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## TOPIC ③

## NEUTRONICS & CORE PHYSICS

### 3.2 Monte Carlo methods

**State-of-the-art and advanced features**

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## Introduction

Radiation and particle transport problems are encountered in various fields of engineering and physics. One of the most rigorous ways to approach these problems is the stochastic Monte Carlo method, which is essentially a simulation technique based on the tracking of individual particles through complicated geometries. The main advantage of Monte Carlo calculation over other, deterministic transport methods, is the capability to handle the physics of nuclear reactions at a very fundamental level. The calculation requires essentially no approximations, and the best available knowledge on nuclear interactions is directly available for the simulation.

The drawback of Monte Carlo calculation is that the simulation requires a lot of CPU time. The method was developed along with the first digital computers in the late 1940's, but it has really started to replace faster deterministic calculation methods during the past few decades. The Monte Carlo method is widely used for criticality safety analyses, radiation shielding and dosimetry calculations, detector modeling and the validation of deterministic transport codes.

Reactor analysis, however, still relies on a multi-stage calculation scheme, consisting of several deterministic sub-steps. The reason why Monte Carlo codes are not widely used for reactor analysis is not only the high computational cost, but that the task requires a certain level of specialization and development in the calculation methods as well.

These lectures focus on two closely connected applications that are standard problems for deterministic lattice transport codes, but relatively new challenges for the Monte Carlo method: homogenization and burnup calculation. The methods introduced are discussed from the practical viewpoint of one Monte Carlo code developer, but they are easily generalized to a broader range of codes and applications.

## Monte Carlo method in reactor analysis

The modeling of an operating power reactor requires dividing the problem into several steps. The first step involves nuclear physics at the level of neutron interactions. As the calculation proceeds, the scale of the modeled system is gradually increased. In order to compensate for the extending boundaries, the physics of the system is simplified after each step. The other end of the chain represents a full-core reactor simulator calculation, typically based on the coupling of few-group nodal diffusion methods to a thermal hydraulics solver.

The crucial part of the chain for neutron transport codes is the lattice calculation, in which high-resolution nuclide-wise interaction data is condensed into a set of homogenized few-group constants that represent the physics inside a single fuel assembly. When Monte Carlo codes are considered for this task, it is seen that not only the advantages, but also the computational challenges differ from traditional Monte Carlo applications to some extent:

1) Instead of dealing with complicated 3D geometries and a number of case-specific user-defined tallies, the system is modeled at the fuel assembly level, surrounded by an infinite lattice of identical assemblies. The code is requested to calculate a set of homogenized multi-group constants and other parameters that are more or less the same for every case.

2) Criticality safety analyses or detector modeling often involves a single calculation case with a few variations, and high computational cost is clearly outweighed by the accuracy of the simulation. Homogenization, on the other hand, requires repeating the calculation for hundreds or even thousands of state points, and the overall CPU time easily becomes, not only a minor inconvenience, but a major practical limitation.

3) The main reason why Monte Carlo codes are used for their traditional applications is the capability to simulate the physics of the transport process to within maximum accuracy. Homogenization starts with a (non-physical) approximation, and the goal is to produce input parameters for the next stage in the calculation chain. The main advantage of using Monte Carlo codes for this task is not the accuracy, but the versatility of the calculation system. The same code and cross section libraries can be used for modeling any fuel or reactor type in two or three dimensions, without losing the close relation to the underlying physics.

The Serpent code, developed at VTT Technical Research Centre of Finland since 2004, was originally developed specifically this task. The code relies on various calculation techniques (Leppänen, 2007, 2009, 2010) that improve the performance in reactor physics and burnup calculations, but also limit the range of applications to some extent. The benefits of focusing in a single field of Monte Carlo neutron transport problems is also one of the main themes in these lectures, and the specific topics are briefly introduced below.

## Homogenization

The theory of homogenization (Koebke, 1978; Smith, 1980) is based on the preservation of integral reaction rates and average surface currents when the calculation proceeds from fuel assembly to full-core level. The generation of homogenized few-group cross sections requires calculating flux- and volume-integrated reaction rates – a task that can be carried out using the standard tally features of any Monte Carlo code. The same applies for assembly discontinuity factors, which are used for coupling each node to its neighbors.

Some parameters, however, require calculation techniques beyond the standard tally capabilities of Monte Carlo codes. A good example is the effective delayed neutron fraction, defined as the adjoint-flux weighed average of the same physical quantity. Approximate methods (Nauchi, 2005; Meulekamp, 2006) have been around for some years, but there has been significant recent development in continuous-energy adjoint calculation techniques as well (Kiedrowski, 2009).

Another problem encountered in homogenization is that the continuous-energy Monte Carlo simulation is not perfectly compatible with the deterministic methods that are used later in the calculation chain. This is especially the case for the calculation of neutron diffusion coefficients, and even though several methods exist (Leppänen, 2007), the results are often less than satisfactory. The problem of methodological incompatibility has recently been approached from a different point-of-view, by performing the homogenization in a leakage-corrected flux spectrum, similar to various deterministic transport codes (Shim, 2008; Fridman, 2011).

## Burnup calculation

Another major task for reactor analysis is the tracking of isotopic changes in fuel materials under irradiation. The problem is relatively straightforward in principle, but it brings the CPU time requirements of Monte Carlo codes to a whole new level, as the transport calculation has to be repeated for each burnup step.

Methods for improving the performance of Monte Carlo burnup calculation codes have been developed over the years (Haeck, 2007; Fridman, 2008). Other important topics include advanced methods for solving the Bateman depletion equations (Pusa, 2010), and improved time integration methods between burnup steps (Isotalo, 2010).

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