

2nd International Workshop on Grid Computing for Complex Problems

GCCP 2006

BOOK OF ABSTRACTS

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A message from the general chair of GCCP 2006

Welcome to the International Workshop on Grid Computing for Complex Problems GCCP 2006. The workshop is a three-day combined event for grid users: workshop with invited lectures, plenary discussions, accompanied by course for administrators of EGEE Grid sites, which is in the scope of EGEE II project – Enabling Grids for E-science 2006-2008, INFOS-RI-031688.

The topics of the workshop are:

- Grid and Cluster Computing
- High Performance Distributed Computing and Large Scale Simulation
- Use of Knowledge and Semantics in Grid and Cluster Computing
- Intelligent and Knowledge oriented Technologies (in the conjunction with WIKT 2006 1st Workshop on Intelligent and Knowledge oriented Technologies).

The next goal of the workshop is 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 aims 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 has attracted 29 paper submissions from Czech Republic, Ukraine and Slovakia. This book is a collection of abstracts of papers from International Workshop on Grid Computing for Complex Problems – GCCP 2006. Workshop's papers will be published after the workshop as edited proceeding.

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 to the workshop.

Ladislav Hluchý
November 2006
Bratislava, Slovakia

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Invited lectures

A Generic Grid Environment for Central Europe

A Study of Rotaxanes Behavior

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Abstract. Grid computing is currently seen as one of the key ingredients for fulfilling up to date science requirements. Requests for extreme computing power together with large storage capacities led to forming a research infrastructure available for everyday scientific work provided by computing/data Grid. This article describes VOCE - Virtual Organization for Central Europe - a production grid infrastructure available for researchers from the Central European region and its successful utilization for accomplishment of large scale computing challenge - detailed investigation of behavior of supramolecular complexes - rotaxanes.

High Performance Methods for Regional Weather Forecasting

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Abstract. A model and computational method is presented for the high performance forecasting regional meteorological processes. Relying on "unilateral influence" relationship of macro- and mesoscale models it suggests avoiding the Cauchy problem in the atmospheric model and replacing it by a boundary-value problem with specific interpolation technique that has a number of advantages of computational efficiency and good suitability for parallelization. The method and its parallel implementation on multiprocessor cluster architecture are considered in this paper. It has been tested by the Hydro-meteorological Centre of Ukraine and successfully applied in regional short- and middle-term weather forecasting for regions of Ukraine.

To modelling of distributed parallel algorithms

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Abstract.

Parallel computing and distributed computing have traditionally evolved as two separate research disciplines. Parallel computing has addressed problems of communication-intensive computation on highly-coupled processors while distributed computing has been concerned with coordination, availability, timeliness, etc., of more loosely coupled computations. Current trends in high performance computing (HPC) and grid computing are to use networks of workstations (NOW) as a cheaper alternative to traditionally used massively parallel multiprocessors or supercomputers suggest the advantages of unifying these two disciplines. To the performance uprising of all common reachable computer means (personal computers, minicomputers, supercomputer etc.) dominate implementation of various forms of parallel principles. In such parallel systems individual workstations are connected through widely used communication standard networks and co-operate to solve one large problem. Each workstation is threatened similarly to a processing element as in a conventional multiprocessor system. To make the whole system appear to the applications as a single parallel computing engine (a virtual parallel system), run-time environments such as PVM (Parallel virtual machine), MPI (Message passing interfaces) are often used to provide an extra layer of abstraction.

Track 1
Grid and Cluster Computing

A conception of parallel graphic architecture for large graphical data volume visualization in grid architecture environment

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Abstract. The paper describes a part of the virtual reality system PROLAND, that was developed on the Department of Computers and Informatics FEI TU Košice. This part is visualizing part, which is oriented to handling and visualization of large data sets on big screen output devices. In first part are described a system for manipulating streams of graphics API commands on clusters of workstations. The next part describes basic conception of our visualization kernel which use multi-screen mode. First practical results are described in the conclusion. This work is supported by VEGA grant project No. 1/3136/06: Research a parallel, distributed and network computer systems applications to solve computational processes in an area of large graphical data volumes processing.

