4th International Workshop on Grid Computing for Complex Problems

GCCP 2008 Proceedings

Associate action to create national Grid initiative:
Making the Grid accessible for electronic science in Slovakia
(Sprístupnenie Gridu pre elektronickú vedu na Slovensku)

October 27 – 29, 2008
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Institute of Informatics, Slovak Academy of Sciences
Dúbravská cesta 9, 845 07 Bratislava, Slovakia
E-mail: {hluchy.ui, dobrucky.ui, peter.kurdel, sebestyenova, sekr.ui}@savba.sk

Proceedings Editors

Ladislav Hluchý
Jolana Sebestyénová
Peter Kurdel
Miroslav Dobrucký

Institute of Informatics, Slovak Academy of Sciences
Dúbravská cesta 9, 845 07 Bratislava, Slovakia
E-mail: {hluchy.ui, sebestyenova, peter.kurdel, dobrucky.ui, }@savba.sk

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Preface

We are pleased to introduce the Proceedings of the 4th International Workshop on Grid Computing for Complex Problems GCCP 2008. The workshop was a three-day combined event for grid users: workshop with invited lectures, plenary discussions, accompanied by course for users of EGEE Grid sites, which was in the scope of EGEE III project – Enabling Grids for E-science 2008-2010, FP7-222667.

The topics of the workshop:
- Distributed Computing and Large Scale Applications
- Computational Chemistry & Material Science
- Grid and Service-oriented Computing
- Grid Workflow and Parallelism
- Astronomy & Astrophysics and High energy Physics
- Grid Tutorials.

The next goal of the workshop was an associate action to create national Grid initiative "Sprístupnenie Gridu pre elektronickú vedu na Slovensku" (Making the Grid accessible for electronic science in Slovakia) which will help to improve the e-Science in Slovakia through the creation of virtual organizations for individual science branches. The associate action aimed to join Grid specialists with complex application users, to provide a medium for the exchange of ideas between theoreticians and practitioners to address the important issues in computational performance and computational intelligence towards Grid computing.

The workshop on Grid Computing for Complex Problems GCCP 2008 has attracted 27 paper contributions and active participations from Austria, Czech Republic, France, Germany, Greece, Hungary, Italy, Ukraine and Slovakia.

Many people have assisted in the success of this workshop. I would like to thank all the members of the Program and Organizing Committees, the workshop Secretariat for their work and assistance of the workshop. I would like to express my gratitude to all authors for contributing their research papers as well as for their participation in the workshop that made our cooperation more fruitful and successful.

Ladislav Hluchý
October 2008
Bratislava, Slovakia

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EGI: Building of a Future Pan-European Grid Infrastructure

Dieter Kranzlmüller

Joh. Kepler University Linz, Austria

Abstract. The European Grid Initiative (EGI) represents an effort to realize a sustainable grid infrastructure in Europe and beyond. Based on the requirements of the user communities and by combining the strength and views of the National Grid Initiatives (NGI), EGI is expected to deliver the next step towards a permanent and common grid infrastructure. The effort is currently driven by the EGI Design Study, an FP7 funded project defining the structure and functionality of the future EGI and providing support to the NGIs in their evolution. The goal is the setup of an organizational model, with the EGI Organization (EGI.org) as the glue between the national efforts, which provides seamless access to grid resources for all application domains.

The DEISA European Supercomputing Ecosystem

Wolfgang Gentzsch

D-Grid coordinator, DEISA project, Regensburg Area, Germany

Abstract. This talk presents an overview of the EU funded project DEISA, the Distributed European Infrastructure for Supercomputing Applications. The key role and aim of DEISA will be to deliver a turnkey operational solution for a future persistent European High Performance Computing ecosystem. Now, the EU FP7 DEISA2 project continues to support and further develop the distributed high performance computing infrastructure and its services. Activities and services relevant for applications enabling, operation, and technologies are continued and further enhanced, as these are indispensable for the effective support of computational sciences in the HPC area. The service provisioning model will be extended from one that supports single projects to one supporting virtual European communities. Collaborative activities will also be carried out with new European and other international initiatives.

Grid Empowered Molecular and Material Science Simulations

Antonio Lagana

Department of Chemistry of the University of Perugia, Italy

Abstract. Molecular and material science is an elective field for computing grid applications. Due to its nanometer nature molecular and material science is able to account for most of the natural and technological structures and processes. For this reason it is an indespensable component of any realistic simulation. Grid empowered Molecular and Material science simulators are being implemented on the production grid of EGEE within the activities of the COMPCHEM virtual organization. They are articulated mainly in three blocks taking care respectively of the construction of an interaction bed built out of electronic structure calculations, the integration of motion equations to determine the time (or space) evolution of the system and of the statistical averaging of the calculated quantities to assemble observable properties. All these steps are being implemented on the computing grid using the appropriate EGEE middleware. The role of the COMPCHEM virtual organization is also evolving from a simple collector of users (who implement their own programs for personal usage) to a coordinator of cooperative work fostering the development of a specific grid community. Examples of the outcomes of all these activities will be illustrated.

Grid computing for Earth Sciences

Monique Petitdidier

CNRS - Centre National de la Recherche Scientifique, Paris, France

Abstract. Earth Science (ES) community has a big potential to exploit nowadays grid infrastructures like EGEE due to their heavy computational simulations. Several members of ES community created a project called DEGREE (Dissemination and Exploitation of GRids in Earth science), which tries to help other ES application developers and users with using such infrastructures. DEGREE also seeks to address the barriers, which stand in the way of a wider uptake of the technology, such as perceived complexity of the middleware, insufficient support for important ES functions and vital additional services. The results will provide feedback to the GRID community and dissemination in the ES community will increase awareness of and involvement with GRID developments. This paper brings an overview of the DEGREE project and its objectives. Other environmental applications can benefit from the roadmap, one of the DEGREE project results.

