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A MATRIX-FREE NEWTON METHOD FOR COUPLED NEUTRONICS THERMAL-HYDRAULICS REACTOR ANALYSIS

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ABSTRACT

A matrix-free Newton-Krylov method is developed for solving the coupled neutron and temperature/fluid field equations for practical nuclear reactor systems models. Results are compared to the traditional explicit "marching" method as well as to a nested iterative method in which the coupled fields are converged at each time step. The applications are first to a simplified example problem using a single fluid, one-dimensional core T-H and neutronics models, and then to a practical two-fluid, multi-dimensional T-H and neutronics model using the coupled codes TRAC-M and PARCS. Results indicate that the Newton-Krylov method has the potential to reduce the computational burden compared to the explicit marching method because of the increased time step size.

Key Words: Matrix-Free Newton-Krylov methods, nonlinear thermal-hydraulics\neutronics coupling

1. INTRODUCTION

The solution of the coupled neutron and temperature/fluid field equations for practical nuclear reactor systems models can be a formidable computational problem. Several hours of computing time have been required to analyze OECD coupled code benchmarks such as the PWR TMI Main Steam Line Break and the BWR Peach Bottom Turbine Trip using the U.S. NRC thermal-hydraulics/neutronics code TRAC-M/PARCS [1, 4]. Currently, an explicit "marching" scheme is used to couple the codes in which the system's thermal-hyraulics equations are first solved in TRAC-M and then the neutronics equations are solved in PARCS [2, 3, 5, 6, 7]. The time steps are kept small enough so that iteration of the coupled field solutions at a given time step is usually not required.

The research reported describes an investigation into more efficient and robust methods in which the coupled non-linear fields at each time step are converged using Newton iterations. In principle this would permit longer time steps and a reduction of the computational burden for solving the coupled field equations. Previous research in solving the coupled field equations with Newton methods for nuclear engineering applications has shown some promise. Most notably, Turinsky et al [17] applied a Newton-Krylov method to the solution of the coupled neutronics and two-fluid problem for BWR reload analysis. In their work, they explicitly formed the Jacobian and employed the BiCGSTAB algorithm for the inner iterations. The method proposed here is to employ a matrix-free, Newton-Krylov technique which avoids explicit formation of the Jacobian matrix [11]. The matrix-free method is well suited to the solution of multi-field problems using "legacy" codes such as TRAC-M and PARCS in which the derivates required to form the Jacobian matrix are not easily available.

The following paper will first compare the traditional marching method to a "nested method" which iterates on the neutron and temperature/fluid fields until convergence is achieved at each time step. The tradeoff is examined in the increased computational cost at each time step because of the additional iterations in the nested method and the reduced computational cost because of the larger time steps possible with the nested method. A matrix free, Newton-Krylov method is then presented and applied to the coupled field equations. The applications here are first to a simplified example problem using a single fluid, one-dimensional core T-H and neutronics models, and then to a practical two-fluid, multi-dimensional T-H and neutronics model using the coupled codes TRAC-M and PARCS.

The paper is organized as follows. In the next section the current methods used to solve the coupled field problem for practical LWR analysis is described using the TRAC-M/PARCS example. In section 3 a matrix-free Newton-Krylov method is proposed for solving the coupled field problem. In section 4, the method is first examined using a simplified 1D neutronics and T-H model with MATLAB, and then the method is examined for practical coupled TRAC-M/PARCS applications. Finally, a summary and conclusions, as well as the direction of future research are provided in section 5.

2. COUPING MODEL OF THERMAL-HYDRAULICS/NEUTRONICS

The traditional method for coupling system thermal-hydraulics and spatial kinetics codes has been to integrate the spatial kinetics code into the systems code and to utilize common variables and memory address space. This approach considerably simplifies code execution but restricts the ability to utilize various combinations of thermal-hydraulics and spatial kinetics codes, as well as complicates the maintenance of the individual codes. The U.S. NRC has adopted the concept of a generic interface that can be used for the various combinations of codes and simplifies code development/maintenance [2]. In the framework of the coupled TRAC-M/PARCS code, TRAC-M is designed to be a self-contained process that communicates with PARCS through the General Interface via the PVM message passing interface. The implementation of the General Interface in the framework of the coupled code is depicted in Figure 1. The coupling of the neutronics module to the thermal-hydraulics module is accomplished via the incorporation of thermal-hydraulic feedback effects into the cross sections. The space-dependent thermal-hydraulic and heat structure variables are mapped from thermal-hydraulics module to neutronics module include moderator temperature (T_m), liquid density (ρ_l), vapor density (ρ_v), void fraction (α), boron concentration (B), average fuel temperature ($\overline{T}_f$), fuel centerline temperature (T_f^{cl}), and fuel surface temperature (T_f^{sf}). The space-dependent powers obtained from the spatial kinetics calculation, which consist of the sum of fission and decay power, are mapped from the neutronics module to both the thermal-hydraulic and heat structure components specified in the mapping input file. Thus, the powers packed into the neutronic vector are power to thermal-hydraulic zones ($Q_{T/H}$) and power to heat structure components (Q_{HS}). In order to reduce the cost of message passing, the General Interface has recently been integrated directly into the PARCS neutronics code. One of the additional advantages of the general interface concept is the ability to easily investigate more advanced code coupling schemes such as the matrix-free Newton-Krylov method proposed in the work here.

