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VERIFICATION OF MULTIPHYSICS SOFTWARE: SPACE AND TIME CONVERGENCE STUDIES FOR NONLINEARLY COUPLED APPLICATIONS

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ABSTRACT

High-fidelity modeling of nuclear reactors requires the solution of nonlinear coupled multi-physics stiff problems with widely varying time and length scales that need to be resolved correctly. A numerical method that converges the implicit nonlinear terms to a small tolerance is often referred to as nonlinearly consistent (or tightly coupled). This nonlinear consistency is still lacking in the vast majority of coupling techniques employed today. We describe a tightly coupled multiphysics framework that tackles this issue and present code verification and convergence analyses in space and time for several models of nonlinear coupled physics.

Key Words: Multiphysics, tight coupling, code verification, manufactured solutions.

1. INTRODUCTION

Over the past decades, high fidelity modeling of nonlinear multi-physics problems has been subdivided into several distinct domains of physics and solved individually as mono disciplinary blocks without rigorous coupling between the different physics, a technique mathematically referred to as Operator-Splitting (OS). Although naïve, this is still the most widely used coupling strategy for nonlinear multi-physics simulations, including in reactor analysis, design and safety. OS is based on coupling several existing specialized single physics codes with a "black-box" strategy, where the input of one code becomes the output of another, thereby producing solutions that are weakly coupled. The strategy is often non-iterative and hence the nonlinearities in the system due to the coupling are not resolved, reducing the accuracy in the time stepping procedure to first order in time, even though high-order time integration might be used in the individual physics components. Although OS allows parts of the problem to be treated implicitly, the lack of

iterations over the nonlinear coupling terms leads to lower accuracy solutions. Despite these drawbacks, this is still one of the major coupling paradigms used today for solving nonlinear coupled multi-physics systems. The explicit linearization of the coupled physics terms in the OS strategy does not resolve nonlinearities between physics over a time step. Such an inconsistent treatment of the nonlinear terms usually results in a loss of the convergence order in the final solution and requires the use of excessively small time steps due to stability constraints and loss of convergence order.

In this paper, an alternate scheme to OS, based on a Newton's method for the whole nonlinear system of equations, is presented and implemented. This Jacobian-Free Newton-Krylov (JFNK) method preserves and resolves the coupling between the physics components, such that high-order accuracy in space and time is retained. The JFNK method enables the solution of the nonlinear equations without the need for the expensive Jacobian matrix. It has been proposed by Brown and Saad, in the early 1990's [1] and has enjoyed much success, see, for instance, the recent JFNK review paper by Knoll and Keyes [2].

The present work is a continuation of the work described in [3, 5, 6] and we present the implementation and verification of the JFNK method for coupled physics applied to reactor analysis and safety. The KARMA computer code developed in that regard serves as a test bed code for methods development and contains the following features:

1. state-of-the-art computer science toolboxes and libraries for efficient spatial discretizations, handling and interfacing of the various physics components, fast and robust linear algebra routines for parallel computing platforms;
2. coarse grain physics models for rapid testing and verification; finer grain models can later replace the existing ones in a straightforward fashion through the common C++ interface.

Past research on the effect of the OS methods in terms of accuracy as compared to fully implicit coupling methods have been analyzed and documented [4]. Mousseau [7] demonstrated that coupled problems with diffusion and two-phase flow using a consistent and accurate numerical scheme based on the JFNK framework is more effective to resolve the nonlinearities than traditional OS methods. Such a scheme will preserve the higher orders of accuracy in time for the whole coupled solution.

2. KARMA, a C(K)ODE FOR ACCIDENT AND REACTOR MODELING ANALYSIS

KARMA is a fully implicit coupled multi-physics transient analysis test bed code that could eventually be used to analyze reactor accidents. The rationale for KARMA is to provide a software environment in which

1. new coupling methodologies can be implemented and verified and
2. code architectures and software design for the next-generation of safety analysis code can be tested.

