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A Newton-based Jacobian-free approach for neutronic-Monte Carlo/thermal-hydraulic static coupled analysis

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ABSTRACT

In the field of nuclear reactor analysis, multi-physics calculations that account for the bonded nature of the neutronic and thermal-hydraulic phenomena are of major importance for both reactor safety and design. So far in the context of Monte-Carlo neutronic analysis a kind of "serial" algorithm has been mainly used for coupling with thermal-hydraulics. The main motivation of this work is the interest for an algorithm that could maintain the distinct treatment of the involved fields within a tight coupling context that could be translated into higher convergence rates and more stable behaviour. This work investigates the possibility of replacing the usually used "serial" iteration with an approximate Newton algorithm. The selected algorithm, called Approximate Block Newton, is actually a version of the Jacobian-free Newton Krylov method suitably modified for coupling mono-disciplinary solvers. Within this Newton scheme the linearised system is solved with a Krylov solver in order to avoid the creation of the Jacobian matrix. A coupling algorithm between Monte-Carlo neutronics and thermal-hydraulics based on the above-mentioned methodology is developed and its performance is analysed. More specifically, OpenMC, a Monte-Carlo neutronics code and COBRA-EN, a thermal-hydraulics code for sub-channel and core analysis, are merged in a coupling scheme using the Approximate Block Newton method aiming to examine the performance of this scheme and compare with that of the "traditional" serial iterative scheme. First results show a clear improvement of the convergence especially in problems where significant coolant density gradients appear.

1. Introduction

Generally, within the scientific community of computational physics there is a strong interest for efficient and flexible techniques able to solve systems of equations in some segregated fashion. Quite efficient techniques are those that allow the distinct treatment of the involved physical problems using black-box solvers, alleviating the need for modification of their algorithms. The main advantage of such methods is that they can link existing solvers relatively easily. As a result, these merged tools can be used for the treatment of complex problems aiming to a higher level of accuracy than that achieved by each solver separately. Furthermore, this philosophy may reduce the required effort for development-verification which can increase extraordinarily when tools are designed and developed from scratch.

Reactor core analysis is traditionally performed handling separately each part of the involved physics using distinct solvers. For example the static-critical neutronic behaviour of the reactor core is analysed either solving the steady-state eigenvalue form of the neutron transport equation in a deterministic way or simulating the corresponding physics in a stochastic (Monte-Carlo) way. In both cases the Thermal-Hydraulic (T-H) conditions are considered fixed. Similarly, the T-H behaviour of the reactor core is analysed using a variety of T-H solvers in various levels (system level, sub-channel, computational fluid dynamics). In this case the neutronic conditions (power distribution) are considered as known. However in a nuclear reactor core the various physical phenomena of different nature are interrelated. In this sense, the neutronic and T-H phenomena are strongly bonded; the

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microscopic neutron cross sections of the core materials are dependent on temperature and the moderation rate is dependent on coolant density. This interrelation induces the need for multi-physics calculations, i.e., calculations which are able to compute the parameters of interest taking these interactions into consideration.

Nowadays, the Monte-Carlo neutronic analysis of the reactor core is extensively used mainly because it allows the detailed geometrical and continuous energy treatment of the analysed model. So far, Monte-Carlo neutronic analysis has been coupled with T-H utilising a "serial" coupling approach that is the simplest and most obvious way to couple two distinct solvers (Gill et al., 2017; Derby et al., 2007). This procedure could be considered as a Picard iteration and generally is the most used technique for coupling distinct solvers. However in some cases within the generalized context of computational physics this approach faces difficulties in obtaining convergence of the overall problem, as reported for example in Gill et al. (2017); Yeckel et al. (2009, 2010). Then, the need for more robust methods arises.

The main motivation of the present work is the interest for a coupling approach that could maintain the distinct treatment of the involved neutronic and T-H fields within a tight coupling context. More specifically, in this work an alternative strategy of coupling neutronic Monte-Carlo and T-H solvers is adopted and investigated. Instead of a PI technique, an Approximate Block Newton (ABN) algorithm, developed in Yeckel et al. (2009), is adapted in a reactor core analysis framework aiming to tightly link stochastic (Monte-Carlo) neutronic with deterministic T-H analysis. Since the performance of such a method is determined by a set of numerical parameters and their combination, one could consider many variations of the algorithm. However, the aim of this work is not to present a very well optimized version but to show that there is room to consider this algorithm as a candidate for Monte-Carlo/T-H static coupled analysis.