Grid Technologies for Earth Observation Applications

Nataliia Kussul[1], Ladislav Hluchy[2], Paul Kopp[3], Evgeny Lupian[4],
Andrii Shelestov[1], Sergii Skakun[1], Oleksii Kravchenko[1], Mykola Ilin[1], Yulia Gripich[1]

[1] Space Research Institute NASU-NSAU, Glushkov Ave 40,
03680 Kyiv, Ukraine
inform@ikd.kiev.ua
[2] Institute of Informatics SAV, Dubravska cesta 9,
84507 Bratislava, Slovakia
hluchy.ui@savba.sk
[3] Centre National d'Etudes Spatiales (CNES), 18 avenue Edouard Belin
F-31401 Toulouse Cedex 9, France
paul.kopp@cnes.fr
[4] Space Research Institute (IKI), 84/32 Profsoyuznaya Str,
117997 Moscow, Russia
evgeny@d902.iki.rssi.ru

Abstract. This paper presents a Grid infrastructure that is being developed in the Space Research Institute NASU-NSAU and integrates the resources of several geographically distributed organizations. The use of Grid technologies is motivated by the need to make computations in the near real-time for fast response to natural disasters and to manage large volumes of satellite data. We show the use of the Grid infrastructure for a number of applications that heavily rely on Earth observation data. The applications include: weather prediction, flood monitoring, biodiversity assessment, and crop yield prediction.

Keywords: environmental applications, Earth sciences, research infrastructure, Grid computing, Earth observations.

Introduction

At present, global climate changes in the world made a rational land use, environmental monitoring and prediction of natural and technological disasters the tasks of a great importance. The basis for the solution of these problems is the integrated use of data of different nature: modelling data, in situ measurements, and indirect observations such as airborne and spaceborne remote sensing data.

Satellite observations have an advantage of acquiring data for the large and hard-to-reach territories, as well as providing continuous and human-independent measurements. Such important applications as monitoring and predictions of floods, droughts, vegetation state assessment etc. heavily rely on the use of Earth observation (EO) data from space. For example, the satellite-derived flood extent is very important for calibration and validation of hydraulic models to reconstruct what happened during the flood and determine what caused the water to go where it did [1].

Using the Grid for forest fire front evolution prediction

Nikos Voutsinas[1], Demetrios V. Manatakis[2], Elias S. Manolakos[2,3]

[1]Network Operations Center (NOC)
University of Athens, Panepistimioupolis, Ilisia Athens, 15784, Greece
nvoutsin@noc.uoa.gr

[2]Department of Informatics and Telecommunications
University of Athens, Panepistimioupolis, Ilisia Athens, 15784, Greece
{dmanatak, eliasm}@di.uoa.gr

[3]Greek Research and Technology Network (GRNET)
GRNET, Mesogion Av. Athens, 11527, Greece

Abstract. We present a Grid computing workflow used by the ongoing EC FP6 SCIER (Sensor and Computing Infrastructure for Environmental Risk) project in order to simulate effectively the evolution of a wildfire front line and the temperature field it induces, under different assumptions for the prevailing wind speed and direction in the area affected by the fire. Our simulation results show that using the Grid allows for the efficient evaluation of a large number of alternative scenarios, as needed to estimate accurately and on time the probability that a specific geographical area will be affected by a spreading fire. These probabilities may be updated periodically, as new temperature measurements from a deployed network of distributed wireless sensors become available at the SCIER computing subsystem.

Keywords: Fire spread modeling, temperature field modeling, Grid simulation

1 Introduction

The global warming due to the green house effect and the drought caused by the elevation of the mean temperature have created favorable conditions for frequent forest fire eruptions. During the last few years huge ecological disasters have been caused by wild fires around the globe (e.g. in Greece, California U.S. etc). Many countries are struggling to find ways of dealing with the management of this catastrophic phenomenon. A major issue that needs to be addressed effectively is the prediction to the fire front line i.e. where the front line of a detected fire will be located in the next few hours and with what probability. A significant effort in that direction currently in progress is the SCIER project [1] that is co-funded by the European Commission under the 6th Framework of R+TD. *SCIER* is combining cutting edge ***S***ensing and ***C***omputing ***I***nfrastructures (namely Wireless Sensor Networks and GRID computing) for ***E***nvironmental ***R***isk monitoring and evolution prediction.

A Graphical Frontend for Utilization of Grid
A CharonGUI Use Case

Vítězslav Plšek, Jan Kmuníček, and Martin Kuba

CESNET z. s. p. o., Zikova 4, 160 00 Prague 6, Czech Republic
Masaryk University, Botanická 68a, 602 00 Brno, Czech Republic
{kmunicek, makub, winsik}@ics.muni.cz

Abstract. The Charon Extension Layer (CEL) is a unique generic system for computational jobs and applications management within grid environments. It provides a sophisticated command-line interface that encapsulates all operations required to control a computational job lifetime - it allows users to submit their jobs, check jobs' statuses and get results using only three basic commands. In this paper we present CharonGUI - a graphical user interface built over the original CEL. CharonGUI adopts all advantages of the CEL with their benefits and turns them into a graphical representation. Moreover, CharonGUI simultaneously brings a set of new interesting features that offers additional comfort for the grid end users. CharonGUI is expected to complement the command-line version of CEL allowing users to have both approaches available in parallel.

1 Introduction

Communities of grid environments users have grown markedly in several last years also due to great effort of scientists and developers who work on many utilities for end users to be able to use advantages of grid environments in more effective way. Nowadays, majority of these tools and utilities provides command-line interfaces. They are advanced and effective on one hand but on the other hand they can seem to be far too complex for complete grid newcomers and for users who prefer graphical interface. One of these utilities is Charon Extension Layer (CEL). It is a unique system for computational job management in grid environment, generic enough for wide range of scientific applications. CEL system creates a layer upon the grid middleware and makes the access to the distinct grid infrastructures uniform. Original CEL system has been built as a command line interface and it unifies the provides the way of utilization multiple middlewares.

CharonGUI is an attempt to demonstrate how an existing command-line system can be enhanced in several directions by graphical extension. There was a simple request for creating utility that can help users to manage computational jobs in a more effective way in the beginning of the CharonGUI development. Therefore, the planned graphical tool was supposed to provide at least the features which can ensure minimally the same comfort as the CEL provides for

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Section 1
Distributed Computing and Large Scale Applications

Performance Analysis of Parallel Algorithm for Backtracking

Karol Grondžák, Penka Martincová, and Matúš Chochlík

Faculty of Management Science and Informatics, University of Žilina
Slovak Republic
{Karol.Grondzak,Penka.Martincova,Matus.Chochlik}@fri.uniza.sk
http://www.fri.utc.sk

Abstract. Different versions of backtracking algorithms are often used to solve combinatorial problems. Combinatorial search, as a subset of combinatorial problems, can be defined as a process of evaluating solutions on discrete, finite mathematical structures. This paper deals with the decision making problem algorithms which attempt to find a solution that satisfies all prescribed constraints. General parallel algorithm for backtracking was implemented using message passing library MPICH2. To study the behaviour of the algorithm, problem of finding Hamiltonian path on a specific graph was solved.

