Monte Carlo simulation of neutron transport applied to criticality

Focus on sources and flux convergence issues

J. Miss[1], Y. Richet[1] and O. Jacquet[2]
[1] IRSN, Study, Research, Codes Development and Validation Laboratory, France
[2] Independent consultant, France

Abstract

Safety studies to determine criticality risk (uncontrolled multiplication of neutrons) in systems containing fissile material require the use of computer codes (software programs) that can simulate neutrons in complex three-dimensional configurations. This article describes the specific features of the Monte Carlo simulation method, used to simulate neutron transport for criticality studies conducted using the MORET code developed at IRSN. It highlights also the flux convergence issues in Monte Carlo depletion simulations.

1. Introduction

Fissile material (such as the isotopes used in the nuclear fuel cycle: uranium, plutonium) may be the source of a nuclear chain reaction. All systems (for industry, research, etc.) that use these materials present therefore a criticality risk, which must be assessed and controlled. The main physical parameter used to quantify this risk is the effective neutron multiplication factor (keff), defined as the ratio between the number of neutrons produced and the number of neutrons lost (through leakage and absorption). In other words, this factor characterizes the "critical state" of the fissile material in question. Since configurations are often complex, keff is generally estimated using a set of software tools (computer codes) that model the fissile material and its geometry, as well as the physical laws governing particle behaviour.

Probabilistic simulation techniques are usually currently used to solve problems in three major areas: criticality, reactor neutronics, and radiation shielding.

Although the same probabilistic simulation method, known as the "Monte Carlo method", is used in all these three areas, the mathematical algorithms used to track particles differ. Radiation shielding or dosimetry simulations are said to be "fixed-source" simulations (the spatial distribution of emitted particles is known and fixed at the beginning of the simulation: fissions, radioactive sources of α, β, γ, X-ray or neutron radiation, etc.). One example of a problem to be solved is the dose rate at a detector placed at a given distance from the source, which has known characteristics. In contrast, criticality or reactor neutronic simulations are said to be "eigenvalue" simulations, where the real position of the sources is not known at the beginning of the simulation, since their position is what determines the solution to the problem (i.e. the desired keff value).

Consequently, finding criticality results cannot be assimilated with finding results in a radiation shielding approach, because the simulation algorithms are not the same. A Monte Carlo criticality simulation is based on an iterative process used to converge on the "real" neutron distribution in the geometry. The population of neutrons is initially positioned in the geometry by the user, with each

new generation of neutrons arising from fissions induced by the previous one. The value of keff is therefore recalculated at the end of each generation.

MORET [1] is a Monte Carlo code for simulating neutron transport, developed and used by IRSN for criticality-safety studies. It can compute the effective multiplication factor of complex three-dimensional systems, neutron flux and reaction rates in various volumes, and neutron leakage from the system. MORET is a precious tool for studying neutron behaviour in configurations containing fissile material. R&D work on this code aims at understanding and controlling the specific parameters of Monte Carlo neutron simulation in critical conditions, which is the focus of this article.

2. Fission source convergence in criticality simulations

For criticality studies, the first part of the Monte Carlo simulation consists in converging the neutron distribution in the phase space. This distribution is initially unknown to the user. To achieve convergence, the neutrons of one generation are tracked until they disappear and their fission daughters are stored. The next generation is sampled among the stored neutrons, which are once again tracked and their daughters stored in turn. This is referred to as a Markov chain Monte Carlo simulation. The convergence phase ends when neutron distribution becomes stationary from one generation to the next. More or less robust criteria to detect stationarity for this type of simulation have been developed and implemented in criticality simulation codes.

It is easy to demonstrate that all events governing neutron flux can be broken down into a Neumann series, leading to the use of an iterative process to solve the Boltzmann equation.

Let Φ (r, E, Ω) be the particle flux at point (r, E, Ω) of the phase space (r: geometric position; E: particle energy; Ω direction of travel). If T is the transport operator, C the collision operator, S the initial neutron sources, and n the neutron generation index, then:

$\Phi_0 = TS$ (flux after transport of initial sources)

$\Phi_n = TC\Phi_{n-1}$

$\Phi_n = (TC)_n TS$

This approach induces a certain statistical correlation from one generation to the next, which can generate bias in the statistical estimators produced by the simulation code. Criticality simulations aim to assess the capability of a system containing fissile material to multiply neutrons and hence to sustain a chain reaction. The value to be determined is therefore keff, which is closely linked to neutron distribution in the configuration under study.

