Dieter Kranzlmüller
Peter Kacsuk
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Recent Advances in Parallel Virtual Machine and Message Passing Interface

11th European PVM/MPI Users' Group Meeting
Budapest, Hungary, September 2004
Proceedings

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Preface

The message passing paradigm is the most frequently used approach to develop high-performance computing applications on parallel and distributed computing architectures. Parallel Virtual Machine (PVM) and Message Passing Interface (MPI) are the two main representatives in this domain.

This volume comprises 50 selected contributions presented at the 11th European PVM/MPI Users' Group Meeting, which was held in Budapest, Hungary, September 19–22, 2004. The conference was organized by the Laboratory of Parallel and Distributed Systems (LPDS) at the Computer and Automation Research Institute of the Hungarian Academy of Sciences (MTA SZTAKI).

The conference was previously held in Venice, Italy (2003), Linz, Austria (2002), Santorini, Greece (2001), Balatonfüred, Hungary (2000), Barcelona, Spain (1999), Liverpool, UK (1998), and Krakow, Poland (1997). The first three conferences were devoted to PVM and were held in Munich, Germany (1996), Lyon, France (1995), and Rome, Italy (1994).

In its eleventh year, this conference is well established as the forum for users and developers of PVM, MPI, and other message passing environments. Interactions between these groups have proved to be very useful for developing new ideas in parallel computing, and for applying some of those already existent to new practical fields. The main topics of the meeting were evaluation and performance of PVM and MPI, extensions, implementations and improvements of PVM and MPI, parallel algorithms using the message passing paradigm, and parallel applications in science and engineering. In addition, the topics of the conference were extended to include cluster and grid computing, in order to reflect the importance of this area for the high-performance computing community.

Besides the main track of contributed papers, the conference featured the third edition of the special session "ParSim 04 – Current Trends in Numerical Simulation for Parallel Engineering Environments". The conference also included three tutorials, one on "Using MPI-2: A Problem-Based Approach", one on "Interactive Applications on the Grid – the CrossGrid Tutorial", and another one on "Production Grid Systems and Their Programming", and invited talks on MPI and high-productivity programming, fault tolerance in message passing and in action, high-performance application execution scenarios in P-GRADE, an open cluster system software stack, from PVM grids to self-assembling virtual machines, the grid middleware of the NorduGrid, next-generation grids, and the Austrian Grid initiative – high-level extensions to grid middleware. These proceedings contain papers on the 50 contributed presentations together with abstracts of the invited and tutorial speakers' presentations.

The 11th Euro PVM/MPI conference was held together with DAPSYS 2004, the 5th Austrian-Hungarian Workshop on Distributed and Parallel Systems. Participants of the two events shared invited talks, tutorials, the vendors' session, and social events, while contributed paper presentations proceeded in separate tracks in parallel. While Euro PVM/MPI is dedicated to the latest developments of PVM and MPI, DAPSYS was a major event to discuss general aspects of distributed and parallel systems. In this way the two events were complementary to each other and participants of Euro PVM/MPI could benefit from the joint organization of the two events.

The invited speakers of the joint Euro PVM/MPI and DAPSYS conference were Jack Dongarra, Gabor Dozsa, Al Geist, William Gropp, Balazs Konya, Domenico Laforenza, Ewing Lusk, and Jens Volkert. The tutorials were presented by William Gropp and Ewing Lusk, Tomasz Szepieniec, Marcin Radecki and Katarzyna Rycerz, and Peter Kacsuk, Balazs Konya, and Peter Stefan.

We express our gratitude for the kind support of our sponsors (see below) and we thank the members of the Program Committee and the additional reviewers for their work in refereeing the submitted papers and ensuring the high quality of Euro PVM/MPI. Finally, we would like to express our gratitude to our colleagues at MTA SZTAKI and GUP, JKU Linz for their help and support during the conference organization.