Statistical response to the point defect of magnetic dot array simulated on a grid platform

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Abstract. The regular square-shaped 5×5 segment of magnetic dot array (MDA) in cyclic magnetic field under the simultaneous thermal activation has been simulated on the NorduGrid platform. The integration of stochastic Landau-Lifshitz-Gilbert equation (SLLG) repeated for many separate hysteretic remagnetization events represents the polynomial time problem. The physical motivation of our simulation study is to identify the most remarkable differences between the remagnetization statistics in defect-free and defect-including geometries.

The model of the current stellar perturbations on the Oort Cloud

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Abstract. In a study of the Oort-Cloud dynamics, the stellar perturbations should be taken into account. A model of the stellar passages around the solar system has to reflect both the frequency and perihelion distribution of the passing stars, in the same time. When the Galactic tide is also considered to influence the stellar trajectories, these become different from the Keplerian hyperbolas and a working out of the model is not trivial.

We provide the model the stellar passages and consequent stellar perturbations for 1 Gyr period assuming the current environment, in which the solar system is situated.

Taking the characteristics of actual stars provided by Garcia-Sanchez et al. in 2001 on the basis of the HIPPARCOS observations available that time, we find the model satisfying the simultaneous validity of the frequency of passages and velocity dispersion for 13 representative stellar spectral types. An agreement of these characteristics is reached through a numerical integration of a variety of 401400 stellar orbits. This extensive task is performed using the European GRID computing system.

The resultant data count the dynamical characteristics of 41594 simulated stars passing the solar system over 1 Gyr. These data will be available in an electronic form at http://www.ta3.sk/~ne/STELLAR_PERTURBATIONS/, soon.

IEPSAS-Kosice: Experiences and advances

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Abstract. The article presents lessons learned in running and maintenance of the cluster IEPSAS-Kosice. We will highlight the history of the high performance computing at the Institute of Experimental Physics (IEP) and provide a brief overview of the high energy physics experiments, where IEP participates. Further, we will present the architecture, configuration and network topology of the cluster and provide details about our day-to-day operations. The process of the integration into the EGEE/LCG2/gLite will be presented, as well as statistics about the past and present usage. We will also briefly describe the supported virtual organizations and the role they have played in the forming of the requirements on the cluster. We will conclude with our plans for the future.

Parallel implementation of Ant Colony Optimization algorithms

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Abstract. Ant Colony Optimization (ACO) is a population-based, nature-inspired metaheuristic that has been successfully applied to a variety of combinatorial optimization problems. ACO takes inspiration from the behaviour of real ant colonies. Despite the fact that sequential version of ACO contains a high level parallelism, little research has been conducted on this aspect. In this paper we give discuss several parallelization strategies for Ant Colony Optimization algorithms and give results that have been obtained using the Parallel Ants strategy on Traveling Salesman Problem.

Keywords: parallel algorithms, ant colony optimization, performance evaluation, traveling salesman problem

Grid Computing in Computational Chemistry

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Abstract. Over the past three or four decades, computational chemistry has developed application software to predict molecular structures, spectral information, and the thermodynamic and kinetic properties at high accuracy and with ever-shorter execution times (better numerical algorithms, improved methods, parallel computing). More recently computer programs covering these methods have successfully been coupled to extend the scope of their applicability. Coupling several autonomous computational steps (molecular structure optimization, transition energy calculation, and solvent effect calculation) makes computations easier to use and more powerful in prediction.

Distributed Solving of Combinatorial Problems

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Abstract. Combinatorial search can be defined as a process of evaluating solutions on discrete, finite mathematical structures. This paper deals with the decision problem algorithms which attempt to find a solution that satisfies all the constraints. This means to evaluate large amount of data. To speed up this operation, an parallel algorithm was proposed and implemented. It is based on the message – passing specification MPI implemented in free–available MPICH2 library. Proposed algorithm was tested on commodity cluster and presented result show significant reduction of execution time.

