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An assessment of coupling algorithms for nuclear reactor core physics simulations *



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ABSTRACT

This paper evaluates the performance of multiphysics coupling algorithms applied to a light water nuclear reactor core simulation. The simulation couples the *k*-eigenvalue form of the neutron transport equation with heat conduction and subchannel flow equations. We compare Picard iteration (block Gauss-Seidel) to Anderson acceleration and multiple variants of preconditioned Jacobian-free Newton-Krylov (JFNK). The performance of the methods are evaluated over a range of energy group structures and core power levels. A novel physics-based approximation to a Jacobian-vector product has been developed to mitigate the impact of expensive on-line cross section processing steps. Numerical simulations demonstrating the efficiency of JFNK and Anderson acceleration relative to standard Picard iteration are performed on a 3D model of a nuclear fuel assembly. Both criticality (*k*-eigenvalue) and critical boron search problems are considered.

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1. Introduction

Determining the steady-state power and temperature distributions within an operating nuclear reactor is an important component of reactor design and analysis. This task requires simultaneously solving equations describing the distribution of neutrons throughout the reactor as well as the transfer of heat through the fuel and structural materials into fluid coolant regions. Current core analysis methods rely on the use of a Picard iteration [1–7], alternating between solving individual physics components. Although this approach offers a simple path to coupling different physics codes due to the minimal code interaction required, there are also significant drawbacks. Picard iteration lacks a global convergence result and, at best, achieves a q-linear convergence rate [8]. Additionally, user-defined relaxation schemes are usually required to achieve convergence. Newton-based methods, however, are shown to be globally convergent with q-quadratic convergence

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rates. The downside to Newton-based methods is that the need for residual and sensitivity information requires more invasive access to application codes. While access to analytical Jacobian matrices is commonly infeasible, Jacobian-free Newton-Krylov (JFNK) methods [9] can be used to realize many of the benefits of Newton-based methods while only requiring evaluation of nonlinear functions. While JFNK methods have been successfully applied in many areas, to date, the application to multiphysics reactor simulations has been limited to few-group diffusion approximations to the transport equation with analytic temperature feedback models not suitable for accurate reactor analyses.

In this study, we investigate the performance of Anderson acceleration and JFNK solvers compared to Picard iteration on multiphysics problems that couple 3D discretizations of the radiation transport and heat transfer equations along with a simple subchannel flow model for modeling of pressurized water reactors (PWRs). Although Newton and JFNK methods have been used previously for neutronics-only problems [10–12] and even for multiphysics problems [13–17], previous studies have used only few-group nuclear cross sections with analytic temperature variation. In this study we consider the impact of utilizing many energy groups with on-line generation of cross section data for use by the neutronics solver. One of the dominant costs associated with the current model is the on-line generation of cross sections; a significant contribution of this paper is development of a low-cost approximate function evaluation for the JFNK approach that mitigates this cross section processing cost. Another notable contribution is the design of a JFNK boron search formulation, allowing direct computation of the critical boron concentration as an alternative to standard indirect searches. Coupling algorithms are evaluated on both criticality (*k*-eigenvalue) and boron search problems.

The remainder of the paper is organized as follows: Section 2 describes the physics models, Section 3 describes various coupling algorithms, Section 4 contains numerical results for a single PWR fuel assembly, and Section 5 presents conclusions and proposals for future areas of investigation.

2. Physics models

In this paper, we consider the solution of multiphysics problems involving coupling between neutron transport and heat transfer. In particular, we focus on the solution of problems involving light water reactors (LWRs). Most of the fundamental ideas described here are applicable to a wide range of reactor types, but certain aspects of the problem, such as geometric features, are particular to LWRs (and possibly PWRs in particular). For nuclear reactor problems, the standard formulation of the neutron transport equation is the *k*-eigenvalue problem

$$\hat{\Omega} \cdot \nabla \psi(\vec{r}, E, \hat{\Omega}) + \sigma(\vec{r}, E, T) \psi(\vec{r}, E, \hat{\Omega})
= \frac{1}{4\pi} \int_{0}^{\infty} dE' \int_{4\pi} d\hat{\Omega}' \, \sigma_{s}(\vec{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega}, T) \psi(\vec{r}, E', \hat{\Omega}')
+ \frac{1}{4\pi k} \chi(\vec{r}, E) \int_{0}^{\infty} dE' \int_{4\pi} d\hat{\Omega}' \, \nu \sigma_{f}(\vec{r}, E', T) \psi(\vec{r}, E', \hat{\Omega}') ,$$
(1)

where \vec{r} is the coordinate vector, $\hat{\Omega}$ is the direction of particle travel, E is the particle energy, T is the temperature of the background material, σ is the total cross section, σ_s is the scattering cross section, $v\sigma_f$ is the neutron production cross section, and χ is the fission spectrum. The goal for solving this equation is to find the largest value of the eigenvalue k and the corresponding eigenvector ψ . Because Eq. (1) represents an eigenvalue problem, the vector ψ has no explicit magnitude. We choose a natural normalization by setting the global heat generation rate (due to nuclear fission occurring in the fuel) to a pre-defined value, i.e.,

$$\frac{1}{4\pi} \int dV \int_{0}^{\infty} dE \int_{4\pi} d\hat{\Omega} \kappa \sigma_f \psi = P^* \,, \tag{2}$$

where κ is the heat generated per fission event, and nonlocal energy deposition (e.g., gamma heating) effects have been ignored.

As noted in Eq. (1), the cross sections are dependent on the temperature of the media, T. Thus, for a reactor not operating at a constant temperature, it is also necessary to solve a heat conduction equation within the solid fuel and clad regions, with fission providing the thermal source, i.e.,

$$-\nabla \cdot K(T)\nabla T = \frac{1}{4\pi} \int_{0}^{\infty} dE \int_{4\pi} d\hat{\Omega} \kappa \sigma_f(E) \psi(E, \hat{\Omega}), \qquad (3)$$

where *K* is the material thermal conductivity. Because no fission occurs in the clad regions, the source in those locations is zero. The exterior surface of the clad is then coupled to the coolant through the subchannel model that solves equations describing the conservation of mass, momentum, and energy,

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