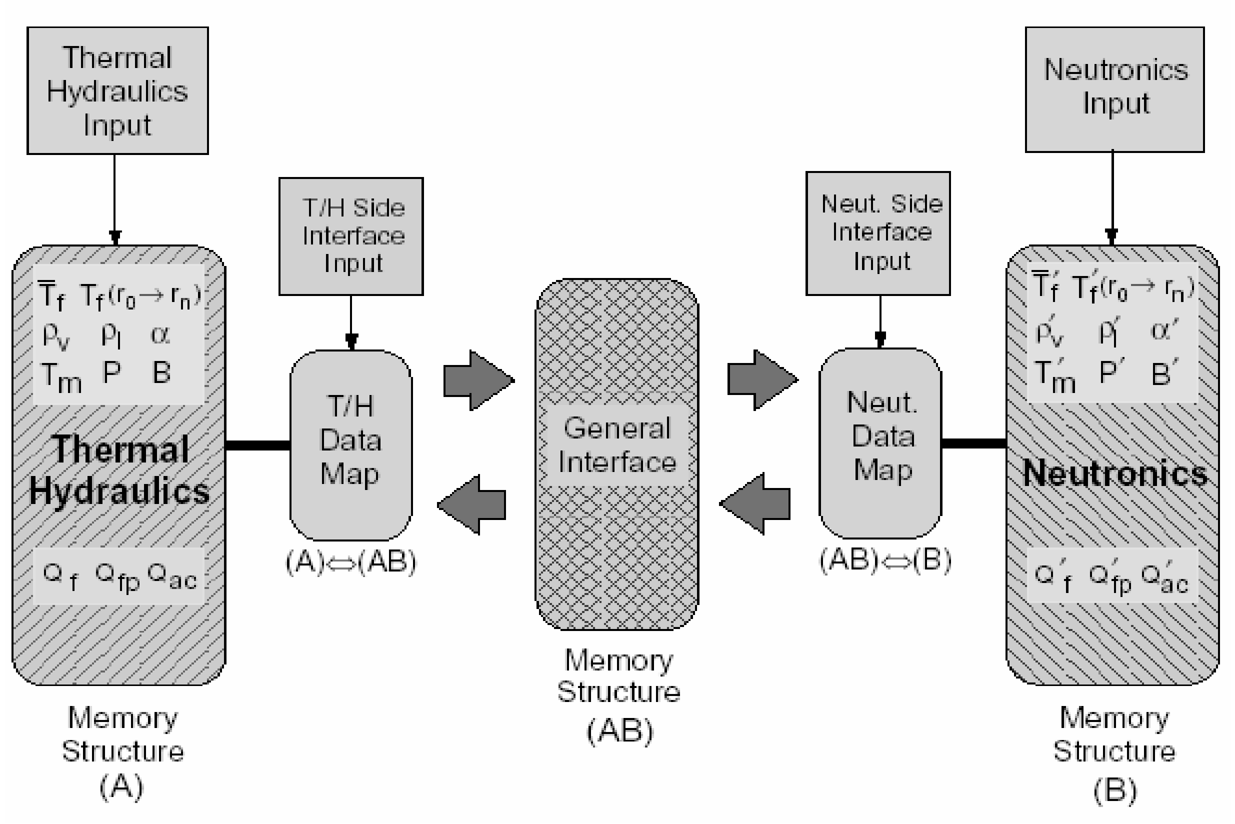


Figure 1. Schematic of General Interface Implementation

The simplest method to time advance the coupled field calculation is to implement an explicit marching-forward feedback model as illustrated in Figure 2. Here "step" represents time step in the transient coupled field solution