In general, regardless of initial positioning, a population of neutrons will eventually converge on a spatial distribution that remains stable from one step to the next. However, in geometries where certain fissile units contribute significantly to system reactivity and are loosely coupled to other fissile volumes (e.g. assemblies in which the irradiation profile is taken into account, models of very large installations such as reactor cores, etc.), this correlation between steps, associated with other parameters such as an insufficient number of source neutrons or inadequate placement of these neutrons in the first generation, can lead to incorrect keff values.

This is a well-known problem among users of Monte Carlo criticality codes and has been an R&D focus for many years, notably through international work groups coordinated by the NEA (Nuclear Energy Agency) of the OECD (Organisation for Economic Co-operation and Development): http://www.nea.fr/html/science/wpncs/convergence .

Developers of the IRSN MORET Monte Carlo code (described in greater detail below) have participated actively in these R&D initiatives [2], particularly by developing and comparing several neutron sampling models, in order to resolve the convergence problems while achieving faster, more robust simulations.

3. MORET, a Monte Carlo code dedicated to criticality studies

MORET5 is a both multi-group and continuous energy criticality Monte-Carlo code. It allows to estimate fluxes, the neutron effective multiplication factor and kinetic parameters for any three dimensional systems. Specially designed to meet the needs of criticality studies, it has been used in most studies of nuclear fuel cycle facilities and fissile material transport in France. Neutron simulation in MORET has been optimized to achieve a good compromise between cost and accuracy, making the code suitable for project studies.

Criticality simulations are usually run in two stages. In the first stage, a deterministic code is used to solve the Boltzmann equation as accurately as possible, not for the entire configuration, but rather for a smaller geometry having only one or two dimensions, e.g. a fuel rod or fuel assembly, in order to determine the physical variables in zones displaying a certain degree of neutron homogeneity. In the second stage, the Monte Carlo code is used to simulate the entire configuration in three dimensions, in a geometry with partial spatial homogenization using results from the first stage. The MORET code has thus been coupled with deterministic codes that take into account local heterogeneities, thereby simplifying Monte Carlo simulation models and reducing computation time, which enables the engineers in charge of criticality studies and expert assessments to rapidly run a large number of verification simulations (Figure 1).

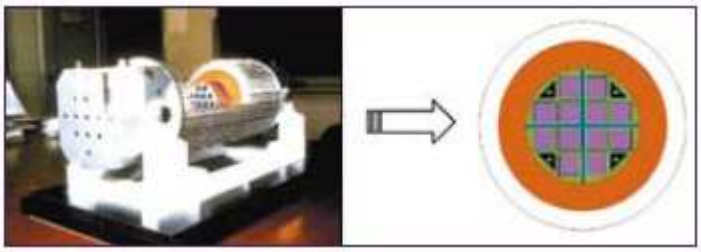

Figure 1: Fissile material transport. Actual configuration and simplified modeling in MORET.

The main results obtained with MORET are as follows:

- keff resulting from neutron tracking during a given generation;
- mean keff and its standard deviation;
- validity indicators for the assumption of a normal keff distribution at each generation;
- per-volume balance, which can be used to obtain reaction rates (absorption, fission, etc.);
- number of source neutrons in each fissile volume at different generations of the simulation;
- various neutron parameters ($k\infty$, average fission group, kinetic parameters, etc.).

It is designed to read any macroscopic multigroup library performed with APOLLO, DRAGON or SCALE systems, and any ACE pointwise library.

Specific functionalities have been implemented in the MORET code to take into account advances in criticality studies (increasingly accurate modeling, integration of in-core fuel irradiation (currently known as burnup [3]), reusability of simulations run by other engineers, etc.).

One of the particularly useful features of the code is its capability to create "modular" geometries, including multiple arrays and arrays of arrays. These geometries consist of modules or "building blocks" that model various parts of the system considered and are independent in terms of geometric description, facilitating reuse from one input file to another. These new developments make it easier to model configurations of increasing complexity, with an ever greater number of volumes. Furthermore, modularity makes it possible to create databases of standard geometries that, once verified, can be easily and safely reused from one configuration to another by different engineers. This option improves the quality of studies conducted. For example, a fissile material container to be routed through several facilities only needs to be modeled and verified once. The resulting model can then be used by the different engineers in charge of the various facilities, without creating new models. The potential risk of error or inconsistency that accompanies each new description is therefore eliminated.

