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Power uprates
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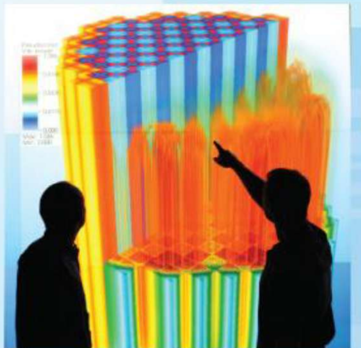

Engineering design
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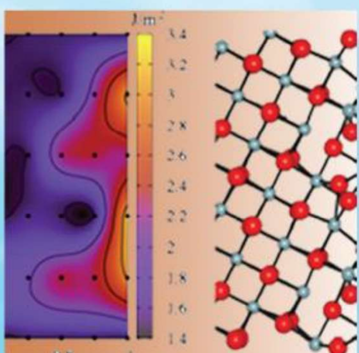
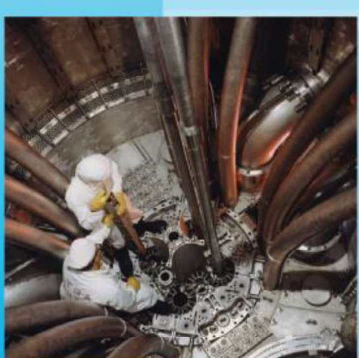


Fundamental science



Plant operational data

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Advanced Multiphysics Strategies for Radiation Transport/Heat Transfer Coupling

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Advanced Multiphysics Strategies for Radiation Transport/Heat Transfer Coupling

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1 Theory

In this document, we are interested in finding solutions to the Boltzmann neutron transport equation coupled with conjugate heat transfer (thermal conduction within fuel pins and cladding plus some description of convective heat transfer to the coolant). The k-eigenvalue form of the transport equation (the standard for for steady-state neutronics calculations [1]) is given by

$$\hat{\Omega} \cdot \nabla \psi + \sigma \psi = \iint d\hat{\Omega}' \, dE' \, \sigma_s \psi + \frac{1}{k} \chi \iint d\hat{\Omega}' \, dE' \, \nu \sigma_f \psi, \tag{1}$$

where $\psi = \psi(\vec{r}, E, \hat{\Omega})$ is the angular flux; k is the multiplication factor; σ, σ_s, and σ_f are the total, scattering, and fission cross sections, respectively; χ is the fission energy spectrum; and ν is the number of neutrons generated per fission. Because the eigenvector has no inherent magnitude, a normalization is applied to set the globally averaged power magnitude to a pre-determined level, i.e.

$$\frac{1}{\int dV} \iiint d\hat{\Omega} \, dE \, dV \, \kappa \sigma_f \psi = \bar{P}, \tag{2}$$

where κ is the heat generated per fission. In operator notation, we can write (1) as

$$(\mathbf{L} - \mathbf{MSD})\psi = \frac{1}{k} \mathbf{MFD} \psi. \tag{3}$$

All cross section quantities depend on the material temperature, T, so we can write (3) with this explicit dependence as

$$(\mathbf{L}(T) - \mathbf{MS}(T)\mathbf{D})\, \psi = \frac{1}{k} \mathbf{MF}(T) \mathbf{D} \psi. \tag{4}$$

Heat transfer within fuel pins and clad is governed by the diffusion equation

$$-\nabla \cdot k \nabla T = q, \tag{5}$$

where $k = k(T)$ is the thermal conductivity and q is the heat generation rate which, in this discussion, is due to fission in the fuel. In operator notation, we can write this as

$$\mathbf{K}(T) T = q. \tag{6}$$

More completely, $\mathbf{K}(T)$ represents the operator for heat transfer within the entire fuel pin, transfer from pellet-to-cladding, and within the cladding. Though not described explicitly, subchannel flow equations can be included in the nonlinear heat transfer operator, in which case the independent variables include both temperature throughout the domain as well as density in the coolant.

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2 Coupling Strategies

The radiation transport and heat transfer systems described in the previous section can be written as a single system of coupled equations as

$$f\begin{pmatrix}\phi\\ k\\ T\end{pmatrix} = \begin{bmatrix}\left(\mathbf{L}(T) - \mathbf{MS}(T)\mathbf{D} - \frac{1}{k}\mathbf{MF}(T)\mathbf{D}\right)\psi\\ \mathbf{RF}(T)\psi - \bar{P}\\ \mathbf{K}(T)T - \mathbf{F}(T)\psi\end{bmatrix} = 0,$$

where $\mathbf{R}$ describes the averaging of a power vector over the entire domain as in (2).

