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New kinetic simulation capabilities for TRIPOLI-4®: Methods and applications

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ABSTRACT

Thanks to the growing computer power, it is now feasible to apply Monte Carlo methods to the solution of non-stationary transport problems in reactor physics and in criticality-safety, which play an instrumental role in producing reference numerical solutions for the analysis of transients occurring during normal and accidental behaviour. In this respect, a major scientific challenge is represented by the very different time scales of neutrons and precursors, which demand distinct strategies and variance reduction techniques with respect to stationary simulations. In this work we will present the principal algorithms and simulation methods that have been explored and selected for the kinetic capabilities of TRIPOLI-4®, the production Monte Carlo code developed at CEA. The efficiency of the tested methods will be demonstrated on simple geometries as well as on step reactivity insertion and extraction due to control rod movements for the experimental reactor SPERT-III E-core. The solutions obtained by using TRIPOLI-4® will be compared to the point-kinetics approximation and to the asymptotic analysis based on alpha eigenvalues.

1. Introduction

The development of reliable and fast numerical tools allowing for the multi-physics simulation of reactor cores (coupling neutron flux with thermal-hydraulics and thermomechanical feedbacks, in stationary and non-stationary regimes) has undergone intensive research efforts in recent years. This is witnessed by the innovation agendas SNETP,[1] NUGENIA[2] and H2020[3], and in particular the European projects FP7 NURESIM,[4] NURISP,[5] NURESAFE,[6] HPMC[7] and McSAFE[8]. Similar initiatives have been undertaken in China and in the USA (for instance, the CESAR [9] project or the CASL[10] consortium). The final goal of these efforts is to pave the way towards a full "numerical reactor core", allowing even extreme (i.e., inaccessible to experimental evidence) conditions to be probed and the associated uncertainties to be quantified.

Until very recently, the simulation of neutron transport in non-stationary conditions was entirely based on deterministic methods (which are usually very fast for stationary conditions). For transient regimes, due to the very large number of unknowns ($\sim 10^{14}$) resulting from a fine discretization of phase space variables (space, angle, energy and time), current state-of-the-art industrial codes employ a two-step approach: a detailed transport calculation at the lattice scale in stationary conditions in two dimensions is followed by a time evolution calculation for the neutron flux at the core scale, based on the cross sections determined in the course of the first step. The time-dependent step is typically carried out in simplified transport models (diffusion or SP_N, for instance) with a coarse energy discretization (D'Auria et al., 2004; Dulla et al., 2008; Larsen, 2011).

Since the approximations introduced in the deterministic approach are problem-dependent (i.e., specific to each reactor type), the validity of the results thus obtained, as well as the assessment of the associated uncertainties, depend on the configuration under analysis (D'Auria et al., 2004; Dulla et al., 2008; Larsen, 2011). Thus, in order to relax these constraints and to consolidate the validation of deterministic codes, it is mandatory to develop a *high fidelity* method (IAEA, 2003). This is especially true in view of the limited number of experimental measurements available for transient reactor operation or accidents (IAEA, 2015).

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[1] Sustainable Nuclear Energy Technology Platform.
[2] Nuclear Generation II & III Association.
[3] HORIZON 2020.
[4] NUclear REactor SIMulation: 2005–2008.
[5] NUclear Reactor Integrated Simulation Project: 2009–2012.
[6] NUclear REactor SAFEty: 2013–2015
[7] High Performance Monte Carlo reactor core analysis: 2011–2014.
[8] High-performance Monte Carlo methods for SAFEty demonstration: 2017–2020; cordis.europa.eu/projects.
[9] Center for Exascale Simulation of Advanced Reactors; cesar.mcs.anl.gov.
[10] Consortium for Advanced Simulation of Light Water Reactors; www.casl.gov.

