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Evaluation of coupling approaches for thermomechanical simulations

S.R. Novascone*, B.W. Spencer, J.D. Hales, R.L. Williamson

Fuel Modeling and Simulation, Idaho National Laboratory, P.O. Box 1625, Idaho Falls, ID 83415-3840, United States

HIGHLIGHTS

- Use consistent convergence criteria when comparing coupling approaches.
- Systems of equations with one-way feedback run faster with loose coupling.
- Two-way feedback equation systems run faster when tightly coupled.
- Examples of two-way feedback are thermal gradients and contact.

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ABSTRACT

Many problems of interest, particularly in the nuclear engineering field, involve coupling between the thermal and mechanical response of an engineered system. The strength of the two-way feedback between the thermal and mechanical solution fields can vary significantly depending on the problem. Contact problems exhibit a particularly high degree of two-way feedback between those fields. This paper describes and demonstrates the application of a flexible simulation environment that permits the solution of coupled physics problems using either a tightly coupled approach or a loosely coupled approach. In the tight coupling approach, Newton iterations include the coupling effects between all physics, while in the loosely coupled approach, the individual physics models are solved independently, and fixed-point iterations are performed until the coupled system is converged. These approaches are applied to simple demonstration problems and to realistic nuclear engineering applications. The demonstration problems consist of single and multi-domain thermomechanics with and without thermal and mechanical contact. Simulations of a reactor pressure vessel under pressurized thermal shock conditions and a simulation of light water reactor fuel are also presented. Problems that include thermal and mechanical contact, such as the contact between the fuel and cladding in the fuel simulation, exhibit much stronger two-way feedback between the thermal and mechanical solutions, and as a result, are better solved using a tight coupling strategy.

1. Introduction

The processes involved in capturing energy from nuclear reactions and converting that to usable form can involve extreme thermal environments. To characterize the thermal and mechanical response of nuclear power plant components subjected to those conditions, one must consider the physics driving both the thermal and mechanical response, as well as the interactions between the two.

Numerical methods for the implicit solution of the partial differential equations that describe physical phenomena typically lead to the solution of a system of discretized equations. If multiple coupled physics are included in a model, the set of equations to be solved includes degrees of freedom from all of these physics. The strategies used to solve coupled sets of physics equations can be generally categorized as loose coupling and tight coupling. In loose coupling, the individual physics in a coupled problem are solved individually, keeping the solutions for the other physics fixed. After a solution is obtained for an individual physics, it is transferred to other physics that depend on it, and solutions are obtained for those physics.

These fixed-point iterations are repeated until convergence is obtained. If there is not a strong two-way feedback between the physics involved, convergence can be obtained quickly with a minimal number of loose-coupling iterations. An advantage of this approach is that it allows for independent codes to be coupled with relatively minor modifications to those codes, and they can each use their own solution strategies that are tailored for their solution domain. The disadvantage of loose coupling is that if there is

* Corresponding author. Tel.: +1 2085263729.
E-mail addresses: Stephen.Novascone@inl.gov (S.R. Novascone), Benjamin.Spencer@inl.gov (B.W. Spencer), Jason.Hales@inl.gov (J.D. Hales), Richard.Williamson@inl.gov (R.L. Williamson).

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strong two-way feedback between the physics, that approach can have an unacceptably slow convergence rate and may encounter convergence difficulty.

In tight coupling solution methods, a single system of equations is assembled and solved for the full set of coupled physics. The nonlinear iterations operate on the full system of equations simultaneously, taking into account the interactions between the equations for the coupled physics in each iteration. In cases where there is strong coupling between the physics, this approach can have faster convergence rates than loose coupling. The primary disadvantage of this approach is that it necessitates tighter coordination between the codes to solve the individual physics.

In thermomechanical problems, in the absence of evolving contact between components, the coupling between the heat conduction and solid mechanics equations is often primarily one-way. The temperatures obtained from the heat conduction equations cause thermal strains, which result in displacement of the mechanical model. These displacements typically have a negligible effect on the thermal model, and such problems can be readily solved using loose coupling strategies, or even by transferring data from a thermal code to a solid mechanics code and completely neglecting the effect of the mechanical solution on the thermal solution. The simulation of the response of a reactor pressure vessel to pressurized thermal shock conditions is a good example of such a problem in nuclear power generation. During an accident, the vessel could be subjected to rapidly decreasing temperature and pressure, potentially followed by a rapid repressurization. High tensile stresses can occur on the interior of the vessel due to the combined effects of thermal gradients and internal pressure. In this problem, temperature changes lead to thermally-induced strains, but the displacement caused by those thermal strains has a negligible effect on the thermal response.

