WORKSHOP ON PARALLEL COMPUTING ALGORITHMS AND APPLICATIONS (PCAA-99)

June 21-25, 1999

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Simulations of both parallel and distributed nature are playing an increasingly critical role in all areas of science and engineering. As the applications of these simulations expand, the demand grows for high-performance computing of increasing power, flexibility, and utility. Parallel processing is making a tremendous impact on many areas of computer application. With the high raw computing power of parallel computers, it is now possible to address many applications that were recently beyond the capability of conventional computing techniques. The demand for performance of large-scale applications is a familiar feature of every aspect of computing. Thus, new types of applications will also be enabled in multidisplinary collaboration environments in near future.

The availability of various parallel computers has created a number of challenges to solve large-scale scientific, engineering and commercial applications. For example: How should parallel computers be programmed? What algorithms and data structures are used? How can the quality of the algorithms be analyzed? How can the tools and libraries be used to extract performance? etc.

To provide an answer to such queries, C-DAC conducted a workshop on PARALLEL COMPUTING-ALGORITHMS AND APPLICATIONS (PCAA-99) at C-DAC during June 21-25, 1999. C-DAC views the PCAA-99 workshop and the Hands-on Session document presentation notes as a continuously evolving resource on parallel computing. The PCAA-99 workshop proceedings, hands-on using PARAM 10000 document and companion software offer bird's eye view of Parallel Computing.

The main objective of PCAA-99 workshop was to promote parallel computing for solving large-scale problems in science/engineering and commercial domains. The Technical programme featured keynote addresses, invited lectures, classroom lectures and hands-on sessions on PARAM 10000. Hands-on sessions provided an opportunity to the participants to work on various numerical and non-numerical parallel algorithms on PARAM 10000. The workshop was meant for beginners as well as advanced level users of parallel computers. The workshop provided an opportunity for participants to learn and use of parallel computing to solve scientific

applications. It also provided an opportunity for interaction among the various participants from different academic institutes and research organizations in the country working in the area of Parallel Computing.

The PCAA-99 workshop proceedings provided a balanced coverage of five aspects: current trends in models of parallel computers, parallel programming of multiprocessors, and network-based cluster platforms, principles of algorithms and design, numerical/non-numerical algorithms and scientific and engineering applications. Hands-on sessions provided an opportunity to the participants to work on various numerical and non-numerical parallel algorithms on PARAM 10000 at National PARAM Supercomputing facility (NPSF).

The classroom lectures in PCAA-99 workshop covered theoretical aspects. The main objective of the classroom lectures was to cover the topics such as models of parallel computers, trends in serial processor computing, scalability and performance studies, principles of message passing programming, principles of parallel algorithm and design, numerical algorithms (dense and sparse matrix computations, and Fast Fourier transformations) and non-numerical algorithms (graph and sorting algorithms).

Invited Lectures on scientific and engineering applications such as weather simulation, ocean modelling, computational fluid dynamics, seisimic data processing, Parallel unstructured mesh computations, parallel genetic algorithms, molecular modelling, chemistry, bioinformatics, graphics visualization, and finite element applications were delivered by experts from research organizations and academic institutes. Some of these applications performance were demonstrated on PARAM 10000 to the participants. Also, popular lectures and key note addresses were delivered by experts from leading academic institutions and research organizations in India on high performance computing in science and engineering during workshop.

The PCAA-99 workshop also focussed on elaborate hands-on session on each day using portable Parallel Programming with the Message Passing Interface (MPI). The PCAA-99 Hands-on Session program provided foundation for application user to write good parallel algorithms and parallel programs to extract performance of large-scale application and libraries on PARAM 10000.

The DAY ONE, DAY TWO, DAY THREE, DAY FOUR, and DAY FIVE hands-on session introduced to the fundamentals of parallel programming by letting the participants to write simple and complex parallel programs in Fortran and C languages for numerical and non-numerical computations. Also, participants were exposed to practical aspects of classroom lectures in the hands-on session. There were three-hour Hands on Session on PARAM 10000 on each day, which focused on writing MPI programs for numerical and non-numerical algorithms. Examples included numerical integration, global summation algorithms on various topologies, matrix vector multiplication, matrix multiplication, direct/iterative methods (gaussian elimination method, conjugate gradient method), sparse matrix multiplication, graph coloring, sorting, search algorithms, finite element and finite difference methods for partial differential equations. Performance evaluation and visualization was an important and useful technique that helped the user to understand and improve complex parallel performance phenomena. A number of performance visualization tools were demonstrated for performance analysis of MPI programs. These performance tools were required in order to help the programmer to understand the behavior of a parallel program.

The workshop proceedings along with hands-on session notes is not only a tutorial on the use of MPI as a language for expressing parallel algorithms but also a handbook for those seeking to understand and improve the performance of large scale applications and libraries.

The DAY ONE hands-on session introduced the fundamentals of parallel programming by letting the participants write simple MPI programs in Fortran and C languages, for PARAM 10000. Programs based on point-to-point

communication, collective communication and computation and Simple MPI programs were included. The DAY TWO and DAY THREE hands-on session introduced the participants to write programs for algorithms involving dense matrix computations in several numerical contexts. Different methods of decomposition of matrices were covered and several MPI programs in Fortran and C languages were provided. Special MPI library calls, which allow user to define virtual topology, were used in matrix-vector and matrix-matrix computations.

The DAY FOUR hands-on session focused on writing programs for direct/iterative methods to solve linear system of matrix equations. Gaussian elimination method without pivoting strategy; Jacobi method and Conjugate Gradient iterative method for the solution of matrix system of equations and MPI programs in and C languages were discussed and provided. Simple algorithms for sparse matrix and vector multiplication using Compressed Row Storage format were included in DAY-FOUR hands-on session. Parallel programs on Sorting, Graph were included in DAY FOUR Hands-on Session. The DAY-FIVE hands-on session also introduced a special class of parallelisation methods to solve partial differential equations. The different decomposition methods can be used for mapping the task onto processors so that the processors are efficiently utilized. The good choice of decomposition depends on the details of the underlying hardware. MPI provides special library calls to perform computations. Advanced MPI point-to-point communication library calls were used and different versions of MPI programs were provided. This helped the application user to use wide variety of MPI special library calls for the solution of parallel differential equations. Simple algorithms for parallelization of solution of partial differential equations by finite element method and coloring of a sparse graph were also discussed.

On Day-FOUR Hands-on Session, we briefly demonstrated the use of various performance visualization tools on PARAM 10000.