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Newton-Krylov method with nodal coupling coefficient to solve the coupled neutronics/thermal-hydraulics equations in PWR transient analysis

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ABSTRACT

This paper presents the solution to the neutronics equations coupled to a parallel channel model containing a 1D heat transfer model in PWR core transient calculation. Unlike traditional coupling techniques where the coupled field equations are solved separately, Newton-Krylov method is implemented to solve the coupled nonlinear field equations simultaneously. The related Jacobian of the nonlinear system is analytically derived based on the nonlinear residual functions and transferred into a compressed format which can be easily handled on a personal computer (PC). Since the Jacobian is explicitly constructed, it is directly passed to a GMRES solver with ILU preconditioning. A new solution strategy is proposed under the framework of Newton's iteration, in which the nodal coupling coefficient (NCC) appeared in the neutronics equations is resolved in the Newton iteration level. The proposed method is studied by simulating all the six cases in the OECD NEACRP PWR rod ejection benchmark. Results indicate that that nonlinearity of NCC can be resolved in the Newton iteration level and can be further controlled by a user specified number, N_{NCC}. Computational simulation also shows that the proposed method is capable to converge to a much tighter level with only a few iterations.

1. Introduction

Reactor core is a complex multi-physics environment, among which the coupling of neutronics, fluids and heat conductions draws the highest attention. Traditionally, the solution of the coupled field equations has been performed in a loose manner by separately solving the individual field equations with independent codes and transferring information between them (Ivanov and Avramova, 2007). For a certain time-step during a transient, if no iteration is being performed between the fields, it is the so-called explicit coupling scheme, otherwise it is called as implicit coupling scheme. These two traditional approaches have been widely used in the past decades and still play an important role nowadays for it is relatively easy to implement. But it is computationally inefficient. For explicit coupling scheme, strict restriction on time-step size is a must to preserve accuracy and stability since the feedback parameters are lagged in time. For implicit coupling scheme, which is essentially a Picard method from mathematic point of view, only possesses a first order convergence rate. Usually, additional damping factor is required to guarantee convergence. Recently, Newton based methods to simultaneously solving all the coupled field equations has become more and more popular.

For any Newton based methods, the key is to calculate or to approximate the action on Jacobian in each Newton's iteration. According to this idea, the Newton based methods applied to reactor simulation can be divided into two categories. First, the Newton-Krylov (NK) method which requires explicitly constructing Jacobian is presented. Then, the second Newton based method is introduced in the followed paragraph.

For the first Newton based method, Kastanya implemented NK method to evaluate the three-dimensional, two-group neutron diffusion equations coupled with a two-phase flow model within a BWR core simulator in Kastanya and Febrian (2002). In his study, a speedup of 1.9 is achieved comparing with traditional nested iteration. In Watson and Ivanov (2012) Watson (2010), the researchers used several one-dimensional problems to demonstrate the ability of NK method to solve nonlinear coupled systems and maintain accuracy while removing time-step dependency of the coupled calculation. But the nodal coupling coefficient is set

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to zero which could lead to low accuracy when neutron flux vary significantly. In Ward (2012), Ward implemented Newton's method to solve the coupled neutronics-porous medium equations for Pebble Bed Modular Reactor (PBMR) in steady state calculation.

The second Newton based method is the Jacobian-Free-Newton-Krylov (JFNK) method whose mathematical basis can be found in Brown and Saad (1990). Leveraged from characteristics of GMRES, JFNK method bypassed construction of Jacobian via a finite difference approximation on matrix-vector product. The feature gives great convenience for code development and have used in many areas. A comprehensive survey of approaches and applications of the JFNK method can be found in Knoll and Keyes (2004). In Gan et al. (2003), the researchers named the method as matrix-free Newton method. They found the method has the potential to reduce computational burden compared to the explicit marching method due to the increased time step size. Founded on the mathematical principle of JFNK method, one typical parallel computational framework MOOSE was developed for multiphysics simulations (Gaston, 2009). A variety of MOOSE-based application were developed including the Pebble-bed reactor simulation tool PRONGHORN (Park et al., 2009), the fuel performance application BISON (Gaston, 2012), the radiation transport application Rattlesnake and the nuclear reactor system safety analysis application RELAP-7 (Wang et al., 2017). Physics-based preconditioning (PBP) is utilized to improve the efficiency of the JFNK solver for the MOOSE-based applications. In Mousseau (2004), JFNK method is implemented to solve the implicit balance equations of the two-phase flow coupled to non-linear heat conduction.