The plug-in architecture employed in KARMA is straightforward to expand in order to incorporate additional physics components. Hence, the KARMA framework can be used to seamlessly integrate its existing numerical models with the new physics models. The idea behind this new code to solve strongly coupled physics using a loosely coupled software methodology. A prime concern in the code design is to achieve a high level of efficiency while still maintaining the object-oriented philosophy. In order to focus on multiphysics coupling schemes, it was decided to use "off-the-shelf" well verified linear algebra and finite element general purpose libraries in order to reduce the overhead in implementation design. This also follows closely the principles of object and code re-use whenever possible, thereby avoiding a significant effort to be spent on verification of lower-level functions.

Some of the supporting libraries include

1. PETSc [8], the Portable, Extensible Toolkit for Scientific computation, developed at Argonne National Laboratory ([9]), which is a general purpose suite of tools for the scalable solution of partial differential equations and related problems.

2. A generic Finite Element (FE) library called LibMesh [10], written in the C++ language. Libmesh has been made to interface with KARMA, makes use of data structures exposed by PETSc, and provides objects to handle and manipulate (a) different types of Finite Elements, (b) the unstructured mesh in the domain, (c) the connectivity of the unknowns and (d) association of material properties to each element. We employ both Continuous Galerkin (CG) method for parabolic equations (neutron diffusion, heat conduction) and Discontinuous Galerkin (DG) method for hyperbolic equations (fluid flow).

3. The SLEPc [11] and ARPACK [12] libraries, for solving generalized eigenvalue problems that occur in nuclear reactor analysis problems.

4. A generic temporal integrator, written for KARMA's framework and employing a the general description based on Butcher-Coefficient matrices. Currently, KARMA can handle Explicit RK (ERK) and Diagonally Implicit RK (DIRK) methods and future efforts will include Fully Implicit RK (FIRK) schemes also. Since the integrator is generic enough, arbitrary orders of temporal accuracy can be obtained using higher order RK schemes without any modifications in the user code.

5. Gmsh [13] is an automatic three-dimensional finite element mesh generator with a built-in CAD engine and pre-, post-processing functionalities. Its design goal is to provide a simple meshing tool with parametric input and advanced visualization capabilities.

6. VisIt [14] is a free interactive parallel visualization and graphical analysis tool for viewing scientific data.

7. ParMETIS [15] is an MPI-based parallel library that implements a variety of algorithms for partitioning unstructured graphs, finite element meshes, and for producing fill-reducing orderings of sparse matrices.

8. Other toolboxes: TinyXML, a small C++ library that can handle reading, manipulation and writing of XML data; CSVParser, another supporting C++ library that acts as a parser to read and write Comma Separated Values (CSV) to aid in reading data from spreadsheets like Excel or from data exported from MATLAB (csvwrite, csvread).

3. JACOBIAN-FREE NEWTON-KRYLOV (JFNK) ALGORITHM

3.1. Introduction

The JFNK method employs Newton's method (outer nonlinear solves) and Krylov methods (inner linear solves) to solve a set of nonlinear equations. The Jacobian-Free approximation implies that the algorithm can be implemented without explicitly building the Jacobian matrix needed in the linear solve. The matrix-free nature of the solvers relies on (i) the fact that Krylov solvers build a solution subspace using matrix-vector operations and (ii) these matrix-vector operations can be approximated using a finite difference formula that does not require knowledge of the matrix at all. Nevertheless, Krylov methods may require a certain number of basis vector to be stored in order to find an accurate solution (i.e., the size of the subspace may become large). The Krylov space size and the overall computing time can be significantly reduced by the use of an appropriate preconditioner. Therefore, the JFNK algorithm consists of 3 levels of iterations: 1) Newton iteration 2) Krylov iteration 3) Preconditioner iteration.

