ARTICLE IN PRESS

Annals of Nuclear Energy xxx (2015) xxx-xxx

Contents lists available at ScienceDirect



Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

Review of multi-physics temporal coupling methods for analysis of nuclear reactors

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ARTICLE INFO

Article history: Received 2 July 2014 Received in revised form 15 January 2015 Accepted 20 January 2015 Available online xxxx

Keywords: Multi-physics Temporal coupling Operator Splitting Jacobian Free Newton-Krylov Approximate Block Newton Review

ABSTRACT

The advanced numerical simulation of a realistic physical system typically involves multi-physics problem. For example, analysis of a LWR core involves the intricate simulation of neutron production and transport, heat transfer throughout the structures of the system and the flowing, possibly two-phase, coolant. Such analysis involves the dynamic coupling of multiple simulation codes, each one devoted to the solving of one of the coupled physics. Multiple temporal coupling methods exist, yet the accuracy of such coupling is generally driven by the least accurate numerical scheme. The goal of this paper is to review in detail the approaches and numerical methods that can be used for the multi-physics temporal coupling, including a comprehensive discussion of the issues associated with the temporal coupling, and define approaches that can be used to perform multi-physics analysis. The paper is not limited to any particular multi-physics process or situation, but is intended to provide a generic description of multi-physics temporal coupling schemes for any development stage of the individual (single-physics) tools and methods. This includes a wide spectrum of situation, where the individual (single-physics) solvers are based on pre-existing computation codes embedded as individual components, or a new development where the temporal coupling can be developed and implemented as a part of code development. The discussed coupling methods are demonstrated in the framework of LWR core analysis.

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1. Introduction

The steady-state and transient analysis of a LWR core is a complex multi-physics problem, involving the intricate simulation of neutron production and transport, heat transfer throughout the structures of the system and the flowing, possibly two-phase, coolant. Such analysis involves the dynamic coupling of separated simulation codes, each one devoted to the solving of one of the coupled physics. Most of the existing coupled code systems apply an Operator Splitting (OS) coupling technique, where one code is iterated first to provide boundary conditions to the second code and so on until the last code of the simulation system completes one overall temporal step. The accuracy of such coupling is generally driven by the one code that uses the least accurate numerical scheme. As a consequence, traditional OS coupling methods can result in theory into 1st order accuracy, but practically less because of round-off errors. Moreover, the non-implicit nature of this step-by-step

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http://dx.doi.org/10.1016/j.anucene.2015.01.019 0306-4549/© 2015 Elsevier Ltd. All rights reserved. decomposition imposes the use of small times steps to ensure the stability of the solution.

In this context, the goal of this paper is to identify areas for improvements of the existing coupling schemes, or to define more accurate coupling approaches, that can be used to perform multiphysics coupling of existing codes. In this case, the solvers would be based on pre-existing computation codes that would be embedded as individual components and would be exchanging information (for instance the T–H and N–K fields for the LWR transient analysis) through a limited set of interfaces and be operated using generic functionalities. These different components (solvers, interfaces, functionalities) would then serve as the basic elements to develop the transient calculation routes.

An OECD report D'Auria et al. (2004) presented the State-Of-the-Art (SOA) as of 2004 of the coupling techniques applied to reactor transient simulations, which can be partially applied to today's situation, especially in respect to the basic issues of Neutron-Kinetics/Thermal-Hydraulic (N-K/T-H) coupling. A detailed presentation of the various N-K and T-H codes used in coupled mode is given in the paper, followed by a description of the coupling issues which are:

Please cite this article in press as: Zerkak, O., et al. Review of multi-physics temporal coupling methods for analysis of nuclear reactors. Ann. Nucl. Energy (2015), http://dx.doi.org/10.1016/j.anucene.2015.01.019

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- Coupling approach integration algorithm or parallel processing.
- Ways of coupling internal or external.
- Spatial mesh overlays.
- Coupled time step algorithms.
- Coupling numerics explicit, semi-implicit or implicit schemes.
- Coupled convergence schemes.

The two first items refer to the different methods than can be used to couple two existing solvers, either integrating one code into the other one (thus resulting into one code), or establishing a dynamic data exchange routine (PVM or MPI based) between the two codes, thus corresponding to a "black-box" interfacing were only limited modifications to the two solvers are needed. The third item, which corresponds to the problem of exchanging coupling fields computed on different meshing schemes, has been the object of dedicated developments during the NURESIM project (Zerkak et al., 2007), and will not be tackled here. The last three items were not discussed in details, except for an interesting development of the SIMTRAN 3D core dynamics code where staggered alternate time step advancement and extrapolation strategies are used between the two physics (N-K and T-H), and which helped transferring the exchanged T-H feedback variables in a nearly implicit manner for the core power calculation (Aragonés et al., 2004).