Key words: Backtracking, combinatorial algorithm, MPI, MPICH2, search tree, Hamiltonian path

1 Introduction

Combinatorial problems still attract researchers attention. There are still some challenges, despite the fact that recently some large unsolved problems have been solved exactly.

As an example let us mention the Symmetric Traveling Salesman problem, solved for more than 10000 cities by Applegate et al.[1]. The progress in Operations Reasearch is one of the keys which allowed this success. Another key is the advance of the computational means. Instead of using one processor, tens of processors were used to perform the search of the tree.

Another example of successfull application of parallel computation is the soultion of the Quadratic Assignment Problem for up to size 32 ([2]). They employed several thousands of heterogeneous workstations in different institutions to solve the problem.

These results demonstrate that application of parallel paradigm is the way how to achieve speed-up of scientific calculations.

1.1 Backtrack Search

Many optimization and decision making problems are solved using combinatorial algorithms. The main challenge when solving these problems is the size of the set which has to be searched.

MULTICORE PROCESSOR ARCHITECTURE FOR FLIGHT SIMULATOR MODELING

Peter KVASNICA[1], Tomáš PÁLENÍK[2]

[1] Alexander Dubček University in Trenčín, Center of information technologies and Faculty of Mechatronics, Department of Informatics,
Študentská č. 2, 911 50 Trenčín, Slovak Republic,
kvasnica@tnuni.sk
[2] Alexander Dubček University in Trenčín, Faculty of Mechatronics, Department of Informatics,
Študentská č. 2, 911 50 Trenčín, Slovak Republic,
palenik@tnuni.sk

Abstract. The paper deals with the method of computing mathematic model of a flight simulator. This modeling is accomplished by programming tool OpenMP on multicore processor, which is able to create a shared-memory of parallel programming. Mathematical modeling of the simulator system is made by equation depending on the architecture computer system. The important part of this article describes the solving mathematic models by different tolls.

Keywords: SMP, OpenMP, mathematic model, parallel task, flight simulator.

1 INTRODUCTION

The simulation of distributed mathematical model can be created using parallel computer architecture. This parallel computer architecture can be based on the multiprocessors and nowadays especially on the multicore processors. The power of such systems is higher in compare of one processor systems. But it is complicated to synchronize the running processes of the parallel model on the multicore processor.
Symmetric multiprocessing (SMP) is a multiprocessor computer architecture where two or more identical processors are connected to a single shared main memory. SMP systems allow any processor to work on any task no matter where the data for that task are located in memory; with proper operating system support [1]. SMP is one of the earliest styles of multiprocessor machine architectures, typically used for building smaller computers with up to 8 processors.
Larger computer systems might use newer architectures such as NUMA (Non-Uniform Memory Access). Other systems include asymmetric multiprocessing (ASMP).
To simulate the system of differential equations – mathematical models, it is necessary to change the mathematical form of the object. Decomposition of the

Static Job Scheduling in the Grid

Penka Martincová, Karol Grondžák and Matúš Chochlík

Penka.Martincova@fri,uniza.sk, Karol.Grondzak@fri.uniza.sk,
Matus.Chochlik@fri.uniza.sk

Abstract. The abstract should summarize the contents of the paper and should contain at least 70 and at most 150 words. It should be set in 9-point font size and should be inset 1.0 cm from the right and left margins. There should be two blank (10-point) lines before and after the abstract. This document is in the required format.

Keywords: Grid computing, grid scheduling, Java simulation

1 Introduction

Grid computing is intended to offer an easy and seamless access to remote resources. The importance of grid computing can be seen by the attention it gained recently in research and industry support. The scheduling task of allocating these resources automatically to user jobs is an essential part of a grid environment.

Grid scheduling is a process of scheduling applications over grid resources. A grid scheduler is different from local scheduler in that a local scheduler only manages a single site or cluster and usually owns the resource. A grid scheduler is in charge of resource discovery, grid scheduling (resource allocation and task scheduling), and job execution management over multiple administrative domains. This paper concerns local grid scheduling and presents the results of our research of grid scheduling algorithms.

2 Scheduling Architecture

The proposed architecture (Fig.1) is suitable for computational grid, which consists of community resources e.g. university or company resources. Resources belong to different administrative domains, which mean that there are different scheduling policies. The users can submit their jobs to a grid through one central point.

The scheduling system has two levels, which means that scheduling is done in two steps by two different schedulers – global broker and local scheduler. Two algorithms for global scheduling were used – Firs_Suitable (FS) and First_Free (FF).

High-resolution visualisation in cluster environment

Branislav SOBOTA, Ján PERHÁČ, Csaba SZABÓ, Štefan SCHRÖTTER

Department of Computers and Informatics
Faculty of Electrical Engineering and Informatics
Technical University of Košice
Letná 9, 040 01 Košice, The Slovak Republic,
Branislav.Sobota@tuke.sk
Jan.Perhac@tuke.sk
Csaba.Szabo@tuke.sk
Stefan.Schrotter@tuke.sk

Abstract. The paper deals with the photorealistic visualisation in cluster environment. The parallel raytracing is the method how to compute 3D scene in photorealistic quality in a cluster computer environment. The first part contains description of the photorealistic visualisation techniques and rendering process. The computation model of parallel raytracing and its implementation is described in this part too. Finally, the second part describes some multi/big-screen visualisation solution. In conclusion are presented some examples of visualisation

1 Introduction

Imagines, ideas, design, construction, realisation, production, benefits, marketing, satisfied customers - there are points of industrial production. It is very important to show these points before production, before money investment, before realisation appropriate goals. One way for these goals achievement is computer modelling and visualisation. During the past several years, high-performance and feature-rich PC graphics interfaces have become available at low cost. This development enables us to build clusters of high-performance graphics PCs at reasonable cost. Then photorealistic rendering methods like raytracing or radiosity can be computed faster and inexpensive. Raytracing is one of computer graphics techniques used to produce accurate images of photorealistic quality from complex three-dimensional scenes described and stored in some computer-readable form. It is based on simulation of real-world optical processes. One great disadvantage of such techniques is that they are computationally very expensive and require massive amounts of floating point operations. Parallel raytracing takes advantage of parallel computing, cluster computing in particular, to speed up image rendering, since this technique is inherently parallel. The use of clusters for computationally intensive simulations and applications has lead to the development of interface standards such as the MPI (http://www.mpi-forum.org) and OpenPBS (http://www.openpbs.org).

