Scientific Programming provides a meeting ground for research results in, and practical experience with, software engineering environments, tools, languages, and models of computation aimed specifically at supporting scientific and engineering computing. Scientific Programming brings together in one place developments that are found in a wide variety of journals, conference proceedings and informal society journals. Scientific Programming publishes papers on language, compiler and programming environment issues for scientific computing. Of particular interest are contributions to programming and software engineering for grid computing, high performance computing, processing very large data sets, supercomputing, visualization and parallel computing. This special issue includes extended versions of eight papers originally presented at the joint International Symposium of Parallel and Distributed Computing (ISPDC) and International Workshop on Algorithms, Models and Tools for Parallel Computing on Heterogeneous Networks (HeteroPar) 2004, held at University College Cork, Ireland from July 5–7, 2004. The conference attracted many excellent submissions, not all of which could be accommodated here. The papers selected for this issue not only contribute valuable insights and results but were felt to have particular relevance to the Scientific Programming Community.

I. Banicescu, R. Carino, J. Harvill and J. Lestrade present “Statistical Analysis of Multiple Datasets on Heterogeneous Clusters”, describing how multiple datasets are analysed simultaneously using a statistical model across a 64-node cluster. Processors were arranged into groups to facilitate efficient communications and the use of a dynamic loop scheduling approach to load balancing. Results from preliminary tests using this strategy to fit gamma ray burst time profiles with vector functional coefficient autoregressive models are presented.

G. Gravannis and K. Giannoutakis present “Parallel Preconditioned Conjugate Gradient Square Method Based on Normalized Approximate Inverses”, describing a new class of normalized explicit approximate factorization procedures for solving sparse linear systems resulting from the finite difference discretization of partial differential equations in three space variables. The results obtained using an MPI implementation of the method are included.

A. Lastovetsky and R. Reddy present “Data Partitioning for Multiprocessors with Memory Heterogeneity and Memory Constraints”, describing a performance model that can be used to optimally distribute computations over heterogeneous computers. The model is application-centric, representing the speed of each computer as a function of the problem size, taking into account processor heterogeneity, memory structure heterogeneity and memory limitations at each level of the memory hierarchy.

B. Clayton, T. Quillinan and S. Foley present “Automating Security Configuration for the Grid”, describing a system that provides automated support for grid administration requests, such as resource reservation and user account management. Trust metrics are proposed to help judge the merits and suitability of each request, and a description of how these metrics can be implemented using trust management techniques is given.

A. Marowka presents “Execution Model of Three Parallel Languages: OpenMP, UPC and CAF”, describing a quantitative evaluation of three parallel languages (OpenMP, Unified Parallel C and Co-Array Fortran). Each language is deconstructed into its basic components, analysed, and compared with the others with the aid of examples. Finally, conclusions are drawn regarding the best language of the three.

D. Petcu, M. Paprzycki and D. Dubu present “Design and Implementation of a Grid Extension for Maple”, describing a software package (Maple2G) that allows Maple applications to take advantage of Grid resources via the Globus toolkit. The design and implementation of the system are described, along with the results of a number of experiments that measured its performance.
R. Byrom et al. present “The CanonicalProducer: An Instrument Monitoring Component of the Relational Grid Monitoring Architecture (R-GMA)”, describing a software component that allows the Relational Grid Monitoring Architecture to be used for instrument monitoring. An example use of this approach in the European CrossGrid Project, SANTA-G, is also presented.

Finally, K. Chmiel, M. Gawinecki, P. Kaczmarek, M. Szymczak and M. Paprzycki present “Efficiency of JADE Agent Platform”, describing a number of experiments conducted to investigate the performance and scalability of the JADE platform. These experiments were conducted using a variety of test scenarios, and the results obtained are discussed and conclusions drawn.

The guest editors would like to especially thank the reviewers for their diligence, insight and hard work put into commenting on the selected papers. Their efforts were much appreciated by the authors and editors alike. Finally, sincere thanks to the editor-in-chief, Ron Perrott, and the journal manager for IOS Press, Marleen Berfelo.

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