3.2. Newton's Method

Let us consider a system of nonlinear equations of the form $F(y) = 0$, e.g., obtained by implicit time differentiation of a system of ordinary differential equations after applying a spatial discretization scheme. Newton's method iteratively seeks a root as follows:

$$J(y^k)\delta y = -F(y^k) \quad (1)$$

$$y^{k+1} = y^k + \delta y \quad (2)$$

where $J(y^k) = \frac{\partial F(y^k)}{\partial y}$ is the Jacobian matrix of the system at the current Newton iterate y^k, δy is the increment update, solution of the linear solve, and the next Newton iterate is given by y^{k+1}.

It is quite clear that the above equation requires forming the Jacobian matrix explicitly in order to solve the system for δy. This can be expensive in terms of computational time if a finite difference procedure to perturb $F(y)$ is used to find J element by element (i.e., numerical Jacobian). Alternately, a different algorithm can be employed in the linear solve such that the Jacobian matrix itself is not required but only its action on a given vector. This operation will be required during the linear solve of (1). For a given vector v, the action of the Jacobian on the vector can be computed using the following equation

$$Jv \approx \frac{F(y + \epsilon v) - F(y)}{\epsilon} \quad (3)$$

where ϵ is a parameter used to control the magnitude of perturbation. An optimal equation for choosing the perturbation parameter ϵ has also been derived in [2]. The class of linear solvers to be employed in the matrix-free algorithm are the Krylov solvers. Since the Jacobian matrix is non-symmetric, a natural choice for the Krylov linear solver is the GMRES algorithm.

4. PHYSICS MODELS

The physics of nuclear systems are usually sub-divided into 4 primary domains for extensive and rigorous calculations based on the nature of the physics. They are given as:

1. Neutronics - Description of the neutron population distribution in the reactor core as a function of position, time, energy and angle.
2. Fuel heat conduction - Description of the temperature fields within the nuclear fuel pin
3. Coolant flow - Description of the coolant flow fields that include density, momentum and total energy

The aim of the current work is primarily focused on testing and verifying accurate numerical methods for coupled multi-physics calculations. Hence, a decision was made to use coarse-grain fidelity physical models rather than investing additional effort into the derivation of high-fidelity models for each of the physics component. The architecture of KARMA allows for straightforward addition of new physics models and should be considered in the future. Some examples of coarse grained physical models including multigroup neutron diffusion, nonlinear heat conduction, Euler's equations for fluid.

5. RESULTS

We present two nonlinear problems solved with KARMA.

5.1. Nonlinear Heat conduction problem

Using the method of manufactured solutions (MMS), 1-, 2-, and 3-D test problems, with a diffusion coefficient varying as $k(T) = T^2$, have been devised, where the exact solution is taken to be $T(r,t) = \tanh(t)\prod_{i=1}^{dim}\sin(\pi r_i)$ where $r = [x, y, z]$. Since the exact solution is known, the spatial and temporal error discretization can be quantified and the solution methodology can be verified to be consistent.

Plots for the spatial order of accuracy are shown in Fig. 1 (top) using linear and quadratic continuous Lagrange shape functions. The temporal order of accuracy is shown in Fig. 1 (bottom) for the following methods: Backward Euler, Crank Nicholson and SDIRK (of order 3). It can be seen that the nonlinear solution method with the JFNK framework is high-order accurate in space **and** time and is consistent with the expected theoretical orders of accuracy based on the discretization.