A special effort has also been made to reach high levels of validation and qualification to consolidate MORET as a code dedicated to safety [4], targeting the following objectives:

- test to ensure non-regression compared to earlier versions, taking into account new developments;
- assess any discrepancies with the real world (benchmarking);
- define the validity range and estimate simulation uncertainty and bias.

Finally, to correct the problem inherent to using the Monte Carlo method in criticality simulations, different techniques of simulating and sampling source neutrons among the fission sites have been studied. These methods (all implemented in MORET) are the subject of in-depth analysis conducted by the NEA/OECD Expert Group on Source Convergence. The sampling [2] and simulation [5;6] methods available in MORET are as follows:

- **The "natural", "conventional" or "analog" (to reality) method**: typically (available and) used in Monte Carlo criticality codes. The number of neutrons produced in a volume, divided by the total number of neutrons produced in the system, represents the proportion of neutrons to be emitted from this volume in the following step.

- **The "stratified sampling" method**: does not allow a zero value for the number of source neutrons to be generated in a fissile volume when the estimated real number of source neutrons is less than 0.5. If this is the case, an additional source neutron is generated with a weight equal to the estimated real number of source neutrons in the volume. The objective of this strategy is to guarantee that each fissile zone (loosely coupled with the rest of the system) contains in each generation at least one source neutron, with a weight that may be less than 1.

- **"Kij" method**: uses the Kij matrix to obtain the number of fission-emitted neutrons in volume i based on one neutron emitted in volume j; the largest eigenvalue of this matrix is equal to the system multiplication factor and the associated eigenvector corresponds to the neutron

distribution in the different volumes. This eigenvector is used to simulate the distribution of source neutrons for the following step in order to accelerate source convergence. This method is very close to the stratified method, except for use of the eigenvector associated with the largest eigenvalue of the Kij matrix to renormalize the source neutron distribution every "Freq" step (Freq is a user-specified integer).

- **The "Importance" sampling**: a simulation option that uses the "greatest eigenvalue function" to estimate source neutron distribution from one step to the next, in order to accelerate convergence. The greatest eignenvalue function uses the eigenvector associated with the largest eigenvalue of the Kij adjoint matrix. It calculates the contribution of each volume in the production of neutrons from one step to the next. This process inhibits the creation of neutrons in volumes less important from the point of view of the reactivity.

- **The "superhistory" method**: a simulation option used to track a source neutron and its daughters over L generations, in order to avoid recalculating source distribution at each generation. For all methods except the superhistory method, the number of neutrons simulated at each generation is constant. This normalization has been shown to cause bias in the computed keff and its variance. A constant number of neutrons at each generation may effectively favor smaller zones. The superhistory method allows the neutron population to be variable for L generations; the number of neutrons is only normalized thereafter.

- **The "Wielandt" method**: a part of fission neutrons emitted during random walk processes are tracked within the current cycle, and thus a fission source distribution used in the next cycle spread more widely.

- **The "Woodcock tracking" method**, also known as the pseudo-scattering or fictitious-scattering tracking method, is an alternate to the “classical” way to perform particle transport in Monte Carlo codes. The idea of the Woodcock method is to virtually homogenize the whole system by giving it a unique total cross-section (Σ^M), that is equal to the maximum value of the total cross-sections for the various material present in the system (Σ_1^T, Σ_2^T, … , Σ_n^T).

4. Flux convergence issues in Monte Carlo depletion criticality simulation

Source convergence issues in Monte Carlo criticality simulation were previously seen as a difficult research problem, fortunately having a marginal impact on real world criticality licensing, which focuses mainly on k-effective estimation. Applied in depletion calculations, Monte Carlo source convergence is now a key point for the reliability and usability of this type of application.

The goal of this paragraph is to highlight these issues through a simple example.

4.1 The VESTA interface

VESTA [7] is a Monte Carlo depletion interface code that is currently under development at IRSN. With VESTA, the emphasis lies on both accuracy and performance, so that the code will be capable of providing accurate and complete answers in an acceptable amount of time compared to other Monte Carlo depletion codes. VESTA has been transmitted to OECD/NEA and RSICC and should be soon available through these information computational centers.

From its inception, VESTA is intended to be a “generic” interface code so that it will ultimately be capable of using any Monte-Carlo code or depletion module and that can be tailored to the user’s needs. For now, the first release of VESTA allows for the use of any version of MCNP(X) and a modified version of ORIGEN 2.2. Support for other Monte-Carlo codes (like the MORET 5 code developed at IRSN) and/or depletion modules (like PHOENIX developed at IRSN) are foreseen in the near future.

