Experiments with Cholesky Factorization on Clusters of SMPs

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ABSTRACT

Summary In this paper we report on experiments with various parallel versions of Cholesky decomposition for dense matrices using different linear algebra software packages on clusters of (symmetric) shared memory multiprocessors (SMPs). Clusters of SMPs can be characterized as hybrid parallel architectures which combine the main architectural features of distributed memory and shared memory parallel computers. SMP clusters consist of a number of nodes each equipped with multiple processors. Each processor has direct access only to the shared memory within its node, while data located on other nodes has to be accessed by means of explicit message passing over the interconnection network. Although the availability of SMP clusters is increasing rapidly within the scientific computing community, currently no generally accepted programming model exists for these machines. As a consequence, most application developers utilize pure distributed memory programming models, usually based on the message passing interface (MPI [7]), and thus may miss a number of optimization opportunities offered by the shared memory available within the nodes of a cluster. In order to address these issues, we have experimented with different parallelization strategies for Cholesky decomposition comparing pure message passing strategies to a hybrid parallelization strategy that combines message passing with shared memory parallelization based on multi-threading.

1 Introduction

The Cholesky factorization, which is usually written as either

\[ A = LL^T \quad \text{or} \quad A = U^TU \]  

(1)

is a factorization of the Hermitian, positive definite matrix \( A \) into a lower triangular matrix \( L \) or an upper triangular matrix \( U \). This factorization is widely used for solving systems of equations or generalized eigenproblems (see, e.g. [1]). It is also an integral part of the program package WIEN2k [2]. Cholesky factorization belongs to the basic numerical algorithms with numerous applications in scientific and engineering computing, ranging from computational fluid dynamic problems to financial modeling problems.

Over the last several years, clusters of shared-memory parallel processors (SMPs) have become the most promising parallel computer architectures. These machines can be characterized as hybrid-parallel systems, combining distributed-memory (DM) and shared-memory (SM) parallel architectures. Clusters of SMPs offer several possibilities for an efficient parallelization of linear algebra algorithms. However, the designers of new parallel algorithms are faced with the challenge of achieving the highest possible performance while ensuring portability across different computing platforms. Recent studies [5] show that there are benefits to be gained by rethinking the parallelization issues and by combining distributed
and shared-memory parallelization models into a hybrid-parallel model. However, until now there is a lack of effective mixed-mode (hybrid) parallel libraries and is unlikely that they will be available soon. It is more likely that libraries which have been designed for distributed memory parallel computers will be adapted for SMP clusters by relying on appropriate SMP-based multithreaded kernels. The PESSL [8] library, which is available for IBM Power 4 clusters, is an example of such a multithreaded library.

2 Parallelization using Linear Algebra Packages

In the full paper we outline the main issues in parallelizing the Cholesky decomposition algorithm using various standard linear algebra libraries, including LAPACK and ScaLAPACK, and discuss performance results obtained on a 64 processor and on a 96 processor SMP cluster.

In our work, we have experimented with different parallel versions of Cholesky decomposition using various combinations of publically available linear algebra libraries. The libraries we used comprise the sequential LAPACK library [3] and its multithreaded versions (optimized with ATLAS [6]), the ScaLAPACK [4] library, which is an MPI-based parallel version for distributed memory machines, the ESSL and Parallel ESSL libraries [8], and the ASCI RED multi-threaded BLAS libraries.

We performed a number of experiments on two parallel machines, on a 64 processor Beowulf SMP cluster located at the University of Vienna, and on an IBM p690 high-end SMP server consisting of 3 SMP nodes with 32 processors each, located at the Parallab, University of Bergen, Norway. Our experiments and performance studies have been performed for various problem and machine sizes. In addition to the analysis of the different parallelization strategies, emphasis has been put on the comparison of distributed memory versions to hybrid parallel versions.

3 Concluding remarks

Clusters of SMP systems increase the complexity of user applications development forcing programmers to deal with shared-memory and distributed memory parallelization techniques in order to achieve the highest possible performance. In our work we studied various parallelization techniques based on the combination of linear algebra libraries in the context of the widely used Cholesky decomposition.

REFERENCES