This study focuses on NK method since analytical Jacobian is available for the physical models used. The paper is arranged as follows: In Section 2, theoretical formulation is given in detail including forming of the coupled nonlinear system, derivation of the Jacobian, and overall solution strategy to consider the nodal coupling coefficient; in Section 3, the proposed method is verified against OECD NEACRP PWR rod ejection benchmark; in Section 4, conclusion is given.

2. Theoretical formulation

2.1. Newton-Krylov method

Newton's method is a classical iterative method to find the root $\mathbf{x}$ to the residual $\mathbf{F}(\mathbf{x})$ of a non-linear system. For the coupled neutronics/thermal-hydraulics equations, after applying discretization, one can always rewrite the non-linear system of equations into its residual form as:

$$\mathbf{F}(\mathbf{x}) = 0, \tag{1}$$

where $\mathbf{x}$ is the solution vector involving the neutronics and thermal hydraulics field variables, such as neutron flux, fuel temperature and flow enthalpy.

The iterative process of Newton's method to solve Eq. (1) follows:

$$\begin{aligned} &\text{Do loop} \quad i = 0 \text{ until convergence}: \\ &\quad \text{Solve} \quad \mathbf{J}_F(\mathbf{x}_i)\delta\mathbf{x}_i = -\mathbf{F}(\mathbf{x}_i), \\ &\quad \text{Update} \quad \mathbf{x}_{i+1} = \mathbf{x}_i + \delta\mathbf{x}_i, \\ &\quad \text{Check if } \|\mathbf{F}(x_{i+1})\| \text{ is small enough}, \\ &\text{End do} \end{aligned} \tag{2}$$

where $\mathbf{J}_F(\mathbf{x}_i) = \mathbf{F}'(\mathbf{x}_i)$ is the system Jacobian evaluated at current approximation $\mathbf{x}_i$. It can be observed from Eq. (2) that each Newton's iterative step yields a linear problem requiring inverse of the Jacobian solving for the update vector $\delta\mathbf{x}_i$. This linear problem can be solved either with a direct method, such as Gaussian elimination, or with an iterative method. Typically, it is impractical to use a direct method. More frequently, an iterative method is adopted. Newton-Krylov method refers to that the inner linear problem is solved with an iterative Krylov method while the over-all problem is solved under the idea of Newton's method.

2.2. Physics models

As described in the previous section, Newton-Krylov method is applied to solve the discretized field equations instead of solving the original equations in partial differential form. The discretized governing equations of the neutronics field and thermal-hydraulics field are given in this section. Detailed derivation from their original form will not be included since it is not the emphasis of this paper.

For simplicity, indices of time-step of current time-step n will be neglected in the following paragraph.

2.2.1. Neutronics field

Time-dependent neutron behavior is described by the neutron kinetics equation set as follows:

$$\begin{aligned} \frac{1}{\upsilon_g}\frac{\partial\phi_g^k(\vec{r})}{\partial t} = {} & D_g^k\nabla^2\phi_g^k(\vec{r}) - \Sigma_{tg}^k\phi_g^k(\vec{r}) + \sum_{g'=1}^{G}\Sigma_{g'g}^k\phi_{g'}^k(\vec{r}) \\ & + (1-\beta)\chi_{pg}\sum_{g'=1}^{G}\nu\Sigma_{fg'}^k\phi_{g'}^k(\vec{r}) + \sum_{i=1}^{I}\chi_{dgi}\lambda_i C_i^k, \end{aligned} \tag{3}$$

$$\frac{\partial C_i^k(\vec{r})}{\partial t} = \beta_i\sum_{g'=1}^{G}\nu\Sigma_{fg'}^k\phi_{g'}^k(\vec{r}) - \lambda_i C_i^k(\vec{r}), \tag{4}$$

where superscript k is the indices of node. All other notations are fairly standard. Eq. (3) is the energy-dependent neutron diffusion equation, and Eq. (4) is the precursor concentration equation.