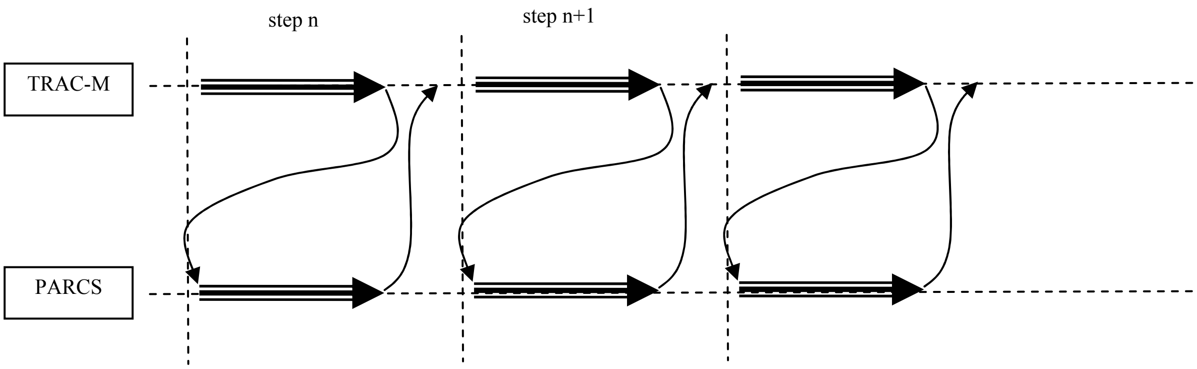


Figure 2. Process Control and Information Flow in "Marching" Method

Since there is no iteration between the fields at a given time step, the size of the time step in the explicit marching method must be constrained to capture the rapidly changing field solution. In principle the time step size can be increased by iterating between the fields until a specified tolerance is achieved. Figure 3 illustrates the "Nested" loop successive iteration. This method will be used in section 3 as a basis for evaluating the Newton-Krylov methods developed in this work.

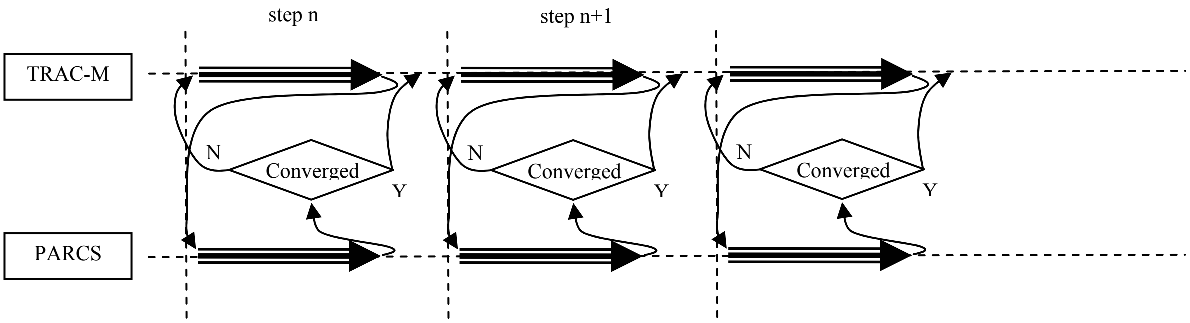


Figure 3. Process Control and Information Flow in "Nested" Method

3. MATRIX-FREE NEWTON-KRYLOV METHODS

Newton methods have been successively employed for many years to solve nonlinear systems of equations similar to the thermal-hydraulics/neutronics equations problem [16]. The problem here can be expressed as:

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

where $F: R^n \rightarrow R^n$ is a nonlinear continuously differentiable mapping, and x is the solution vector involving thermal-hydraulics and neutronics field variables, such as moderator temperature, liquid density, and neutron flux distribution.

3.1. Classical Matrix-Free Newton-Krylov Methods

Application of Newton's method to solve (1) results in the following iterative process:

```
FOR $i$ = 0 until "convergence" DO:                    (2)
    Solve  $J(x_i)\,\delta_i = - F(x_i)$,
    Set    $x_{i+1} = x_i + \delta_i$,
```

where $J(x_i) = F'(x_i)$ is the Jacobian matrix. However, it can be expensive to compute the exact solution of the Jacobian using a direct method such as Gaussian elimination if the number of unknowns is large. Therefore indirect methods are most often used such as the Generalized

Minimal RESidual (GMRES) iterative algorithm [10]. The GMRES iterative residual is given by

$$r_i = J(x_i)\ \delta_i + F(x_i). \tag{3}$$

Since the use of an iterative scheme to solve the linear system (2) yields an approximate solution, the resulting method is classified as an *inexact Newton method* [8, 9]. The convergence criteria is generally based on the size of the relative residual $|| r_i || / || F(x_i)||$:

$$|| r_i || < \gamma ||F(x_i)||, \tag{4}$$

where γ is used to control the level of accuracy and the amount of work per iteration. There exists a trade-off between the accuracy with which the Newton equations are solved and the effort required to solve the linear system (2). A relatively large convergence limit, γ, will result in less work for the iterative solver to archive the solution of the delta vector in Eq. 2, but more nonlinear Newton iterations are required to converge the final solution vector. In the next section a parametric study is discussed and an appropriate γ is applied for the practical coupled code problem.