Key words: Backtracking, combinatorial algorithm, MPI, commodity cluster

Support for object-oriented parallel programs for grids and clusters

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Abstract. MPI is one of the most important standards for communication in parallel applications running on grids and clusters. The already widely accepted version 1.x defines a clear interface for communication operations required by most of the parallel algorithms. This version is however functional rather than object-oriented. While other forms of decomposition are suitable for many parallel applications, there are several classes of applications where object-oriented decomposition is the most natural. Version 2.0 tries to address the issue of limited support for objects in MPI, it introduces object-oriented C++ language bindings, Remote Memory Access and synchronization mechanisms, API for process spawning and management, support for dynamic connection of different process groups, etc. This article will show how to exploit these MPI extensions by using meta-programming and reflection facilities in C++. These facilities are not a part of the ISO C++ standard but can be added in a portable way.

Digital Market for Non-dedicated Cluster

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Abstract. Fast progress in computer technologies allows to build personal computers and workstations that are very cheap and powerful at the same time. However, their utilization is often very low. The concept of non-dedicated clusters allows to join such poorly utilized computers into one virtual cluster machine that can be used for high-performance parallel and distributed computing. The decentralized resource allocation in such systems is a hard problem, classical centralized scheduling algorithms cannot be used. A promising approach is to use microeconomic mechanisms.

We have designed and implemented a micropayment infrastructure and auction mechanisms on top of the non-dedicated cluster architecture CLoNDIKe. The resource holders can join the cluster and profit from selling its resources. This profit can later be used for allocation other resources contributed by other participants in the cluster. Such approach leads to high utilization. The satisfied users will cultivate the cluster, without the need of some central authority. In this paper, we describe a market-based process scheduling in a non-dedicated cluster. We discuss the principles of such a solution, describe the architecture and the decisions during its design, the prototype implementation, and results of experiments.

Medigrid infrastructure - services and portal

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Abstract. In this paper we present the architecture and infrastructure employed in the Medigrid project in order to enable easy remote access to earth science data and simulation models in heterogenous environment (Windows and Linux). We describe design and implementation of the Data transfer and Job submission services. The management and lookup of data sets is leveraged by integrating the Data transfer service with centrally deployed third-party Replica location and Metadata catalog services. Our services are implemented in the Java language and are based on the Globus toolkit's implementation of the WSRF standard what makes them instantly or at least easily portable to any system that can run Java VM. Users can access and use these services using either command line tools or web-based user interface implemented as a set of portlets on top of the Gridsphere portal framework.

Earth Science going into the Grid - DEGREE project

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Abstract. Earth Science (ES) community has a big potential to exploit nowadays grid infrastructures like EGEE due to their heavy computational simulations. A lot of ES applications is waiting for missing features in Grid, that should be provided to attract more ES application developers and users to go into the 'Grid world'.

Therefore several members of ES community created a 6FP project called DEGREE (Dissemination and Exploitation of GRids in Earth science). DEGREE project seeks to address the barriers which stand in the way of a wider uptake of the Grid technology, such as perceived complexity of the middleware, insufficient support for important ES functions and vital additional services.

The project results, whitepaper - roadmap, will provide a feedback both to the Grid and the ES communities, to increase awareness of and involvement with Grid developments.

This paper brings an overview of the DEGREE project and its challenges and objectives.

Interactive application support - Int.eu.grid project

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Abstract. Grid infrastructures that are used nowadays are oriented mostly to batch jobs, i.e. complex jobs that need to be steered during their run have very limited support. The consortium from 13 European countries is trying to improve this situation by developing and deploying an interoperable production-level e-Infrastructure for demanding interactive applications. This will impact the daily work of researchers using distributed parallel MPI interactive computing by user friendly access. This will be achieved through a Grid interactive desktop with powerful visualization, with its support for virtual organizations, collaborative environment, execution and monitoring tools and tools for discussion of results. This paper brings an overview of the Interactive European Grid project, of its pilot applications and more about one of its potential applications – Decision Support Tool for Environmental Assessment of Climate-Change driven Risks in Landscape.