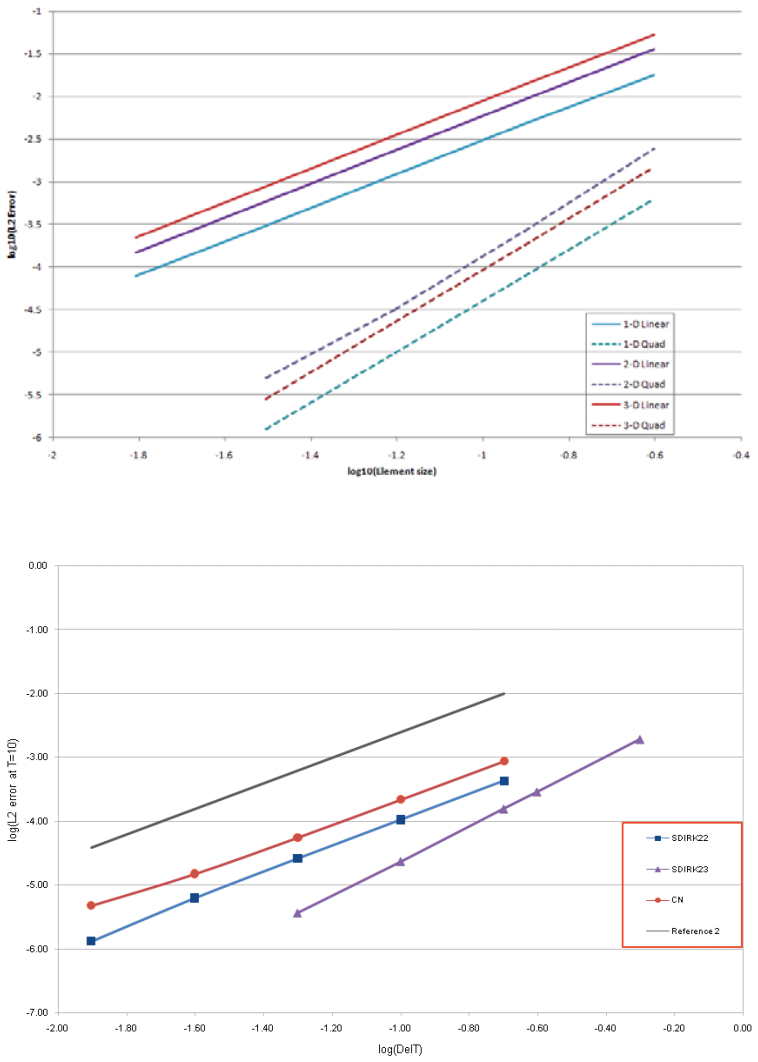

Figure 1. Spatial accuracy (top), temporal accuracy (bottom), nonlinear heat conduction problem.

5.2. Coupled Neutronics/Heat-conduction problem

Making use of the MMS techniques again, a coupled nonlinear heat conduction/neutronics problem was devised to verify convergence of the method to exact solutions. Since the coupling between neutronics and conduction is nonlinear, and due to the fact that the conduction physics is nonlinear by itself, a script in MATLAB was written to obtain the forcing functions based on the following assumptions.

First, the exact solution for the fields are taken to be

$$\phi(x, y, z) = (1 + \tanh(t)) \sin(\pi x) \sin(\pi y) xy \tag{4}$$

$$T(x, y, z) = (1 + \tanh(t)) \sin(\pi x) \sin(\pi y) \tag{5}$$

In this test, the neutron precursors are not considered in the calculation. Hence, the transient is dominated by the prompt neutrons and is strongly affected by the Doppler effects. The coupling coefficients between the two physics are given by

$$\Sigma_f(T) = \Sigma_{f0}(T) + \frac{\partial \Sigma_f}{\partial T}(T - T_0) \tag{6}$$

$$\Sigma_a(T) = \Sigma_{a0}(T) + \frac{\partial \Sigma_a}{\partial T}(T - T_0) \tag{7}$$

and the linearized conductivity coefficient

$$k(T) = k_0 + \frac{\partial k}{\partial T}(T - T_0) \tag{8}$$

With these parameters, the problem was tested for spatial and temporal accuracy. It is quite clear that the coupled solutions in all physics are high order accurate. By varying the coupling coefficients in Equations (6, 7, 8), stiffer transients were created and convergence to the true solution was still observed. The higher order temporal schemes are efficient and allow the usage of larger time steps as compared to say a first order Backward Euler scheme which might be traditional used for coupled physics problems.

