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Algorithms that Enable Newton Coupling of Multi-Physics Simulations

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Sandia National Laboratories has successfully developed many physics simulation codes, whose potential for impact is greatly increased when coupled together to enable high fidelity, complex multi-physics simulations (*e.g.*, fluid-structure interaction problems). Within this context, the codes have traditionally been coupled using "weak" solution methodologies based on successive substitution. This involves computing a solution from one code while keeping variables from all other codes fixed and sequentially stepping through each code in this manner – a numerical procedure with unreliable convergence properties.

As part of our LDRD, "Multi-Physics Coupling for Robust Simulation," we have recently developed more advanced coupling solution methodologies that improve robustness and rates of convergence, yet do so without placing additional burdens on the codes being coupled. Our methodologies approximate Newton's method, the gold-standard for nonlinear solution methods, using the same information from each code needed for weak coupling. We have demonstrated improvements in both robustness and rates of solution convergence in real-world code-coupling environments for problems of interest to Sandia. The algorithms have been incorporated in the Trilinos nonlinear solver package NOX, taking advantage of Trilinos' software quality infrastructure.

The algorithmic innovations in this work were motivated by Sandia applications being very large scale, being written for distributed memory HPC platforms, and often involving poor conditioning of the equations. We verified the implementation of our Newton-based algorithms, one step of which is shown in Table 1. This table shows results for a prototype problem involving two linear problems whose interdependence is controlled by the coupling parameter, β. The Newton-based approach achieves its theoretical performance: one-step convergence for all values of β. A marked improvement in algorithm robustness and time-to-solution compared to weak coupling is already evident in this test problem.

β	Weak	Strong
0.40	33	1
0.45	66	1
0.49	253	1
0.60	FAIL	1

Table 1: Number of coupling iterations required for convergence for a coupling prototype problem involving two linear problems whose interdependence is controlled by parameter, β.

The application of this technology has continued, under ASC Algorithms funding, to impact state-of-the-art application codes where we have deployed our strong coupling algorithms within the Sierra framework. Figure 1 shows results for a MEMS thermal actuator simulation requiring solution for coupled electric potential, temperature, and material displacement fields. For a mild voltage load, our Newton algorithm achieves rapid quadratic convergence rates, as compared to only linear convergence associated with traditional weak coupling. At higher voltage loads, the weak coupling fails while our strong coupling algorithm continues to obtain converged solutions (not shown).

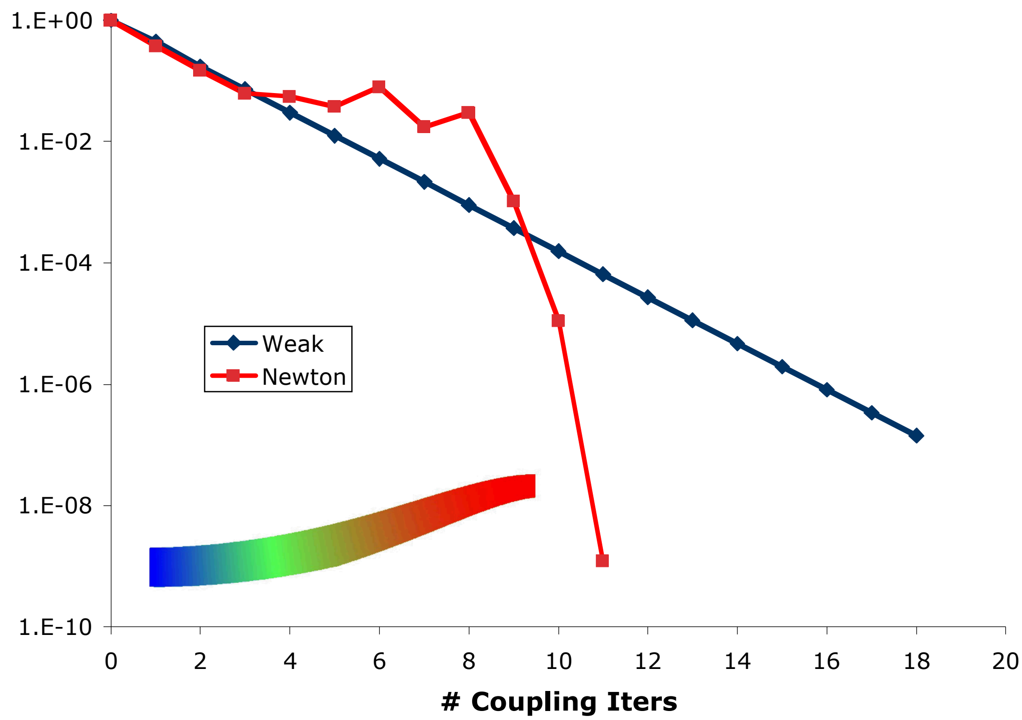

Figure 1: Convergence behavior of Newton (strong) coupling and weak coupling algorithms for simulation of a MEMS Actuator device. The model involves Electro-Thermal-Mechanical coupling solved using the Aria code within the Sierra framework.

