Multi-Physics Coupling for Robust Simulation

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Objectives and Approach

Motivation

- Many current and future modeling applications at Sandia, including ASC milestones, will critically depend on the simultaneous solution of vastly different physical phenomena.
- Issues due to code coupling are often not addressed, understood, or even recognized.

Objectives:

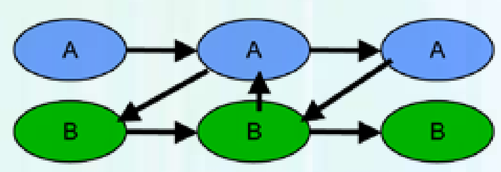
- Provide fundamental analysis of coupling.
- Enable tighter coupling strategies:
  - –leverage existing functionality
  - –minimize requirements
- Provide guidance and software for coupling codes and evaluating the "best" coupling techniques.

Approach:

- Develop a prototype test framework.
- Develop analysis tools.
- Demonstrate and evaluate techniques on systems of interest at Sandia.

Loose Coupling:

- Solves tailored to individual physics
- Minimal coding (transfer functions)
- Linear convergence rate
- No globalization techniques
- Convergence criteria – global norm?



Strong (Full) Coupling:

- Quadratic convergence rate
- Globalization techniques
- Invasive – Jacobian Matrix generation

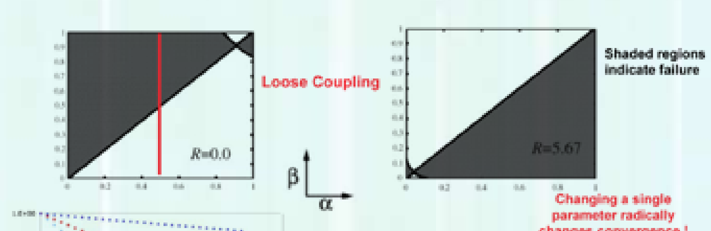
Intermediate Coupling (JFNK):

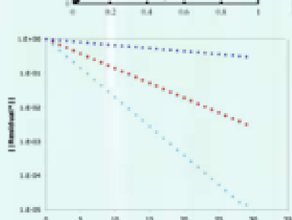
- Quadratic convergence rates?
- Optional Jacobian Dependencies
- Jacobian not required
- Accuracy/convergence issues?

Loose Coupling Convergence Issues

Prototype from: Yeckel et al., IJNME, v 67, n 12, 2006.
Implemented in Trilinos (NOX): http://trilinos.sandia.gov, Trilinos/packages/nox/test/epetra/MultiPhysics

Convergence and convergence rate of loose-coupling can be strongly problem-dependent





α	β	Fixed-pt Iters, R=0
0.50	0.40	33
0.50	0.45	60
0.50	0.49	253
0.50	0.60	N/A

$$\left\| \left. \frac{\partial \mathbf{R}}{\partial \mathbf{T}} \right|_{\mathbf{T}^*} \right\|$$

Fixed-point theory predicts linedar convergence rates that are parameter-dependent are typically observed in practice.

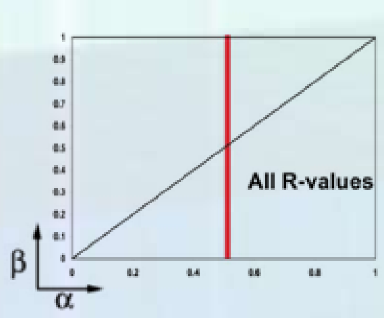
Intermediate, Newton-based Coupling using JFNK

- Jacobian-Free Newton-Krylov (JFNK) is a Newton method:

$$\mathbf{R}(\mathbf{x}_h + \epsilon\mathbf{p}) = \mathbf{R}(\mathbf{x}_h) + \mathbf{J}(\epsilon\mathbf{p}) + \mathcal{O}\left(|\epsilon\mathbf{p}|^2\right)$$

$$\mathbf{J}\mathbf{M}^{-1}\mathbf{p} \approx \frac{\mathbf{R}(\mathbf{x} + \epsilon\mathbf{M}^{-1}\mathbf{p}) - \mathbf{R}(\mathbf{x})}{\epsilon}$$

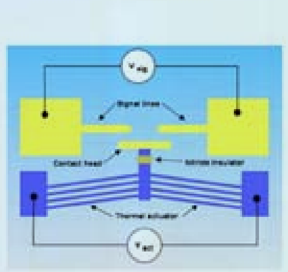
- It is a Newton method that employs Krylov-based linear solves (eg CG, GMRES) without requiring formation of the Jacobian matrix.
- It leverages loose-coupling to provide an approximate preconditioner, M



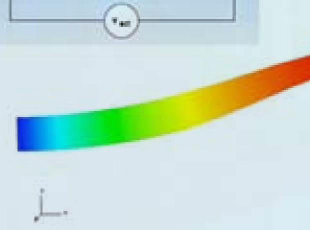
- We recover Newton-like convergence behavior
- We have also taken first step in providing software to drive JFNK

