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Parareal in time 3D numerical solver for the LWR Benchmark neutron diffusion transient model

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ABSTRACT

In this paper we present a time-parallel algorithm for the 3D neutrons calculation of a transient model in a nuclear reactor core. The neutrons calculation consists in numerically solving the time dependent diffusion approximation equation, which is a simplified transport equation. The numerical resolution is done with finite elements method based on a tetrahedral meshing of the computational domain, representing the reactor core, and time discretization is achieved using a θ-scheme. The transient model presents moving control rods during the time of the reaction. Therefore, cross-sections (piecewise constants) are taken into account by interpolations with respect to the velocity of the control rods. The parallelism across the time is achieved by an adequate use of the parareal in time algorithm to the handled problem. This parallel method is a predictor corrector scheme that iteratively combines the use of two kinds of numerical propagators, one coarse and one fine. Our method is made efficient by means of a coarse solver defined with large time step and fixed position control rods model, while the fine propagator is assumed to be a high order numerical approximation of the full model.
The parallel implementation of our method provides a good scalability of the algorithm. Numerical results show the efficiency of the parareal method on large light water reactor transient model corresponding to the Langenbuch–Maurer–Werner benchmark.

1. Introduction

Accurate knowledge of the time-dependent spatial flux density in nuclear reactors is required for nuclear safety and design. The motivation behind the development of methods for solving the energy-, space-, and time-dependent kinetics equations is not only the challenge of developing a method for solving a large set of coupled partial differential equations,

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but also a real need to predict the performance and assess the safety of large commercial reactors, both those presently operating and those being designed for the future.

Modern reactor core design and safety depend heavily on the simulation of the reactor core and plants dynamics as well as their mutual interaction. Significant progress has been made during the last fifteen years in developing accurate techniques to simulate the computationally expensive reactor core models. Modeling the reactor core involves solving a large set of coupled time-dependent partial differential equations (PDEs), where the exact kinetic transport equation is simplified to a multi-group diffusion approximation equation. This model of neutron transport provides a scientific insight and is sufficiently realistic to study the energy of the reactor core for long time scale. The time-dependent multi-group neutron diffusion equation is used to model the scalar flux density. In the time dependent form, we take into account the delayed dynamic of neutrons caused by the presence of so-called *precursors*. Control rods are inserted to absorb neutrons and control the energy during the reaction.

Due to the limitation of the read–write memory in serial computers, it is relevant to propose parallel methods, which solve these large scale system with massively parallel computers. Much successful work has been done in the parallelization of neutron model simulations. For instance [1] studies the static case (eigenvalue problems) with space domain decomposition methods. A very nice strategy employed in [2] and [3] uses quasi-stationary approach to accelerate the simulation.

This paper focuses on neutrons behavior. We investigate the application of the parareal in time algorithm [4,5] on the neutron diffusion equation that governs the time-dependent flux density in the reactor core. The parareal in time algorithm is an iterative scheme, which improves computational time with parallel simulation. In several cases, parareal in time algorithm gives impressive rates of convergence, this is the case for example for linear diffusion equations and also for non-linear case [6]. Stability and convergence results for this algorithm are given in [7–11] particularly for diffusion system and others. The algorithm remains efficient in parallel computer simulation. We find a variety [8,12–24] of versions of this scheme that adapt the original algorithm to tackle new settings. Furthermore the parareal algorithm can be easily coupled with other iterative schemes such as domain decomposition methods (DDM) for instance the basic Schwarz algorithm or more complex ones [25], and optimal control based steepest descent algorithms [26–28].

The paper is organized as follows: After this introduction, we present the model of the kinetics of neutrons inside the reactor core. Section 3 gives a brief introduction of the parareal in time algorithm. Numerical tools are presented in Section 4 and adapt the parareal algorithm to the resolution of the handled problem. Finally, in Section 5, we present and discuss the numerical experiments that demonstrate the speedup following the fully-parallel implementation of the parareal algorithm in a parallel architecture.

