Cyberinfrastructure was proposed in a report of the NSF Blue-Ribbon advisory panel in 2003. Cyberinfrastructure will provide a unified environment to access and manage cyber resources, e.g. supercomputers, data archives, software services, scientific instruments and virtual organizations. In this book, the authors review latest research and development and discuss new technologies and applications involved in building Cyberinfrastructure. The purpose of this book is to provide a detailed summary of early experiences, practices and lessons learned in building Cyberinfrastructure from multiple perspectives: software development and maintenance, resource integration and sharing, cyber environment construction, operation and management, testing and troubleshooting, application enabling, security and QoS ensuring. Consequently, this book can serve as a valuable source of reference and indispensable reading for researchers, educators, engineers, graduate students, and practitioners in the field of design and implementation of Cyberinfrastructure systems.
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Chapter 1

PARALLEL DENSE LINEAR ALGEBRA SOFTWARE IN THE MULTICORE ERA

Alfredo Buttari
Department of Electrical Engineering and Computer Science, University of Tennessee, Knoxville, Tennessee

Jack Dongarra
Department of Electrical Engineering and Computer Science, University of Tennessee, Knoxville, Tennessee
Oak Ridge National Laboratory, Oak Ridge, Tennessee
University of Manchester, Manchester UK

Jakub Kurzak
Department of Electrical Engineering and Computer Science, University of Tennessee, Knoxville, Tennessee

Julien Langou
Department of Mathematical Sciences, University of Colorado Denver, Denver, Colorado

Abstract

The recent emergence of multicore and hybrid microprocessor designs marks the beginning of a forced march toward an era of computing in which research applications must be able to exploit parallelism at an unprecedented scale. This chapter presents a new generation of dense linear algebra libraries that achieve the fastest possible time to an accurate solution on multicore systems.

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1 E-mail address: buttari@cs.utk.edu
2 E-mail address: dongarra@eecs.utk.edu
3 E-mail address: kurzak@cs.utk.edu
4 E-mail address: langou@math.cudenver.edu
Abstract

Cyberinfrastructure (CI) for instrument sharing is an infrastructure that aims to facilitate effective resource sharing of expensive scientific instruments, e.g. telescopes and observatories, through a system of grid services. This cyberinfrastructure consists of three components: an instrument pool alliance, instrument pools, and physical instruments. When a user submits an experiment to the CI environment, the instrument pool alliance is responsible to allocate instruments in related instrument pools to conduct the experiment. After the experiment is finished and results are returned, the user will appraise performance of corresponding services.

In this chapter, fuzzy random scheduling algorithms are proposed in instrument pools when a job is submitted to one of instruments within a pool. The randomness lies in the probability of which
Chapter 3

AN INTEROPERABLE INFORMATION SERVICE SOLUTION FOR GRIDS

Anand Padmanabhan¹
CyberInfrastructure and Geospatial Information Laboratory (CIGI)
National Center for Supercomputing Application (NCSA)
University of Illinois at Urbana-Champaign

Eric Shook²
CyberInfrastructure and Geospatial Information Laboratory (CIGI)
University of Illinois at Urbana-Champaign

Yan Liu³
Shaowen Wang⁴
CyberInfrastructure and Geospatial Information Laboratory (CIGI)
National Center for Supercomputing Application (NCSA)
University of Illinois at Urbana-Champaign

Abstract

Information services are a critical piece of Grid infrastructure, they collect, aggregate, and organize sources of Grid resource information, and provide the information to applications to schedule computational tasks, and enable Virtual Organizations (VO) to share distributed computing resources. To be successful an information provider needs to be able to aggregate diverse information from numerous sources, publish information into different Grid monitoring

¹ E-mail address: apadmana@uiuc.edu
² E-mail address: eshook2@uiuc.edu
³ E-mail address: yaniu@uiuc.edu
⁴ E-mail address: shaowen@uiuc.edu
Chapter 4

