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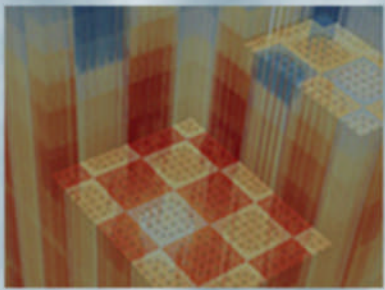
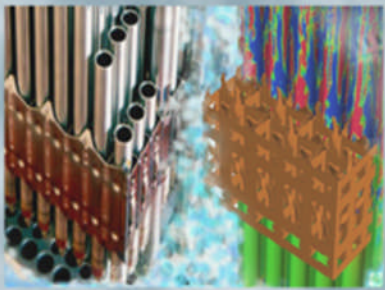
Whitepaper on Uncertainty Quantification for MPACT





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1. INTRODUCTION

The MPACT code provides the ability to perform high-fidelity deterministic calculations to obtain a wide variety of detailed results for very complex reactor core models. However MPACT currently does not have the capability to propagate the effects of input data uncertainties to provide uncertainties in the calculated results. This white paper discusses a potential method for MPACT uncertainty quantification (UQ) based on stochastic sampling.

Stochastic sampling methods determine the uncertainty in any calculated result by repeated passes through the computational sequence, each with a randomly perturbed sample of all input variables of interest. Because the input data are perturbed prior to the beginning of the computations, this approach requires little or no modification to the underlying computational algorithms. The distributions of the perturbed output values provide mean values, standard deviations, as well as correlation coefficients between various types of results. ORNL has implemented this approach in the SAMPLER module that will be included in the next release of SCALE (version 6.2). SAMPLER can propagate uncertainties in all types of cross sections, fission product yields, and decay data, as well as modeling parameters, for any type of SCALE multigroup (MG) computational sequence. This white paper presents a possible Sampler-based methodology for performing uncertainty calculations with MPACT to address cross sections uncertainties. Other types of uncertainties (transmutation and modeling parameters) can be addressed in a future whitepaper. This methodology is only for UQ and does not provide sensitivity coefficients.

2. POTENTIAL UQ METHODOLOGY FOR IMPACT

The proposed approach is to pre-compute 500-1000 randomly perturbed MPACT libraries by varying the multigroup (MG) and continuous energy (CE) data used by the processing codes that generate the libraries. UQ analysis would then just be a matter of running MPACT for the desired number of samples (i.e., libraries) and performing statistical analysis on the output distributions. This can be done using Sampler, or another Sampler-like wrapper code could be developed explicitly for MPACT.

The first step in this procedure is create a new sequence for AMPX that combines all the current processing modules that generate self-shielding data, such as IR lambda values, homogeneous and heterogeneous f-factors, and subgroup parameters. This requires developing a driver routine that reads user input options, loads existing MG and CE libraries into memory using SCALE resource routines, and calls APIs for the processing modules to compute self-shielding data for the specified nuclides. Some modifications to the individual modules are also likely necessary so they fit together logically. The shaded box in Fig. 1 indicates this sequence. Aside from its utility for producing perturbed MPACT libraries, the sequence is very desirable for the standard AMPX library processing because it simplifies the overall procedure by reducing the number of independent steps, and improves maintainability. A single run would accomplish what 3 or 4 independent runs currently do. The sequence execution could probably be completed in a day. After developing this new sequence, perturbed MPACT (or AMPX) libraries can be produced by executing Clairol-plus and Crawdad-plus prior to running the sequence for each desired sample, as indicated in Figure 1. Each perturbed library can be processed independently, so these runs can be done simultaneously on different computing nodes. Thus the entire set of perturbed libraries could probably be produced over a single weekend, if not a single day. The perturbed libraries only need to be processed once and saved for the future UQ analysis.