The explicit construction of the Jacobian can become a formidable computational burden when the size of the problem becomes large and when the complexity of the nonlinear relationships increases, as in the case of large "legacy" codes used to solve the thermal-hydraulic problem. An attractive feature of the GMRES method (as well as other Krylov methods) is that only the action of the Jacobian J on a vector ν is required, and it is not necessary to form J explicitly. This action of matrix-vector products can be approximated by finite differences:

$$J_i v^j \approx \frac{F(x_i + \varepsilon v^j) - F(x_i)}{\varepsilon}, \tag{5}$$

where v^j is a j-th GMRES iteration vector, and ε is an appropriately chosen small perturbation.

The approximation of (5) is the basis for the matrix-free method since it preserves the action of the Jacobian without explicitly forming or storing the Jacobian matrix [11, 12, 15]. In most applications, however, an approximate Jacobian matrix is still required for preconditioning the Krylov subspace methods [13, 14].

3.2. Non-Residual Construction Matrix-Free Newton-Krylov Methods

The objective of implementing a matrix free Newton-Krylov method here is to construct a general implicit method for practical coupled thermal-hydraulics / neutronics code without revising the basic structures of the existing neutronics and TH codes. In the traditional matrix-free Newton-Krylov methods, however, it is unavoidable to generate the residual vectors and to construct the approximate Jacobian as a preconditioner. In the work here an innovative method is proposed which avoids this by appropriately selecting the preconditioner.

The method can be demonstrated using the nested loop successive iteration algorithm:

$$A(x_i)^* x_{i+1} - b(x_i) = 0, \tag{6}$$

where A is the linearized system coefficient matrix and b is the source term. The Newton iterative residual can be expressed in terms of the linearized system (6):

$$F(x) = A(x)x - b(x). \tag{7}$$

And the residuals in the Jacobian matrix-vector product approximation (5) can be expressed as follows:

$$\begin{aligned} F(x_i) &= A(x_i)x_i - b(x_i) \\ F(x_i) &= A(x_i)x_i - b(x_i) - \left(A(x_i)g(x_i) - b(x_i)\right) \\ F(x_i) &= A(x_i)\left(x_i - g(x_i)\right) \end{aligned} \tag{8}$$

or

$$F(x_i + \varepsilon v^j) = A(x_i + \varepsilon v^j)\left(x_i + \varepsilon v^j - g(x_i + \varepsilon v^j)\right), \tag{9}$$

where g(x) is the definition of solution vector of the linearized system (6):

$$g(x) \equiv A(x)^{-1} b(x). \tag{10}$$

The approximation of the action of the Jacobian matrix times a vector in (5) can then be rewritten via (8) and (9) after using the linearized system matrix $A(x_i)$ as the proconditioner:

$$\begin{aligned} A^{-1}(x_i)J_i v^j &\approx A^{-1}(x_i)\frac{F(x_i + \varepsilon v^j) - F(x_i)}{\varepsilon} \\ A^{-1}(x_i)J_i v^j &= A^{-1}(x_i)\frac{A(x_i + \varepsilon v^j)\left((x_i + \varepsilon v^j) - g(x_i + \varepsilon v^j)\right) - A(x_i)\left(x_i - g(x_i)\right)}{\varepsilon} \\ A^{-1}(x_i)J_i v^j &\approx \frac{\left((x_i + \varepsilon v^j) - g(x_i + \varepsilon v^j)\right) - \left(x_i - g(x_i)\right)}{\varepsilon} \\ A^{-1}(x_i)J_i v^j &= v_j + \frac{g(x_i) - g(x_i + \varepsilon v^j)}{\varepsilon} \end{aligned} \quad . \tag{11}$$

Here the approximation of perturbed linearized system, $A(x_i + \varepsilon v^j)$, is applied. Since the small perturbation scalar ε is restrained in size by the finite difference approximation of the Jacobian and vector product, it is not expected that significant errors will be introduced by this approximation. Here the linearized coefficient matrix, A, is a good preconditioner for the coupled code solution since the nonlinear residual can be separated into thermal-hydraulics and neutronics fields as:

$$F(x) = \begin{bmatrix} F^N(x) \\ F^T(x) \end{bmatrix} \qquad \begin{array}{l} F^N(x) = M(T)\Phi - S \\ F^T(x) = N(T)T - Q(\Phi) \end{array}, \tag{12}$$