PHOENIX is a standalone version of the point depletion module implemented in VESTA. The core of PHOENIX is a generic point depletion module because it can be adapted to any type of incident particle (neutrons, protons, etc.), reaction type (fission, capture, particle emission, etc.) and decay mode. In its current form, the PHOENIX module is capable of calculating the evolution of materials through radio-active decay and neutron induced activation using ORIGEN 2.2 data libraries.

The validation/qualification of the first release of VESTA has now been initiated using chemical assay data (like for instance from the SFCOMPO database [8]). Comparison with other depletion codes (both based on deterministic and stochastic codes like TRITON in SCALE or MONTEBURNS) have been performed in the past.

4.2 A simple Monte Carlo discrepancy benchmarking

The VESTA depletion interface is used to simulate isotopes composition histories on a parametric ill-conditioned benchmark of infinite lattice of PWR fuel pins modeled with MORET 5 Monte Carlo code (figure 2). Besides initial random seeds, several simulation parameters (neutrons population size, number of batches, time sampling and geometrical binning) are compared in terms of simulation cost versus time compositions discrepancy.

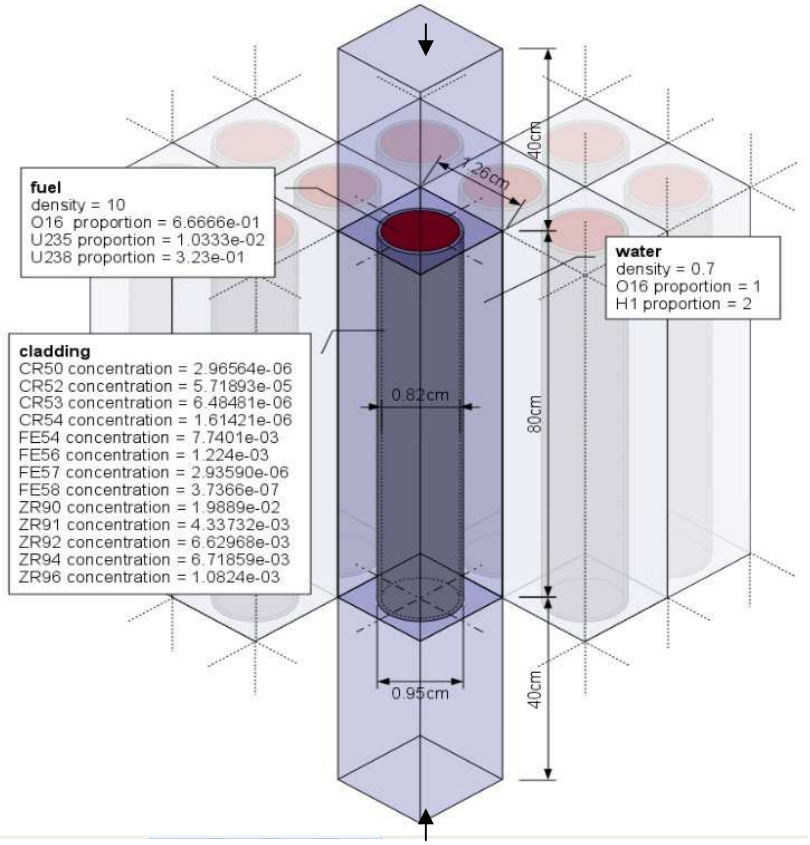

Figure 2: Benchmark model: rod split axially in 8 zones

To summarize Monte Carlo neutron simulation provides fluxes or reaction rates which mean is used as best estimate value. We performed 20 identical calculations with different initial random seed lead to different composition output. The main tools used are: VESTA(ORIGEN-MORET) and PROMETHEE [9].

PROMETHEE (http://www.irsn.org/promethee) is a generic computing environment for any code allowing using grid for parametric calculations. It efficiently parallels and dispatches calculations over all connected servers and has an user friendly front-end intended to be used for both day-to-day engineering or research. It may embed algorithms for advanced computing tasks (uncertainty propagation, sensitivity analysis, optimization, calibration...).

