Models, algorithms, and software: tradeoffs in the design of high-performance computational simulations in science and engineering

Speaker: Phil Colella
Applied Numerical Algorithms Group, Lawrence Berkeley National Lab
Time: 3:30-4:30 in COB 267
Date: Oct. 22, 2010

Abstract: Many important problems for DOE such as combustion, fusion, systems biology, and climate change, involve multiple physical processes operating on multiple space and time scales. In spite of the physical diversity of these problems, there is a great deal of coherence in the underlying mathematical representations. They are all described in terms of various versions of the elliptic, parabolic and hyperbolic partial differential equations (PDE) of classical mathematical physics. The enormous variety and subtlety in these applications comes from the way the PDE are coupled, generalized, and combined with models for other physical processes. The complexity of these models and the need to represent multiple scales lead to a diverse collection of requirements on the numerical methods, with many open questions about stability of coupled algorithms. Finally, the complexity of models and algorithms, combined with uncertainties about the correct combination to use, compli cates the problem of designing high performance software. In this talk, I will attempt to describe the tradeoffs between the models, the discretizations, and the software in the development of high-performance computational simulations in science and engineering involving PDE, including some motivating applications, and the combination of analysis and computational experiments that are used to explore the design space.