where the source term, S, in the neutronics filed is determined by the previous time step solution vector, and the source term, Q, in the thermal-hydrulics filed is also determined by the current reactor power in the coupled calculation. Both linearized coefficient matrices depend on the current thermal-hydraulics filed solution vector. Therefore the Jacobian in the coupled code can be expressed as:

$$J = \nabla F = \begin{bmatrix} \dfrac{\partial F^N}{\partial \Phi} & \dfrac{\partial F^N}{\partial T} \\ \dfrac{\partial F^T}{\partial \Phi} & \dfrac{\partial F^T}{\partial T} \end{bmatrix} = \begin{bmatrix} M & \dfrac{\partial M}{\partial T}\Phi \\ -\dfrac{\partial Q}{\partial \Phi} & N + \dfrac{\partial N}{\partial T}T \end{bmatrix}. \tag{13}$$

Thus the linearized system matrix, A, is the block diagonal of the Jacobian matrix:

$$A = \begin{bmatrix} M & 0 \\ 0 & N \end{bmatrix}. \tag{14}$$

In this manner a good preconditioner is provided for the Newton-Krylov method without modifying the basic structure of the existing codes.

4. APPLICATIONS

In this section the performance of the proposed algorithms is examined, first for a simplified model and then for a practical coupled code problem using TRAC-M/PARCS.

4.1. One-Dimensional Simplified Problem

A simplified single fluid, one-dimensional thermal-hydraulics model was coupled to a one-dimensional, one-group neutronics model and evaluated using MATLAB scripts in order to simplify the examination of the numerical behavior of the proposed method. The problem simulates a control rod ejection transient and the system consists of a single fuel rod and flow channel which are divided into 10 nodes using the same nodalization. The one-group kinetics cross sections are updated by the T/H feedback using fuel temperature, moderator temperature and density:

$$\Sigma = \Sigma_0 + \frac{\partial \Sigma}{\partial \sqrt{T_F}}\Big|_0 (\sqrt{T_F} - \sqrt{T_{F0}}) + \frac{\partial \Sigma}{\partial T_M}\Big|_0 (T_M - T_{M0}) + \frac{\partial \Sigma}{\partial \rho_M}\Big|_0 (\rho_M - \rho_{M0}). \tag{15}$$

Other features of the model include:

- heat conduction in the fuel and clad;
- Newton's law of heat convection in the gas gap and cladding wall;
- heat convection in the T/H channel – single phase flow;
- Crank-Nicholson method for time differencing and central spatial differencing.

Since the solution vector involves significant differences in the magnitude of the variables, two scaling matrices are applied in the linear system, one for solution vector, and the other for residual vector:

$$(\Lambda_2^{-1} J \Lambda_1)(\Lambda_1^{-1}\delta\vec{X}) = -\Lambda_2^{-1} F \quad \Longrightarrow \quad \tilde{J}\delta\tilde{X} = -\tilde{F}\,. \qquad (16)$$

This serves an important role in improving the numerical performance since the condition number of the Jacobian is reduced several orders of magnitude by scaling.

In the following performance study we first examine the effect of the inner GMRES iteration convergence criteria, γ, on the overall convergence of the Newton method. The results for the first time step of the transient calculation are shown in Table I. There is a clear trade-off between the accuracy with which the Newton equations are solved and the effort required to solve the linear system. This is shown more clearly in Figures 4 and 5, which also show the impact of preconditioning. A relatively large γ will result in less work for the iterative solver to achieve a converged solution of the inner iteration, but more outer Newton iterations are then required to achieve convergence of the final solution vector. Since the most expensive operation is the inner GMRES iterations, the best performance is achieved with a relatively loose inner tolerance value of 10^{-2}.

Table I. Effect of Convergence Criteria in Inner GMRES Iteration

Method	Exact Newton Method	Inexact Newton Method with GMRES Inner Iteration					
		10^{-1} *	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}
Newton's Iterations	3	7 (5) **	4 (4)	4 (4)	3 (3)	3 (3)	3 (3)
Inner Iterations	-	79 (15)	76 (17)	106 (23)	115 (21)	141 (24)	172 (27)

