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Development of an efficient tightly coupled method for multiphysics reactor transient analysis

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ABSTRACT

Picard Iteration is a widely used coupling method for multiphysics simulations. This method allows one to directly leverage existing and well-developed single-physics programs without re-writing large portions of the codes. In Picard Iteration, single-physics codes just iteratively pass solutions to each other as inputs until each code has reached a converged solution. However, multiphysics computation linked by Picard Iteration is susceptible to over-solving, which can make the overall computation much less efficient. Over-solving means that each single-physics code provides an accurate solution in each Picard Iteration, which is not necessary in practice. Solving the single-physics codes in an inexact manner, i.e. with relaxed termination criteria, can help avoid this problem. This work develops a modified Picard Iteration coupling method with adaptive, inexact termination criteria for the underlying single-physics codes. Also, nested within the inexact Picard Iteration, inexact Newton methods were applied in the single-physics codes. The effect on the overall computation efficiency due to the inexact (relaxed) termination criteria at both levels is investigated by applying them to solve reactor transient problems. A reactor dynamics problem with temperature feedback in one-dimensional slab geometry is used to scope the behavior of nested inexact solvers. Then these methods are applied to a larger two-dimensional Boiling Water Reactor (BWR) problem. Computational time savings reach 55% for the two-dimensional problem. Additionally, applying an inexact termination criterion (inexact Newton method) to each single-physics code results in a further time savings of up to 18%.

1. Introduction

Multiphysics modeling and analysis of nuclear reactor core and system designs is one of the current thrusts in nuclear energy research. New computational frameworks and codes have been developed to execute multiphysics simulations incorporating coupled neutronic, thermal-hydraulic, and mechanical behaviors in nuclear reactors (Gaston et al., 2015; Palmtag et al., 2014; Siegel et al., 2007; Magedanz et al., 2015; Chanaron et al., 2015). A multiphysics analysis that accurately incorporates feedbacks from each physics process allows for the best predictions of realistic system behaviors. This is in contrast to conventional single-physics analysis where other physical processes are approximated with fixed input parameters. For the analysis of nuclear reactor transients, which are inherently "multi-physical," the motivation for developing multiphysics codes is obvious. Rather than using simplified thermal models and linear feedback coefficients, sophisticated high-fidelity codes can be linked together for detailed analysis. Much work is being done along these lines to enable multiphysics reactor simulations. Readers can find many examples in literature (Ivanov and Avramova, 2007; Bennett et al., 2016; Zerkak et al., 2015; Yilmaz et al., 2017; Kochunas et al., 2017; Mahadevan et al., 2014; Leppänen et al., 2015; Ellis et al., 2017; Herman et al., 2015; Mylonakis et al., 2014).

Conceptually, multiphysics coupling can be implemented in two ways. One is the monolithic approach. All the equations that represent different physics are formulated into a single solution scheme. The different single-physics problems are treated as a single problem and are solved simultaneously (Keyes et al., 2012). The coupling of different physical models is implicitly accounted for in the solution scheme. The monolithic approach is suitable for solving strongly coupled multiphysics problems. The other coupling method is called the partitioned approach. Multiple solvers are used and each tackles a different single-physics problem. These solvers explicitly communicate their answers to each other until the final converged solutions are obtained for all the solvers (Tautges et al., 2011). Each solver has its own solution scheme and is linked to other solvers by a coupling scheme (method). The partitioned approach is much more popular because it allows the reuse of legacy codes (Keyes et al., 2012; Ganine et al., 2013). This is

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important because the separate legacy codes use specialized methods (Herman et al., 2015) and meshes (Hansen and Owen, 2008), which may differ greatly between the single-physics problems. Using different meshes for each single-physics problem greatly complicates (but does not prevent (Mahadevan et al., 2012)) the utilization of the monolithic approach. Furthermore, not all single-physics problems are strongly coupled to each other, in which case the monolithic approach is superfluous (Gaston et al., 2015). Of the partitioned methods, we focus on Picard Iteration (also referred to as fixed-point iteration (Birken, 2015) or Block Gauss-Seidel (Hamilton et al., 2016)), which iterates between the single-physics problems until the coupled problem has converged. But because each single-physics problem is solved independently and repeatedly, Picard Iteration may suffer from poor performance (Keyes et al., 2012). The poor performance stems from two aspects. One is that Picard Iteration only attains a linear convergence rate. Acceleration schemes can be applied to improve the multiphysics convergence rate and stability. Several schemes have been developed (Macleod, 1986; Walker and Ni, 2011) to address the issue of slow linear convergence rates. The other primary cause of poor performance is generally referred to as over-solving, which is the focus of, and is addressed in, this paper.

