Predictive Simulation of Contemporary Large-Scale Coupled Multiphsics-Multiresolution Problems

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Abstract.
In this lecture we first take a brief look back at the evolution of computer simulation in science and engineering to set the stage for the present discussion of "contemporary" work in predictive simulation of complex nonlinear coupled field problems that exhibit interactions at different spatial and temporal scales. A further complication of growing importance is the need to certify results and assess risk or more generally quantify uncertainty in predictive simulations.

Part of this talk will describe theory and methodology underlying the integrated approach to such issues as well as algorithm and software needed to realize reliable predictive simulations with practical error bounds on model, discretization and other sources of error. Related aspects of "verification and validation" will also be briefly discussed.

The use of parallel mesh adaptive strategies and software libraries for efficient solution on this expanded problem domain of contemporary will be examined and illustrated using the open source software library 'libmesh' (Kirk et al, 2006) developed primarily in our Computational Fluid Dynamics laboratory (CFDLab) at the University of Texas.

Results from a variety of interesting nonlinear-coupled systems will be used to demonstrate the central ideas. These include new results from collaborations in recent years with several research associates on cellular patterns in Rayeigh-Benard-Marangoni heat and fluid flow problems, superconductivity (Carey and Knezevic (2008)), biomedical and biological models (Peterson et al (2007)), high speed compressible gas dynamics (Kirk and Carey (2007, 2008)), and material separation with phase field interfacial models (Stogner et al, 2008). Use of the Lonestar and Ranger parallel supercomputer systems at TACC has been made in the large-scale simulations. Some work in progress with Libmesh coupled to Sandia software DAKOTA will also be described. This involves Latin Hypercube Sampling (LHS) in Monte Carlo studies of forward uncertainty propagation and related polynomial chaos studies (Carey et al, 2008).

Finally, I will briefly outline the re-entry space vehicle application and risk analysis of the associated thermal protection system being undertaken by our new PECOS Center in ICES under a Department of Energy grant initiated this year.

Some recent and forthcoming journal papers in which more details are available concerning the above research and application studies are provided below.

*Collaborative References (cited for detailed results):

Carey, G.F., “A Perspective on Adaptive Modeling and Meshing (AM&M)”, *CMAME* (Special Issue from ADMOS ’03 Conference), 195, 214-235, 2006.

Kirk, B., J.W. Peterson, R. Stogner, and G.F. Carey, “libMesh: A C++ Library for Parallel Adaptive Mesh Refinement/Coarsening Simulations”, *Engineering with Computers*, Vol. 22, 237-254, 2006.

Barth, Bill and Carey, G. F., “On a Natural Convection Benchmark Problem in Non-Newtonian Fluids”. *Numerical Heat Transfer, Part B*, 50: 193-216, 2006.

Peterson, J.W., G.F. Carey, D.J. Knezevic and B.T. Murray, “Adaptive finite element methodology for tumor angiogenesis modeling”, *Int’l J. Numer. Meth. In Flds*, Vol. 69, No. 6, 1212-1238, 2007.

Kirk, B. and G. F. Carey, “Development and Validation of a SUPG Finite Element Scheme for the Compressible Navier-Stokes Equations using a Modified Inviscid Flux Discretization”, *IJNME*, Vol. 57, No. 3, 265-293, May 2008

Carnes, B. and G. F. Carey, “Local Boundary Value Problems for the Error in FE Approximation of Non-Linear Diffusion Systems”, *IJNME*, Vol. 73, No. 5, 665-684, January 2008.

Stogner, R., G. F. Carey and B. T. Murray, “Approximation of Cahn-Hilliard Diffuse Interface Models Using Parallel Adaptive Mesh Refinement and Coarsening with C1 Elements", *IJNME*, Vol. 76, No. 5, 636-661, October 2008.

Kirk, B. and G.F. Carey, “A Parallel Adaptive Finite Element Scheme for Modeling Chemotactic Biological Systems”, *CNME*, in press, 2008.

Carey, G.F and D. Knezevic, “Nonuniqueness and Hysteresis Effects for Superconducting Vortex Patterns Computed with Local Adaptive Mesh Refinement, NMPDE, in review, 2008.

Carey ,G.F., V. Garg and R. Stogner “ Forward uncertainty propagation studies in Flow and Transport simulation via LHS Monte Carlo and Polynomial Chaos strategies in parallel adaptive simulation”, in preparation, 2008.

Valli, A.M.P., G. F. Carey and Coutinho, A.L.G.A., “On Decoupled Time Step/Subcycling and Iteration Strategies for Multiphysics Problems”, *CNME*, Published online, January 2008.

Peterson, J. W., G. F. Carey and B. T. Murray, “Multi-Resolution Simulation of Double-Diffusive Convection in Porous Media”, submitted to *IJNMHFF*, August 2008.

Kirk, B. and G.F. Carey, “Validation Studies of Fully-Implicit, Parallel Finite Element Simulations of Laminar Hypersonic Flows”, *AIAA*, In review, 2008.