PERFORMANCE-ORIENTED WORKLOAD MANAGEMENT FOR MULTICLUSTERS AND GRIDS

Ligang He1
Stephen A. Jarvis2
Department of Computer Science, University of Warwick
Coventry, CV4 7AL, UK

Abstract

This chapter addresses the dynamic scheduling of parallel jobs with QoS demands (soft-deadlines) in multiclusters and grids. Three performance metrics (over-deadline, makespan and idle-time) are combined with variable weights to evaluate the scheduling performance. These three metrics are used for measuring the extent of jobs’ QoS demands compliance, resource throughput and resource utilization, respectively. Therefore, clusters situated in different administrative organizations can utilize different weight combinations to represent their different performance requirements. Two levels of performance optimisations are applied in the multicluster. At the multicluster level, a scheduler, (which we call MUSCLE), allocates parallel jobs with high packing potential to the same cluster; MUSCLE also takes the jobs’ QoS requirements into account and employs a heuristic to allocate suitable workloads to each cluster to balance the performance. At the local cluster level, a workload manager, called TITAN, utilizes a genetic algorithm to further improve the scheduling performance of the jobs sent by MUSCLE. The extensive experimental studies are conducted to verify the effectiveness of the scheduling mechanism in MUSCLE; the results show that comparing with the traditional workload allocation policies in distributed systems (Dynamic Least Load and Weighted Random), the comprehensive scheduling performance (in terms of over-deadline, makespan and idle-time) of parallel jobs is significantly improved and well balanced across the multicluster.

1 E-mail address: liganghe@dcs.warwick.ac.uk
2 E-mail address: saj@dcs.warwick.ac.uk
Virtualizing Scientific Applications and Data Sources as Grid Services

Siegfried Benkner¹
Gerhard Engelbrecht²
Martin Köhler³
Alexander Wöhrer⁴

Institute of Scientific Computing, University of Vienna, Austria

Abstract

Service-oriented Grid computing promises to change the way scientists will tackle future research challenges by offering advanced data and application services, providing transparent access to distributed heterogeneous data sources and to high-end computing facilities for performing computationally demanding and data-intensive modeling, simulation and analysis tasks. In this article we describe the Vienna Grid Environment (VGE), a service-oriented Grid infrastructure based on standard Web Services technologies for virtualizing scientific applications and data sources as Grid services that hide the details of the underlying software and hardware infrastructure. The VGE service provision framework adopts a component-based approach which supports the configuration of application and data services from a set of basic service components providing capabilities like job or query execution, data transfers, QoS negotiation, data staging, and error recovery. VGE relies on a business-oriented model to Grid computing based on a flexible QoS infrastructure, dynamic negotiation of service-level agreements, and on-demand access to Grid services. VGE has been developed and utilized in the context of several European projects for the realization of Grid infrastructures within medical and bio-medical application domains.

¹ E-mail address: sig@par.univie.ac.at
² E-mail address: gerry@par.univie.ac.at
³ E-mail address: kohler@par.univie.ac.at
⁴ E-mail address: woehrer@par.univie.ac.at
Chapter 6

GRID RESOURCE BROKER FOR SCHEDULING
COMPONENT-BASED APPLICATIONS ON
DISTRIBUTED RESOURCES

Xingchen Chu¹
Srikumar Venugopal²
Rajkumar Buyya³

Grid Computing and Distributed Systems Laboratory
Department of Computer Science and Software Engineering
The University of Melbourne, Australia

Abstract

This chapter presents the design and implementation of seamless integration of two complex systems component-based distributed application framework ProActive and Gridbus Resource Broker. The integration solution provides: (i) the potential ability for component-based distributed applications developed using ProActive framework, to leverage the economy-based and data-intensive scheduling algorithms provided by the Gridbus Resource Broker; (ii) the execution runtime environment from ProActive for the Gridbus Resource Broker over component-based distributed applications. It also presents the evaluation of the integration solution based on examples provided by the ProActive distribution and some future directions of the current system.