We focused our study on estimation of U_{235}, Pu_{239}, Xe_{135} composition histories, and irradiated the rod (**split axially in 8 identical zones**) during 20 days with a constant power. **As zones are identical and as the rod is totally reflected to simulate an infinite height, we should have theoretically for each isotope a uniform density in the whole rod**. The other parameters are:

- The number of cycles n = {100, 400} (+30 non active)
- The number of neutrons N = {800, 3200}
- The depletion time step dt = {6, 24, 96} hrs

Some results are presented on the following figures (figures 3-7).

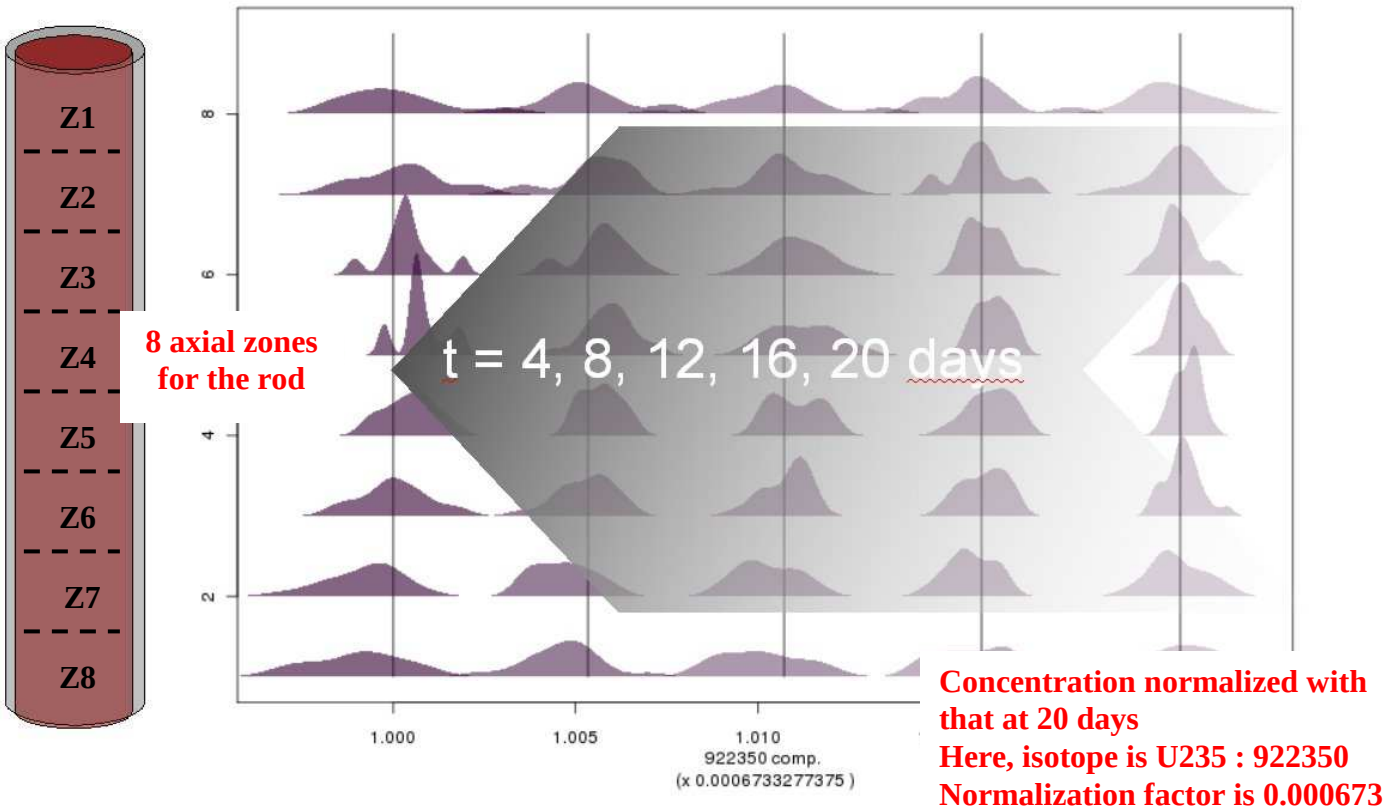

Figure 3: Presentation of the visualization of results

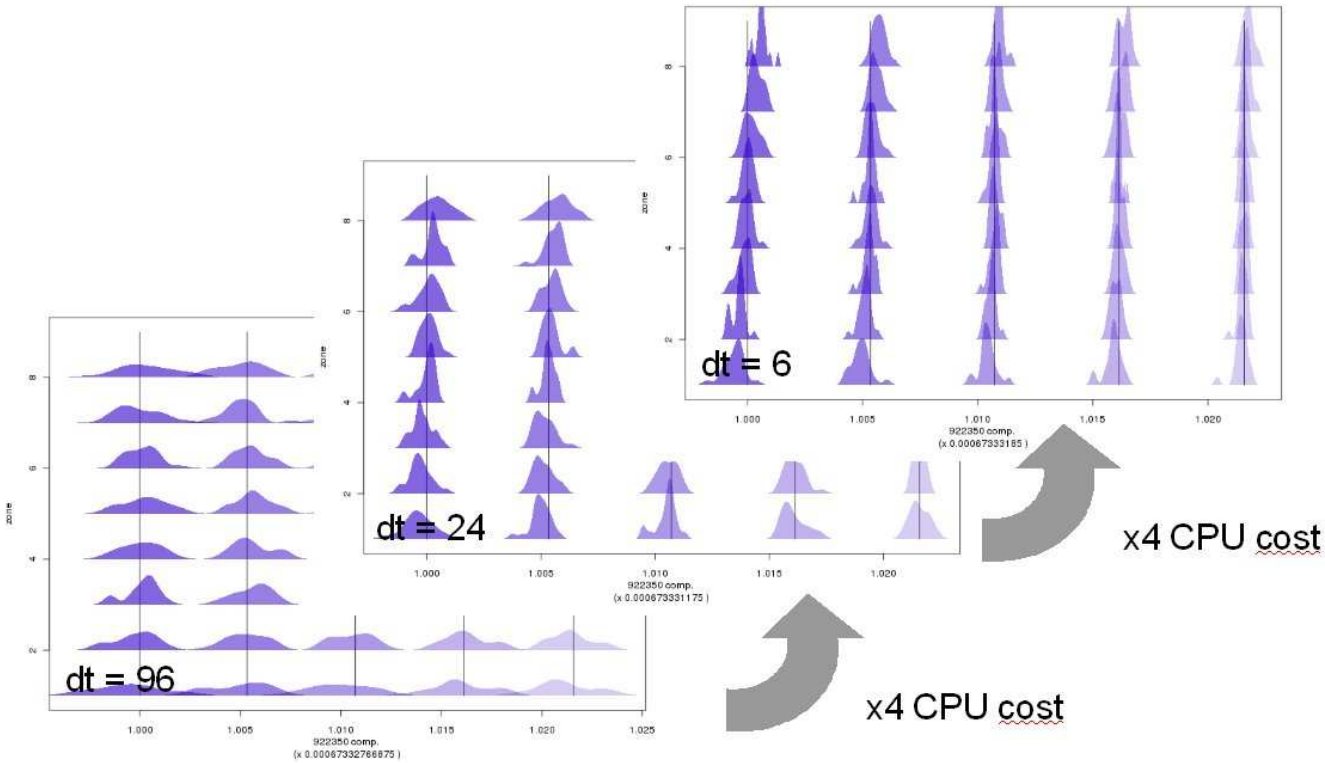

Figure 4: Time step (dt) effect for U_{235}

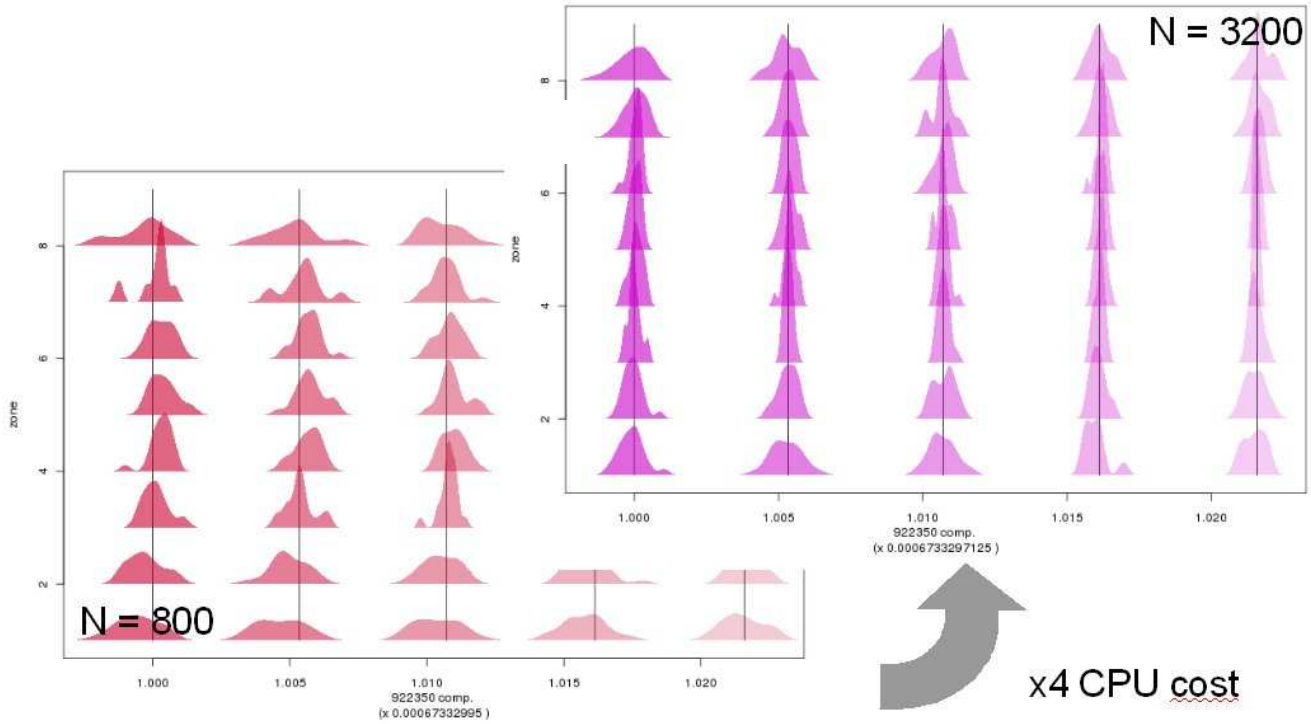

Figure 5: Number of Monte Carlo sources (N) effect for U_{235}

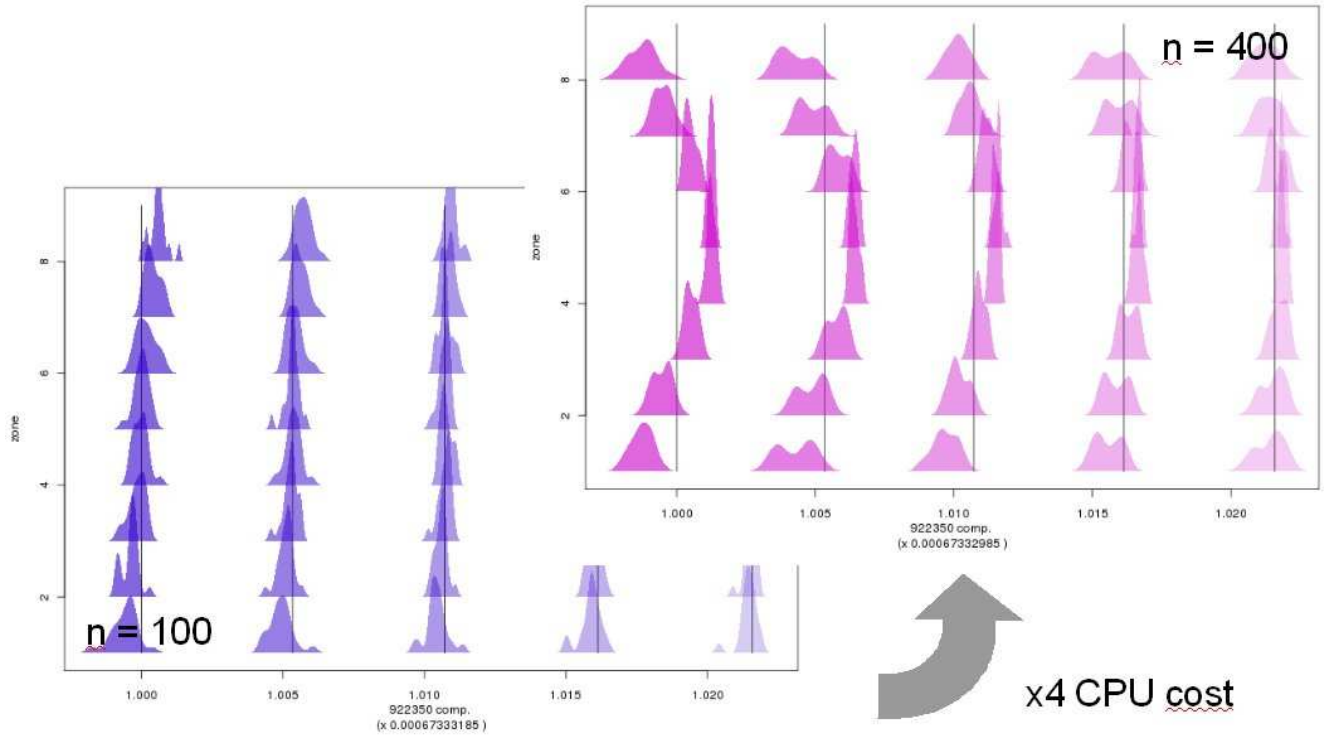

Figure 6: Number of Monte Carlo cycles (n) effect for U_{235}

We observed:

- For depletion time step (dt), spreading seems to stabilize after some time steps;
- High number of sources (N) limits spreading;
- Number of Monte Carlo cycles (n), combined with Z reflections, seems to lead **to bias of composition expectation and large uncertainty**;