Numerical study on a solid bar with and without plastic heating – Further way to improve our energy conservation equation

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Abstract. In this paper a numerical study on a solid bar is presented using fully coupled thermal structural analysis with finite element method (FEM). The analysis is based on the most recent energy conservation equation, which was further improved to take into consideration the effect of plastic heating. In the study loading cases with and without plastic heating were investigated. The paper shortly outlines the mathematical model used in the analysis, compares the calculation results and highlights the major differences between them. In spite of the fact that the energy conservation equation is much more complex than any other before and its experimental verification is not easy, the author believes that the study will play an important role in understanding the real thermo-dynamical processes of a solid body.

Effective Distributed Query Processing on the Grid

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Abstract. Distributed query processing has been widely used in data intensive applications where data are stored at multiply geographically separated locations. Mapping the operators of query tree to available CPU with respect to minimum response time and effective utilization of resources is combinatorial task, solved using heuristics. This paper deals with query tree operator scheduling on the grid with respect of those criteria, using intra-operator parallelism. New heuristics are proposed and tested for two data sets. Results show that exploiting intra-operator parallelism can lead to reducing of response time.

Keywords: Query processing, intra-operator parallelism, operator scheduling, distributed processing.

Technické riešenie výpočtových prostriedkov pre kláštrové počítanie na báze PC komponentov.

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Abstrakt. Tento dokument popisuje konkrétne technické riešenie realizácie výpočtových prostriedkov pre kláštrové počítanie. Je zameraný na výstavbu výpočtového klástra, pozostávajúceho zo šestnástich výpočtových uzlov, prepojovacej komunikačnej siete a jedného riadiaceho počítača. Samotná realizácia jednotlivých častí výpočtového klástra je založená na maximálnom využití štandardných komponentov PC. Dokument ďalej popisuje jednotlivé funkčné časti klástra, ich implementáciu a optimalizáciu, podľa ekonomických a technických kritérií. V závere je uvedený prehľad doterajších riešení týkajúcich sa výstavby klástrov, ktoré boli realizované v rámci vedecko-technických projektov na našom ústave.

Abstract. This paper describes a concrete technical solution of the computing resources realization for the cluster computing. It is aimed at the building of the computing cluster consisting of sixteen computing knots, interconnecting communication network and one control computer. The building of the individual parts of the computing cluster itself is based on the maximum utilization of the standard PC components. The paper also describes individual functional parts of the cluster, their implementation and optimization according to the economic and technical criteria. In the conclusion there is introduced the review of the prior solutions considering cluster building which were realized within the solution of the scientific and technical projects at our institution.

About Knowledge Management and Distributed Computing in Grid Infrastructure

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Abstract. E-science is collaborative science that is made possible by the sharing across the Internet of resources that is often very compute intensive, often very data intensive and crosses organizational and administrative boundaries. The semantic grid annotates the grid with metadata describing the resources it makes available. Semantic grid aims to incorporate the advantages of the grid, semantic web and web services. The aim of VVT information portal is to provide information about possibilities to use high performance computing available for the research and scientific workers of Slovak academy of sciences.

Keywords: Distributed systems, Grid infrastructure, Services, e-Science, Knowledge, Semantics, Ontology, Web portal

Overview of The Grid Authorization

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Abstract. The Authentication together with Authorization cast significant role in Grid environment. The present security infrastructures implement these key concepts by different methods. This paper intends to map them, overview them and compares present approaches of Grid Authorization and focuses on its requirements and problems. It also points on Advanced Grid Authorization Infrastructures and their properties.

Track 2
Use of Knowledge and Semantics
in Grid and Cluster Computing

Knowledge-based Approach to Service Performance Estimation for Grid Workflows

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Abstract. As Grid technology becomes more service oriented and the distributed applications are constructed as complicated Grid service workflows, many new challenges arise during the composition and execution of such workflows. One of such problems is the selection of most suitable web service (WS) deployments for a concrete workflow task execution during the process of work-flow scheduling. A service is needed which is able to estimate the behavior of each web service deployment in the Grid. Herein we present the design of such service capable of estimating WS behavior and performance measures including run time, availability, accessibility, stability and others. This work exploits many scientific concepts and methodologies such as instance based learning and case based reasoning. Presented prediction service also implements a novel approach to WS performance prediction through the refinement of case retrieval process through semantic description of discrete features and service input data.