Nodal methods had been widely used and shown great success for PWR core calculation in the past decades. In this paper, the discreted neutronics equation derived from non-linear iteration semi-analytical nodal method (NLSANM) (Liao and Xie, 2003) is utilized.

By integrating over a node and applying finite difference to Eq. (3), the residual form of the nodal neutron balance equation with two group approximation can be expressed as:

$$\text{group1}: \left(\widehat{\Sigma}_{r1}^k - \widehat{\chi}_1\nu\Sigma_{f1}^k\right)\phi_1^k - \widehat{\chi}_1\nu\Sigma_{f2}^k\phi_2^k + L_1^k - \widehat{S}_{eff,1}^{k,n-1} = 0, \tag{5}$$

$$\text{group2}: -\Sigma_{12}^k\phi_1^k + \widehat{\Sigma}_{r2}^k\phi_2^k + L_2^k - \widehat{S}_{eff,2}^{k,n-1} = 0, \tag{6}$$

where $\widehat{\Sigma}_{rg}^k = \frac{1}{\upsilon_g}\left(\frac{1}{\theta\Delta t^n} + \alpha\right) + \Sigma_{rg}^k$ is the equivalent removal cross-section, $\widehat{\chi}_g = \left((1-\beta)\chi_{pg} + \sum_{i=1}^{I}\chi_{dgi}\lambda_i F_{i1}^{k,n}\right)$ is the equivalent fission spectrum,

$L_g^k = \sum_{u=x,y,z}\frac{1}{\Delta u_k}\begin{bmatrix} -D_{gu+}^{k,FDM}\left(\phi_g^{ku+} - \phi_g^k\right) - D_{gu+}^{k,NOD}\left(\phi_g^{ku+} + \phi_g^k\right) \\ +D_{gu-}^{k,FDM}\left(\phi_g^k - \phi_g^{ku-}\right) + D_{gu-}^{k,NOD}\left(\phi_g^k + \phi_g^{ku-}\right) \end{bmatrix}$ is the leakage term, $\widehat{S}_{eff,g}^{k,n-1} = \left[\left(\frac{1}{\upsilon_g\theta\Delta t^n} - \Theta\frac{\alpha}{\upsilon_g}\right)\phi_g^{k,n-1}(\vec{r}) + \Theta R_g^{k,n-1}(\vec{r})\right]e^{\alpha\Delta t^n} + \sum_{i=1}^{I}\chi_{dgi}\lambda_i C_i^{k,n-1}(\vec{r})e^{-\lambda_i\Delta t^n} + \sum_{i=1}^{I}\chi_{dgi}\lambda_i F_{i0}\cdot\sum_{g'=1}^{G}\nu\Sigma_{fg'}^{k,n-1}\phi_{g'}^{k,n-1}(\vec{r})$ is the transient fixed source (TFS) yields from temporal discretization which only contains information of previous time-step, $\theta \in (0,1]$ is the user specified theta method parameter, $\alpha = \frac{1}{\Delta t^{n-1}}\ln\frac{\left\|\phi^{n-1}\right\|_2}{\left\|\phi^{n-2}\right\|_2}$ is the exponential transformation parameter, $D_{gu+}^{k,FDM} = \frac{2D_g^k D_g^{k+1}}{D_g^k\Delta u_{k+1} + D_g^{k+1}\Delta u_k}$ is the equivalent diffusion coefficient derived from finite difference, D^{NOD} is the nodal coupling coefficient (NCC) which is calculated via the