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Monte Carlo simulation is intrinsically based on the realization of a large number of stochastic neutron trajectories, whose probability laws are determined in agreement with the underlying physical properties (the probability of particle-matter interaction, energy and angle distributions after collision, and so on), and an exact treatment is possible for the reactor geometry (Lux and Koblinger, 1991). Accordingly, Monte Carlo simulation is considered as the "golden standard" for neutron transport calculations (Bell and Glasstone, 1970; Lux and Koblinger, 1991). To this day, Monte Carlo methods have been almost exclusively applied to the solution of stationary problems, due to the very high computational cost (in terms of both memory and CPU time) required for generating the particle trajectories (Lux and Koblinger, 1991). However, thanks to the growing available computer power, Monte Carlo methods can now be also applied to the solution of non-stationary transport problems, as witnessed by the increasing number of scientific publications on this subject (Legrady and Hoogenboom, 2008; Sjenitzer and Hoogenboom, 2011; Leppänen, 2013; Sjenitzer and Hoogenboom, 2013; Sjenitzer et al., 2015; Mylonakis et al., 2017). The two major scientific challenges towards this goal are represented by *i*) the very different time scales of neutrons and precursors during long transients (Legrady and Hoogenboom, 2008; Sjenitzer and Hoogenboom, 2011; Sjenitzer and Hoogenboom, 2013) and *ii*) the presence of physical feedbacks during the transients: the energy released by fission induces temperature and density variations that in turn affect neutron transport (Leppänen, 2013; Sjenitzer et al., 2015). This paper deals with the challenge *i*) and describes the implementation of the *kinetic Monte Carlo* methods. The solution of the problem *ii*) requires the coupling of a kinetic Monte Carlo with other physics solvers (resulting in the *dynamic Monte Carlo*) and is left as the subject of future work.

We have recently investigated Kinetic Monte Carlo in view of its implementation in TRIPOLI-4®, the 3D continuous-energy Monte Carlo transport code developed by CEA, Saclay (Brun et al., 2015). This paper describes the most important algorithms and simulation strategies that have been adopted in TRIPOLI-4. The final goal of this work is to prepare TRIPOLI-4 for the future implementation of dynamic methods, which will require coupling stochastic neutron transport with thermal-hydraulics and/or thermomechanics simulation codes so as to take into account physical feedbacks.

This paper is structured as follows: Section 2 recalls the general context and mathematical formalism of the time-dependent behaviour of neutrons and precursors in nuclear reactors. Section 3 introduces the kinetic Monte Carlo methods that allow dealing with time-dependent neutron transport problems, and details the variance-reduction techniques specific to these simulations. Section 4 presents a set of verification tests for the kinetic algorithms performed with TRIPOLI-4 on Spert III-E core in several configurations, including rod-drop and rod-ejection. Some examples of transient simulations are also presented for the case of Flattop-Pu. Conclusions are finally drawn in Section 5.

2. Time-dependent neutron transport

In many technological applications, encompassing reactor start-up analysis and reactivity measurements, one is interested in determining the time behaviour of the neutron flux φ in a system, starting from a given initial condition (Keepin, 1965; Bell and Glasstone, 1970; Pfeiffer et al., 1974; Hansen, 1985; Pázsit and Pál, 2008; Persson et al., 2008; Cao and Lee, 2010). The full description of such behaviour is provided by the time-dependent Boltzmann equation, possibly coupled with the equations for the precursors concentrations $c_{i,j}$, which read (Bell and Glasstone, 1970)

$$\frac{1}{v}\frac{\partial}{\partial t}\varphi(\mathbf{r},\boldsymbol{\upsilon},t)+L\varphi(\mathbf{r},\upsilon,t)=F_p\varphi(\mathbf{r},\boldsymbol{\upsilon},t)+\sum_{i,j}\chi_d^{i,j}(\mathbf{r},\upsilon)\lambda_{i,j}c_{i,j}(\mathbf{r},t)+\mathcal{S} \tag{1}$$

and

$$\frac{\partial}{\partial t}c_{i,j}(\mathbf{r},t)=\int \nu_d^{i,j}(\upsilon')\Sigma_f^i(\mathbf{r},\upsilon')\varphi(\mathbf{r},\boldsymbol{\upsilon}',t)\,\mathrm{d}\boldsymbol{\upsilon}'-\lambda_{i,j}c_{i,j}(\mathbf{r},t). \tag{2}$$