K-Wf Grid portal: A portal for semantic workflows.

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Abstract. The aim of this paper is to provide a description of Web and portal technologies used in the K-Wf Grid portal. The K-Wf Grid portal provides a central user interface, point of interaction and access to various resources. The K-Wf Grid portal provides users with access to the components developed within the K-Wf Grid project and other requested resources. This covers the components for workflow specification, workflow management and visualization, components dealing with the metadata management and components for accessing the other Grid services. Moreover, the K-Wf Grid portal includes collaborative feature provided by lightweight discussion portlet. Architecture of K-Wf Grid portal is based on the Gridsphere portal framework that serves as an open-source portlet container that wraps user management and application logic. The portal components are made using various technologies from pure portlet through included Java applets up to technologies such as JavaScript and AJAX.

Keywords: Workflow, Gridsphere, ontology, portlet, Java applet, AJAX..

Workflow and Knowledge Support for Flood Forecasting

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Abstract. This paper* presents the tools and concepts, used to provide support and intelligent management to a complex flood forecasting application, which employs grid resources in a series of hydro-meteorological simulations. These simulations are exposed as web services. The tools provide for ontological descriptions of the application's services, management of these services and their composition into user-defined workflow. The whole support system is driven by ontologies and knowledge management technology. It also supports user collaboration and experience management, and enables control of the application through a globally accessible web portal.

Keywords: Flood Forecasting, Grid Computing, Ontologies, Workflow Management

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Semantic Analysis of Grid Workflows

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Abstract. In this contribution we present semantic analysis of workflows in grid environment. The contribution describes a tool WXA (Workflow Xml Analyzer) that enables semantic analysis of workflows (not only in grid applications). The tool is based on analysis of xml files that represent activities in grid workflows. WXA is programmed as a generic tool. It uses Xpath technique, and queries are read from property file which can be edited by a user. As a result, there is no problem of adjusting this tool to any workflow in which activities are represented by Xml files. The tool is used and being developed for K-WfGrid EU RTD IST FP6-511385 and RAPORT APVT-51-024604 (here is called ACoMA – Automated Content-based Message Annotator) projects.

Keywords: grid workflow, query, semantic analysis, tool, xml, xpath technique

Track 3
High Performance Distributed
Computing
and Large Scale Simulation

Simulation of avalanche dynamics in a computational grid

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Abstract. We study an inhomogeneous sandpile model in which two different toppling rules are defined. For any site only one rule is applied corresponding to either the Bak, Tang and Wiesenfeld model [Phys. Rev. Lett. 59, 381 (1987)] or the Manna two-state sandpile model [J. Phys. A 24, L363 (1991)]. The goal of this contribution is to show that this application is suitable for decentralized grid computational model.

Clusters, grids, molecules: why virtual screening should forego real HTS

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Abstract. High-throughput screening (HTS) of large molecular libraries is a common practice used in biopharmaceutical research in order to detect lead molecules (inhibitors) of the target enzymes. This can be quite an expensive procedure based on the price/performance of the HTS robots and additionally on the price of screened libraries. Although the price of a single entity from the libraries is quite low, the screening of libraries composed of tens of thousand compounds can be prohibitive. Virtual screening using calculation protocols thus becomes a complimentary approach.

The most common methods for virtual screening are either ligand or receptor based. Molecular properties are calculated during the ligand-based screening, scored and filtered according predetermined criteria. Receptor-based screening is more complex and the interaction energies between the ligand and the amino-acids in the active site of the protein are calculated. Although such computation for a single ligand-receptor complex can be completed within few minutes on an ordinary PC, when one considers the size of real libraries (usually around one hundred thousand compounds), the screening of the entire library becomes quite a time demanding task and parallel processing is the only way to get sound results in a reasonably short time period.

