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A genetic algorithm for multigroup energy structure search

Mattia Massone *, Fabrizio Gabrielli, Andrei Rineiski

Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

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ABSTRACT

The generation of multigroup neutron cross-section libraries is a key issue of the multigroup transport calculations in reactor physics. The correct choice of the boundaries of the energy groups, in particular, is decisive for obtaining reliable results. Knowledge of the reactor physics, general and specific of the studied reactor, along with long and refined analyses are required for finding out a reasonable energy structure, which is specific for the considered reactor and might be unsuitable for other systems. The genetic algorithm presented in this work aims to choose the most appropriate energy structure for the considered system to collapse a fine multigroup library into a few-groups one, usable for transient transport calculations. The user is free to choose the number of energy groups of the final library, which is in direct relation with the precision required and the time available for the simulation. The methodology is coupled with SIMMER-III code and applied to 3 reactor systems: ESNII+ ASTRID, ESFR and MSFR. The results show that the algorithm can find representative energy structures, providing accurate results on the multiplication factor. The results of each test are analyzed, showing how different compositions, geometries and neutron spectra guide the algorithm choices, so demonstrating the effectiveness of the method.

1. Introduction

The multigroup theory is an important approach to neutron cross section energy dependence representation in deterministic codes for neutron transport (or diffusion) equation solution (Duderstadt and Hamilton, 1976; Stacey, 2001). The energy space and the neutron cross section (XS) libraries are discretized on several intervals, called energy groups, and the generation of such libraries with small number of groups is a crucial step for core calculations. The choice of the energy groups' boundaries is a key issue of this process, as all energy dependent quantities, including the neutron flux and current, are to be described according to the chosen discretization. Hence from a non-optimal energy structure (ES) may easily follow an inappropriate representation of the spectrum, possibly leading to significant deviation of the simulation results with respect to the real behavior.

Unfortunately, the methods currently employed to do such an important choice are neither user-friendly nor precise, as they are mostly based on expert judgement (Cacuci, 2010). This, of course, presumes a deep knowledge of the reactor physics of the considered system and a highly specific competence in the XS-related nuclear science, which might not be the case for many code users. This difficulty in the generation process promotes the creation (and the use) of "general-purpose" few-groups XS libraries, which energy structure, however, might be unsuitable to particular reactor design. In fact, as the neutron spectrum plays a major role in the energy discretization and homogenization procedure, XS libraries should be considered specific to the reactor they have been designed for, and should not be applied to systems too distant from the proper one. In fact, a XS library can adequately model a reactor transient, even with a limited number of groups, if it has been correctly designed for the considered system.

The solution to these issues would be an automatization of the energy boundaries selection which, combined with a XS-collapsing procedure, would make possible the creation of highly-specific XS libraries for each reactor starting from a unique and general fine-group library. Due to the high non-linearities involved, this automatic choice cannot be achieved through a deterministic procedure, but an evolutionary algorithm can overcome the problem and attain the goal.

Among the family of evolutionary algorithms, based on Darwinian selection and evolution principles, a genetic algorithm (GA) has been chosen for the present study. In GAs possible solutions are considered as individuals of a population, each characterized by a genotype and a phenotype; as time passes, the features, or genes, of successful solutions are perpetuated and, appropriately mixed, better individuals are found. The GA concept dates from the

* Corresponding author.
E-mail address: mattia.massone@kit.edu (M. Massone).

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1960s, when it has been proposed by Holland (1962) and is widely used in a number of fields.

Similar approaches to the multigroup energy mesh search, based on metaheuristic optimization, have been proposed by Mosca and Mounier (2008), Mosca et al. (2011a,b) and by Yi and Sjoden (2013). The studies are based on swarm algorithms rather than evolutionary ones and are applied to a predefined set of infinite homogeneous medium problems for fast reactors or to a single pin in a thermal system.