September 2004

Dieter Kranzlmüller
Peter Kacsuk
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PVM Grids to Self-assembling Virtual Machines

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Abstract. Oak Ridge National Laboratory (ORNL) leads two of the five big Genomes-to-Life projects funded in the USA. As a part of these projects researchers at ORNL have been using PVM to build a computational biology grid that spans the USA. This talk will describe this effort, how it is built, and the unique features in PVM that led the researchers to choose PVM as their framework. The computations such as parallel BLAST are run on individual supercomputers or clusters within this P2P grid and are themselves written in PVM to exploit PVM's fault tolerant capabilities.
We will then describe our recent progress in building an even more adaptable distributed virtual machine package called Harness. The Harness project includes research on a scalable, self-adapting core called H2O, and research on fault tolerant MPI. Harness software framework provides parallel software "plug-ins" that adapt the run-time system to changing application needs in real time. This past year we have demonstrated Harness' ability to self-assemble into a virtual machine specifically tailored for particular applications.
Finally we will describe DOE's plan to create a National Leadership Computing Facility, which will house a 100 TF Cray X2 system, and a Cray Red Storm at ORNL, and an IBM Blue Gene system at Argonne National Lab. We will describe the scientific missions of this facility and the new concept of "computational end stations" being pioneered by the Facility.

1 Genomics Grid Built on PVM

The United States Department of Energy (DOE) has embarked on an ambitious computational biology program called Genomes to Life[1]. The program is using DNA sequences from microbes and higher organisms, for systematically tackling questions about the molecular machines and regulatory pathways of living systems. Advanced technological and computational resources are being employed to identify and understand the underlying mechanisms that enable living organisms to develop and survive under a wide variety of environmental conditions.

ORNL is a leader in two of the five Genomes to Life centers. As part of this effort ORNL is building a Genomics Computational Grid across the U.S. connecting ORNL, Argonne National Lab, Pacific Northwest National Lab, and

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Lawrence Berkley National Lab. The software being deployed is called The Genome Channel[2]. The Genome Channel is a computational biology workbench that allows biologists to run a wide range of genome analysis and comparison studies transparently on resources at the grid sites. Genome Channel is built on top of the PVM software. When a request comes in to the Genome Channel, PVM is used to track the request, create a parallel virtual machine combining database servers, Linux clusters, and supercomputer nodes tailored to the nature of the request, spawning the appropriate analysis code on the virtual machine, and then returning the results.

The creators of this Genomics Grid require that their system be available 24/7 and that analyses that are running when a failure occurs are reconfigured around the problem and automatically restarted. PVM's dynamic programming model and fail tolerance features are ideal for this use. The Genome Channel has been cited in "Science" and used by thousands of researchers from around the world.

2 Harness: Self-assembling Virtual Machine

Harness[3] is the code name for the next generation heterogeneous distributed computing package being developed by the PVM team at Oak Ridge National Laboratory, the University of Tennessee, and Emory University. The basic idea behind Harness is to allow users to dynamically customize, adapt, and extend a virtual machine's features to more closely match the needs of their application and to optimize the virtual machine for the underlying computer resources, for example, taking advantage of a high-speed I/O. As part of the Harness project, the University of Tennessee is developing a fault tolerant MPI called FT-MPI. Emory has taken the lead in the architectural design of Harness and development of the H2O core[4].

Harness was envisioned as a research platform for investigating the concepts of parallel plug-ins, distributed peer-to-peer control, and merging and splitting of multiple virtual machines. The parallel plug-in concept provides a way for a heterogeneous distributed machine to take on a new capability, or replace an existing capability with a new method across the entire virtual machine. Parallel plug-ins are also the means for a Harness virtual machine to self-assemble. The peer-to-peer control eliminates all single points of failure and even multiple points of failure. The merging and splitting of Harness virtual machines provides a means of self healing.

The project has made good progress this past year and we have demonstrated the capability for a self-assembling virtual machine with capabilities tuned to the needs of a particular chemistry application. The second part of this talk will describe the latest Harness progress and results.

3 DOE National Leadership Computing Facility

In May of 2004 it was announced that Oak Ridge National Laboratory (ORNL) had been chosen to provide the USA's most powerful open resource for capability