¹ E-mail address: xchu@csse.unimelb.edu.au
² E-mail address: srikumar@csse.unimelb.edu.au
³ E-mail address: raj@csse.unimelb.edu.au
CROWN: A SERVICE GRID MIDDLEWARE FOR E-SCIENCE

Jinpeng Huai¹
Chunming Hu²
Beihang University, Beijing 100083, P. R. China

Abstract

In the past few years, the Grid computing paradigm has emerged as an instance of cyber infrastructure, promising to enable resource sharing and collaborating across multiple domains. In the research community there has been an intense interest in designing and studying of such system. CROWN (China R&D Environment Over Wide-area Network) project is an e-Science project funded by China Natural Science Foundation Committee, and China 863 High-tech Program. The main goal of CROWN project is to empower in-depth integration of resources and cooperation of researchers nationwide and worldwide. CROWN was started in late 2003. The main goal of CROWN project is to build the middleware infrastructure and wide area testbed to support computation intensive, data centric e-Science applications.

Recently, with the evolution of Web services, the service-oriented architecture has become a significant trend for grid computing, with OGSA/WSRF as the de facto standards. CROWN has adopted the service-oriented architecture, connecting large amount of services deployed in universities and institutes. Up till mid 2007, lots of applications in different domains have been deployed into CROWN grid, such as gene comparison in bioinformatics, climates pattern prediction in environment monitoring, etc. The long-range goal for CROWN is to integrate home user resources in a fully decentralized way with a robust, scalable grid middleware infrastructure.

In this chapter, based on a proposed Web service-based grid architecture, a service grid middleware system called CROWN is introduced. As the two kernel points of the middleware, the overlay-based distributed grid resource management mechanism is proposed, and the policy-based

¹ E-mail address: huaijp@buaa.edu.cn
² E-mail address: hucm@buaa.edu.cn
Chapter 8

SEMANTICS-ENABLED SERVICE DISCOVERY FRAMEWORK IN A PAN-EUROPEAN PHARMACEUTICAL GRID

Changtao Qu
Falk Zimmermann
IT Research Division, NEC Laboratories Europe, NEC Europe Ltd.
Rathausallee 10, D-53757 Sankt Augustin, Germany

Kai Kumpf
Fraunhofer Institute for Algorithms and Scientific Computing
Schloss Birlinghoven, D-53754 Sankt Augustin, Germany

Richard Kamuzinzi
Valérie Ledent
Robert Herzog
Department of Molecular Biology, Universite libre de Bruxelles
Rue des Professeurs Jeener et Brachet 12, B-6041 Gosselies, Belgium


2 E-mail address: qu@it.neclab.eu
3 E-mail address: zimmermann@it.neclab.eu
4 E-mail address: kumpf@scai.fraunhofer.de
5 E-mail address: rkamuzinzi@ulb.ac.be
6 E-mail address: vledent@ulb.ac.be
7 E-mail address: rherzog@ulb.ac.be
Chapter 9

SERVICE COMPOSITION AUTOMATION WITH AI PLANNING

Maozhen Li
Electronic and Computer Engineering, School of Engineering and Design
Brunel University, Uxbridge, UB8 3PH, UK

Bin Yu
Level E Limited, Edinburgh, EH9 3JL, UK

Man Qi
Department of Computing, Canterbury Christ Church University
Canterbury, Kent, CT1 1QU, UK

Abstract

Grid computing is rapidly evolving a service-oriented computing infrastructure that facilitates resource sharing and large-scale problem solving on the Internet. It is envisioned that many resources on the grid will be exposed as services for a wide use by the community. Service discovery and composition has thus become a vitally important component in utilising grid facilities. This chapter focuses on discovery of composite services. One challenge in service composition is how to automate the composition process in terms of a large number of services (atomic services or component services) and a variety of user requests. It presents a novel Hierarchical Two Directions Partial Order Planning Algorithm (H2POP) aiming to automate service compositions. A use case is given to illustrate the application of the H2POP algorithm for travel planning service composition automation.