Introducing evolving mechanical and thermal contact to thermomechanical problems transforms thermomechanical problems from being essentially one-way coupled problems to strongly two-way coupled problems. This is because the heat conductance across gaps between adjacent bodies is highly dependent on the distance between those bodies, which is a function of the mechanical deformation. A good example of this type of problem is the simulation of the performance of a light water reactor (LWR) fuel rod. Heat generated by fission is transferred through the fuel pellet, across the gap between the fuel and cladding, and through the cladding to the coolant. The conductance across the gap is strongly dependent on the composition of the gas in that gap and the size of that gap, which is driven by the mechanical response of the fuel system. The fission gas released from the fuel has a strong influence on the composition, and thus, the conductivity of the gas in the gap. The mechanical effects driving the evolving gap size include thermal expansion, swelling, densification and relocation of the fuel, and cladding creep. Because the gap conductance has a strong effect on the thermal response of the fuel system, the ability to efficiently and robustly solve the strongly coupled thermal and mechanical equations in the presence of evolving contact conditions is critical for a successful fuel performance modeling code.

This paper describes the solution environment used to enable tightly and loosely coupled simulations of thermomechanical problems, provides a review of the equations governing thermal and mechanical response, and demonstrates the performance of loose and tight coupling strategies on simple thermomechanical problems with varying degrees of feedback between the two systems. Following these simple demonstrations, the performance of these solution strategies is demonstrated on real-world nuclear engineering problems, first on a simulation of reactor pressure vessel response during pressurized thermal shock conditions and then on a fuel performance simulation. This work extends similar studies presented by the authors in Novascone et al. (2013) and Novascone et al. (2013).

2. Multiphysics solution environment

The work performed in this paper was done using codes built on the open source Multiphysics Object-Oriented Simulation Environment (MOOSE) (Gaston et al., 2009), developed at Idaho National Laboratory (INL). MOOSE is a parallel computing environment for solving general systems of coupled partial differential equations based on the finite element method. MOOSE provides the framework for rapid development of physics simulation codes as well as access to solvers appropriate for nonlinear multiphysics problems.

To solve a nonlinear system of equations, it is common to begin with a residual statement (Hales et al., 2012)

$$\boldsymbol{r}(\boldsymbol{x}) = 0 \tag{1}$$

where $\boldsymbol{r}$ is the residual with $\boldsymbol{x}$ as the unknown solution. The Jacobian is written as

$$\boldsymbol{J}(\boldsymbol{x}) = \frac{\partial \boldsymbol{r}(\boldsymbol{x})}{\partial \boldsymbol{x}}. \tag{2}$$

Newton's method is then

$$\text{Compute } \boldsymbol{J}(\boldsymbol{x}_k), \boldsymbol{r}(\boldsymbol{x}_k) \tag{3}$$

$$\text{Solve } \boldsymbol{J}(\boldsymbol{x}_k)\boldsymbol{s} = -\boldsymbol{r}(\boldsymbol{x}_k) \text{ for } \boldsymbol{s} \tag{4}$$

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \boldsymbol{s} \tag{5}$$

which is continued until the update is sufficiently small or some other criterion is met.

The Jacobian-free Newton Krylov (JFNK) method evaluates the action of the Jacobian through a finite difference approximation,

$$\boldsymbol{J}(\boldsymbol{x}_k)\boldsymbol{v} \approx \frac{\boldsymbol{r}(\boldsymbol{x}_k + \epsilon \boldsymbol{v}) - \boldsymbol{r}(\boldsymbol{x}_k)}{\epsilon}. \tag{6}$$

This is an attractive form since neither the full Jacobian nor its element-by-element contributions are required. Despite not requiring the analytic Jacobian, the effect of the full Jacobian is seen from the first iteration of the iterative solver, unlike modified Newton or quasi-Newton algorithms. Thus, with only GMRES (Saad and Schultz, 1986) (which does not require $\boldsymbol{J}$ but $\boldsymbol{Jv}$) and a function that computes the residual, JFNK finds solutions to nonlinear coupled equations with the convergence rate of a traditional Newton algorithm.

JFNK, like Newton's method, is a general technique for solving nonlinear equations. As such, it provides flexibility in selecting which phenomena are active in a given simulation as well as flexibility in choosing which model to activate for a given phenomenon. This generality is due to the fact that the approach is based on the evaluation of the residual, which is done according to whatever models and options are active for a given analysis.

Efficient solves using iterative methods require good preconditioners. The purpose of preconditioning is to decrease the condition number of the system being solved. In JFNK, it is common to use right preconditioning,

$$\boldsymbol{J}(\boldsymbol{x}_k)\boldsymbol{M}^{-1}(\boldsymbol{M}\boldsymbol{s}) = -\boldsymbol{f}(\boldsymbol{x}_k) \tag{7}$$

where $\boldsymbol{M}$ is the preconditioner or preconditioning process. In this form, the solution approach involves two steps. First, solve $\boldsymbol{J}(\boldsymbol{x}_k)\boldsymbol{M}^{-1}\boldsymbol{w} = -\boldsymbol{f}(\boldsymbol{x}_k)$ for $\boldsymbol{w}$. Then, compute $\boldsymbol{s} = \boldsymbol{M}^{-1}\boldsymbol{w}$. Note that if $\boldsymbol{M}^{-1} = \boldsymbol{J}^{-1}$ the iterative solve will converge in one iteration. However, computing $\boldsymbol{J}^{-1}$ is equivalent to solving the original system and so is not advantageous. It is necessary, therefore, to choose a preconditioner that reflects the character of $\boldsymbol{J}(\boldsymbol{x}_k)$ in order to