Time = 0.01 sec, Δt = 0.01 sec

* tolerance for inner GMRES iteration

** the results included in the brackets are solved with preconditioning

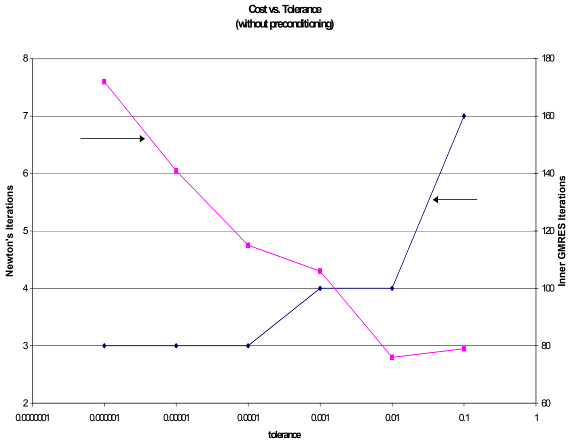


Figure 4. Effect of GMRES Tolerance without Preconditioning

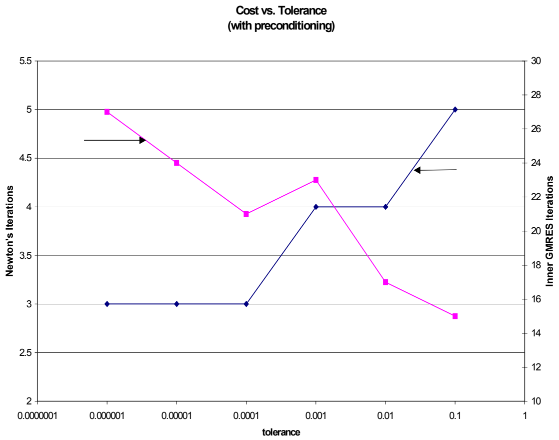


Figure 5. Effect of GMRES Tolerance with Preconditioning

The performance of the Inexact Newton Method with a relaxed convergence criteria for the inner GMRES iteration was then compared to the performance of the "Nested Method" and the Matrix Free Newton Method discussed in the previous section. The results are shown in Table II and illustrated in Figure 6.

Table II. Comparison of Methods

Method	Iterations
Nested Method	111
Exact Newton's Method	4
Inexact Newton Method w/ GMRES	5 (23)
Matrix-Free Newton Method w/ GMRES	5 (24)

* the results included in the brackets are the iteration numbers of inner preconditioned GMRES

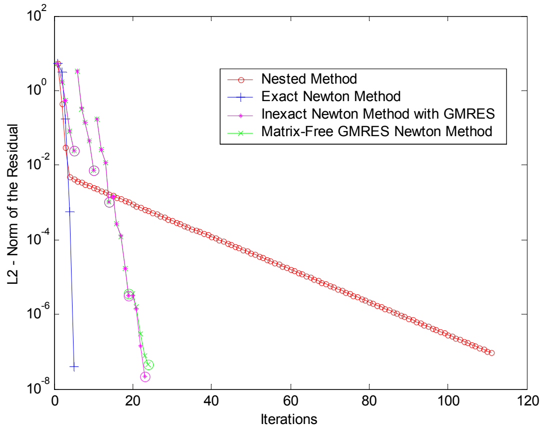


Figure 6. Comparison of Methods for Sample Problem

As indicated in Table II and Figure 6, the nested method converges linearly and requires many more iterations to converge. On the other hand, Newton's method demonstrates superlinear convergence in all cases. The exact Newton's method requires the fewest Newton iterations, but as noted earlier, direct solution of the Jacobian can be expensive for practical problems. The convergence of the inexact Newton Method is slightly better than the matrix-free Newton-Krylov method, but also as noted previously, the effort required to construct the Jacobian can be formidable for practical problems.

The method discussed in the previous section which does not require explicit construction of the residual was then applied to the sample problem. The approximate inner GMRES residual can be estimated using an expression similar to Eq (11):

$$\begin{aligned} r^0 &= P^{-1}F(x_i) \\ r^0 &= A(x_i)^{-1}\{A(x_i)\bullet x_i - b(x_i)\}, \\ r^0 &= x_i - g(x_i) \end{aligned} \tag{17}$$

$$\begin{aligned} r^j &= P^{-1}F(x_i) - P^{-1}J(x_i)\bullet \delta x_i^j \\ r^j &\approx r_0 - P^{-1}\frac{F(x^{n+1,i} + \varepsilon\delta x_i^j) - F(x_i)}{\varepsilon} \quad . \\ r^j &\approx r_0 - \frac{\{(x_i + \varepsilon\delta x_i^j) - g(x_i + \varepsilon\delta x_i^j)\} - r_0}{\varepsilon} \end{aligned} \tag{18}$$

The convergence history for the sample problem is summarized in Figures 7 and 8 for the approximate and exact residuals, respectively.