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Section 2
Computational Chemistry & Material Science

Trying to model the dissipative processes inside a material using a universal constitutive equation with internal damping for fully coupled thermal-structural analysis

Ladislav Écsi[1] , Pavel Élesztős[1], Viera Šipková[2] , Miroslav Dobrucký[2], Ján Astaloš[2]

[1] Institute of Applied Mechanics and Mechatronics, Faculty of Mechanical Engineering,
Slovak University of Technology in Bratislava, Námestie slobody 17
812 31 Bratislava, Slovakia
ladislav.ecsi@stuba.sk

[2] Institute of Informatics, Slovak Academy of Sciences
Dúbravská cesta 9
845 07 Bratislava, Slovakia
viera.sipkova@savba.sk

Abstract. Dissipative processes that take place outside thermal equilibrium play an important role in a material behaviour. One of such a dissipative process is an internal damping of a material which can essentially affect the construction behaviour under mechanical loadings. Contemporary theories don't pay too much attention to the problem and the induced thermo-mechanical processes are not sufficiently understood. In the presented paper a universal constitutive equation with internal damping is presented. The model adapts the idea of a spring-dashpot system connected in parallel for continuum utilizing appropriate deformation measures, which are independent of a rigid body motion and thus it presuppose more accurate numerical simulation. Although the constitutive equation is primarily intended for materials under dynamic and cyclic loadings, it can also be helpful in understanding the thermo-mechanical processes inside a construction material under static loadings. In the presented paper the equation application is shown on cross-shaped specimen under biaxial tension using fully coupled thermal-structural finite element analysis (FEA).

1 Introduction

Dissipative processes that take place in material outside thermal equilibrium play an important role in deformable body behaviour. One such dissipative process is an internal damping which can essentially affect the construction behaviour. Contemporary theories don't pay too much attention to the problem and the induced thermo-mechanical processes are not sufficiently understood. In the presented paper, a universal constitutive equation with internal damping is presented using a fully coupled thermal-structural analysis with one of our latest variational formulation of conservation of energy [6]-[8]. The model adapts the idea of a spring-dashpot system

Material tension stress-strain curve determination via inverse analysis using finite element method in computational Grids – Implementation of the mathematical model

Ladislav Écsi[1] , Pavel Élesztős[1], Viera Šipková[2] , Miroslav Dobrucký[2], Ján Astaloš[2]

[1] Institute of Applied Mechanics and Mechatronics, Faculty of Mechanical Engineering, Slovak University of Technology in Bratislava, Námestie slobody 17
812 31 Bratislava, Slovakia
ladislav.ecsi@stuba.sk

[2] Institute of Informatics, Slovak Academy of Sciences
Dúbravská cesta 9
845 07 Bratislava, Slovakia
viera.sipkova@savba.sk

Abstract. Tensile stress-strain curve of a material represents a significant material property for elastic-plastic finite element analysis (FEA). The curve can easily be determined in the framework of small strain elastoplasticity using a standard uniaxial tensile test. The accurate stress-strain curve determination is almost impossible, when in the specimen large deformation takes place locally during notch development. In this paper an alternative method of the aforementioned material characteristic determination is presented using an inverse analysis in Grid computing environment. The idea is based on a repeated finite element analysis (FEA) execution varying the slope of a multilinear stress-strain curve until the best results are reached. In the numerical simulation a finite element code utilizing the updated Lagrange formulation was used, which was run on a uniprocessor computer in order to study the convergence and accuracy of the finite element (FE) code. In this paper first results of an ongoing research project are presented.

1 Introduction

The majority of contemporary engineering theories for mathematical description of physical phenomena were derived using a phenomenological approach which relates different empirical observations of phenomena to each other in a way which is consistent with fundamental theory, but is not directly derived from theory. In other words the phenomenological theory expresses mathematically the results of observed phenomena without paying detailed attention to their fundamental significance. A typical representative of the phenomenological theory is the theory of elasto-plasticity, which describes the plastic behaviour of a material mostly via a stress-strain controlled yield surface. As a result the stress-strain curve accurate determination is essential for the success of elastoplastic numerical simulations [1]-

Computational "virtual laboratory" tools for biomolecular and drug design

István Komáromi[(1)], László Tóth[(1)] and Tibor Kožár[(2)]

[(1)]University of Debrecen, Medical and Health Center, Clinical Research Center, Debrecen, Hungary
[(2)]Department of Biophysics, Institute of Experimental Physics, Slovak Academy of Sciences, 04001 Košice, Slovak Republic
komaromi@med.unideb.hu
tibor@saske.sk

Abstract. Although the concept of virtual laboratories (VL) was well established several years ago, the building and realization of target-oriented VLs with user-friendly environment is still in its infancy. VLs have cardinal importance for several fields, especially for those, where computer-aided design can speed up the discovery and development (D&D) process. Drug design and nanodesign are typical examples falling in this area. VLs are not intended to replace real laboratories, the intention of VLs is to help and guide experimental work. International collaborations are one of the basic prerequisites for efficient VLs. Our effort culminated in building of a molecular modeling related VL, thus allowing carry out delicate tasks as virtual screening and pharmacophore modeling. Overall, this will provide us additional level for data sharing and information integration.

