Phase 1 Project Summary

Firm: CFD Research Corporation
Contract Number: NNX09CF66P
Project Title: Benchmark Numerical Toolkits for High Performance Multiphysics Computing

Identification and Significance of Innovation: (Limit 200 words or 2,000 characters whichever is less)

Computational analysis encompasses a wide range of diverse scientific disciplines, including fluids, structurals, thermal, electromagnetics, astrophysics, biology, etc. Even though these fields are quite different in their underlying physics, the computational procedure used in each field is similar. Namely, the equations describing the relevant physical processes are discretized over a physical domain using one of many different approaches. This discretization process results in a set of algebraic equations that must be repeatedly solved during the simulation.

Thus, one thing that virtually all the various computational analysis disciplines have in common is the need for a linear equation solver. These solvers consume a significant amount of the total CPU time and memory. Choosing a non-optimum solver can result in CPU times up to a factor of 10 more than is possible with optimum solvers. Choosing the correct solver is imperative for efficient computational analyses, but this is rarely known a priori. A procedure for efficient testing and evaluation of these linear algebra tools would be an important addition to the toolbox of any computational analyst.

The Phase I work developed a proof-of-concept numerical benchmarking toolkit that will greatly aid computational analysts in choosing the optimum linear algebra library for their application.

Technical Objectives and Work Plan: (Limit 200 words or 2,000 characters whichever is less)

The objective of the Phase I work was to demonstrate a proof-of-concept numerical benchmarking tool that will allow numerical analysts to easily and intuitively evaluate different linear algebra packages for their specific applications. The intent is to have the numerical toolkit generate some representative problems automatically, so that users do not need to learn any new computational analysis software to use the tool.

The Phase 1 work plan was organized into six main tasks:

- Critical review of existing benchmarks and selection of new test problems.
- Technical specification and evaluation of test problems and toolkits
- Adaption of existing CFDRC and TACC toolkits for automated benchmark problem generation
- Perform computational benchmark simulations using adapted toolkits
- Web-based benchmark generation and demonstration of test problems
- Final report summarizing accomplishments and Phase II plans

Technical Accomplishments: (Limit 200 words or 2,000 characters whichever is less)

During the Phase I work, several benchmarking analysis cases were run using both iterative and direct linear equation solvers. The results of these analyses showed significant differences in CPU time and memory requirements between different solvers, and even with the same solver using different solver options. We also demonstrated that there is considerable difference in solver performance between serial and parallel solutions. The results of the benchmarking analyses demonstrated the need for a numerical benchmarking toolkit which would allow easy linear solver and preconditioner evaluation for different problems.

After need for the toolkit was clearly established, a proof-of-concept numerical benchmark toolkit was developed, using CFDRC's in-house multiphysics solver as the numerical engine. An intuitive and easy-to-use interface was developed so that users do not need to know how to use the multiphysics solver to set up sample problems. The fluid dynamics and structural dynamics modules of the multiphysics software were incorporated into the toolkit. Two demonstration test cases, a fluid dynamics and and solid dynamics test case, were demonstrated in the toolkit.

NASA Application(s): (Limit 100 words or 1,000 characters whichever is less)

Many NASA scientists and engineers are involved in the development and use of advanced computational codes (for instance NASA's Cielo code) that use linear algebra libraries for applications in physics, engineering, biotechnology, information processing, and other disciplines using parallel computing. This project will develop and deliver a tool for simplified testing and benchmarking of linear algebra libraries for use in these computational codes. These benchmarking tools will improve the efficiency and robustness of the computational codes by helping to identify optimal linear algebra libraries (linear equation solvers, eigenvalue solvers, etc.) for specific types of problems.

Non-NASA Commercial Application(s): (Limit 200 words or 2,000 characters whichever is less)

Scientists and engineers in a wide range of physical disciplines, such as mechanics, medicine, cosmology, nano-technology, etc., employ computational analysis to solve governing equations that are too difficult to solve analytically. Virtually all of these computational disciplines use some type of linear algebra package as a linear equation solver, eigenvalue solver, etc. Experts in these disparate fields are not necessarily experts in linear algebra, so the benchmarking tool developed in this project will serve as an important aid for these researchers to find the optimum linear algebra solution(s) for their particular problem(s).

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