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Parallel Programming of Industrial Applications

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SuperComputing '98 Tutorial Proposal:

Parallel Programming of Industrial Applications

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Abstract

In the introductory material, we overview the typical MPP environment for real application computing and the special tools available such as parallel debuggers and performance analyzers. Next, we draw from a series of real applications codes and discuss the specific challenges and problems that are encountered in parallelizing these individual applications. The application areas drawn from include biomedical sciences, materials processing and design, plasma and fluid dynamics, and others. We show how it was possible to get a particular application to run efficiently and what steps were necessary. Finally we end with a summary of the lessons learned from these applications and predictions for the future of industrial parallel computing. This tutorial is based on material from a forthcoming book entitled: "Industrial Strength Parallel Computing" to be published by Morgan Kaufmann Publishers (ISBN 1-55860-540-1).

Breakdown: (25% Beginner, 50% Intermediate, 25% Advanced)

Tutorial Material and Intended Audience

All major supercomputing centers around the world have powerful parallel programming platforms that are available to the general user community. In fact, for most users who want to do large-scale computations, these platforms are the only viable option to consider for getting their work done. Thus, all applications programmers today are faced with the dilemma surrounding the move to a parallel machine. In contrast to the environment of the University, where the porting and performance of the application is important research in itself, in the competitive application world the porting and design of applications must be relatively seamless to the application's customers. This is particularly important for industrial applications where the change must be made in a timely fashion, or not at all.

In this tutorial, we draw from a database of over 20 actual "industrial strength" applications which were successfully either ported or re-designed for parallel computers. We show which of the many available parallel tools, i.e. languages, debuggers, performance tools, etc. proved useful to the applications programmer. This data base is derived from a set of applications codes based in part on the "Parallel Applications Technology Program" of Cray Research. This program, which started in the mid-1990's and ended in early 1998, paired Cray analysts with applications programmers at a variety of sites throughout the world to promote the simultaneous development of the applications and the appropriate programming tools and models.

In the introductory material, we overview the parallel computing environment using as examples the National Energy Research Supercomputer Center and similar sites in Europe which support a diverse set of applications programmers. This overview will give the newcomer a sense of the resources that are available. In the core of the tutorial, we describe the actually experiences of the applications programmers in a lessons learned fashion. This material is aimed at both the intermediate and advanced levels. We start with the simple choices such as parallel programming paradigm, and show which choices proved judicious. For the advanced level, we show how once these decisions are made, what steps are necessary to achieve high level of performance and give a yardstick for what that level of performance should be given the restrictions of the application. Finally, we return to a level that should appeal to all members of the audience and give our predictions for the future of industrial parallel supercomputing.

Tutorial Outline (1/2 Day or 3 hours)

- The Parallel Computing Resources (1 1/2 hours)
    - Parallel Architecture Overview
        - The cost/speed/memory pyramid
        - Case Studies: Computer Center Choices
    - Performance: What does it really mean for me?
        - Performance Issues
        - Measuring and Reporting Performance
        - Case Studies: Application Speedup
    - Programming Models and Languages: Pros and Cons of Each
        - Message Passing Choices
        - Shared Memory Paradigms
        - High Performance Fortran
        - Other Options: Nested and Mixed-Model Methods, POSIX Threads and Mixed Models, Compiler Extensions for Explicit Parallelism, Work-Sharing Models
        - Case Studies: What Models do the Developers Really Use?

- More Tools of the Trade
  - Performance Analysis Tools
  - Debuggers: How hard is this part?
  - Single CPU Optimizing issues
  - Case Studies: How Much Can Performance Be Increased in a Real Application?
- Putting it all together: How to Design Real Applications (45 minutes)
  - Case Studies
- Future Directions (45 minutes)
  - The Role of Parallel Computing in Industry
  - Micro-architecture Issues
  - Macro-architecture Issues
  - System Software Issues
  - Programming Environment Issues
  - Summary Lessons Learned from the Applications
  - Looking Forward: The Role of Parallel Computing in the Digital Information Age

Sample Slides 10 slides

Presenters' Biographies

Alice E. Koniges is a Physicist and Leader of Multiprogrammatic and Institutional Computing Research at the Lawrence Livermore National Laboratory in California. She is currently on a loan to the Max-Planck Institute in Garching, Germany (Computer Center and Plasma Physics Institute) where she is helping users at this institute with the conversion of applications codes for MPP computers. From 1995 to 1997, she was leader of the Parallel Applications Technology Program at Lawrence Livermore Lab. This was Livermore's portions of the largest ($40Million) CRADA (Cooperative Research and Development Agreement) ever undertaken by the Dept. of Energy. The scope of the agreement provided for the design of parallel industrial supercomputing codes on MPP platforms. She is also under contract with Morgan Kaufmann Publishers of San Francisco as Editor of a book on "Industrial Strength Parallel Computing." She has a Ph.D. in Applied and Numerical Mathematics from Princeton University, an MA and an MSME from Princeton, and a BA from the University of California, San Diego. See online CV for more info.

Mike Heroux has recently joined Sandia National Laboratories as a Principal Member of Technial Staff in the Applied and Numerical Mathematics Group. Previously, he was leader of the Scalable Applications and Capability Prototyping Groups in the Applications Division of SGI/Cray. His primary interests are in the design and implementation of new applications technologies for high performance scientific computing (HPC), with the particular goal of demonstrating and promoting new approaches for the use of HPC in science and industry. Dr. Heroux joined Cray Research in 1988 after obtaining a Ph.D. in Numerical Methods at Colorado State University. He worked in the Math Software Research Group at Cray for five years, focusing on high performance numerical linear algebra. For the next five years, he led groups whose efforts addressed some of the challenging problems in HPC, e.g., large-scale automatic mesh generation, scalable applications technology, and integration of high performance computing, data management, and graphics. Currently he is working on parallel applications development for Sandia, with a special emphasis on modern numerical linear algebra software for current and future large-scale parallel computers. See online CV for more info.

Horst D. Simon has been Director of the NERSC (National Energy Research Scientific Computing) Division located at Lawrence Berkeley National Laboratory in Berkeley, CA since 1996. NERSC is the principal supplier of production high-performance computing services to the nationwide energy research community. From 1994-1996, Dr. Simon was with the Advanced System Division of Silicon Graphics in Mountain View, California, where he managed SGI's university and research laboratory programs. From 1987-1994, he was with Computer Sciences Corporation at the NAS Division at NASA Ames Research Center, Moffett Field, California, leading a research department with groups in parallel applications, scientific visualization, and numerical grid generation. Dr. Simon's algorithm research efforts were honored with the 1988 Gordon Bell Award for parallel processing research. He participated significantly in the development of the NAS Parallel Benchmarks. He holds a Diploma in Mathematik from the TU Berlin, Germany (1978) and a Ph.D. in mathematics from the University of California (1982), Berkeley, CA. See online CV for more info.

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