Monte Carlo Methods and Simulations in Nuclear Technology

Convergence of the Fission Source, Bias in the Fission Source and k-eigenvalue, Optimising the Source Convergence

Jan Dufek

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KTH Royal Institute of Technology

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Convergence of the fission source

Convergence of the fission source

A criticality equation can be written even for the fission source as

$$ks = \mathbb{H}s$$

where $\mathbb{H}s$ gives the next generation fission source.

Solutions to the criticality equation

Many eigenvalues k_i and eigenfunctions s_i of $\mathbb{H}$ can satisfy the eigenvalue equation $ks = \mathbb{H}s$. Let's order them so that

$$k_0 > |k_1| > |k_2| > \dots$$

- The k_0 eigenvalue and its corresponding s_0 eigenfunction represent the so-called fundamental mode.
- Other eigenvalues and eigenfunctions represent higher modes. E.g., s_1 is the first higher-mode eigenfunction.
- Only the fundamental mode eigenfunction s_0 is non-negative in the whole system, and represents (together with k_0) a physical solution.

Convergence of the fission source

Fundamental mode

The fundamental mode source and eigenvalue can be computed iteratively by the power iteration (that represents the cycles in MC criticality simulation) as

$$s^{(n)} = \frac{\mathbb{H}s^{(n-1)}}{k^{(n-1)}}$$

$$k^{(n)} = \frac{< \mathbb{H}s^{(n-1)} >}{< s^{(n-1)} >} = \frac{k^{(n-1)} < s^{(n)} >}{< s^{(n-1)} >}$$

where $<>$ integrates over the whole space, energy and all directions, and $k^{(0)}$ and $s^{(0)}$ (initial values for the initial cycle) must be guessed.

Convergence of the fission source

Initial fission source

Any real function in domain of $\mathbb{H}$, and so also the initial fission source $s^{(0)}$ (the one that a user must guess in order to start the MC criticality simulation), can be written as a weighted sum of eigenfunctions s_i:

$$s^{(0)} = \sum_i \gamma_i s_i$$

Convergence of the fission source

Let's investigate the rate at which the source shape converges

The source shape would converge over the cycles even if we didn't normalise it by the eigenvalue:

$$s^{(n)} = \mathbb{H}s^{(n-1)}$$

which can be written as

$$s^{(n)} = \mathbb{H}^n s^{(0)}$$

which can be written as

$$s^{(n)} = \mathbb{H}^n \sum_i \gamma_i s_i$$

Convergence of the fission source

Let's investigate the rate at which the source shape converges

$$s^{(n)} = \mathbb{H}^n \sum_i \gamma_i s_i$$

can also be written as

$$s^{(n)} = \sum_i \gamma_i \mathbb{H}^n s_i$$

which (when combined with the eigenvalue equation) gives

$$s^{(n)} = \sum_i \gamma_i k_i^n s_i$$

Convergence of the fission source

Let's investigate the rate at which the source shape converges

When the equation

$$s^{(n)} = \sum_i \gamma_i k_i^n s_i$$

is divided by k_0^n then it can be written as

$$s^{(n)} \sim \gamma_0 s_0 + \left(\frac{k_1}{k_0}\right)^n \gamma_1 s_1 + \left(\frac{k_2}{k_0}\right)^n \gamma_2 s_2 + \dots$$

Convergence of the fission source

Let's investigate the rate at which the source shape converges

Since

$$1 > |k_1/k_0| > |k_2/k_0| > \dots$$

The source $s^{(n)}$,

$$s^{(n)} \sim \gamma_0 s_0 + \left(\frac{k_1}{k_0}\right)^n \gamma_1 s_1 + \left(\frac{k_2}{k_0}\right)^n \gamma_2 s_2 + \dots$$

must converge to s_0 as $O((k_1/k_0)^n)$.

Dominance ratio

The term k_1/k_0 is called the **dominance ratio**.

Remember!