There are several docking programs, that allow one to calculate the position of the ligands in the protein active site. The quality of the ligand-receptor match is measured by scoring functions. These can be based on force field scoring, on empirical free energy scoring, or on knowledge-based scoring. Consensus scoring is a feature of some modern programs.

We were using two docking programs, FlexX and AutoDock for receptor-based virtual screening. We will compare the results from virtual screening with data from real HTS to illustrate how the so called “cherry-picking” approaches can help to improve the quality of obtained results while simultaneously significantly decreasing the funds required to purchase compounds.

Modelling speed the Aircraft at the single computer and MPI of the simulator

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Abstract. The content of this article summarises the authors' experience from time consuming mathematic modelling of decomposed information systems of a simulator. The knowledge arises from a theory of design computer control systems. These are derived from computers that create a distributed computer system of a flight simulator. Modelling the time precision of mathematic model speed of the simulator system is done by description equations depending on architecture of computer systems. An important part of this article is the implementation computation speed of aircraft, on the single-processor architecture and MPI on the two one processors.

Mobile Networks System Level Simulations with Grid Computing

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Abstract. System level simulations in mobile networks are important means for evaluating existing and also new developed technologies for mobile systems. In Siemens PSE s.r.o. Bratislava flexible libraries which form mobile simulation platform are used and further developed. Although simulations are carried out on powerful Linux based systems, simulation time is long and ways of solving this problem should be found. Some improvements have been reached by more efficient coding of the critical parts and by using special algorithms. Further analysis has shown that there are more promising improvements by using DSP technologies or parallel computing. The last one with a help of grid computing is in preparation and because of a lack of knowledge a contact with an appropriate research organisation is desirable.

Parallel Grid Implementation for Laplacean Equation Computation by Gauss-Seidel Method

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Abstract. Parallel computer systems, parallel programming and algorithms are widely studied and used in the world. This article is devoted to the task of development and implementation of real algorithm for parallel computation. The individual example demonstrates the methods, the tools and also the influence of parallel system communication overheads.

Tutorials and Courses

Utilizing E-Science through Charon Extension Layer Toolkit

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Přednáška o systému Charon

Lecture with hands-on (in Czech language)

Course for administrators of EGEE Grid sites Kurz pre administrátorov uzlov EGEE Gridu

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1. Introduction - *Jan Astalos* (20 min)

- Basics of EGEE Grid operation - infrastructure, node types, job flow, etc.
- Authentication - X509 certificates, Certification Authorities, proxy certificates
- Authorisation - Virtual Organisations

2. Design of grid site - *Marian Babik* (20 min)

- HW design - required/optional nodes, structure of grid site, cooling, etc.
- SW design - operating system, batch systems
- things that site designer must be aware of

3. Installation and setup of grid nodes - *Tomas Daranyi* (20 min)

- common steps - installation of NTP, Java
- YAIM - installation and configuration of nodes
- how to prepare site configuration
- configuration of nodes and post-installation steps

4. Registration of site into EGEE infrastructure - *Jan Astalos* (20 min)

- EGEE organisation - federations, support units, ROC
- registration procedure - Security Policies, GOCDB, site certification, dteam VO
- site testing - SAM tests, job submission, data management, accounting

5. EGEE Grid site operation - *Jan Astalos* (10 min)

- site administration - updates, GGUS tickets
- solving problems - 1st line support
- most common problems

6. Discussion

gLite

Lightweight Middleware for Grid Computing

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Abstract. During the past few years, advances in networking and distributed computing allowed the establishment of production Grid infrastructures, such as EGEE in Europa, OSG in the US, and NAREGI in Japan, which offer their services to many scientific and industrial applications. For any Grid computing effort, middleware is a critical component. The Grid middleware provides a set of services to facilitate and control the resource sharing - allowing resources to be discovered, accessed, allocated, monitored and accounted for, regardless of their physical locations. This paper gives an overview of the *gLite - the Lightweight Middleware for Grid Computing*, which is deployed and used in the EGEE Grid infrastructure.