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Optimised Iteration in Coupled Monte Carlo – Thermal-Hydraulics Calculations

J. Eduard Hoogenboom*[1] and Jan Dufek[2]

[1]*Delft Nuclear Consultancy, IJsselzoom 2, 2902 LB Capelle aan den IJssel, The Netherlands*
[2]*Royal Institute of Technology (KTH), Nuclear Reactor Technology, AlbaNova University Center, 10691 Stockholm, Sweden*

We address the problem of an efficient solution to the coupled Monte Carlo and thermal-hydraulic steady-state problem. Depending on the strength of the feedback between the power and thermal-hydraulic conditions this problem can become highly non-linear, requiring a stable iteration scheme to achieve convergence, such as the stochastic approximation scheme derived in our previous work. This scheme varies the relaxation factor and the sample size (number of simulated neutron histories) at each iteration step to ensure stability and efficiency. In this paper we provide detailed and practical instructions as to how the scheme can be implemented. The scheme is demonstrated for a BWR type fuel pin cell problem with axially varying fuel enrichment. Results are shown for the axial power distribution during the iteration steps and the behaviour of the number of simulated neutron histories in all iteration steps, which shows a nearly linear increase per iteration.

KEYWORDS: Monte Carlo, Thermal-hydraulics, stochastic approximation

I. Introduction

As Monte Carlo calculations do not need approximations with regard to the neutron transport model, reactor geometry or nuclear data as in deterministic calculations, it is used more and more often for full-size reactor analysis. In coupled Monte Carlo–thermal-hydraulic steady-state reactor calculations a Monte Carlo (MC) criticality calculation will provide the spatial power distribution in the reactor given the spatial distribution of temperatures and coolant densities. The power distribution is then input to the thermal-hydraulic (TH) calculation to produce updated temperatures and coolant densities, which can be fed back into the Monte Carlo criticality calculation to update the power distribution. This represents a non-linear problem that may diverge when solved with the standard fixed-point iteration scheme. We base our method on the stochastic approximation - the relaxation scheme derived in our previous work.[(1)]

As the MC calculation will normally take the major part of the necessary computing time, it is of utmost important to optimise the Monte Carlo runs in the MC-TH iteration process. Optimisation regards two main points: the number of neutron histories simulated in each iteration step and the way the results are combined over all iterations steps.

The specific coupling procedure[(2)] consists of a Python script that drives the iterations and calls the MC and TH codes successively. To prepare the input for the TH code a conversion program reads the output file from the MC calculation to obtain the estimated power distribution and include it in the proper format in the input file for the TH calculation. After the TH run the driver script calls another conversion program to read the output of the TH code, selects the axial temperature distributions for the fuel, cladding and coolant, as well as the density distribution of the coolant, for each fuel rod in the problem and prepares with these data a new input file for the next MC run.

II. Method

To determine optimised relaxation parameters for the MC-TH iterations, the method of stochastic approximation[(1)] is applied. We denote the number of simulated neutron histories in iteration step n by s_n. The cumulative number of histories up to and including step n is

$$S_n := \sum_{i=1}^{n} s_i.$$

The number of histories simulated determines implicitly the statistical accuracy of the estimated power distribution. If $p_n(\vec{r})$ is the spatial power distribution calculated by the Monte Carlo code in the n^{th} iteration step, it can be used as input to the next thermal-hydraulic calculation. However, it will be a waste of all Monte Carlo criticality runs in previous iterations not to use their results. Therefore, we define the relaxed power distribution $P_n(\vec{r})$ for iteration step n as:

$$P_n(\vec{r}) = (1 - \alpha_n)P_{n-1}(\vec{r}) + \alpha_n p_n(\vec{r}) \tag{1}$$

with α_n the relaxation coefficient with $\alpha_1 = 1$ for the first iteration. The relaxation coefficient is taken as[(1)]

$$\alpha_n = \frac{s_n}{S_n} \tag{2}$$

As the best convergence rate possible with Monte Carlo algorithms is of the order of $S^{1/2}$, this leads to