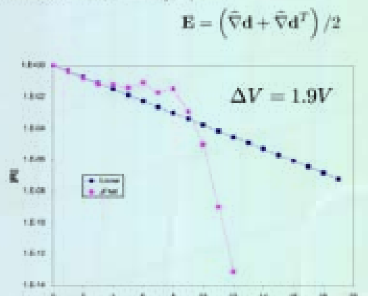
α	β	Fixed-pt Iters, R=0	JFNK Iters, R=0	JFNK Iters, R=5.67
0.50	0.40	33	1	3
0.50	0.45	60	1	3
0.50	0.49	253	1	3
0.50	0.60	N/A	1	3

Impact Part 1: Sierra Aria Multiphysics Studies



$$\nabla \cdot \sigma \nabla V = 0$$
$$\nabla \cdot \kappa \nabla T = \sigma (\nabla V \cdot \nabla V)$$
$$\nabla \cdot [\lambda E_{kk}\mathbf{I} + 2\mu\mathbf{E} - \beta(T - T_{ref})\mathbf{I}] = 0$$
$$\mathbf{E} = \left(\tilde{\nabla}\mathbf{d} + \tilde{\nabla}\mathbf{d}^T\right)/2$$



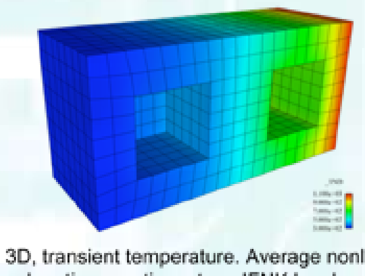


Loose coupling fails for higher potential loading (2.7 V)

Impact Part 2: Sierra Coupled Thermal-Radiation Multi-physics

$$\begin{aligned} K\,u_h + B\,J_h &= F(u_h) \quad // \text{ Calore} \\ M\,J_h &= G(u_h) \quad // \text{ Chaparral} \end{aligned}$$

Thermal conduction (Calore), enclosure radiation (Chaparral), u = temperature, J=radiosity

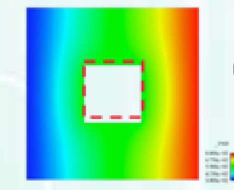


3D, transient temperature. Average nonlinear solver time per time step. JFNK has largest impact for implicit solvers and large time steps.

Elements/ timesteps	8	15	60
1289	3.88 (2.38)	2.60 (2.60)	0.63 (0.42)
10312	23.4 (15.9)	15.3 (12.5)	6.87 (6.37)

Equivalent reduced temperature residual (Calore)

$$R(u_h) \equiv K\,u_h + B\,\underbrace{M^{-1}G(u_h)} - F(u_h) = 0$$

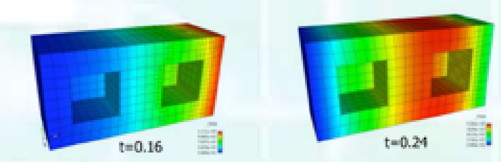


2D, steady state temperature

Elements	Nonlin. Iter	Total time
128	352 (5)	2.5 s (0.2)
512	311 (5)	4.3 s (0.5)
2048	267 (5)	9.2 s (1.5)
8192	222 (5)	33.3 s (5.1)
32768	176 (5)	127 s (21.3)

Speedup for JFNK (blue) over loose coupling (red) for uniformly refined spatial meshes.

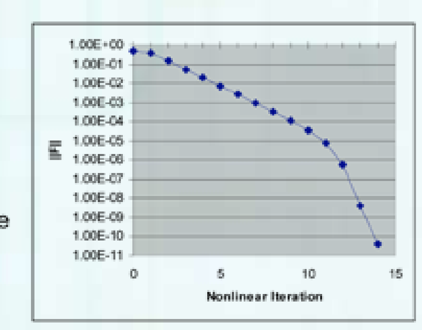
Impact Part 3: Other work influenced by this LDRD



- Transient, 3D, h-adaptive, coupled thermal-radiation
- Adjoint-based error estimation
- FY08 ASC Algorithms projects

Xyce-Charon Coupling via Nonlinear Elimination:

- Fully coupled, robust, flexible
- Well suited to multi-physics simulations which use two separate simulation codes
- Nearly quadratic convergence



Intermediate JFNK Coupling Summary

- Demonstrable improvement in both robustness and efficiency overloose coupling ⟶ Preconditioning is key
- Little to no added application requirements beyond loose-coupling
- Generally applicable through object-oriented extensions of existing nonlinear solver library (NOX in Trilinos)

It is possible to provide the benefits of strong, Newton-based coupling while respecting modularity of existing applications codes !

We have delivered this technology in several key application environments at Sandia.

LDRD Impact Summary

- Identified a set of prototype applications and critical Sandia applications.
- Developed a prototype multi-physics module implemented in Trilinos (NOX)
- Implemented and evaluated multiple nonlinear coupling techniques:
  - – Successive Substitution, Picard, JFNK, Newton.
  - – Identified failure modes and efficiency issues.
  - – Developed several methods for preconditioning JFNK in the context of multi-physics
- Kept this effort at the cutting-edge via dialogues at conferences and with international and academic researchers doing multi-physics coupling
- Delivered coupling algorithms in key impact areas at Sandia with demonstrable improvements in convergence robustness and simulation times
- Maintained working relations with other multi-physics coupling efforts at Sandia to deploy and tailor this work for maximum impact
- 2 Proceedings papers, 5 Presentations, 2 SIAM Mini-Symposia, 1 Paper (in prep.), Final SAND Report (in prep.)

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