Key words: Virtual laboratory, high-throughput computing, molecular modeling, computer-aided molecular design, molecular dynamics simulations

1. Introduction

The concept and the definition of the "Virtual Laboratory" (VL), is as follows *"an electronic workspace for distance collaboration and experimentation in research or other creative activity, to generate and deliver results using distributed information and communication technologies"* [1]. Although the referred definition is clear, the building and realization of a target-oriented VL with user-friendly environment is still not an easy task. VLs have cardinal importance for several fields, especially for those, where computer-aided design can speed up the discovery and development (D&D) process. Drug design and nanodesign are typical examples which fall into this area. Computational VL can facilitate the D&D process to proceed faster and more efficiently in comparison to the standard protocols of the wet laboratories. Although the importance of the standard laboratories is unquestionable and VLs are not aimed to replace them, the intention of VLs is to help and guide experimental work. Filtering out molecules with unwanted ADME/T properties is a particular example for economic impact of VL on the D&D cycle. Our effort, in

Parallelization of algorithms of stochastic reaction kinetics

Zdenko Turčan[1], Jozef Uličný[1]

[1] Faculty of Science, P.J.Šafárik University,
Jesenná 5, 040 01 Košice, Slovakia
{zdenko@turcan.sk, ulicny@bioflab.upjs.sk}

Abstract. Stochastic algorithms for simulation of reactive kinetics based on ideas of D. Gillespie have become more popular with increasing speed of computers, allowing simulations of increasingly complex systems, including those encountered in simulations of biomolecular interaction networks. Iterative refinement of computational models created within the frame of systems biology requires extreme computer performance, unavailable for single, even very performant computer. The time necessary for such computations can be significantly shortened by proper choice of algorithm parallelization. In the present contribution we propose new algorithm based on stochastic Gillespie algorithm, suitable for the parallel implementation on current distributed computational architectures. The essence of the algorithm consists in controlled-phase mixing of reactants within a split-reaction system, where the computational problem is decomposed along reaction boundaries. The algorithm shows promissing speedup against serial version.

Keywords: Stochastic kinetics, molecular interaction networks

1 Introduction

There are many intracellular processes represented by network of coupled reactions involving molecular species at very low concentrations. Often these reactions play decisive role at various life processes. Simulation of kinetics of such reactions involving low number of molecules using traditional continuous deterministic models is not adequate, since it does not take into account the discrete nature of the concentration and the random character of reactions. The application of traditional, ODE-based simulations leads sometimes even to serious qualitative disagreement between the stochastic and deterministic kinetic models [1]. In such cases, the simulations based on stochastic reaction kinetics is the preferred methodology. With the growing experimental possibilities of single molecule detection and the increased knowledge about the molecular interaction networks, the stochastic kinetics approach is becoming more popular, as evidenced by the exponential growth of scientific

Section 3
Grid and Service-oriented Computing

Establishing Semantic Annotation and Execution of the Text-mining Services

Marian Babik[1], Martin Sarnovsky[2], Zoltan Durcik[2] *

[1] Department of Parallel and Distributed Computing, Institute of Informatics, Slovak Academy of Sciences
[2] Center for Information Technologies, Technical University, Kosice
Marian.Babik@saske.sk, Martin.Sarnovsky@tuke.sk, Zoltan.Durcik@tuke.sk

Abstract. Recently, there are several proposals to combine text mining and semantic web technologies. The main aim is to leverage the existing advances in the Semantic Web to establish an automated framework for mining the existing relational and Web-based data. Semantic description of text mining service should be a key-enabling technology for such frameworks by providing methods for automated discovery, composition and execution of the complex text mining processes. In this paper we provide an overview of our effort towards establishing an automated execution of a set of text mining services by initially providing a semantic description of services in OWL-S and later describing a corresponding mapping of OWL-S processes to Petri-net based workflow and BPEL.

1 Introduction

In the presented paper we introduce a semantic model intended to describe text mining web services, whereby the semantic information about the functional models and data can be utilized to construct the resulting executable workflow. When text mining tasks are represented as a web services, such approach opens ways to a plenty of various possibilities for building the text mining scenarios that can be represented as a workflows. The paper presents two various approaches to workflow execution, the first one based on Perti-Nets and BPEL. BPEL is very well supported by the software vendors as the choice for the execution of the web services, but on the other hand, it is not designed for addressing the challenges of the semantic web. Our approach is based on models of the semantics of the system, that are expressed in OWL-S and the execution is conducted in BPEL standard.

2 Web Ontology of Services (OWL-S)

OWL-S is an ontology-based approach to the semantic web services [1]. The structure of the ontology consists of a service profile for advertising and discov-

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Secure Management of Crisis Situations Using Mobile Code in Untrustworthy Distributed Computing Environment

Zoltán Balogh, Ivana Budinská, Branislav Šimo, Ladislav Hluchý

Institute of Informatics, Slovak Academy of Sciences,
Dúbravská cesta 9, 845 07 Bratislava, Slovakia
{zoltan.balogh, ivana.budinska, branislav.simo, ladislav.hluchy}@savba.sk

Abstract. This article deals with a challenge of secure execution of processes in untrustworthy distributed computing environment. Our solution to this problem is based on mobile code, which would be executed in a secure trusted hardware module. This module could be connected to any computational unit through a common interface. The code mobility is envisaged to be implemented as mobile services designed based on patterns known from the field of multi-agent systems. The article was inspired by the need for secure execution of processes for management of crisis situations. We also present a generic architecture for untrustworthy distributed environment for which we plan to implement our proposed solution. This article is a "work in progress".

Keywords: mobile code, agents, web services, trusted platforms.

1 Introduction

Recently there still exist data and computation security matters, which are not satisfactory solved. These problems mostly relate to distributed nature of computation execution and data processing. Many security problems are already solved such as secure communication tunneling through encryption or authorization and authentication using asymmetric cryptography. Security challenges for distributed computing can be generally divided into the following two groups: privacy and trust. Both of these security areas can be solved either on the side of clients (initiators) or on the side of executors (servers). In chapter 2 of this article we mainly discuss the trust and privacy of computation and data processing on the side of executor (server).

Communication, security and accessibility of information are the key factors during management of crises situations. Secure communication is a technological challenge which must be solved in a complex manner. It is important to solve interconnection of multiple communication channels but also protection from misuse of information and communication flows. In this article we present architecture of a distributed system for secure execution of mobile code implemented as mobile services in untrustworthy computing environment using secure hardware platform module for the management of crises situations.

SLA-based monitoring of quality in dynamic food supply-chains

Eugen Volk, Ansger Jacob

Extended Abstract

As food supply chains became more dynamic today and become in future, the problem of monitoring of quality of food during the production, transformation process and especially transport becoming increasingly important.

One major difficulty to overcome in order to enable secure monitoring of quality in dynamic supply chains consists of sharing the information about food trade units between supply chains partners in fast, secure and easy way, enabling access to contracted partners only for each particular supply chain.

