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An alternative algorithm for the linearization process of transmutation and decay networks

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Abstract

To modelling the changes occurring in the nuclear reactor's fuel composition, it is necessary to solve a coupled system of first order differential equations, known as the Bateman equations. Nowadays, there are two main methods to accomplish this task: the linear chain method and the matrix exponential method. The general procedure for the linear chain method consists in breaking a transmutation network into independent depletion chains (also known as "linear chains") and then solving each one analytically. The common way to build these linear chains is using a Depth-First-Search (DFS) algorithm, which consists in finding every possible path in a network, tracking the decay and transmutation reactions for a set of isotopes until one stable appears or there is no more information to continue. At this point, the algorithm moves backwards searching a branch or an untraveled path, and then the procedure is repeated. In the present work, an alternative new algorithm for building linear chains is developed, which uses a special notation and reduces the problem of finding paths to the problem of ordering a sequence of characters. Unlike the DFS, the algorithm developed has not a backward routine, but it has a "fill" procedure instead. The last property decreases the computation time spent in build linear chains and is useful with cyclic chains. We carry out a comparative analysis including computational schemes based on the running time of the algorithms, versus the length of the linear chains built. We considered two kinds of networks: 1) where the initial element is a heavy isotope that undergoes fission reaction and 2) where the first element is a fission product. In all the practical scenarios the proposed algorithm is faster than the DFS's, nevertheless when the values of the chain's length are large enough, the running times converge, being necessary to use a more complex and advanced sorting method.

1. Introduction

Changes occurring in the fuel isotopic composition during nuclear reactors operation modify the fuel neutronic properties. As a result, there is an effect in the reactivity and safety parameters of the reactor core, and therefore it is necessary a detailed knowledge of the depletion and distribution of the fuel. These changes are due to three main reactions and transformations in the isotopes: 1) radioactive decay, 2) capture, and 3) fission process. The simulation of them in a nuclear reactor is known as burnup calculation.

The change of the isotope concentration over time can be described by the following differential equation (Isotalo,2013):

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