Benchmark Numerical Toolkits for High Performance Computing: This topic addresses the need for well defined benchmarks to test and verify numerical toolkits for linear algebra applied to large problems running on serial and parallel computers. The goal of this work is to deliver a comprehensive numerical test suite that can be used in current and future high performance computing benchmarking activities. The toolkits can be either from public domain, for example PETSCi or LAPACK or from commercial vendors like Boeing Computer Services (BCS) or CASI.

Today’s models reach sizes of millions of degrees of freedom. Parallel processing is used to achieve acceptable turn-around time. Although most of the public domain packages for numerical methods are well tested for small standard problems, little experience and published benchmarks exist for parallel processing of large models. Computations with explicit solvers, for example in the area of crash dynamics or fluid dynamics, do not require matrix based equation solvers and inherently exhibit good scalability on large numbers of processors. Analyses requiring implicit solvers, for example in the computation of thermally driven structural response, utilize large matrix equation solvers. In most cases, the matrices are sparse. However, in thermal radiation exchange problems, the matrices may be dense and unsymmetric. The proposed work must address the latter cases.

Subtopics

T5.01 Benchmark Numerical Toolkits for High Performance Computing

Lead Center: JPL

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The work must include:

- Benchmarks of models with analytical solutions;
- Benchmarks for indefinite matrices and pathological cases;
- Benchmarks of implicit solution algorithms with production models in the area of thermal and structural analysis;
- Document the strengths, weaknesses, and limitations of the toolkits used together with recommendations;
- Comparison of solutions on serial and parallel hardware;
- Study of wall clock performance with respect to the number of processors;
- Precision and round-off studies on serial and parallel machines.

The number of processors should be varied based on common architectures (64, 256, 512, 1024 etc.). The study should also include performance comparisons between distributed and shared memory machines as well as machines with a mixed memory architecture. Phase 1 can include the selection of problem sets and research with respect to the current state of the art (particularly identifying areas of insufficient coverage). Phase 2 will include implementation and demonstration of the problem set on selected architectures.