The convergence rate of the source power iteration is governed by the dominance ratio. The closer the dominance ratio is to unity the slower the source converges and the more inactive cycles are needed.

Which systems have a large dominance ratio?

- Typically, large reactors have a dominance ratio very close to unity.
- Coupled systems (systems consisting of similarly reactive components, like a field of containers with nuclear waste)

Which systems have a small dominance ratio?

- Typically, small research reactors.
- Large reactors with a very asymmetrical configuration of control elements.

Convergence of the fission source

Is it possible to decrease the dominance ratio of a system in order to accelerate the convergence of the fission source?

- Nuclear reactor cores usually have a symmetrical configuration of fuel assemblies.
- In such a case, it is possible to model only a small part of the core, and apply reflective boundary conditions on the relevant radial surfaces.
- This will remove certain higher modes from the system, which will reduce the dominance ratio.

Bias in the Fission Source and k-eigenvalue

Bias in the Fission Source

Errors in the fission source

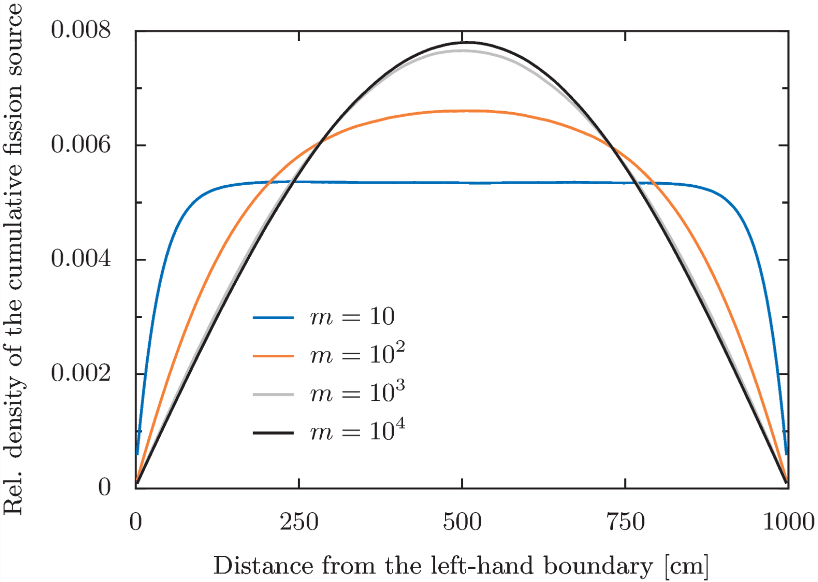
The fission source is sampled at a limited number m of points in the system (m is the batch size). Therefore it always contains a statistical error of the order $O(1/\sqrt{(m)})$.

Bias in the fission source

- Though it is difficult to derive mathematically, it is a fact that the normalisation of the fission source at each cycle introduces a bias (a systematic error) into the computed fission source and the multiplication factor in criticality simulations.
- The expected source $E(s^{(n)})$ thus converges not to s_0 but to a biased stationary distribution $s_{0,m}$.
- The difference between $s_{0,m}$ and s_0 is of order $O(1/m)$.