Having this in mind a GA has been developed and proposed in the paper to perform the energy groups' boundaries search in neutron transport problems. The developed GA has then been joined together with the SIMMER-III code (Yamano et al., 2003; Kondo et al., 2000), as a complement to the XS collapsing extension already proposed in 2014 (Massone et al., 2014), and tested on 3 reactor systems: the Advanced Sodium Technological Reactor for Industrial Demonstration (ASTRID) developed in the framework of the European Sustainable Nuclear Industrial Initiative (ESNII+) (SNETP, 2014), the Working Horse (WH) core (Fiorini, 2009) of the European Sodium Fast Reactor (ESFR) (Andriolo, 2015), and the Molten Salt Fast Reactor (MSFR) considered for the Evaluation and Viability of Liquid Fuel Fast Reactor System (EVOL) project (EVOL, 2011). The obtained results are then analysed and compared to demonstrate the effectiveness of the approach and to study the physical implications underlying the GA choices.

2. Method description

2.1. First approach

The first attempt to produce an automated procedure for energy structure choice has been the transposition into an algorithm of the study on the flux spectrum, which is the basis of the current methods used for energy structure determination. Hence, adjacent energy groups characterized by similar values of the neutron population should be collapsed together, while avoiding averaging together peaks and valleys in the spectrum profile. Essentially, this represents a *greedy approach* (Cormen et al., 2000), i.e. at each step the best option available at the moment is chosen. The main step is the collapsing of the two close energy groups with the lowest difference in neutron population, repeated until the desired number of groups is achieved.

Due to the poor results obtained in this way, different options for the collapsing criterion (while keeping the greedy approach) have been explored:

- Least difference in neutron flux;
- Least difference in reaction rate;
- Least difference in $\frac{\Delta\varphi}{u}$.

In all cases the results were far from being acceptable. Moreover, the solutions with the best match in the k_{eff} looked very counterintuitive, when contrasting them with the flux spectrum.

A better approach, also based on the greedy algorithm but focused on the final result (k_{eff}) rather than on the spectrum, has then been envisioned:

I. The k_{eff} of the uncollapsed solution is calculated and taken as objective;
II. The k_{eff} related to each possible solution with $N-1$ energy groups is calculated;
III. The best option is picked;
IV. Procedure continues with Step II, considering all now possible solutions ($N-2$);

This algorithm, however, would have required a large number of calculations performed with a large number of groups (very computationally expensive), associated with a high probability of obtaining a sub-optimal result (greedy algorithms do not explore adequately the solution space) or even the worst option (Bang-Jensen et al., 2004).

The risk of obtaining unacceptable results can be prevented using an evolutionary algorithm, such as a GA. It would require a large number of calculations before convergence, like the proposed greedy algorithm, but these would be characterized by a limited number of energy groups, i.e. they would be computationally cheap.

2.2. The genetic algorithm

Genetic algorithms are a particular group of evolutionary algorithms, which working principle is the same of Darwinian selection and evolution. John Holland introduces first the concept of genetic algorithm in the 1960s (Holland, 1962) and then develops it and provides a theoretical basis in the next years (Holland, 1975). Since then this technique has been widely proven and exploited in a number of fields, including different sectors of the nuclear engineering.

The central point of the algorithm is the fitness function, which correlates each possible solution (denoted as *individual* using the analogy of biology, very diffused in the evolutionary methods terminology) with a measure (the *fitness* indeed) of the suitability in solving the problem. The fitness of each individual of an initial randomly generated set (*population*) is evaluated and a new population is produced; the next generation originates from the individuals of the old one, but the ones with better fitness have more chances of handing their properties (*genes*) on to their descendants. In this way the quality of the population progressively improves and the solution space is explored, eventually reaching the optimum (or a close enough problem solution).

2.3. Chromosome representation

The representation of each individual's genes set (*chromosome*) is a highly problem-specific issue, and it is useful specifying the constraints of the case before dealing with it:

I. Each energy cut of the final library (FL) ES must correspond to one of the starting fine-groups library (SL) ES. Hence, being G the gene pool

$$\#G < \aleph_0 \tag{1}$$

i.e. G is finite;
II. All solutions must have the same number of energy groups, fixed in advance.

While constraint *I* attains to the problem nature (and so cannot be relaxed), the second one has a practical reason: leaving the user with the freedom to set the number of groups to use, information which is directly associated with the precision required from the calculation and with the amount of time available for the calculation. Moreover, the natural tendency of the algorithm to a better fitness would privilege solutions with a larger number of energy groups over individuals with less ones, so potentially removing the really most interesting solutions from the population. A possible answer to this issue is the introduction of a penalty factor (Goldberg, 1989) in the fitness calculation based on the number of groups tuned to make fair the competition, but it has been preferred not to investigate this issue.