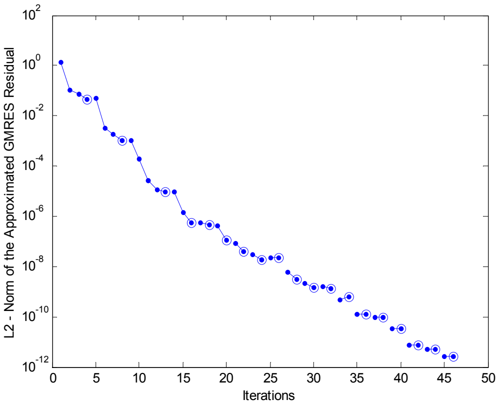


Figure 7. Approximate Residual

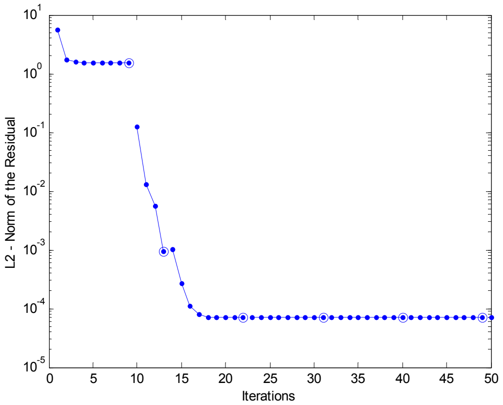


Figure 8. Exact Residual

The approximate GMRES residual converges very quickly as shown in Figure 7, while the exact nonlinear residual, *F*, stalls at about 10^{-4} because of the perturbation coefficient matrix approximation in (11). However, this tolerance is comparable to the traditional matrix-free Newton-Krylov method illustrated in Figure 6 and should not impact the convergence of the outer iteration.

4.2. TRAC-M/PARCS Solution of the OECD Main Steam Line Break

The nested and matrix free Newton-Krylov methods were then applied to a practical coupled code problem using TRAC-M/PARCS. Some modifications were required in order to implement an independent function to control calculation flow. However, because the matrix free method was employed, no modifications were required to TRAC-M or PARCS in order to implement Newton's Method. The thermal-hydraulics and neutronics codes were only used to pass the solution vector (with or without perturbation) to the global flow control function.

The OECD PWR main steam line break benchmark problem is a well established benchmark and well suited to analyze the performance of the methods proposed here. Because of its simplicity, the second of the three separate exercises of the OECD MSLB benchmark was chosen here. This problem consists of a spatial kinetics model of the core with the plant response modeled with time-dependent core thermal-hydraulic boundary conditions. The core neutronics problems simulates the TMI-I nuclear power plant at the EOC, 177 FA, 2772 MW_{th}, with 24 axial layers. The system nodalization is depicted in Figure 9:

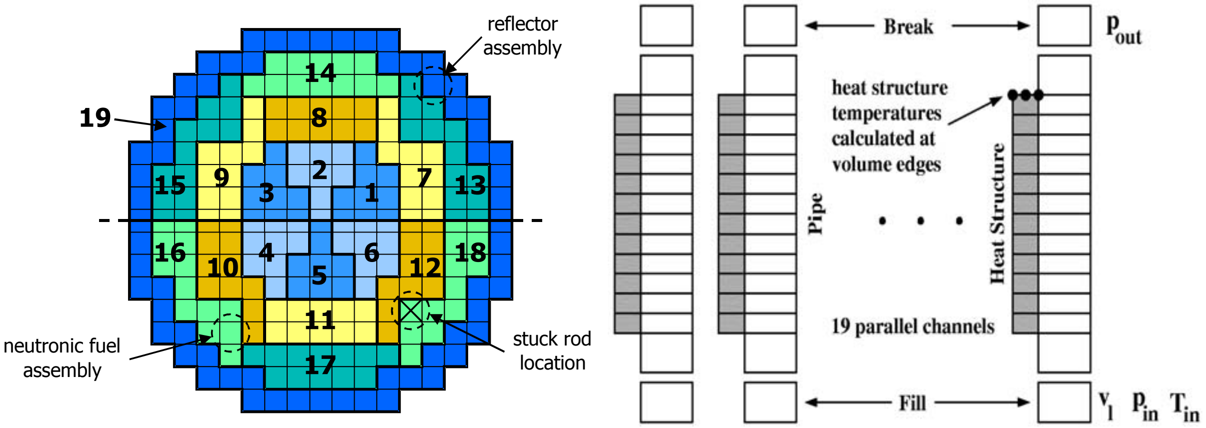
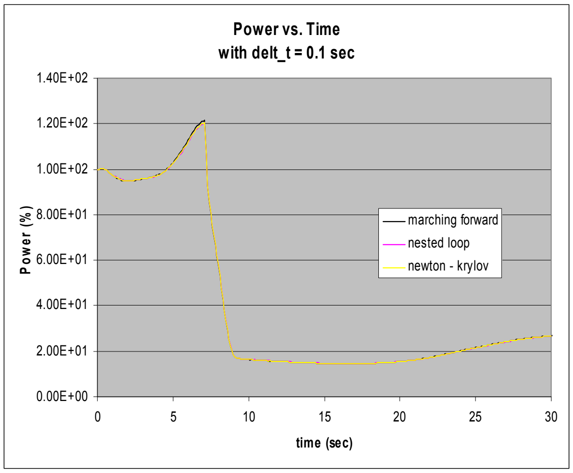


