CYBERINFRASTRUCTURE TECHNOLOGIES AND APPLICATIONS

EDITOR: JUNWEI CAO

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 leaned 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

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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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Chapter 2

SHARING SCIENTIFIC INSTRUMENTS FOR HIGHER EDUCATION AND RESEARCH IN CHINA

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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

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Chapter 3

AN INTEROPERABLE INFORMATION SERVICE SOLUTION FOR GRIDS

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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

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Chapter 4

PERFORMANCE-ORIENTED WORKLOAD MANAGEMENT FOR MULTICLUSTERS AND GRIDS

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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.

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Chapter 5

VIRTUALIZING SCIENTIFIC APPLICATIONS AND DATA SOURCES AS GRID SERVICES

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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.

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Chapter 6

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

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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.

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Chapter 7

CROWN: A SERVICE GRID MIDDLEWARE FOR E-SCIENCE

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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

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Chapter 8

SEMANTICS-ENABLED SERVICE DISCOVERY FRAMEWORK IN A PAN-EUROPEAN PHARMACEUTICAL GRID[1]

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[1] This chapter is an extended version of "C. Qu, F. Zimmermann, K. Kumpf, R. Kamuzinzi, V. Ledent, and R. Herzog, Semantics-Enabled Service Discovery Framework in the SIMDAT Pharma Grid, IEEE Trans. on Information Technology in Biomedicine, vol. 12, to appear in 2008".

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Chapter 9

SERVICE COMPOSITION AUTOMATION WITH AI PLANNING

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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.

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Chapter 10

WORKFLOW IN A SERVICE ORIENTED CYBERINFRASTRUCTURE/GRID ENVIRONMENT

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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

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Chapter 11

FEDERAL MANAGEMENT OF VIRTUAL ORGANIZATIONS WITH TRUST EVALUATION

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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 discinplines

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Chapter 12

COMMUNITY-SCALE CYBERINFRASTRUCTURE FOR EXPLORATORY SCIENCE

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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.

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Chapter 13

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

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Chapter 14

THE BRIDHING DOMAIN MULTISCALE METHOD AND ITS HIGH PERFORMANCE COMPUTING IMPLEMENTATION

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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.

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Chapter 15

CYBERINFRASTRUCTURE FOR AGRICULTURAL DATA AND KNOWLEDGE SHARING IN CHINA

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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.

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