- Small uncertainties for U_{235} concentration results (standard deviation ~ 0.3%);
- Significant uncertainties for Pu_{239} concentration results (standard deviation ~ 2%)
- Large uncertainties for Xe_{135} concentration results (standard deviation ~ 5%)

5. Conclusion

Criticality studies have conventionally focused on determining keff (an integral quantity), while more local information (flux, dose rate, etc.) is targeted in neutronic and radiation protection studies. Advances in criticality codes, such as increasingly accurate modeling of configurations, consideration of burn-up which are non-uniform along fuel assemblies, and broader use of these codes (e.g. to simulate various types of reactor core), have introduced new problems. In Monte Carlo criticality simulation algorithms, source neutrons are sampled from one generation to the next, which tends to favor the neutron population in the most reactive areas of the system studied. This correlation effect between generations makes it difficult to perform statistics estimations with a sample of neutrons that have passed through certain areas in the system, particularly for keff or neutron flux determinations. Research and development is thus underway on the MORET code, aiming to solve these convergence problems and gain complete control over all actions that contribute to a criticality result obtained with a Monte Carlo code, from evaluating nuclear data and creating cross-section libraries to running probabilistic simulations and estimating the propagated uncertainty. A way currently being explored involves the five sampling methods described in this article. The goal of implementing these methods is to identify the most effective among them and move toward an "ultimate" method of neutron convergence. MORET developments thus build knowledge at all stages of the simulation process, making this code an invaluable tool.

Concerning Monte Carlo depletion issues, the probability density of resulting compositions obtained on such "crude" Monte Carlo propagation of simulation noise due to Boltzmann equation Monte Carlo solving process tends to arise numerical instability which leads to false neutronic oscillations similar to (physically true) Xenon effect. The density functions observed are investigated to suggest some explanations based on Monte Carlo neutron simulation characteristics and convergence issues.

6. References

[1] J. Miss, O. Jacquet, F. Bernard, B. Forestier, Massive evolution in the MORET Monte Carlo code. A new multigroup-continuous energy version, ICNC 2007, Saint Petersburg, Russia, May 28-June 01, 2007.