A straightforward approach to solving this system is to loosely couple the equations by alternating between solving the individual physics components. This fixed point, or Picard, iteration can be written as

$$\begin{aligned}\left(\mathbf{L}(T^j) - \mathbf{MS}(T^j)\mathbf{D}\right)\psi^{j+1/2} &= \frac{1}{k^{j+1}}\mathbf{MF}(T^j)\mathbf{D}\psi^{j+1/2}\\ \psi^{j+1} &= \frac{\psi^{j+1/2}}{\mathbf{RF}(T^j)\psi^{j+1/2}}\\ \mathbf{K}(T^{j+1})T^{j+1} &= \mathbf{F}(T^j)\psi^{j+1}.\end{aligned} \tag{7}$$

Each Picard iteration thus requires solving a radiation transport eigenvalue problem and a nonlinear heat transfer problem. The eigenvalue problem can be solved with standard strategies used for stand-alone radiation transport problems such as power iteration, Arnoldi's method, or a generalized Davidson solver. The heat transfer problem, being itself nonlinear, requires the use of an inner nonlinear solver such as Newton's method. A significant drawback to the use of Picard iteration is that the iteration as written in (7) is often not convergent due to oscillations that arise in the solution vector between iterations. It is often necessary to introduce an under-relaxation, or damping factor, to achieve convergence. Figure 1 shows the convergence behavior of Picard iteration on a coupled neutronics problem, where the damping is applied to the temperature component of the solution vector. Several studies have indicated the need for damping parameters in the range of 0.3-0.6 and resulting iteration counts of 10-20 [2, 3, 4].

An alternative approach to Picard iteration is to use a more tightly coupled solver to solve (7) as a monolithic system. One possibility is to use a Jacobian-free Newton-Krylov method (JFNK) [5]. JFNK is a variant of Newton's method in which matrix-vector products involving the Jacobian of the nonlinear system are approximated using only nonlinear function evaluations using a relationship of the form

$$\mathbf{Jv} \approx \frac{1}{\epsilon}\left[f(\mathbf{x} + \epsilon\mathbf{v}) - f(\mathbf{x})\right]. \tag{8}$$

Because Krylov linear solvers typically only require access to the linear operator in terms of matrix-vector products, JFNK methods allow the solution of nonlinear systems of equations using only function evaluations. Thus, JFNK methods are very attractive for multiphysics problems in which construction of the relevant Jacobian matrices may be intractable.

3 Results

In this section we consider a sample problem to demonstrate the performance of Picard iteration and JFNK. The problem is a single fuel pin 150 cm in height containing 3.1% enriched UO_2, zircaloy cladding, and natural water coolant/moderator. For the radiation transport component, the simplified P_N (SP_N) discretization implemented in Denovo is used. SP_N provides an attractive approach for testing algorithms because, unlike

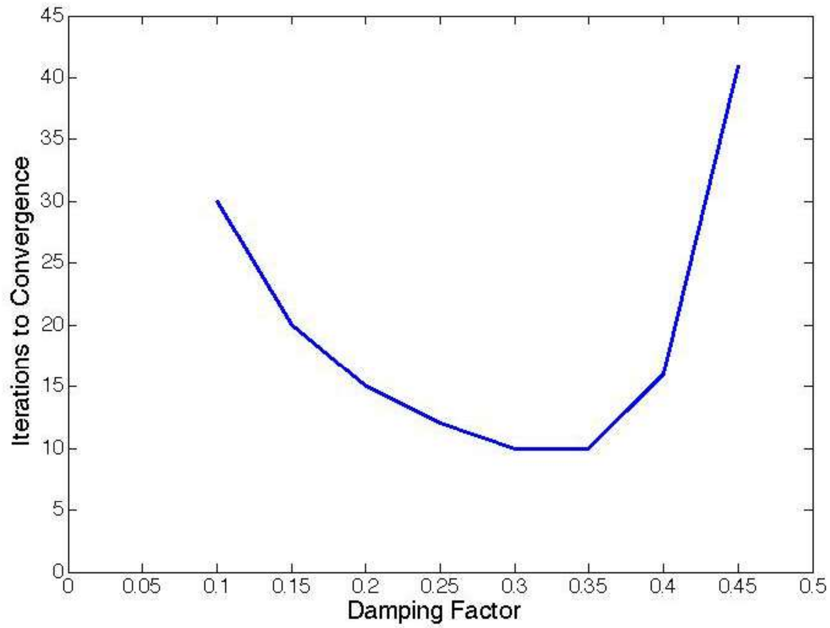

Figure 1: Convergence behavior for Picard iteration as a function of damping factor.