2. The coupled Monte-Carlo/T-H problem

The k-eigenvalue form of the neutron transport steady-state equation is given by the following relation:

$$\begin{aligned}\boldsymbol{\Omega}\cdot\nabla\psi(\boldsymbol{r},\boldsymbol{\Omega},E)+\Sigma_t(\boldsymbol{r},E)\psi(\boldsymbol{r},\boldsymbol{\Omega},E)\\ =\iint\Sigma_s(\boldsymbol{r},E',\boldsymbol{\Omega}'\rightarrow E,\boldsymbol{\Omega})\psi(\boldsymbol{r},E',\boldsymbol{\Omega}')d\Omega'dE'\\ +\frac{\chi(E)}{k_{eff}}\iint\nu(E')\Sigma_f(\boldsymbol{r},E')\psi(\boldsymbol{r}',E',\boldsymbol{\Omega}')d\Omega'dE'\end{aligned}\tag{1}$$

where $\boldsymbol{r}$ represents a point in R^3, $\boldsymbol{\Omega}$ is a unit vector in R^3 showing the direction of the neutron motion, E is the neutron energy, ψ is the angular flux that is connected with the total flux ϕ by the relation $\phi=\int_{4\pi}\psi d\Omega$, and k_{eff} is the effective multiplication factor. Σ_t,Σ_s and Σ_f are the total, scattering and fission macroscopic cross-sections, ν is the mean number of neutrons produced per fission and χ is the fission energy distribution function. When this eigenvalue problem is solved as is, in a standalone way, temperature and density fields are considered as given; as a result, the dependence of neutronics on the temperature and density fields is not properly handled.

If the dependence on T-H conditions is desired to be taken into account, the problem described by Eq. (1), when spatially discretized, can be represented as:

$$\boldsymbol{f}(\boldsymbol{x},\boldsymbol{y})=\boldsymbol{0}\tag{2}$$

where the vector $\boldsymbol{x}$ contains the vector of the fluxes and the scalar k_{eff} while $\boldsymbol{y}$ contains the temperature and density fields. The T-H problem that corresponds to the calculation of the temperature and density fields is written as

$$\boldsymbol{g}(\boldsymbol{x},\boldsymbol{y})=\boldsymbol{0}\tag{3}$$

Therefore, the solution of the global problem described by Eqs. (2) and (3) is desired to be found. If it is assumed that the solution of the sub-problems $\boldsymbol{f}$ and $\boldsymbol{g}$ is segregated, i.e., if $\boldsymbol{x}$ is the solution of $\boldsymbol{f}$ and $\boldsymbol{y}$ is the solution of $\boldsymbol{g}$, the problem can be written in the following way:

$$\boldsymbol{f}(\boldsymbol{x},\widetilde{\boldsymbol{y}})=\boldsymbol{0}\tag{4}$$

$$\boldsymbol{g}(\widetilde{\boldsymbol{x}},\boldsymbol{y})=\boldsymbol{0}\tag{5}$$

where the tilde represents the coupling terms. Assuming monodisciplinary solvers available for the solution of each sub-problem, the global problem takes the following form:

$$\boldsymbol{x}=N(\boldsymbol{x},\widetilde{\boldsymbol{y}})\tag{6}$$

$$\boldsymbol{y}=T(\widetilde{\boldsymbol{x}},\boldsymbol{y})\tag{7}$$

where N and T represent respectively the action of the neutronics and the T-H solver on the vectors $\boldsymbol{y}$ and $\boldsymbol{x}$. At this point, an important decision on the exact methodology that will be utilised for the numerical solution of this problem is to be made.

3. Numerics of coupling

So far, most of the attempts to couple Monte-Carlo and T-H have utilised a kind of serial coupling that is actually a serial application of the involved solvers until some measure of convergence is achieved. Such a scheme could be considered as a Picard iteration and is described below. A more advanced approach of solving the global problem is to use a gradient-based method such as a Newton method. The potential advantages are the higher convergence rates and the simultaneous calculation of the whole set of the involved unknowns, features that are desirable in tightly coupled systems. However the implementation of a Newton method in its original form is inappropriate when the distinct nature of different solvers is desired to be preserved and more strictly when neutronics is analysed by a Monte-Carlo solver for reasons that are explained later. Therefore only modified versions of the general Newton methodology could be considered in this framework.

3.1. The Picard iteration

So far, most of the attempts to couple stochastic neutronic with T-H solvers for coupled static analysis use a kind of serial coupling like Joo et al., 2004; Waata et al., 2005; Ivanov and Avramova, 2007; Seker et al., 2007; Grieshemer et al., 2008; Hu, 2008; Shan et al., 2010; Kotlyar et al., 2011; Cardoni, 2011; Vasquez et al., 2012; Li et al., 2012; Li and Wang, 2012; Chaudri et al., 2012; Espel et al., 2013; Guoa et al., 2013; Bettencourt et al., 2013; Mylonakis et al., 2014; Bernnat et al., 2014; Wu and Kozlowski, 2015. This type of coupling is a Picard Iteration (PI). For two individual single-physics solvers the PI can be described by Eqs. (8) and (9). In these equations only the exchanged variables appear since the internal variables at the current iteration are inaccessible and are treated as invisible.

$$\boldsymbol{y}^{k+1}=T(\boldsymbol{x}^{k})\tag{8}$$

$$\boldsymbol{x}^{k+1}=N(\boldsymbol{y}^{k+1})\tag{9}$$

N and T represent the neutronics and the T-H solvers that receive as inputs the vectors $\boldsymbol{y}$ and $\boldsymbol{x}$, respectively. The T-H information (part of the output of the T-H solver that passes to neutronics) is symbol-