A more complicated example is shown in Figure 2, where now the coupling is between two codes that use different discretization methods to solve fundamentally different physics, and that are coupled at a shared interface. The compressible flow code Premo uses a finite volume discretization to simulate flow and heat transfer over an airfoil, while the thermal code Calore utilizes a finite element discretization to solve for heat transfer within the airfoil. With this multi-physics model, the temperature and heat flux fields along the surface of the airfoil are solved for naturally as part of the simulation, not artificially specified by a boundary condition.

The above work highlights the success of our strategy of seeing our fundamental algorithm research through to deployment in application codes, not only in impacting the applications but also in generating new and relevant algorithmic research ideas. This problem motivated research into a variant of the strong coupling algorithm tailored to systems where the problem coupling involves considerably fewer unknowns than the whole system, *e.g.* at an interface.

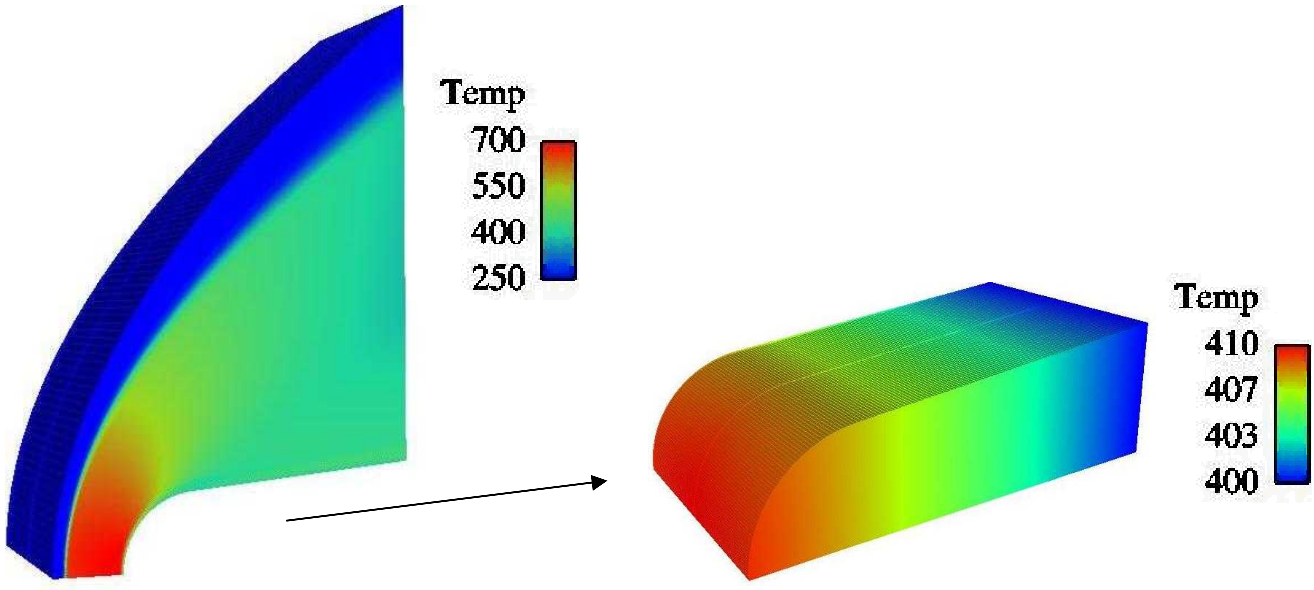

Figure 2: Mach 3 Shock over a thermally interacting airfoil. Simulations involve coupled compressible flow and heat transfer using the Premo and Calore codes in Sierra.

The impact of this work will grow well beyond improved robustness and computational efficiency of running a multi-physics simulation. The Newton algorithm supplied by the strong coupling algorithm is the kernel of most sophisticated analysis and design capabilities: sensitivity analysis, parameter continuation, stability analysis, global error control, and PDE-constrained optimization. For more information, contact: Russell Hooper, Applied Computational Methods Dept (1416), rhoope@sandia.gov. Collaborators include: Roger Pawlowski (1416), Matt Hopkins (1514), Harry Moffat (1514), Tom Smith (1433), and Pat Notz (1514).

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