4th International Workshop on Grid Computing for Complex Problems

GCCP 2008
BOOK OF ABSTRACTS

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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

Proceeding 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

Preface

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

The topics of the workshop are:
- 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 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 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. This book is a collection of abstracts of papers from International Workshop on Grid Computing for Complex Problems – GCCP 2008. 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 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.

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

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.

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

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.

Static Job Scheduling in the Grid

Penka Martincova, Karol Grondzak, Matuš Chochlík

Faculty of Management Science and Informatics, University of Zilina, Slovak Republic

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

Abstract. In this paper we study *static job scheduling algorithms* in grid environments when each job is submitted before a schedule is made. The scheduling goal is to minimize a makespan. Scheduling is made in two steps – in first step global scheduler allocates jobs to local scheduler and in second step local schedule is prepared. Performance of the designed algorithms MS_SJF and MS_LJF is compared with known algorithms with local searching – Tabu search, Hill climbing and Genetic algorithm. The results obtained show, that algorithms MS_SJF and MS_LJF are fastest and suitable for static scheduling.

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

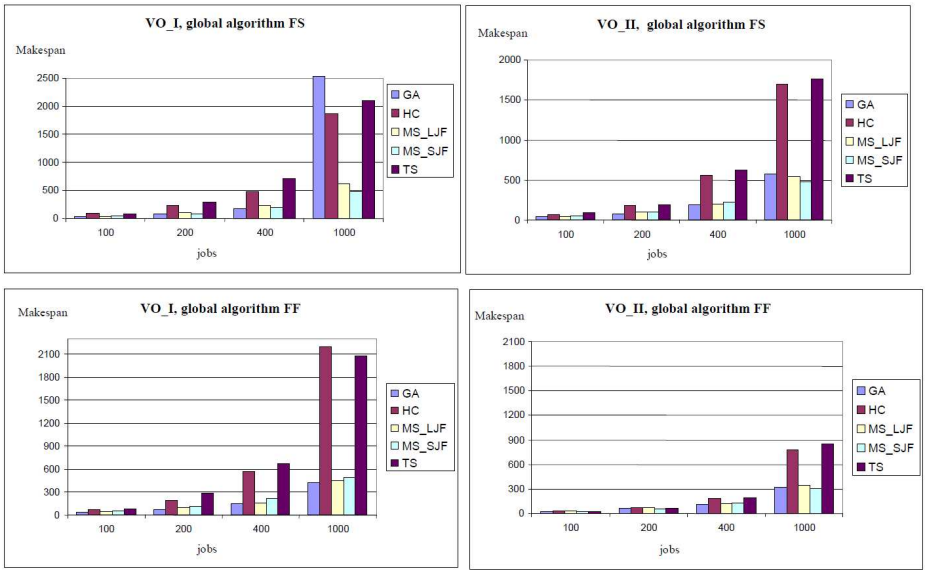
The proposed architecture is suitable for computational grid, which consists of community resources e.g. university or company resources. Resources belong to different administrative domains, which mean that there are different scheduling policies. The users can submit their jobs to a grid through one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

3 Local scheduling algorithms

After the tasks are assigned to resources, local scheduler computes schedule in order to optimize an objective function. In our experiments the objective function was minimum makespan. As the scheduling is NP – complete [2], the suboptimal schedule is found. Five local scheduling algorithms were used. Three of them belong to local search based algorithms: Hill Climbing algorithm (HC), Tabu Search (TS) and Genetic algorithm (GA). These algorithms are well known and they are often used in optimization problem solving.

Next two algorithms we proposed for purposes of local grid scheduling. These algorithms - Most Suitable_Longest Job First (MS_LJF) and Most Suitable_Shortest Job First (MS_SJF) are so called list scheduling algorithms. Their common feature is that they create list of tasks and order them using some rule - in our case for MS_LJF the rule is longest job first and for MS_SJF the rule is shortest job first. The tasks from the list are assigned to most suitable resources.



4 Result Analysis

The Performance comparison of static local scheduling algorithms GA, HC, TS, MS_LJF a MS_SJF shows, that our proposed algorithms MS_LJF a MS_SJF achieved the best results – shortest makespan. These results are better when our global algorithm FF is used. This algorithm creates better initial schedule and thus better local Schedule is created. Genetic algorithm (GA) achieved similar results, but the scheduling time of GA is very long.

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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

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).

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.