We have here defined the net disappearance operator

$$Lf=\boldsymbol{\Omega}\cdot\nabla f+\Sigma_t f-\int\Sigma_s(\mathbf{r},\boldsymbol{\upsilon}'\to\boldsymbol{\upsilon})f(\mathbf{r},\boldsymbol{\upsilon}')\,\mathrm{d}\boldsymbol{\upsilon}', \tag{3}$$

and the prompt fission operator

$$F_pf=\sum_i\chi_p^i(\mathbf{r},\upsilon)\int\nu_p^i(\upsilon')\Sigma_f^i(\mathbf{r},\upsilon')f(\mathbf{r},\boldsymbol{\upsilon}')\,\mathrm{d}\boldsymbol{\upsilon}'. \tag{4}$$

Notation is as follows: $\boldsymbol{\upsilon}$ is the velocity, $\mathbf{r}$ is the position vector and $\boldsymbol{\Omega}$ is the angular direction vector, $\upsilon=\boldsymbol{\upsilon}\cdot\boldsymbol{\Omega}$ is the neutron speed, Σ_t is the total cross-section, Σ_s is the differential scattering cross-section, χ_p^i is the normalized spectrum for prompt fission neutrons of isotope i, ν_p^i is the average number of prompt fission neutrons of isotope i, Σ_f is the fission cross-section, $\chi_d^{i,j}$ is the normalized spectrum of delayed neutrons emitted from precursor family j of isotope i, $\lambda_{i,j}$ is the decay constant of precursor family j of isotope i, $\nu_d^{i,j}$ is the average number of delayed fission neutrons of precursor family j of isotope i, and the double sum is extended over all fissile isotopes i and over all precursor families j for each fissile isotope. The equations above are completed by assigning the proper initial and boundary conditions for φ and $c_{i,j}$. The quantity $\mathcal{S}$ represents the contribution due to an external source. We have assumed here that all physical parameters (such as cross-sections, velocity spectra, and so on) are time-independent (Keepin, 1965; Akcasu et al., 1971). If N fissile isotopes are present, each associated to M precursors families, Eqs. (1) and (2) form a system of $1+N\times M$ equations to be solved simultaneously. In order to keep notation simple, we will only consider one isotope in the following and we will drop the index i.

2.1. Eigenmode decomposition

The k eigenmodes φ_k associated to the Boltzmann equation emerge by imposing that the system should be exactly critical without external sources and asking by which factor k the fission terms should be rescaled in order to make this happen (i.e., to make the time derivative vanish) (Bell and Glasstone, 1970; Cullen et al., 2003). This leads to the following eigenvalue system

$$L\varphi(\mathbf{r},\boldsymbol{\upsilon})=\frac{1}{k}F_p\varphi_k(\mathbf{r},\boldsymbol{\upsilon})+\sum_j\chi_d^j(\mathbf{r},\upsilon)\lambda_jc_j(\mathbf{r}) \tag{5}$$

and

$$\frac{1}{k}\int\nu_d^j(\upsilon')\Sigma_f(\mathbf{r},\upsilon')\varphi_k(\mathbf{r},\boldsymbol{\upsilon}')\,\mathrm{d}\boldsymbol{\upsilon}'=\lambda_jc_j(\mathbf{r}). \tag{6}$$

By replacing the precursor equations into that for the neutron flux, we get the k eigenvalue equation in its standard form, namely,

$$L\varphi_k(\mathbf{r},\boldsymbol{\upsilon})=\frac{1}{k}F\varphi_k(\mathbf{r},\boldsymbol{\upsilon}), \tag{7}$$

where we have defined the total production operator $F=F_p+F_d$, with the delayed fission operator

$$F_df=\sum_j\chi_d^j(\mathbf{r},\upsilon)\int\nu_d^j(\upsilon')\Sigma_f(\mathbf{r},\upsilon')f(\mathbf{r},\boldsymbol{\upsilon}')\,\mathrm{d}\boldsymbol{\upsilon}'. \tag{8}$$