One can also recall one conclusion of the report (D'Auria et al., 2004), in respect to the trend in using more advanced simulation techniques in the different domains (physics), such as computational fluid dynamics (CFD), and Monte-Carlo and transport methods for the T–H and the N–K, respectively. Progress was made in applying these higher order methods to LWR steady-state and transient problems, but these new approaches are still experimental and will not be discussed here, also for the very reason that the required higher order simulation tools (CFD, neutron transport) are not included in this paper. But the coupling methodologies that will be discussed here could also be applied using these higher-order simulation tools.

Therefore, this paper will consist of further discussing the issues associated with the last three items listed above. Another review paper was published (Mylonakis et al., 2014), however in view of recent developments in code coupling methodologies, the objective here is to consider how one could improve the convergence of the existing coupling techniques (OS based), and to discuss how more accurate coupling methodologies could be applied. This paper is composed of several sections which represent the different methods discussed in this paper. First, an overview of the state-of-the-art on code coupling in the nuclear domain and on the latest developments on code coupling optimization methods is presented. Then, following this review, Section 3 discusses the advantages and disadvantages of each one of them.

2. Coupling methods

2.1. Operator Splitting coupling method

The purpose of the so-called multi-physics simulation methods is to combine into one single solution scheme the different "physics" of the problem, which are obtained by numerical solvers of the separate sets of PDEs of the different physical phenomena of interest. In such segregated configuration, the different sets of PDE cannot be solved simultaneously (i.e. within one stationary or nonstationary iteration step), since the result from one set of PDEs (physics) is to be used as boundary condition to the other one and vice versa. To overcome this problem, Operator Splitting (OS) methods were developed, also referred to as Fractional Time-Stepping methods (FTS). The first OS method was the Chorin's projection method which consisted in solving the incompressible nonstationary Navier–Stokes equations by decoupling the pressure and velocity fields and solving them iteratively within one single time step (Chorin, 1968).

To put it simply, the OS methods follow the "divide-and-conquer" strategy, in which the set of PDEs of the overall problem is decomposed into simpler sub-problems that can be discretized independently and be treated thus individually using dedicated numerical algorithms. After one time step iteration on a subproblem, the partial solution is then used as a new estimate for the boundary conditions and derivatives of the next sub-problem. OS methods can be applied even within one single set of PDEs, where the spatial derivative operator is decomposed in groups of operators that represent different individual physical phenomena. For instance, one can consider the time-dependent 1-D convection-diffusion problem:

$$\frac{\partial u}{\partial t} + Lu = f(x, t) \tag{2.1}$$

where $L = v \frac{\partial}{\partial x} - d \frac{\partial^2}{\partial x^2}$.

0...

In this case, one simple OS method would consist of decomposing the operator *L* into the sum of two operators $L_1 = v \frac{\partial}{\partial x}$ (convection term) and $L_2 = -d \frac{\partial^2}{\partial x^2}$ (diffusion term), and divide the discretized full problem into two sequentially solved sub-problems:

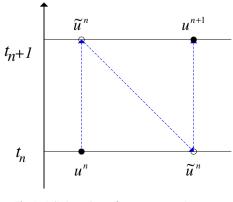
1.
$$\frac{\widetilde{u}^n - u^n}{\Delta t} + L_1 \widetilde{u}^n = 0$$
(2.2a)

2.
$$\frac{u^{n+1} - \widetilde{u}^n}{\Delta t} + L_2 u^{n+1} = f^n$$
 (2.2b)

as illustrated on Fig. 1.

This example results in a 1st order temporal accuracy, but 2nd order accuracy can be obtained as will be described later by using temporal midpoint rule corrections, or staggered time grids, or by nesting the OS method into a predictor–corrector loop. These different techniques are not uniquely defined, and their implementation would also depend on the type of problem to be solved, but the overall splitting strategy is always the same, whether it is in the differential operators, the meshing grids or the physics.

In the context of the steady-state and transient simulation of LWR, the complex multi-physics problem involves the temporal coupling of separated codes. In this case, the OS method approach is applied to the extent that one code would correspond to one sub-problem, e.g. PARCS/RELAP5 (Barber et al., 1999a), CRONOS2/ FLICA4 (Royer and Toumi, 1998), SIMULATE-3K/TRACE (Nikitin et al., 2010), SIMULA/COBRA and SIMULA/RELAP5 (Aragonés





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