Bias in the Fission Source

Example of biased source in a slab reactor



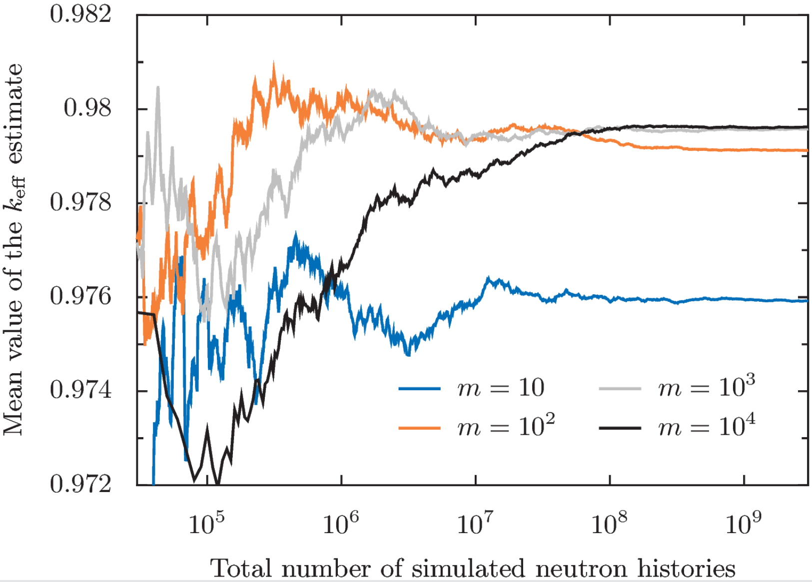
Bias in the Fission Source

Bias in k-eigenvalue

- The biased fission source causes a bias in the k-eigenvalue of the order $O(1/m)$.
- The biased source is usually flatter than the fundamental source, causing a larger neutron leakage from the system.
- The biased k-eigenvalue is therefore *usually* smaller than the correct value.
- This creates a risk of under-estimating the reactivity of the system, which is an important safety issue (a super-critical system could be found to be safely sub-critical by the MC calculation).
- The source bias also depends on the size of the system. The source bias is larger in large systems than in small systems (having the same number of neutrons per cycle in both systems).

Bias in the Fission Source

Example of the biased eigenvalue of a slab reactor



Bias in the Fission Source

How to lower the bias in the fission source and k-eigenvalue?

- The bias can be lowered only be increasing the batch size m.
- For usual systems, the batch size should not be smaller than 500 - 1000 neutrons.
- A bigger batch size may be needed for systems where the fundamental mode source departs considerably from a flat distribution.

Optimising the Source Convergence

Optimising the Source Convergence

Efficiency of criticality calculations

We wish to optimise the **batch size** m so that we obtain results with the required precision in the shortest computational time.

What are the advantages/disadvantages of setting a low batch size?

When m is small then

- many inactive and active cycles can be simulated within the allocated time, so the source can get converged during the inactive cycles in systems with dominance ratio close to unity.
- the bias in source and k may be so large that the accuracy of the result will be poor. The difference between the correct and the calculated value (i.e., accuracy) cannot be estimated, so the problem will be hidden.

Optimising the Source Convergence

What are the advantages/disadvantages of setting a large batch size?

- Due to the large batch size it may not be possible to simulate many inactive and active cycles, so the source may not converge, and results may contain large errors due to the un-converged fission source.
- The source bias (systematic error) will be small, but the source will contain errors of the initial fission source distribution since few cycles were simulated.

Optimising the Source Convergence

What should we consider when we optimise the batch size?

You have to look at the system you are modelling, and estimate:

- whether the system may have a dominance ratio close to unity (then many inactive cycles need to be specified (e.g. a thousand) -> that may call for a small batch size [e.g. 1000]),
- whether the fundamental source may differ much to a flat distribution (which would mean the source bias could be large -> a large batch size is needed [e.g. 5000 or more]),
- whether the initial fission source can be sampled from a distribution close to the fundamental mode (then the source is practically converged already and the number of cycles can be reduced and the batch size can be increased [e.g. to 50,000 or more])

You have to decide on the choice of the number of cycles vs the number of neutrons per cycles considering the computed time allocated for your simulation.

Can we do some tricks to improve the efficiency of criticality calculations in large systems prone to the source bias?

Yes. You can also divide the inactive cycles of the criticality calculation into several stages:

- Start with a small batch size of about 1000 neutrons, and simulate many cycles.
- In each stage increase the batch size several times, and simulate fewer cycles, starting with the source iterated in the previous stage.
- After several stages, start active cycles with a large batch size. This will allow you to make many inactive cycles while reducing the bias in active cycles. (And, you can indeed lower the DR if the system geometry is symmetrical.)