Fortunately there exists such a platform called GTNet® [2] which allows sharing of information about trade units in such a way and enables tracking and tracing of trade-units in static supply chains. Based upon such a platform, we introduce the "AgroGrid Framework" – developed within the Business Experiment AgroGrid in EU research project BEinGRID [1] - for monitoring and evaluation of food quality in dynamic supply chains.

In order to meet the specific requirements to monitor and evaluate quality of foods in dynamic supply chains, the solution introduced and to be implemented in AgroGrid is built on the development of the VO-Management, SLA-Monitoring and SLA-Evaluation services, enabling monitoring and evaluation of bipartite SLAs between contracted parties.

A negotiated and contracted SLA between two parties in AgroGrid contains SLA-terms defining not only the amount, quality, and price of food products to be delivered, but also environmental conditions, under which they are stored and shipped. These SLA-terms define monitoring-metrics which are used to monitor the quality and especially environmental condition of incoming, stored or shipped food trade units. Every supply-chain partner publishes the monitoring data about incoming, stored or shipped food trade unit in his/her local-database, allowing access only to the buyer of the food trade unit, after receiving the trade-unit-id (which serves as a security token) shipped with the food trade unit. The access to his/her local database is managed by each partner locally, based on the GTNet® access mechanisms already available.

As a consequence of restricted access, the approach proposed in AgroGrid is based on the hierarchical SLA-Monitoring and SLA-Evaluation, deployed within each partner of the supply-chain separately. The SLA-Monitoring service within each partner query GTNet® for the unique trade unit-id (corresponding to the security token) shipped with the food trade unit. As a result, the monitoring data from the database of the product provider or logistic company, which delivered the product, is returned. The monitored data are evaluated against the SLA-terms contracted in the SLA. If

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Section 4
Grid Workflow and Parallelism

Visual support of workflow composition involving collaboration

Peter Bartalos, Ivan Kapustík, Viera Rozinajová

Institute of Informatics and Software Engineering, Faculty of Informatics and Information Technologies, Slovak University of Technology in Bratislava
Ilkovičova 3, 842 16 Bratislava, Slovakia
{bartalos,kapustik,rozinajova}@fiit.stuba.sk

Abstract. In this paper we deal with visual support of workflow composition involving user collaboration. Our aim is to present some ideas how such a support should be realized using a multiuser workflow editor. The aim is to create a workflow by multiple users. We propose a solution how to avoid inconsistencies in the workflow during its editing arising from the multiple user manipulation with a shared object – workflow.

1 Introduction

Nowadays a lot of companies operating in different domains need to adapt and restructure their business processes often. To support this requirement workflow systems are usually employed.

The array of domains where workflow systems can take place is wide. Their common characteristics are:

- workflow adaptation: flexible reaction to the changes of real processes which are realized by workflows, without the need of system reimplementation
- dynamic workflow composition: the desired goal and the world may change during the composition and execution of workflows
- user interaction: users should be seen as parts of the system which control the composition and execute some operations
- different, distributed users: in the environment there are distributed different kind of users which must collaborate to make decisions

From these characteristics it comes out that a workflow system has to support the following activities:

- workflow composition support
- group work and collaboration support
- composition and execution process monitoring

Workflow composition is currently being a popular way how to deal with complex goals requiring execution of several related operations. Web and GRID services bring a convenient technology wrapping these operations into standardized, remotely invocable, distributed software systems [1, 5, 7, 8, 11]. The aim of

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A Survey of Approaches to Automatic Workflow Composition[1]

Branislav Simo

Institute of Informatics, SAS
branislav.simo@savba.sk

This paper presents the survey of the existing approaches to the automatic workflow composition. The individual tasks of the workflow can be web or grid services, (grid) jobs or some general activities. The actual process and protocol for the invocation of the workflow tasks is not important.

Introduction

A workflow composition problem is just another name for the planning problem studied in the artificial intelligence, i.e. trying to decide what actions to use to achieve some set of objectives. Automated Planning [1], as an area of artificial intelligence, deals with finding a sequence of steps to apply to the state of the problem domain in order to reach a predefined goal, starting from the known initial state. In contrast to an ordinary problem-solving using standard search algorithms, automated planning tries to design algorithms that would more efficiently handle large problems.
Workflow composition approach can be divided into two main groups: a process oriented composition and data oriented composition. In the process oriented composition the goal is specified by the global behavior, such as desired conversations or process flow. Data oriented composition uses a goal specified by the final result, such as a data to be produced or state to be reached.

Planning Problem

Planning itself is quite old discipline. The first major planning system was STRIPS [2], developed in 1971. This system gave later the name to the formal language used to represent the actions for the system. The variants of the language have been then used in the majority of the planning systems.

A planning problem is specified by three components: a system or domain where the planning takes place, an initial state and a goal. The system is usually represented as a

[1] This work was supported by the Slovak national project SEMCO-WS APVV-0391-06 and EU FP7 project Secricom SEC-2007-4.12-04.

Towards an Advanced Distributed Computing

V. Šipková and M. Dobrucký

Ústav Informatiky, Slovenská Akadémia Vied
845 07 Bratislava, Dúbravská cesta 9

Abstract. In recent years grids and peer-to-peer networks have gained popularity as favourable platforms for the next generation of parallel and distributed computing. Although grid computing was conceived in research organizations to support initially compute-intensive scientific applications, enterprises of all types are beginning to recognize this technology as a foundation for the flexible management and use of their internal resources. The rapid enhancements in web services technology, semantic technology, and standards, have provided an evolutionary path from the architecture of the early grid to the advanced *Cyberinfrastructure* that will constitute a standardized, general-purpose, service-oriented, knowledge, enterprise-class Grid of the future. This paper[1] outlines the latest technology trends encountered in distributed computing, with particular emphasis on grids, services, and the envisioned utility-based Cloud computing, which have a massive impact on the development of complex applications in both the scientific and business scene.