Over-solving is working to obtain a precise solution to an imprecise problem. For example, there is no need to find an extremely precise temperature distribution until the flux/power distribution has been solved to a commensurate level of precision. However in standard Picard Iteration, each single-physics problem is solved to full precision at every iteration. This is not necessary because the solution keeps changing as a function of the feedback from the other solver(s). Only approximate solutions are needed until all of the solvers approach their final converged solutions (in the last few Picard iterations). Over-solving is well-known in Newton methods where it is not necessary to solve the linear system for the next update to great precision when the current guess is still far from the exact solution (Dembo et al., 1982). Over-solving in Newton solvers has been addressed with a variety of strategies (Dembo et al., 1982; Eisenstat and Walker, 1996; Cai et al., 1994; An et al., 2007; Ter, 2007), referred to as inexact Newton methods. However, over-solving has not been thoroughly treated for multiphysics problems and it presents more complexity than what a single Newton solver faces. In multiphysics simulations using Picard Iteration, there is a plurality of single-physics solvers interacting with each other by iteratively exchanging solutions. Within these Picard iterations, each constituent single-physics solver, depending on its solution method, may have multiple levels of nested iterations—as is the case with Newton-based methods. If so, over-solving may occur within the single-physics solvers as well. Thus over-solving should be dealt with at each level to attain better performance. Over-solving in multiphysics is often addressed only as an afterthought in multiphysics problems (Lipnikov et al., 2013; Clarno et al., 2015; Jareteg et al., 2013), until recently (Birken, 2015). Our previous work (Senecal and Ji, 2017) focused solely on methods for reducing over-solving in partitioned multiphysics problems, here we build upon that progress. The present study focuses on multiphysics problems involving only two single-physics solvers, each implementing a Newton-based method. The basic strategy is to employ inexact methods to relax the termination criteria at each level of iteration.

Inexact methods (methods that do not solve the inner level of a nested problem to a tight numerical tolerance) are acceptable because they still arrive at the correct solution. Assuming that the coupled problem converges with standard termination criteria, Birken has shown that the exact answer can still be obtained by using relaxed tolerances in the constituent solvers, provided the tolerance approaches zero as the simulation progresses (Birken, 2015). He also provided numerical results to support this conclusion; and in all of our example problems the inexact methods arrive at the same solution as the exact methods.

In our previous work (Senecal and Ji, 2017, 2015, 2016), several methods were introduced that reduce over-solving. In addition to applying the best of these methods (the Residual Balance method) to nuclear reactor transient problems, further improvements have been developed in order to make it more broadly applicable. A further novel contribution of the present work is to demonstrate the combined benefit of removing over-solving on multiple levels (within both the multiphysics and single-physics solvers).

Before proceeding further, several terms are defined for the sake of clarity. “Global iterations” refer to solving each of the single-physics problems and performing the associated data mapping operations. “Constituent iterations” denote the iterations performed to solve a single-physics problem. “Linear iterations” solve for the update step in the Newton method. Throughout this paper the norm operator, $\|\cdot\|$, refers to the Euclidean norm.

2. Numerical methods

A brief background on Picard Iteration is provided before describing the Residual Balance method. Afterwards, inexact Newton methods are discussed as a means to reduce over-solving in the single-physics solvers.

2.1. Picard Iteration

Picard Iteration (PI) is a commonly used method for coupling multiple physics codes. At each time step (steady-state problems have only one “time step”), the algorithm executes the solvers sequentially and iteratively. Because the constituent single-physics codes are executed sequentially, they can be independent codes that have been developed previously (Mylonakis et al., 2014). Fig. 1 portrays the general solution scheme for a Picard Iteration-based multiphysics solver involving two single-physics solvers. Generally, weakly coupled problems require few global iterations to resolve the feedbacks between the

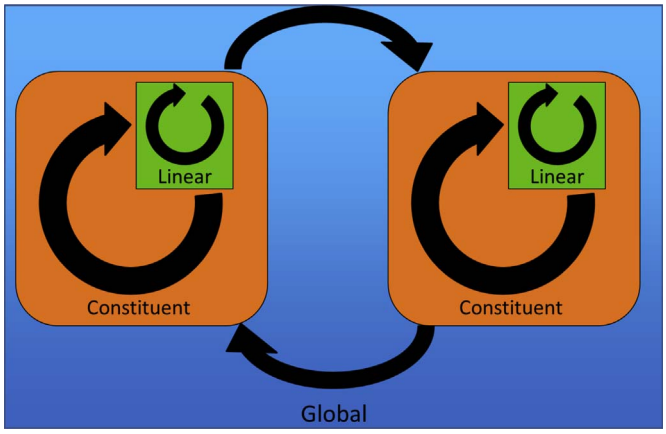

Fig. 1. Schematic diagram of a partitioned multiphysics solver. The “Global” loop refers to the Picard Iteration scheme that connects the single-physics codes. Each single-physics solver is executed in a series of “Constituent” iterations. Finally the “Linear” iterations are nested within the constituent iterations.