from information in the experimental database EXFOR and a set of simple rules. A proof that such weights give a consistent implementation of Bayes' theorem is provided. The impact of the weights is mainly studied for a set of integral systems/applications, *e.g.*, a set of shielding fuel assemblies which shall prevent aging of the pressure vessels of the Swedish nuclear reactors Ringhals 3 and 4.

In this implementation, the impact from the weighting is small for many of the applications. In some cases, this can be explained by the fact that the distributions used as priors are too narrow to be valid as such. Another possible explanation is that the integral systems are highly sensitive to resonance parameters, which effectively are not treated in this work. In other cases, only a very small number of files get significantly large weights, *i.e.*, the region of interest is poorly resolved. This convergence issue can be due to the parameter distributions used as priors or model defects, for example.

Further, some parameters used in the rules for the EXFOR interpretation have been varied. The observed impact from varying one parameter at a time is not very strong. This can partially be due to the general insensitivity to the weights seen for many applications, and there can be strong interaction effects. The automatic treatment of outliers has a quite large impact, however.

To approach more justified ND uncertainties, the rules for the EXFOR interpretation shall be further discussed and developed, in particular the rules for rejecting outliers, and random ND files that are intended to describe prior distributions shall be generated. Further, model defects need to be treated.

1. Introduction and Total Monte Carlo

Nuclear data (ND) underpins all nuclear science and technology (Forrest, 2014), and its accuracy is hence paramount. As for any scientific quantity, ND (and results derived from it) should be presented with both best estimates and with uncertainties.

Total Monte Carlo (TMC, Koning and Rochman, 2008) is an ND uncertainty propagation method based on the idea of sampling nuclear reaction model parameters to a nuclear reaction code, typically the TALYS code system T6 (Koning and Rochman, 2012), which complements TALYS (Koning et al, 2013) results with, *e.g.*, resonance data.

An overview of the methodology is seen in Fig. 1. By feeding T6

* Corresponding author. Dpt. of Phys. and Astronomy, Box 516, 751 20 Uppsala, Sweden.
E-mail address: petter.helgesson@physics.uu.se (P. Helgesson).