1 Introduction

In recent years grids and peer-to-peer high-speed networks have gained popularity as favourable platforms for the next generation of parallel and distributed computing. Although grid computing was conceived in research organizations to support initially compute-intensive scientific applications, enterprises of all types are beginning to recognize this technology as a foundation for the flexible management and use of their internal resources enabling them to better meet business objectives. It has become clear that there is a considerable overlap between the goals of grid computing and benefits of the emerging Service Oriented Architecture used in common by business and industry. The rapid enhancements in the web services technology, semantic technology, and standards, have provided an evolutionary path from the architecture of the early grid to the advanced *Cyberinfrastructure* that will constitute a standardized, general-purpose, service-oriented, knowledge, enterprise-class grid of the future supporting the collaborative high-performance computing and data sharing, as well as the adaptive enterprise, and the envisioned utility-oriented *cloud* computing, which will allow users and developers to utilize services without knowledge of, expertise with, and nor control over the technology infrastructure. Cloud computing is a general concept [7, 8] that incorporates the SOA (Service Oriented Architecture), SaaS (Software-as-a-Service), PaaS (Platform as a Service), Outsourcing, Virtualization, Web 2.0, and other recent known technology models, where the common theme is reliance on the

[1] The content of the paper was elaborated pursuant to the several documents presented by experts in grid computing on conferences, in journals, and as Web Blogs.

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Section 5
Astronomy & Astrophysics and High energy Physics

Extended modeling of the Oort cloud formation from the initial proto-planetary disc.

T. Paulech[1], M. Jakubík[2], L. Neslušan[2], P. A. Dybczyński[3], and G. Leto[4]

[1] Astronomical Institute of the Slovak Academy of Sciences, Dúbravská cesta 9, 84504 Bratislava, Slovakia
astrotom@savba.sk

[2] Astronomical Institute of the Slovak Academy of Sciences, 05960 Tatranská Lomnica, Slovakia
mjakubik@ta3.sk; ne@ta3.sk

[3] Astronomical Observatory of the A. Mickiewicz University, Słoneczna 36, 60-286 Poznań, Poland
dybol@amu.edu.pl

[4] Catania Astrophysical Observatory, Via Santa Sofia 78, I-95123 Catania, Italy
gle@astrct.oact.inaf.it

Abstract. *Aims* : A fraction of small bodies from the once existing proto-planetary disc were ejected, by the giant planets, to large heliocentric distances and became to constitute the comet Oort cloud. Considering four models of initial proto-planetary disc, we attempt to roughly map the dependence between the initial disc's structure and some properties of the Oort cloud.

Methods : We use the resultant data of our previous simulation of the Oort cloud formation (Dybczyński P.A. et al. 2008, A&A, 487, 345) for the first 2 Gyrs. New disc models, consisting of a set of representative test particles, are created subtracting a fraction of the particles in a way to obtain the required heliocentric-distance distribution. Specifically, we focus on the situations, in which a part of the particles is assumed to be already spent in the previous process of the giant planet formation. We omit the particles, from an original smooth profile, in the regions adjacent to the planet orbits. With the reduced data, we construct the comet cloud characteristics we are interested in.

Results : At first, we find that it is difficult to construct the proto-planetary disc if the following three assumptions have to be simultaneously valid: (i) the material in the vicinity of planet orbits is assumed to be already spent for the planet formation, (ii) the amount of heavy chemical elements in the Jupiter and Saturn is as high as currently accepted (≈ 20 and $\approx 29\,M_\oplus$, respectively), and (iii) the total mass of the minimum-mass solar nebula is assumed to be lower than $\approx 0.05\,M_\odot$. The behaviour of the Oort cloud formation does not crucially depend on the initial disc model. Some differences in its structure are obvious: since the cloud is known to be filled mainly by the Uranus and Neptune, the efficiency of its formation is higher when the initial amount of particles in the Uranus-Neptune region is relatively higher. A significantly large number of Jupiter Trojans in our simulation appears, however, only in the case of the initially non-gapped disc, with the particles situated also close to the Jupiter's orbit.

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Visualization tool for Grid-based applications

Eva Pajorová[1], Marián Jakubík[2], Luboš Neslušan[2], Peter Slížik[1], Ladislav Hluchý[1]

[1]Institute of Informatics, Slovak Academy of Sciences
Dúbravská cesta 9, 845 07 Bratislava, Slovakia
[2]Astronomical Institute, Slovak Academy of Sciences
059 60 Tatranská Lomnica, Slovakia

utrrepaj@savba.sk, mjakubik@ta3.sk, ne@ta3.sk,
peter.slizik@savba.sk, ladislav.hluchy@savba.sk

Abstract. Grid-based applications that generate visualization outputs on-the-fly require a unified application framework. That motivates the research of software architectures that would be optimal in this kind of applications. The computations that generate data for visualization run in high-performance Grid environment. Visualization outputs are displayed in a computationally limited environment of an ordinary PC or a graphical station, or a special graphical device. For this reason, it makes sense to split up applications supporting the Grid-based visualization of partial and final results of simulations into three phases. We have tried to come up with a unified framework for Grid tools and control scripts. The aim of this article is to present one of these tools – the Visualization Tool and discuss its integration into the Grid infrastructure, or, more specifically, its integration into the proposed framework. Our case study was based on the application. It is an astronomical simulation program, which is designed to integrate a set of mutually gravitationally interacting bodies together with a group of test particles which feel the gravitation influence of the massive bodies but do not affect each other or the massive bodies [1].

Key words. Grid application, visualization tool, Oort cloud

1 Introduction

The tools of visualization tools of the running Grid applications rendering a monitoring of the intermediate or final results in the client application were based on more applications computed in our institute, or applications solved in some of international projects[6]. One of them is an astronomical simulation program, which is an astronomical simulation program, which is designed to integrate the motion of a set of test particles gravitationally influenced by the giant planets, Galactic tide,passing star. The test particles are influenced by the smasive bodies, but do not affect each other or the masive bodies. The simulation program is developed using the standard MERCURY package for the integration of orbits [1]. There are some related works concerned with the problems to visualize the applications in Grid environment in which computations are exceedingly long. One of them is GRID visualization Kernel developed in the Johannes. Kepler Univ. Linz in Austria [4],[7]. There is an

Using the GRID Infrastructure for Local Hadronic Calibration of the Experiment ATLAS Calorimetric System.

Pavel Šťavina[1], Tibor Ženiš[1], Pavol Stríženec[2], Pavol Bartoš[1], Lucia Báťková[1], Pavol Federič[1], Viliam Pažma[1], Martin Pécsy[1], Július Vanko[1], and Matej Zagiba[1]

[1] Faculty of Mathematics, Physics and Informatics, Mlynská dolina, 842 48 Bratislava
[2] IEP SAS, Watsonova 47, Košice

Abstract. Calibration of the experiment ATLAS calorimetric system requires lot of data and therefore a large scale simulation and data analysis jobs were performed. The mentioned jobs utilize extensively all existing grid infrastructure. Since the beginning of the official production in 2006 more than 4.5 millions production jobs were successfully finished and more than 1 PetaByte of data was produced by the VO ATLAS. For the largest grid centers the average data transfer can reach more than 100 MB/s.