many discretizations (i.e. discrete ordinates), it is possible to explicitly construct the transport matrices rather than only accessing the operators via matrix-vector products. Additionally, treatment of boundary conditions is far simpler in SP_N and overall computational cost is significantly less relative to discrete ordinates transport. Although the SP_N equations do not represent a consistent discretization of the transport equation (i.e. they cannot be expected to converge to the true solution of the transport equation), they have nonetheless been shown to produce accurate solution for many problems, particularly light water reactor problems. It should be noted that in no way are the methods used here limited to SP_N, the SP_N equations simply provide a convenient test bed for an initial implementation. Cross sections are processed using the XSProc module of the SCALE package using an 8 group cross section library. The heat transfer component of the problem uses the AMP multiphysics framework. AMP solves 3D nonlinear thermal diffusion equations within the solid regions of the problem (fuel pellets and clad) and uses a gap conductance model from FRAPCON to describe heat transfer across the pellet-clad gap. Material models from the MATPRO material library are used to evaluate the thermal conductivity. Therefore, computational requirements are significantly higher than the coarse-mesh, 2D heat transfer within COBRA-TF.

Table 1 shows the behavior of both Picard iteration and JFNK on this sample problem. The convergence criteria for both strategies is a decrease in the residual norm by four orders of magnitude, resulting in very good agreement between the computed eigenvalues. The JFNK approach leads to a moderate decrease in the number of heat transfer function evaluations, a dramatic decrease in the number of radiation transport evaluations, and a sizeable increase in the number of cross section processing steps. For this problem, the run time is largely dominated by the heat transfer evaluations and so the difference in total execution time is only slightly different between the two cases. The use of a larger cross section library or a higher order Denovo discretization could lead to a significantly different timing distribution. The large increase in the number of XSProc evaluations with JFNK is due to the fact that new cross sections are required for every

Table 1: Convergence comparison between Picard iteration and JFNK.

	Solver	
	Picard	JFNK
Eigenvalue	1.1777081	1.1777085
Nonlinear Iterations	17	6
Thermal Evaluations	245	172
Core Neutronics Evaluations	5718	172
Cross Section Processing Evaluation	17	172
Total Time (s)	780	720

nonlinear function evaluation, which for JFNK is performed at ever linear iteration. Future work will evaluate the possibility of performing this cross section update only at nonlinear iterations rather than every linear iteration.

4 Implications and Conclusions

The choice of codes used in this study were related to ease of analysis, rather than consistency with the primary CASL software components. The specific timing of each portion is relatively irrelevant because there are several options for components to use for both neutronics and heat transfer. Therefore, the relative comparison of JFNK and Picard depends on the particular timing of the codes that are composed to solve a particular problem. All estimates within this section are arbitrary and used for discussion purposes only.

For the conjugate heat transfer solve, several options exist, including (i) COBRA-TF, (ii) COBRA-TF (fluid) + Peregrine (2D solid), (iii) COBRA-TF (fluid) + Peregrine (3D solid), and (iv) Hydra (fluid) + Peregrine (3D solid); there will be many orders of magnitude difference between (i) and (iv). However, because (iv) could provide an efficient residual evaluation, as opposed to (i) - (iii), it might be able to provide the evaluation at a more reasonable cost than (iii).

The neutronics calculation includes two components: the core neutronics and the cross section processing. The cross section processing step must be solved at each nonlinear iteration and at least estimated at each linear iteration. For the cross section processing solve, two primary options exist: (i) XSProc (1D pin cells) and (ii) MOC (2D core slices); however, it is likely that (iii) a simple function evaluation, or table evaluation, could be used to approximate the cross section dependence for the thermal iterations. If (iii) were used for the linear solves, the accuracy of (i) or (ii) could be maintained and only require a solve at each nonlinear iteration.

For the core neutronics solve, the three-dimensional core neutronics can be solved with (i) SPn, (ii) CMFD, (iii) Sn, and (iv) continuous-energy Monte Carlo. (i) and (ii) are likely to be relatively similar in run time and both able to provide a true residual. The Denovo Sn solver could be modified to provide a residual, but in its current form would require a full solve. It is not clear how (iv) could provide an inexpensive residual evaluation, thus require a full solve.

In the current test problem, the time to solution is dominated by the cross section processing, thus making the JFNK comparable in cost to the Picard iterations. However, if the cross section processing can be accelerated with an approximate method for the linear iterations using a functional evaluation, then both the JFNK and Picard iterations would be dominated by the total number of nonlinear iterations, thus showing a great benefit of JFNK. Similarly, if the transport or heat transfer components become more expensive by using advanced methods, such as Sn and 3D Peregrine, then the relative cost of the cross section processing is reduced and the JFNK becomes much more attractive.

In general, if the global residual can be evaluated, the convergence of the problem will be much more stable and predictable, because it does not rely on a multilevel convergence scheme that may lead to false convergence as is common with Picard iteration. Therefore, the choice in the future direction of the coupled-physics solves will significantly affect the decision to continue pursuing the exploration of advanced algorithms for coupling.

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