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Iterative Methods for Nonsymmetric Systems on MIMD Machines *

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A wide variety of physical phenomena arising within many scientific disciplines can be described by systems of coupled partial differential equations (PDEs). The numerical approximation of these PDEs often involves the solution of a system of algebraic equations (possibly nonlinear) which are typically large, sparse and nonsymmetric. The increasing computational demands required by the solution of such complex scientific applications has motivated the current direction toward large-scale parallel computers. We, therefore, consider solution techniques of representative systems of equations on large scale MIMD machines.

Our primary emphasis in this study is the evaluation of iterative methods for the solution of nonsymmetric systems. In particular, we discuss two Krylov subspace methods, the conjugate gradient squared algorithm (CGS) and the generalized minimum residual method (GMRES), along with the multigrid algorithm (MG) on massively parallel MIMD architectures. The focus of

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this evaluation considers the performance of various algorithm and implementation variations over a broad selection of problems using a parallel machine. In conjunction with the Krylov subspace methods, a number of classical preconditioners are considered including Gauss-Seidel, Jacobi, and polynomial based methods as well as the more recent multilevel preconditioners such as multigrid and multilevel filtering. In conjunction with the multigrid method a number of relaxation schemes are considered including Jacobi, and Gauss-Seidel (point, line, and block). Additionally, the parallelization tradeoffs associated between the full multigrid variant and the standard 'V' cycle method will be discussed. Some of the key issues that are considered in the context of both the Krylov subspace and multigrid methods include tradeoffs between inner product, matrix multiplication and approximate factorization operations (such as ILU or line relaxation) and their effects on numerical performance, load balancing, and communication overhead.

An important aspect of this work is the application of these algorithms to relatively complex phenomena. To facilitate the programming and implementation of the various methods for a relatively wide range of problems, a distributed sparse matrix format is used. In particular, the format considered is similar to other sparse matrix specifications proposed for serial/vector machines. The primary difference is that the matrix data structure is distributed over all the processors in such a way that each processor contains a local discretization of the PDE problem within a specific subdomain. In this fashion, the different solution algorithms can be designed relatively independently of the specific application. This implies that many of the low level parallelization routines (e.g. communication, data shuffling and preconditioners) need not be redesigned for each new application.

Timing results and comparisons between the methods are given based on implementations on an NCUBE/6400 1024 processor hypercube. A wide variety of PDE applications are considered in making these evaluations including a nonlinear system of equations arising from a CFD application. Emphasis is placed on issues and results specific to nonsymmetric systems (such as the role and effect of preconditioners as well as the explicit orthogonalization issues in Krylov subspace methods). In addition, we offer observations regarding the robustness of each algorithm and the corresponding programming effort (serial and parallel) required to apply them to complex problems. Based on the NCUBE results a timing model is developed for the majority of these algorithms which describes the execution time and efficiency of each method as a function of the number of processors, size of the grid, computation speed and communication costs. Using this model, general conclusions are made corresponding to other parallel machines (including more massively parallel systems).

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