Figure 9. OECD MSLB Exercise 2 System Nodalization

The thirty-second transient simulation was performed using two time step sizes (0.1 and 0.5 sec) and results are summarized in Figures 10 and 11. During the scram of the reactor at about 5 seconds, small time steps are required to capture the mechanical movement of the control rods and there would be no advantage to employing Newton's method. Therefore, the SCRAM time phase of the transient is excluded from the analysis and the comparisons in the figures are for the time in the transient in which the control rods are not moving.



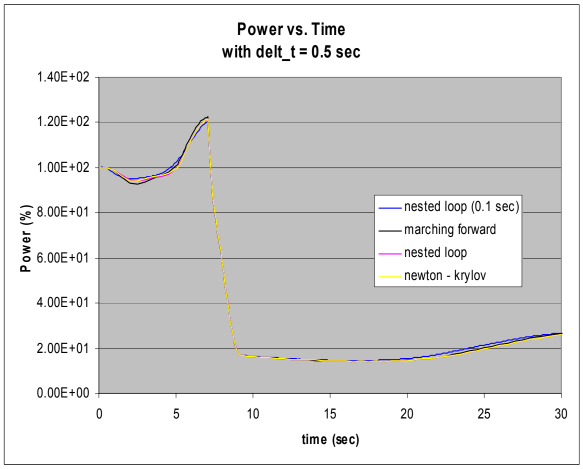


Figure 10. Reactor Power with t=0.1 sec

Figure 11. Reactor Power with t=0.5 sec

First, it is worth noting in Figure 11 that with the larger time size (t=0.5 secs) the solution accuracy is improved with the implicit Newton-Krylov method. The computing costs of various methods are compared in Tables III and IV. The CPU-time ratios are normalized to the original marching forward method for which the small (t=0.1 sec) time step size are listed in the gray cells.

Table III. CPU Summary for Various Solvers: time step size: 0.1 sec, time steps: 250

Numerical Solver	Diff. Power (%)	CPU-Time				Iterations		
		TRAC-M		PARCS		NESTED	NEWTON	GMRES
		Time (sec)	Ratio	Time (sec)	Ratio			
Marching Forward	0.153	69.3	1.0	298.6	1.0	250	-	-
Nested Loop Method	-	253.7	3.7	582.7	2.0	971	-	-
Newton Method	0.0511	602.6	8.7	1686.7	6.6	2351	693	774

Table IV. CPU Summary for Various Solvers: time step size: 0.5 sec, time steps: 50

Numerical Solver	Diff. Power (%)	CPU-Time (sec)				Iterations		
		TRAC-M		PARCS		NESTED	NEWTON	GMRES
		Time (sec)	Ratio	Time (sec)	Ratio			
Marching Forward	2.97	15.9	0.2	90.5	0.3	50	-	-
Nested Loop Method	1.26	61.1	0.9	165.96	0.6	223	-	-
Newton Method	1.35	334.9	4.8	1564.6	5.2	1251	192	480

At the larger time step (t=0.5 sec), the computational time required for the nested method is about 10% less than the marching method with the smaller time step size (t=0.1 sec) with minor reduction in solution accuracy. However, the computational time for the matrix-free Newton method at the larger time step size is about a factor of 5 larger than the marching method at the smaller time step size. However, the Newton method convergence has not been optimized and the relatively small TH model in exercise 2 of this benchmark does not highlight the potential savings in TRAC-M calculations. These preliminary results are encouraging because they demonstrate the successful implementation of the matrix free Newton method for practical applications. Work is continuing to optimize the Newton method and to apply the method to exercise 3 of the benchmark.

5. CONCLUSIONS AND PROSPECTS

The matrix-free Newton-Krylov method has been demonstrated to provide an alternate method for solving nonlinear thermal-hydraulics / neutronics coupled code problems. An innovative non-residual construction matrix-free Newton-Krylov with preconditioning was presented, which considerably simplifies the implementation of Newton's method into existing codes. The preliminary applications demonstrate the numerical robustness of the method and the feasibility of implementing the algorithm in practical coupled codes such as TRAC-M/PARCS.

Work is continuing on optimizing the numerical behavior of the nested and Newton methods using a convergence study via Fourier analysis. Also a trade-off in accuracy vrs CPU time will be examined for a wider range of coupled transient systems with more complicated thermal hydraulics model, such as OECD MSLB EX3 and a BWR Peach Bottom Turbine Trip Transient.

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