2. Model

The neutron dynamics in a reactor core are governed by the kinetic transport Boltzmann equation [29]. The solution to this equation, denoted by Ψ, represents the directional neutron flux. It is a function of time t, the position $\vec{r}$ within the reactor core $\mathcal{R} \subset \mathbb{R}^3$, and the velocity of neutrons $\vec{V} = \sqrt{2E/m}\vec{\Omega}$, where $\vec{\Omega}$ is a unit vector indicating the direction of the velocity, E stands for the energy of the neutron and m for its mass. For computational reason, a simplification of the model has been proposed in [29, Chap. XXI, Section 5] that consists in averaging over the velocity directional variable leading to the introduction of the new function $\phi(\vec{r}, t, E) = \frac{1}{4\pi}\int_S \Psi(\vec{r}, t, E, \vec{\Omega})\, d\vec{\Omega}$ where S is the unit sphere. This method leads to accurate results in standard cases, unfortunately the computational time remains excessively long. Further simplifications consist in also averaging over the energy variable: the energy interval $[E_{\min}, E_{\max}]$ is divided into $\hat{g}$ non-overlapping intervals around a set of discrete energies $\{E^g\}_{g=1}^{\hat{g}}$ and leads to a new unknown $\Phi \equiv \Phi(\vec{r}, t) = \{\phi^g(\vec{r}, t)\}_{g=1}^{\hat{g}}$ composed of the set of the neutron average flux over each subinterval around E^g. This approach is known as the multi-group theory [30] where for each energy group $g = 1, \ldots, \hat{g}$ and any position $\vec{r} \in \mathcal{R} \subset \mathbb{R}^3$, the equations are a set of coupled three-dimensional multi-energy-group neutron kinetics equations involving time delayed contributions due to the fission of some isotope precursors, denoted by $C \equiv C(\vec{r}, t) = \{C^k(\vec{r}, t)\}_{k=1}^{K}$. The set of partial differential equation that govern the kinetics of neutrons in the reactor core is

$$\begin{cases} \frac{1}{V^g}\frac{\partial}{\partial t}\phi^g(\vec{r}, t) = \operatorname{div}(D^g \nabla\phi^g(\vec{r}, t)) - \Sigma_t^g \phi^g(\vec{r}, t) + \chi_p^g \sum_{g'=1}^{\hat{g}} (1-\beta^{g'})\nu^{g'}\Sigma_f^{g'}\phi^{g'}(\vec{r}, t) \\ \qquad\qquad + \sum_{g'=1}^{\hat{g}} \Sigma_s^{g'\to g}\phi^{g'}(\vec{r}, t) + \sum_{k=1}^{K} \chi_d^{k,g}\lambda_k C^k(\vec{r}, t), \quad \forall g \in \{1..\hat{g}\},\ t \in [0, T] \text{ and } \vec{r} \in \mathcal{R}, \\ \phi^g(\vec{r}, t) = 0 \quad \text{on the boundary of the reactor core: } \forall g \in \{1..\hat{g}\},\ t \in [0, T],\ \vec{r} \in \partial\mathcal{R}, \\ \phi^g(\vec{r}, 0) = \phi_0^g(\vec{r}) \quad \text{the initial condition: } \forall g \in \{1..\hat{g}\},\ \vec{r} \in \mathcal{R}. \end{cases} \tag{1}$$

The delayed neutron concentrations satisfy $\forall k \in \{1..K\}$:

$$\frac{\partial C^k}{\partial t}(\vec{r}, t) = -\lambda_k C^k(\vec{r}, t) + \sum_{g'=1}^{\hat{g}} \beta^{k,g'}\nu^{g'}\Sigma_f^{g'}\phi^{g'}(\vec{r}, t), \quad t \in [0, T] \text{ and } \vec{r} \in \mathcal{R}. \tag{2}$$

In Eqs. (1) and (2), the neutron velocity is defined as $V^g = \sqrt{2E^g/m}$, the diffusion coefficient is denoted by D^g. The total and production cross-sections are denoted by Σ_t^g and $\nu\Sigma_f^g$ respectively, and $\Sigma_s^{g'\to g}$ stands for the transfer cross-section