$$\alpha_n = \sqrt{\frac{s_1}{S_n}} \tag{3}$$

Elimination of α_n shows that

$$s_n = \sqrt{s_1 S_n} \tag{4}$$

As S_n depends on s_n we can solve s_n from a quadratic equation and find

$$s_n = \frac{s_1 + \sqrt{s_1^2 + 4 s_1 S_{n-1}}}{2} \tag{5}$$

At the start of the calculation the number s_1 of simulated histories for the first Monte Carlo run can be chosen. Mostly the number of successive (active) cycles (or batches) must be input to the MC code, as well as the number of histories per cycle (batch). One of these quantities can be chosen and the other follows from s_1. For all successive iteration steps the number of histories follows from Eq. (5), from which the number of cycles or the number of histories per cycle can be deduced for that iteration. Once the MC run provides the estimate of the power distribution $p_n(\vec{r})$, the input for the TH code can be composed from Eq. (1) with the relaxation coefficient given by Eq. (2).

III. Application

1. Description

The MC-TH iteration scheme is applied to a single BWR pincell problem with axially varying enrichment in the fuel. MCNP5[3] is used as the Monte Carlo code and SubChanFlow[4] as the thermal-hydraulics code. To start the coupled calculation an axial cosine distribution was chosen for the initial thermal-hydraulics run. In the MC runs the number of histories per cycle was fixed at 1000. For each run the results from the first 30 cycles were skipped to let the fission source distribution converge. Due to the stochastic behaviour of the results, the convergence criterion was taken as

$$\frac{\Delta T_f(z_i)}{T_f(z_i)} < 0.5\% \quad \text{for all axial zones } z_i \tag{6}$$

for two successive iteration steps.

2. Results

The MC-TH iteration process took 58 iterations to satisfy the convergence criteria. Fig. 1 shows the normalised axial power distribution at various iteration steps. Initially some oscillatory behaviour can be noticed. The tight convergence criterion forces a relatively large number of iterations. Fig. 2 shows the number of active cycles in successive iteration steps. It increases almost linearly.

IV. Conclusions

The presented optimised iteration scheme for Monte Carlo calculations when coupled with thermal-hydraulic calculations has shown to be an effective tool for this type of reactor calculations. The procedure can be implemented relatively easy, once a coupling scheme for Monte Carlo and thermal-hydraulic reactor calculations is available.

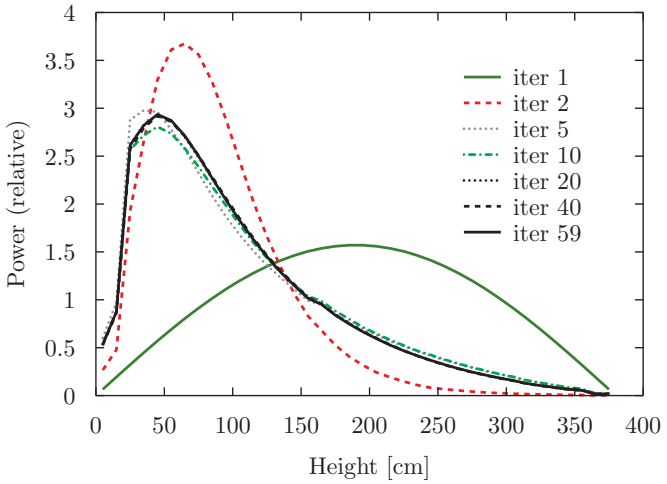

Figure 1: Normalised axial power distribution for successive MC-TH iterations

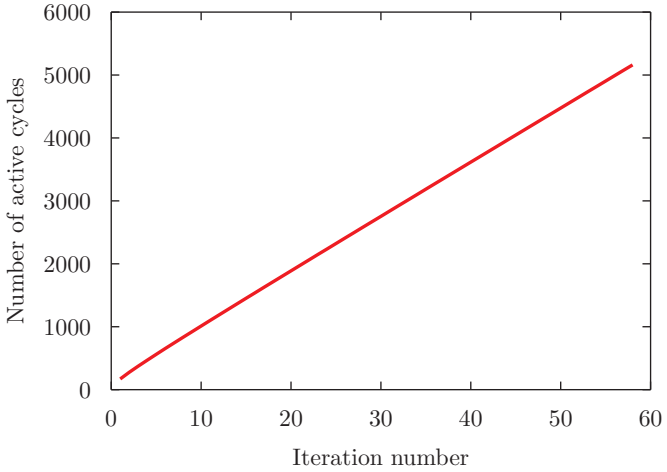

Figure 2: Number of active cycles in MC calculation for successive MC-TH iterations

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