Figure 2 shows the MPACT UQ calculation procedure using the pre-generated perturbed libraries inside of a Sample-type wrapper. Sampler is used to load a perturbed library for a given Sample, to scrap the desired responses from the MPACT output, and perform statistical analysis,

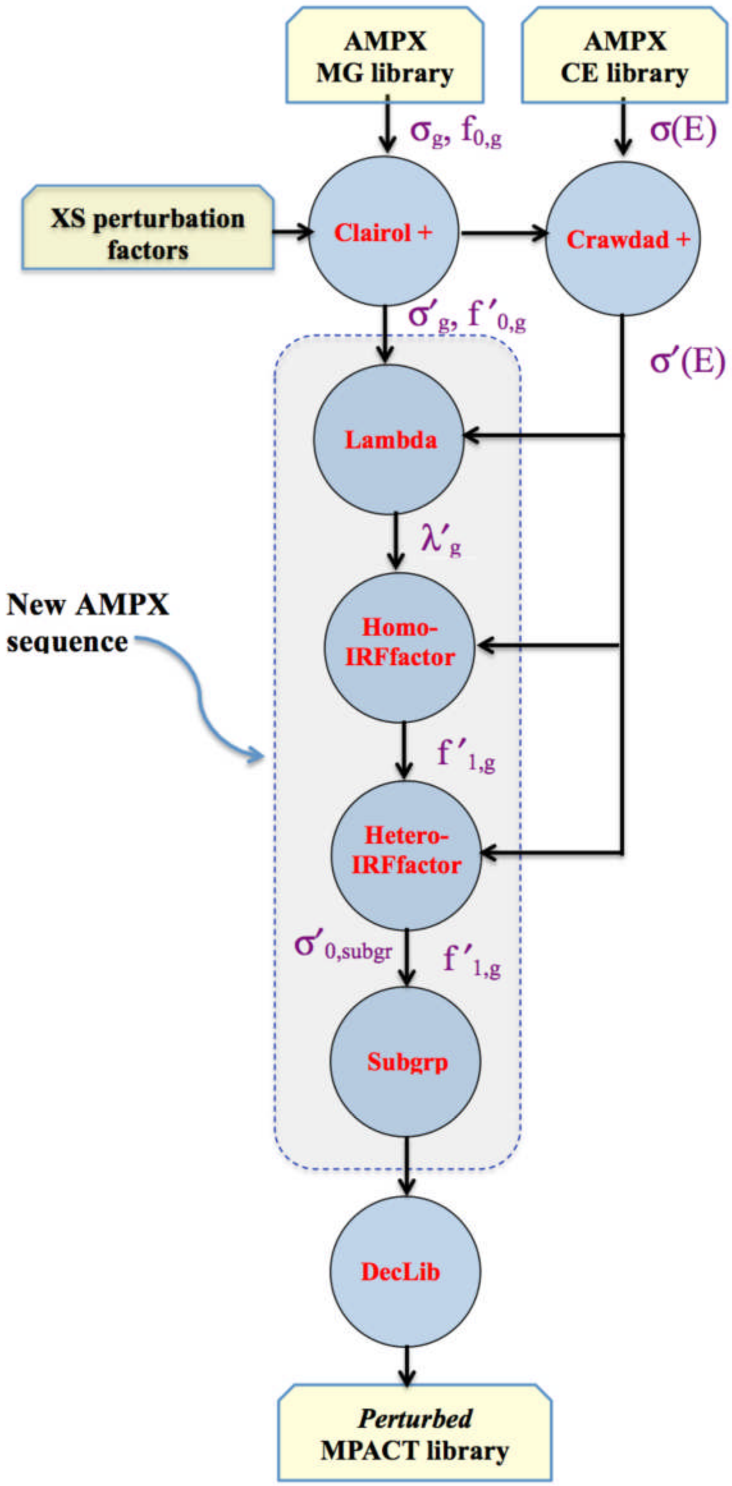

Figure 1. Generation of a Perturbed MPACT Library

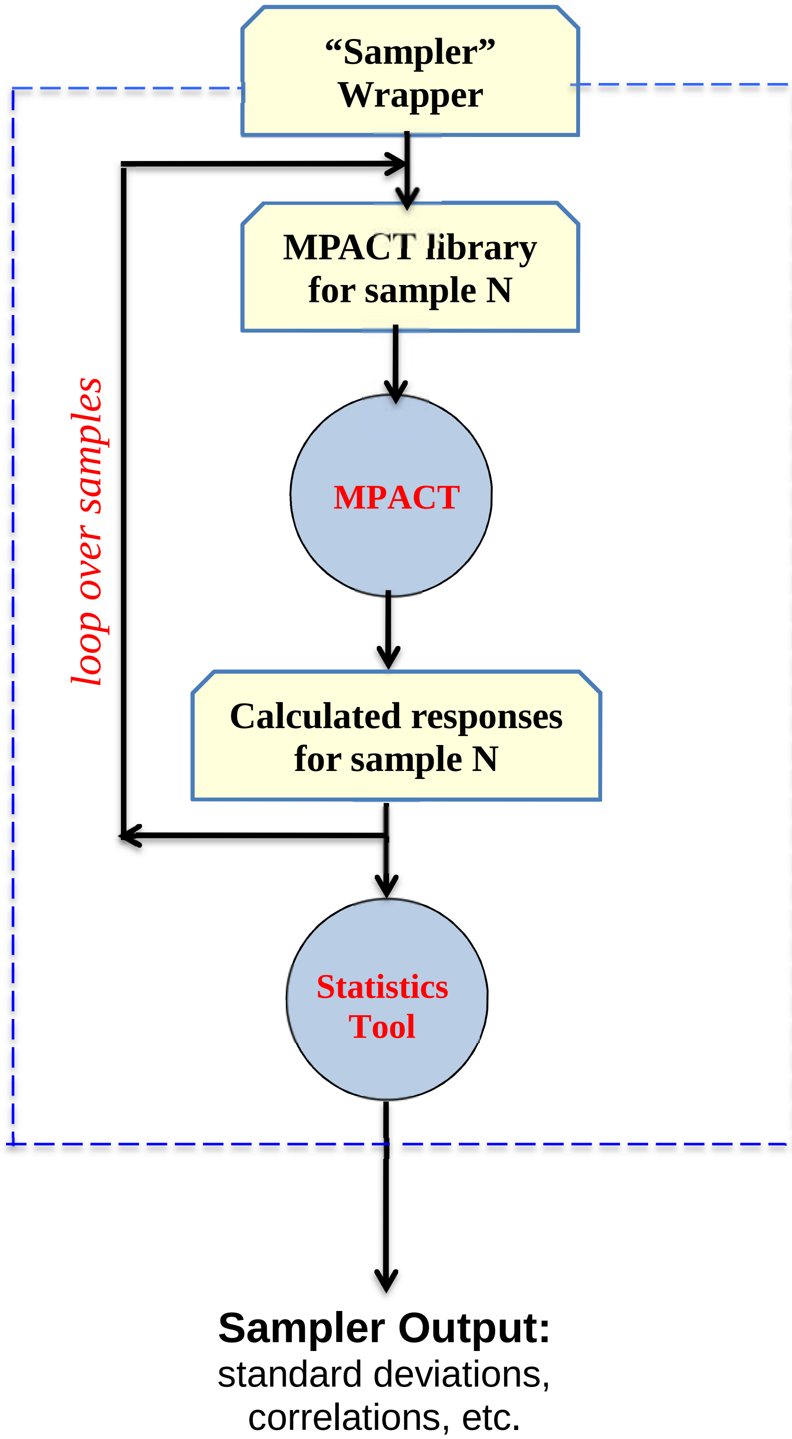

Figure 2. UQ Analysis with MPACT

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