1 E-mail address: Maozhen.Li@brunel.ac.uk
2 E-mail address: Bin.Yu@levelelimited.com
3 E-mail address: mq4@canterbury.ac.uk
Chapter 10

WORKFLOW IN A SERVICE ORIENTED CYBERINFRASTRUCTURE/GRID ENVIRONMENT

Wei Tan
Computation Institute, University of Chicago and Argonne National Laboratory Chicago, IL, USA

Yushun Fan
Department of Automation, Tsinghua University, Beijing 100084, P. R. China

Ian Foster
Computation Institute, Argonne National Laboratory and University of Chicago Chicago, IL, USA

Ravi Madduri
Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL, USA

Abstract

With the emergence of Service Oriented Computing, workflow has become an important method to compose services and reuse existing resources in the Cyberinfrastructure (CI) and the Grid. In this chapter, we first summarize research activities in the field of workflow in service oriented computing. We discuss five major research topics, i.e., languages and tools for service orchestration, automatic service composition, mediation-aided service composition, verification of service workflow, and decentralized execution of workflow. Although some of this work was originally targeted at the area of business process management, they can be adopted by the CI
Chapter 11

FEDERAL MANAGEMENT OF VIRTUAL ORGANIZATIONS WITH TRUST EVALUATION

Zhen Wang¹
Junwei Cao²
Research Institute of Information Technology
Tsinghua National Laboratory for Information Science and Technology
Tsinghua University, Beijing 100084, P. R. China

Abstract

Dynamical and flexible resource aggregation tools are required in 21st century research. Scientists need to aggregate various digital equipments and cooperate with each other in different organizations through Virtual Organizations (VO) on the Internet in a flexible and dynamical way. In this cooperation and resource sharing process, trust evaluation is of great importance for flexible VO management. Traditional tools such as VOMS for grids are short in dynamism and trust evaluation. In this chapter, we propose a new scheme providing federal VO membership management based on trust evaluation, with which researchers can achieve appropriate trust relationships with each other and establish a particular VO dynamically to aggregate resources for their own purposes.

1. Introduction

1.1. Background

Modern science research has great requirement for experimental instruments, computational and storage capability, and cooperation across organizations and disciplines

¹ E-mail address: zhen-wang07@mails.tsinghua.edu.cn
² E-mail address: jcao@tsinghua.edu.cn
COMMUNITY-SCALE CYBERINFRASTRUCTURE FOR EXPLORATORY SCIENCE

Peter Bajcsy¹
Rob Kooper²
Luigi Marini³
Jim Myers⁴

National Center for Supercomputing Applications (NCSA)
University of Illinois at Urbana-Champaign (UIUC)

Abstract

This chapter presents some of the key aspects of Cyberinfrastructure (CI) research and development targeting community-scale exploratory science. The motivation comes from the fact that successful software for CI is increasing scientific productivity of a single investigator, small groups of scientists as well as dispersed teams spanning multiple institutions. Community scale scientific activities and their informatics requirements are driving the development of new CI solutions. It becomes critical to follow CI design principles based on past, present and future efforts. In addition, data- and hypothesis-driven explorations are fundamental scientific activities leading to discoveries. In this work, our focus is on informatics requirements and CI design principles behind existing software for CI. We have included our experiences and described several prototype CI solutions to support exploratory science.