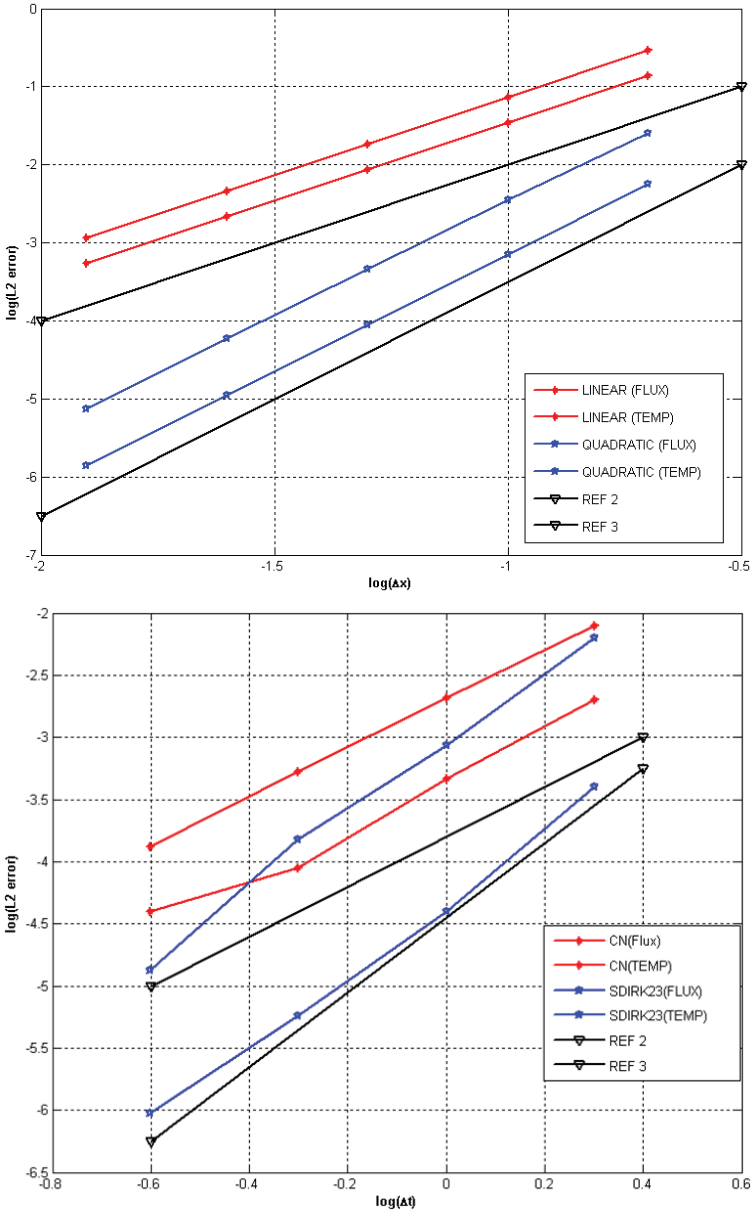

Figure 2. Spatial accuracy (top) and temporal accuracy (top); Coupled neutronics/heat conduction.

6. CONCLUSIONS

KARMA, a new test bed code for multi-physics applications in reactor analysis, is being developed and implemented. The rationale for KARMA is to provide a software environment in which

1. new coupling methodologies can be implemented and verified and
2. code architectures and software design for the next generation of safety analysis code can be tested.

KARMA is written in C++, with object oriented principles, and future extensions to add new physics in the future are straightforward. KARMA's method is based on a Jacobian-Free Newton-Krylov technique. The numerics are based on state-of-the-art libraries, such as PETSc (linear and nonlinear algebra), LibMesh (finite element spatial discretization), Gmsh (mesh generation) and high-order Runge Kutta time integrators. Some coarse grain multi-physics models have been implemented and tested. Further analysis is necessary to quantify the accuracy vs efficiency of the fully implicit JFNK scheme in comparison to traditional OS methods for problems of interest in LWR and SFR.

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