Computational “virtual laboratory” tools for biomolecular and drug design

István Komáromi[a], László Tóth[a] and Tibor Kožár[b]

[a]Clinical Research Center, Medical and Health Center, University of Debrecen, Debrecen, Hungary

[b]Department of Biophysics, Institute of Experimental Physics, Slovak Academy of Sciences, Košice, Slovakia

The concept and the definition of the “Virtual Laboratory” (VL), i.e. VL being *“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] was well-established several year ago. 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 falling in this area. Computational VL can facilitate the D&D process to proceed faster and more efficiently in comparison to the standard protocols of the real wet laboratories. Although the importance of the standard laboratories is unquestionable and VLs are not intended to replace them, the intention of VLs is somehow 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 accord with the promising VL approach in drug discovery [2] was devoted to build a VL with following assumptions:

a) allow international remote collaboration,
b) build joint molecular databases (originating from both, molecular collections from commercial vendors and huge, in-house combinatorial-generated target-specific molecular datasets),
c) provide virtual screening environment to evaluate the protein-ligand interaction profiles,
d) allow the integration of information related to small-molecules with information on protein targets, e.g. characterize and refine the protein-ligand interaction patterns,
e) link experimental activity data (when available) with protein-ligand complexes,
f) allow information storage, data mining and borderless information sharing.

We started the international collaboration with evaluation of the suitability of the software tolls for use in remote (grid) environment. Although the molecular docking calculations were efficiently running on the grid, clusters in local computational laboratories were preferably used for the more complex QC/MM calculations. Virtual private network (VPN) was tested to provide the safest option to link such dedicated laboratories. In addition, VPN was shown to become an efficient VL environment to build hypotheses and evaluate them (e.g. pharmacophore modeling), providing thus additional layer for data sharing and information integration.

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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

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[3] *

[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.

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Secure management of crises situations using mobile code in untrustworthy distributed computing environment

Zoltán Balogh, Ivana Budinská, Branislav Šimo

Institute of Informatics, Slovak Academy of Sciences, Bratislava
balogh@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 web 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 crises situations. We also present a generic architecture for untrustworthy distributed environment for which we plan to implement our proposed solution. This article is presented as "work in progress" so we conclude with our plans for the near future.

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

Management of Distributed Metadata

Ondrej Habala[1], Branislav Šimo[1], Ladislav Hluchý[1]

[1] Institute of Informatics, Slovak Academy of Sciences, Dúbravská cesta 9, 84507 Bratislava, Slovakia
{Ondrej.Habala, Branislav.Simo, Ladislav.Hluchy}@savba.sk

Abstract. Metadata, long being a second-class citizen in the data management world, is gaining prominence in the last couple of years. Whether it is grid computing, large-scale service-oriented infrastructures, or the elusive Web 2.0, metadata is the key to information lookup and retrieval in all these areas. This paper discusses a system, enabling seamless access to metadata in a distributed environment. The metadata is in the form of RDF triples, so it can be used not only to describe files or other pieces of data (which is the traditional role of metadata), but also to store semantic information on any object relevant to the domain of the application, in whose context the system is deployed. The system is being developed and tested in the project SEMCO-WS[*].

Keywords: distributed metadata, metadata management, grid computing, RDF

[*] This work is supported by projects ADMIRE FP7-215024, VEGA No. 2/6103/6, SEMCO-WS APVV-0391-06.

European X-ray Free Electron Laser Facility - the Project, the Machine parameters, the Data Acquisition System. A message for Slovakia: to build up the top GRID infrastructure for computing and huge data storing

Pavel Murín

UPJŠ Košice

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

SLA violations are detected, the affected parties are informed immediately. The result of SLA-Evaluation is stored in the local database and is offered to hierarchically higher settled partner in the supply-chain – buyer of the buyer, after the shipment of the processed or transformed food trade unit.

The paper will describe in detail the architecture of the AgroGrid framework, consisting of the SLA-Management, VO-Management services and portals, used to enable forming of the dynamic food supply-chains and monitoring of quality in such dynamic supply-chains.

The approach proposed in AgroGrid enables food industry to build and extend supply-chains (managed within AgroGrid as dynamic VO) by new partners, in flexible and dynamic manner, while ensuring monitoring of food-quality on each level and all sub-levels of the supply-chain hierarchy, determined by the order of the supply-chain partners. The quality management mechanism proposed in AgroGrid establishes trust-building commercialization support mechanism between all partners in the supply-chain.

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Abbreviation:

SLA	Service Level Agreement
BEinGRID	Business Experiments in Grid
VO	Virutal Organisation

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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.

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 composition we are interested in can deal with web or grid services, (grid) jobs or some general activities.

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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.

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.

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

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 Bátťková[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.

ATLAS on Slovak GRID

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

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

Abstract. ATLAS – one of experiments on LHC – will produce enormous amount of data about 1PB 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.

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.

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)