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List of symbols

$:=$	Defined by, 5
$\langle \cdot \rangle$	Expected value, 5
$\langle \cdot \rangle_g$	Expected value with respect to PDF g, 5
$\mathbf{C}_\mathrm{E}$	"Experimental covariance matrix"4, **6**
$\mathbf{C}_{\mathrm{E}(j)}$	Covariance matrix corresponding to j'th experiment, 7
$\chi^2_{(j),\mathrm{central}}$	χ^2 for comparison of j'th experiment to $\overline{\tau}_{(j)}$, 7
χ^2_k	Generalized χ^2 for k'th random file (parameter set $\mathbf{p}^{(k)}$), 4
$\mathbf{C}_{\tau(j)}$	Covariance matrix inherent in random files for j'th experiment, 7
$\Delta E_{0,i}$	Uncertainty in $E_{0,i}$, 6
$\Delta E'_i$	"Energy spectrum width", 6
δ_{ij}	Kronecker delta (1 if $i \neq j$, 0 otherwise), 7
$E_{0,i}$	Mean neutron energy of experimental point, 6
ε_ℓ	Random variable describing normalized error due to ℓ'th systematic contribution, 7
$f_0(\mathbf{p})$	Prior PDF for $\mathbf{p}$, 4
$F_{\chi^2(m_j)}$	Distribution function for χ^2-distributed random variable with m_j degrees of freedom, 7
$f(\mathbf{p})$	PDF for $\mathbf{p}$, 4
$f(\mathbf{p}\|\mathbf{x})$	PDF for $\mathbf{p}$ given $\mathbf{x}$, 4
f_W	Probability density for generic random variable W (if W is a random variable), 6
$f_\mathbf{X}(\mathbf{x}\|\mathbf{p})$	PDF for $\mathbf{X}$ given $\mathbf{p}$ evaluated at $\mathbf{x}$, 5
k_eff	Neutron multiplication factor, 3
k_∞	k_eff neglecting neutron leakage, 10
$L(\mathbf{p}^{(k)};\mathbf{x})$	Likelihood function for $\mathbf{p}^{(k)}$ under $\mathbf{x}$, 4
M	# of experiments, 7
m	# of experimental points, 4
$M_{(j)}$	Random vector describing the true values corresponding to $\mathbf{X}_{(j)}$, 7
$m_{(j)}$	Observation of $M_{(j)}$, 7
m_j	# of experimental points in j'th experiment, 7
N	# model parameters, 4
n	# random ND files, 3
ν	# systematic contributions, 6
$\mathbf{p}$	Vector with model parameters, 4
P_j	Estimated p-value for j'th experiment, 7
p_j	Model parameter (element of $\mathbf{p}$), 4
P_tol	Tolerance used for rejection of outliers, 7
q	Generic integral quantity, 4
$\widehat{q^j(\mathbf{p})}$	Estimate of j'th moment of q given $\mathbf{x}$, 5
σ_i^2	Random variance of X_i, 6
$\sigma^2_\mathrm{observed}(q)$	Estimate of total variance of q, 5
$\sigma^2_\mathrm{stat}(q)$	Estimated variance in q due to statistics of Monte Carlo code, 5
$\sigma_\text{fully correlated}$	Added uncertainty, fully correlated for all experimental points for the same reaction channel (and nuclide), 6, 9
$\sigma_{i\ell}$	Uncertainty in X_i due to ℓ'th systematic contribution, 6
$\sigma_\mathrm{ND}(q)$	Estimated standard deviation due to ND uncertainty, 5
$\sigma_\text{stat,extra abs}$	Added absolute random uncertainty, 6, 11
$\sigma_{\text{stat,extra rel to }\sigma}$	Added random uncertainty, relative to random uncertainty, 6, 11
$\sigma_{\mathrm{stat},min}$	Minimum random uncertainty, 6, 11
$\sigma_\text{sys,extra abs}$	Added absolute systematic uncertainty, 6, 11
$\sigma_\text{sys,extra rel}$	Added relative systematic uncertainty, 6, 11
$\sigma_\mathrm{sys,min}$	Minimum systematic uncertainty, 6, 11
$\varsigma(E')$	Theoretical cross section at E', 6
$(\cdot)^\mathrm{T}$	Transpose, 4
$\tau_i^{(k)}$	Value in k'th random file corresponding to x_i (element of $\tau^{(k)}$), 4
$\overline{\tau}_{(j)}$	Mean value of values in random files corresponding to $\mathbf{x}_{(j)}$, 7
τ	Vector with values in k'th random file corresponding to $\mathbf{x}$, 4
$V(\cdot)$	Variance, 6
$V_{\Delta E}(\tau_i^{(k)})$	Variance in $\tau_i^{(k)}$ due to energy resolution, 6
w_k	Weight for k'th random file, 5
$\mathbf{X}$	Random vector describing the experimental points, 4
$\mathbf{x}$	Vector with observed experimental values, 4
X_i	Random variable describing i'th experimental point, 7
x_i	i'th experimental value (element of $\mathbf{x}$), 4
$\mathbf{x}_{(j)}$	Vector with experimental results for j'th experiment (sub-vector of $\mathbf{x}$), 7
$\mathbf{X}_{(j)}\Big\vert(\mathbf{M}_{(j)}=\mathbf{m}_{(j)})$	$\mathbf{X}_{(j)}$ given that $\mathbf{M}_{(j)}=\mathbf{m}_{(j)}$, 7
Y_i	Random variable describing expected value and random uncertainty of i'th experimental point, 7

with n randomly sampled sets of parameters, n ENDF (Trkov et al., 2011) libraries with ND are produced, referred to as random files in this text. By using each such random file in a simulation of a nuclear system of interest, n results for all output quantities are obtained. The output quantities could, *e.g.*, be grouped macroscopic cross sections, power distribution, k_eff, decay heat, dose rate, inventories, *etc.*, to mention a few possible examples. If the ND which is varied has any relevance to the system, the results will have a spread because of the varying ND. Using statistical inference one can then estimate the propagated ND uncertainty in any of the output quantities.

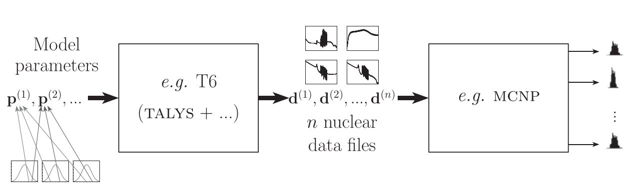

Fig. 1. An overview of the TMC methodology.

TMC has been applied to numerous different cases, ranging from shielding models (Sjöstrand et al., 2014a), thoroughly studied pin cells (Helgesson et al., 2014) and a wide range of criticality safety benchmarks (Rochman et al., 2009) to full core neutronics simulations (van der Marck and Rochman, 1051) and even to models including thermo-hydraulics (Cabellos et al, 2013) and transients (da Cruz et al., 2014).

The methodology has a number of advantages compared to the conventional use of covariance matrices and sensitivities to propagate ND uncertainties; for example, non-Gaussian output distributions can be observed (examples of which can be seen in Koning and Rochman (2008) and Alhassan et al. (2015), it allows for non-linearities and also for more complete input distributions than simply central values and covariances. Another important advantage is the transparency compared to how the covariance data in the ND evaluations are produced. Finally, there is no need to process covariance matrices and to keep track of them in all codes in the entire chain of simulations.