¹ E-mail address: pbajcsy@ncsa.uiuc.edu
² E-mail address: kooper@ncsa.uiuc.edu
³ E-mail address: lmarini@ncsa.uiuc.edu
⁴ E-mail address: jimmyers@ncsa.uiuc.edu
Chapter 13

CYBERINFRASTRUCTURE FOR BIOMEDICAL APPLICATIONS: METASCHEDULING AS AN ESSENTIAL COMPONENT FOR PERVERSIVE COMPUTING

Zhaohui Ding
Xiaohui Wei
College of Computer Science and Technology, Jilin University
Changchun, Jilin, 130012 P. R. China

Osamu Tatebe
Department of Computer Science, Tsukuba University
Tsukuba, Ibaraki, 3058573, Japan

Peter W. Arzberger
National Biomedical Computation Resource, University of California
San Diego, CA 92093, United States

Philip M. Papadopoulos
Wilfred W. Li
National Biomedical Computation Resource, San Diego Supercomputer Center
University of California, San Diego, CA 92093, United States

1 E-mail address: zhaohui.ding@email.jlu.edu.cn
2 E-mail address: weixh@email.jlu.edu.cn
3 E-mail address: tatebe@cs.tsukuba.ac.jp
4 E-mail address: parzberg@ucsd.edu
5 E-mail address: phil@sdsc.edu
6 E-mail address: wilfred@sdsc.edu
Chapter 14

THE BRIDGING DOMAIN MULTISCALE METHOD AND ITS HIGH PERFORMANCE COMPUTING IMPLEMENTATION

Shaoping Xiao1
Department of Mechanical and Industrial Engineering, Center for Computer-Aided Design, The University of Iowa, Iowa City, IA 52242

Jun Ni2
Department of Mechanical and Industrial Engineering, Department of Radiology
The University of Iowa, Iowa City, IA 52242

Shaowen Wang3
CyberInfrastructure and Geospatial Information Laboratory (CIGI)
National Center for Supercomputing Application (NCSA)
University of Illinois at Urbana-Champaign, Urbana, IL 61801

Abstract

This chapter presents a study on the feasibility of applying high performance computing (HPC) to the Bridging Domain Multiscale (BDM) method, so that featured scalable multiscale computations can be achieved. Wave propagation in a molecule chain through an entire computational domain is employed as an example to demonstrate its applicability and computing performance when multiscale-based simulations are conducted in a large-scale parallel computing environment. In addition, the conceptual idea and computing framework using Grid computing technologies is proposed to enhance future multiscale computations in nanotechnology.

1 E-mail address: shaoping-xiao@uiowa.edu
2 E-mail address: jun-ni@uiowa.edu
3 E-mail address: Shaowen@uiuc.edu
Chapter 15

CYBERINFRASTRUCTURE FOR AGRICULTURAL DATA
AND KNOWLEDGE SHARING IN CHINA

Chunjiang Zhao¹
National Engineering and Research Center for Information Technology for Agriculture,
Beijing 100097, P. R. China

Yuxin Wan²
Department of Automation, Tsinghua University, Beijing 100084, P. R. China

Huarui Wu³
National Engineering and Research Center for Information Technology for Agriculture,
Beijing 100097, P. R. China
School of Computer Science, Beijing University of Technology, Beijing 100022, P. R. China

Wen Zhang⁴
Department of Automation, Tsinghua University, Beijing 100084, P. R. China

Abstract

During the last decade, billions of national investment has been spent in China on building
agricultural information systems for data collection, integration, analysis and processing. Each
province has built its own technology platform for information sharing and access. However,
since data sources are separate and corresponding applications are developed by different
organizations, cross-domain data and knowledge sharing becomes very difficult. A
Cyberinfrastructure (CI) for agricultural data and knowledge sharing in China is proposed in this
work and funded by the Ministry of Science and Technology of China under the national 863
high-tech R&D program. In this work, related work is summarized and our system structure is
described in details. Heterogeneity of different operating systems and databases has to be
addressed. System performance can be improved by avoiding large-scale data transferring by
introducing an application server within each domain for local data processing.

¹ E-mail address: zhaocj@nercita.org.cn
² E-mail address: wanyx04@mails.tsinghua.edu.cn
³ E-mail address: wuhr@nercita.org.cn
⁴ E-mail address: wen-zhang05@mails.tsinghua.edu.cn