1 Calibration of the Experiment ATLAS Calorimetric System

The ATLAS experiment is the general purpose experiment in a field of particle physics. The main physics goal of the experiment is to discover Higgs boson if it exists and to investigate the structure of Higgs sector. The other goals are the precise measurements of the top quark physics, discovery of SUSY particles and searching for any other new physics beyond the Standard Model.

To reach the desired goals very fine adjusting of all sub-detectors is required. One of the crucial sub-systems is the calorimetric system (see Figure 1) [1], [2]. Precise calibration of this system is inevitable for successful operation of the experiment. The calibration of such complex system is in generally very complicated task due to the heterogeneous structure and complicated readout electronics of the system. Nevertheless taking into account the LHC luminosity and the nature of the physics at LHC without very precise calibration it is almost impossible to reach the desired goals.

One of the possible approaches for the global calorimetric system calibration is so called *local hadronic calibration*.

The basic idea is to obtain for each readout cell the optimal energy assignment, i.e. to get locally the best estimate of deposited energy. This guarantees that the calibration is not biased towards some specific interpretations of the given event, but provides the best possible measurement of energy for all physics hypotheses. Given the fact that the ATLAS calorimeter is non-compensating, a

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ATLAS on Slovak GRID

Tibor Ženiš[1], Pavel Šťavina[1], Pavol Stríženec[2], Pavol Bartoš[1], Lucia Báťková[1], Pavol Federič[1], Viliam Pažma[1], Martin Pecsy[1], Július Vanko[1], and Matej Zagiba[1]

[1] Faculty of Mathematics, Physics and Informatics, Mlynská dolina, 842 48 Bratislava
[2] IEP SAS, Watsonova 47, Košice

Abstract. ATLAS – one of experiments on LHC – will produce enormous amount of data about 1 PB each year. Reconstruction of all stored data requires 10000 CPUs. Analysis is not possible by conventional way a distributed computing must be used. Project LHC Computing Grid was created to support experiments on LHC. Two laboratories of Slovakia participate in ATLAS. Both institutions actively cooperate with LCG. Dedicated computer farms were built and the farms are used to compute ATLAS jobs.

1 Introduction to Experiment

The Large Hadron Collider (LHC) is a particle accelerator of the European Organization for Nuclear Research (CERN)[2]. The LHC is the world-s largest and highest-energy particle accelerator. The collider is contained in circular tunnel with a circumference of 27 km (Fig. 1). The accelerator will boost the energy of protons to 7 TeV. The protons will be formed to 2808 bunches. The bunches of two contrarotating beams will collide every 25 ns. One of the LHC's intersection points is occupied by the ATLAS experiment.

1.1 Description of ATLAS

ATLAS (A Toroidal LHC ApparatuS) is a general-purpose particle detector[2]. ATLAS is 46 m long 25 m in diameter and weighs 7000 tonnes (Fig. 2). The project involves 2000 scientists at 165 institutions in 35 countries. ATLAS is intended to investigate many types of physics that might become detectable in the collision at LHC. The most important goals of ATLAS are Higgs boson - the missing piece of the Standard Model, CP-violation, top quark. ATLAS has the potential to discovery signature of physics beyond the Standard Model. Some kinds of the new physics are microscopic black holes, technicolour, supersymmetry.

ATLAS is designed to capture particles born in collisions of protons accelerated by LHC. A lot of created particles are unstable and decay. ATLAS records the path of particles passing layers of detectors (Semi-Conductor Tracker, Transition radiation tracker, Muon spectrometer) and energy of particles absorbed inside calorimeters. ATLAS has over 160 million readout channels. The detector

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Tutorials and Courses

Developing and executing complex applications on production grids with P-GRADE Portal

Robert Lovas

MTA SZTAKI Computer and Automation Research Institute Hungarian Academy of Sciences, Budapest, Hungary

Abstract. P-GRADE Portal provides an intuitive and service rich graphical environment for the development, execution and monitoring of grid application. Tools of P-GRADE act as extensions of the gLite and Globus middleware services and implement user centric services that ease the management of complex data and task parallel applications on these platforms.

The tutorial will demonstrate the services of P-GRADE Portal, including the compiler, file manager, workflow and parameter study manager, grid application editor and certificate manager tools. For further information on the open source P-GRADE Portal please visit http://www.portal.p-grade.hu.

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Training course (including tutorial) for Grid users and application developers

Miroslav Dobrucký, Viera Šipková, Viet D. Tran

Institute of Informatics, Slovak Academy of Sciences, Bratislava

Participants of the hands-on tutorial should have a Linux user background and must bring their own laptops with an ssh client (e.g. PuTTY).

Programme schedule:

- Introduction to Grid and EGEE infrastructure (15-20min / Dobrucký)
- Grid security and getting the access to the Grid (15-20min / Dobrucký)
- Grid computing - principles of parallel and distributed computing (15-20min / Šipková)
- Development of Grid applications (15-20min / Tran)
- Overview of the Grid middlewares and high-level tools (15-20min / Tran)
- gLite middleware (30min / Šipková)

Hands-on tutorial
Basic practicals with the gLite middleware (security, job, and data management) using both the Command Line Interface and Genius portal. (1h 30min)

Presentations

Hardware Platform Designed for GRID Computing Applications and High Performance Computing Environments

Jan Ostrochovský

Hewlett-Packard Slovakia, Bratislava

Abstract. The HP ProLiant BL2x220c provides extreme density for customers where compute performance and power efficiency are at a premium. With up to 32 server nodes per enclosure each capable of supporting 2 Quad-Core CPUs and up to 32GB of RAM, the BL2x220c scales to provide up to 1024 cores and 4TB of RAM per 42U rack. Two Gigabit Ethernet ports are provided per server node as standard with options available to upgrade to 10Gbit Ethernet or Infiniband for high performance, low latency interconnects. The BL2x220c provides industry leading compute density and unmatched power efficiency.

Sponsor

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