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High Performance Computing for Computational Science -VECPAR 2006

7th International Conference Rio de Janeiro, Brazil, June 10-13, 2006 Revised Selected and Invited Papers



Volume Editors

Michel Daydé

Institut de Recherche en Informatique de Toulouse, France

E-mail: Michel.Dayde@enseeiht.fr

José M. L. M. Palma

Faculdade de Engenharia da Universidade do Porto, Portugal

E-mail: jpalma@fe.up.pt

Álvaro L. G. A. Coutinho

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Center for Parallel Computations and Dep. of Civil Engineering, Brazil

E-mail: alvaro@nacad.ufrj.br

Esther Pacitti

LINA-Laboratoire d'Informatique de Nantes-Atlantique, France

E-mail: Esther.Pacitti@univ-nantes.fr

João Correia Lopes

Universidade do Porto/INESC-Porto, Portugal

E-mail: jlopes@fe.up.pt

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Preface

Following the practice of all previous editions of the VECPAR series of conferences, the most significant contributions have been organized and made available in a book, edited after the conference, and after a second review of all orally presented papers at VECPAR 2006, the seventh International Meeting on High-Performance Computing for Computational Science, held in Rio de Janeiro (Brazil), June 10–13, 2006.

After the conference is finished this is what is left, a document that, we hope, can be a reference to a wide range of researchers in computational science. For the first time, and reflecting the conference programme of the seventh edition of the VECPAR series, this book includes some of the presentations at the two workshops, namely:

WCGC 2006 — Workshop on Computational Grids and Clusters: Models, Middlewares, Testbeds, Architectures, User Feedback

HPDGrid 2006 — International Workshop on High-Performance Data Management in Grid Environments

Both the workshops and the conference programme evidence the current trends in computer and computational science, with an increasing importance of the Grid technologies.

The book contains 57 papers, organized in seven chapters, with the two last chapters entirely devoted to the workshops. Chapter 1 opens with six papers dealing on current issues such as the scheduling of workflows on grids, their use in structural analysis or peer-to-peer models in large-scale grids. Chapter 2, with a total of 14 papers, is concerned with aspects closer to computer science, which includes computation on volatile nodes, the evaluation of decentralized parallel I/O scheduling strategies for parallel file systems. Chapter 3 is devoted to numerical techniques; it opens with the invited lecture by Bruce Hendrickson on combinatorial scientific computing, followed by 15 papers mostly in the field of linear algebra; application of BlockCGSI algorithm, parallel processing of matrix multiplication in a CPU and GPU heterogeneous environment or construction of a unit triangular matrix with prescribed singular values are examples of subjects that can be found in this chapter that represents a major mainstream in all VECPAR conferences. Chapter 4 contains a set of five papers more concerned with applications in physics, ranging from cosmological simulations to simulations of laser propagations. Chapter 5 is made of three papers on bioinformatics, a topic of greater importance over the last few years that announces the impact of computational methods in life sciences.

Best Student Paper

The best Student Paper Award initiated in the third edition of VECPAR, in 1998, has always been the opportunity to reward high-quality research studies by newcomers and highly promising students. This year, and after a difficult selection among the 11 candidates, the prize was awarded to Jacques Bahi for his work, entitled:

JaceV: a Programming and Execution Environment for Asynchronous Iterative Computations on Volatile Nodes

Acknowledgements

The seventh edition of VECPAR was the second organized outside Portugal, and the first outside Europe. This time and after the interest shown by our colleagues in Brazil, who volunteered to organize the conference, VECPAR took place in the beautiful city of Rio de Janeiro, at IMPA (Applied Mathematics Institute), located over the Botanic Garden and overlooking the beautiful Rodrigo de Freitas lagoon.

This was a true multi-continent organization, made possible by current computer technologies, where the organizational aspects were dealt with by colleagues in Brazil, a joint collaboration between IMPA and the Institute Alberto Luiz Coimbra of Research and Post-Graduate Studies of the Federal University of Rio de Janeiro (COPPE/UFRJ). Paper submission and selection were managed via the conference database, held and managed by the Faculty of Engineering of the University of Porto. Vítor Carvalho created and maintained the conference Web site.

The success of the VECPAR conferences and its long life are a result of the collaboration of many. This time, given the widespread organization, a larger number of collaborators were involved. We mention only some, and through them we thank many others who offered most of their time and commitment to the success of the conference and workshops: Mara Prata (COPPE/UFRJ, Brazil) Conference Secretary, Marta Mattoso (COPPE/UFRJ, Brazil) and Patrick Valduriez (INRIA and LINA, France).

For their contribution to the present book, we must thank all the authors for meeting the deadlines and all members of the Scientific Committee who helped us so much in selecting the papers.

December 2006

Michel Daydé José M. L. M. Palma Álvaro L.G.A. Coutinho Esther Pacitti João Correia Lopes

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Workshop on Computational Grids and Clusters

The WCGC2006 Workshop followed the VECPAR 2006 Conference and focused on cluster and grid environments and tools for efficient management of computations.

The objectives of the workshop were to bring together researchers, practitioners and people with less experience in grid and clusters, to report on recent advances, and to share user feedback.

The topics of the workshop included (but were not restricted to):

- Hardware issues for clusters and grids
- Middlewares, distributed systems, runtime systems
- Interoperability issues
- Programming environments
- Communication protocols
- User experience in deploying grids and testbeds
- Grid and cluster management
- Performance evaluation
- Scheduling, load balancing, scalability, fault-tolerance issues
- Web applications, peer-to-peer
- Design of high performance clusters

The program of the workshop consisted of two invited talks and nine papers. One invited talk and six papers are included in the present book. A wide range of important topics in grid computing are covered (management of clusters, management of services, and deploying applications on computational grids).

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International Workshop on High-Performance Data Management in Grid Environments

Initially developed for the scientific community as a generalization of cluster computing using the Web, grid computing is now gaining much interest in other important areas such as enterprise information systems. This makes data management more critical than ever. Compared with cluster computing which deals with homogeneous parallel systems, grids are characterized by high heterogeneity, high autonomy and large-scale distribution of computing and data resources. Managing and transparently accessing large numbers of autonomous, heterogeneous data resources efficiently is an open problem. Furthermore, different grids may have different requirements with respect to autonomy, query expressiveness, efficiency, quality of service, fault-tolerance, security, etc. Thus, different solutions need be investigated, ranging from extensions of distributed and parallel computing techniques to more decentralized, self-adaptive techniques such as peer-to-peer (P2P).

The objective of this one-day workshop was to bring together researchers and practitioners from the high-performance computing, distributed systems and database communities to discuss the challenges and propose novel solutions in the design and implementation of high-performance data management in grid environments.

The Program Committee received 19 paper submissions. Each paper was reviewed by three PC members. The following program is the result of the paper selection, with nine papers presented in three sessions: (1) data grid applications, (2) replication and consistency in data grids, (3) design and implementation of data grids. In addition, we had one keynote session on "Enterprise Grids: Challenges Ahead" by Ricardo Jiménez-Peris, Marta Patiño-Martinez and Bettina Kemme. The authors of the papers are from five different countries (Brazil, Canada, France, Spain and USA), thus reflecting the true international nature of the workshop.

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