

# Multi-Physics Coupling for Robust Simulation

SAND2007-5960P

Sandia National Laboratories

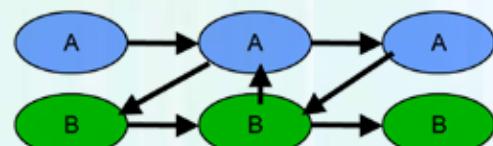
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## OBJECTIVES AND APPROACH

### 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.



### Strong (Full) Coupling:

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

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

### Intermediate Coupling (JFNK):

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

### Approach:

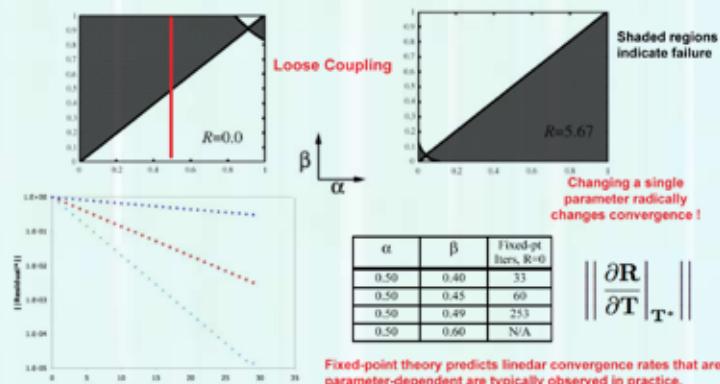
- Develop a prototype test framework.
- Develop analysis tools.
- Demonstrate and evaluate techniques on systems of interest at Sandia.

## 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



## INTERMEDIATE, NEWTON-BASED COUPLING USING JFNK

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

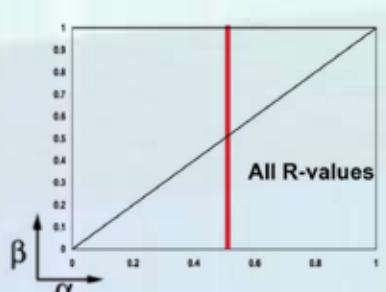
$$\mathbf{R}(\mathbf{x}_h + \epsilon \mathbf{p}) = \mathbf{R}(\mathbf{x}_h) + \mathbf{J}(\epsilon \mathbf{p}) + \mathcal{O}(|\epsilon \mathbf{p}|^2)$$

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

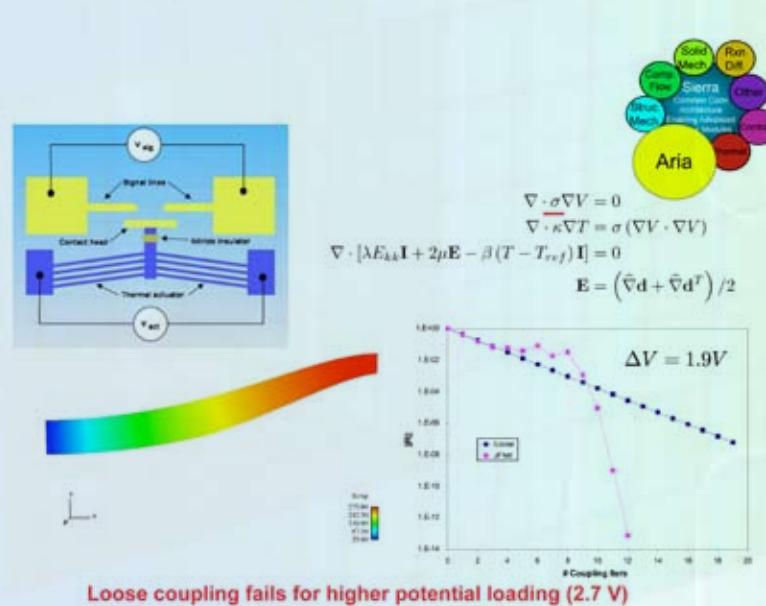
- It is a Newton method that employs Krylov-based linear solves (eg CG, GMRES) without requiring formation of the Jacobian matrix.
- It leverages loose-coupling to provide an approximate preconditioner, M

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

$\alpha$	$\beta$	Fixed-pt Iter, R=0	JFNK Iter, R=0	JFNK Iter, 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

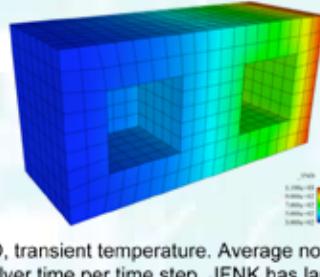


## IMPACT PART 2: SIERRA COUPLED THERMAL-RADIATION MULTIPHYSICS

$$K u_h + B J_h = F(u_h) \quad // \text{Calore}$$

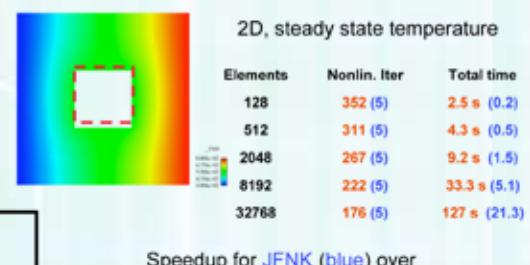
$$M J_h = G(u_h) \quad // \text{Chaparral}$$

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.

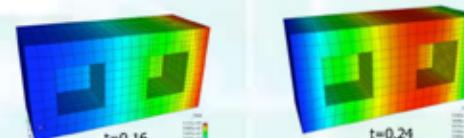
$$\text{Equivalent reduced temperature residual (Calore)} \\ R(u_h) \equiv K u_h + B M^{-1} G(u_h) - F(u_h) = 0$$



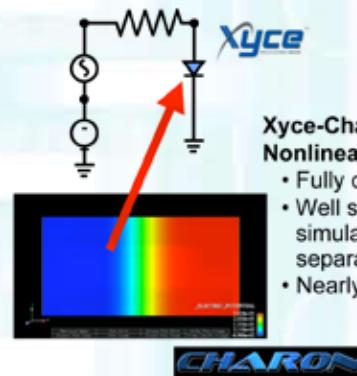
Elements/timesteps	8	15	60
1289	3.88 (2.38)	2.60 (2.60)	0.63 (0.42)
10312	23.4 (15.9)	15.3 (12.5)	6.87 (6.37)

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

## IMPACT PART 3: OTHER WORK INFLUENCED BY THIS LDRD

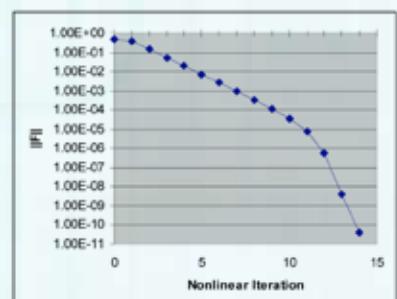


- Transient, 3D, h-adaptive, coupled thermal-radiation
- Adjoint-based error estimation
- FY08 ASC Algorithms projects



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 over loose 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 application 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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