[2] R. Blomquist, M. Armishaw, D. Hanlon, N. Smith, Y. Naito, J. Yang, Y. Mioshi, T. Yamamoto, O. Jacquet, J. Miss. Source convergence in criticality safety analyses –Phase 1: Results for four test problems.

[3] J. Raby, C. Lavarenne. La prise en compte du credit burnup dans les études de criticité, IRSN, Rapport scientifique et technique 2005.

[4] I. Duhamel, E. Létang, G. Daumen, I. Lebars. Processus de qualification des formulaires de criticité et exemple d'utilisation dans le domaine de l'expertise de criticité, IRSN, Rapport scientifique et technique 2006.

[5] T. Yamamoto, Y. Miyoshi - method for fission source convergence of Monte Carlo criticality calculation with Wielandt method – J. Nucl. Sci. Technol., Vol 41, No2, p99-107 (2004)

[6] B. Forestier et al. Criticality calculations on pebble-bed HTR-PROTEUS configuration as a validation for the pseudo-scattering tracking method implemented in the MORET 5 Monte Carlo code, PHYSOR 2008, Interlacken

[7] W. Haeck, "VESTA User's Manual - Version 2.0.0", IRSN DSU/SEC/T/2008-331 - Indice A, Institut de Radioprotection et de Sûreté Nucléaire, France (2009)

[8] http://www.nea.fr/sfcompo

[9] http://promethee.irsn.org