International Workshop on Grid Computing for Complex Problems

GCCP2005

BOOK OF ABSTRACTS

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International Workshop on Grid Computing for Complex Problems GCCP2005 is organized by:

- Institute of Informatics, Slovak Academy of Science
- Faculty of Electrical Engineering and Informatics, Technical University of Košice

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- Miroslav Dobrucký, IISAS
- Giang Nguyen, IISAS
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A message from the general chair of GCCP2005

Welcome to the International Workshop on Grid Computing for Complex Problems GCCP2005. The workshop is three-day combined event for grid users: workshop with invited lectures, plenary discussions, accompanied by induction and grid application developer course, which is in the scope of EGEE project - Enabling Grids for E-science 2004-2006, INFSO-RI-508833.

The topics of the workshop are:

- High performance applications
- Tools and services for grid computing
- Knowledge mechanisms applicable in grid computing

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 ideas between theoreticians and practitioners to address the important issues in computational performance and computational intelligence towards Grid computing.

The workshop has attracted 28 paper submissions from Austria, Czech Republic, Hungary, Poland, Slovakia and Ukraine. This book is a collection of abstracts of papers from International Workshop on Grid Computing for Complex Problems - GCCP2005. 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 member of the Programme 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 2005, Bratislava, Slovakia

Grid Computing in Projects of IISAS
(Gridové počítanie v projektoch ÚI-SAV)

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The paper presents history of grid computing at the Institute of Informatics, Slovak Academy of Sciences, and current grid projects, activities and applications. The ANFAS project has developed the support decision system for flood prevention and protection, integrating the most advanced techniques in data processing and management. The CrossGrid project has developed, implemented and exploited new Grid components for interactive computation- and data intensive applications. Project EGEE (Integrated Infrastructure Initiative) is aiming at creating and deploying Grid technologies to enable the widespread uptake of e-Science applications throughout the European Research Area. The K-Wf_Grid project addresses the need for a better infrastructure for the future Grid environment; in order to address the complexity in using and controlling the next generation Grid, the consortium will adopt the approaches envisioned by semantic Web and Grid communities in a novel, generic infrastructure, to assist its users in composing powerful Grid workflows by means of a rule-based expert system. The MEDIGRID project aims at creating a distributed framework for multi-risk assessment of natural disasters; it will integrate models of forest fire behaviour and effects, flash floods and landslides, which will be upgraded to web applications.

Interactive Result Visualization on the Grid

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Considering the nowadays important role of grid computing within the domain of computational science and related applications the visualization of results produced on the grid becomes a crucial task. Since grid-based simulations commonly produce result data of significant size visualization is in most cases required to support the users understanding. On the other hand the size of the datasets to be visualized turns the visualization itself into a suitable grid application. However the present status of visualization on the grid is not really satisfying. In contrast to other grid services, such as batch processing, data transfer, and resource scheduling, visualization is still commonly utilized in the traditional point-to-point fashion, with applications integrating visualization as subroutine calls or even post-mortem. This situation is addressed by the Grid Visualization Kernel GVK, which proposes a fully grid-enabled approach to interactive scientific visualization. The infrastructure of GVK enables visualization and interactive steering of a remote simulation while the actual processing of the data within the visualization pipeline is transparently performed on the available grid resources.

For delivering visualization services GVK relies on glogin which offers interactive direct connections to grid resources. Within GVK-based applications glogin serves as data transportation layer and additionally supports interactive application steering over secure connections. Another important building block of GVK is grid-enabled modules based on Visualization Toolkit (VTK) classes. For performing the visualization task which is represented as a pipeline it is decomposed into multiple data conversion stages which can be executed on different resources within a grid testbed. The GVK approach has been used within several different application domains in the scope of the EU CrossGrid and Austrian Grid projects. We have realized GVK-based prototypes for disaster management, medical applications and astronomical data visualization.

P-GRADE Portal: Towards a User-friendly Grid Environment

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The rapid evolution of Grid systems in the last ten years has made the life of their users quite difficult. As each new system is deployed, users have to adapt to a whole new set of operating methods. Users working with the world.s various Grid systems have to learn new sets of commands for each system they utilise. Typically these commands are low-level, tedious to memorise and error-prone to use. Learning these commands demands significant effort and time from the user before they even get to use the system.

P-GRADE, P-GRADE Grid portal and Mercury Grid monitor are a family of tools developed by MTA SZTAKI to specifically combat these problems. P-GRADE breaks down the barriers between incompatible Grid systems, helping the user to develop parallel code that can be used on both supercomputers, clusters and in various Grids. P-GRADE hides the complexity of the Grid from the user, making it transparent. Users no longer have to worry about which service or resource they are accessing, as they will use the same high-level graphical environment and tools. The P-GRADE Grid Portal is a workflow-oriented Grid portal that enables the creation, execution and monitoring workflows in grid environments through high-level, graphical Web interfaces. Components of the workflows can be sequential and parallel (MPI, PVM) jobs. The P-GRADE Grid Portal hides the low-level details of Grid access mechanisms by providing a high-level Grid user interface that can be used for any Grid. Workflows developed in the P-GRADE portal are portable between different Grids without any re-learning of the features of the new Grid system. In this way P-GRADE Grid Portal helps the user to cope with the large variety of Grid systems. More than that P-GRADE portal can be configured to access several Grids and if a user has valid certificate for several Grids, then she can exploit all those Grids simultaneously during the execution of her workflow. Accessing Grid resources with the P-GRADE Grid Portal is as easy as never before, thus the P-GRADE Grid Portal is a perfect tool to anyone who would like to effectively solve computational intensive problems and avoid complicated grid protocols and commands at the same time.

P-GRADE Grid portal is already the entry point of four Grid systems: SEE-Grid, HunGrid, VOCE and the UK National Grid Service. SEE-Grid is the South-East European Grid infrastructure, while HunGrid is the Hungarian VO and VOCE is the Central European VO of the EGEE Grid.

Virtual Laboratory - closer the eScience

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An advanced scientific research becomes more and more expensive nowadays. It concerns especially experimental science, where the major cost of the research and development belongs to the experiment. Additionally the laboratory equipments that are used during the experimental work are very expensive and therefore unique as well, i.e. spectroscopes, radio telescopes or CAT scanners.

Only big regional or national centers can afford to purchase and use it, but on a very limited scale. That is a real problem that disqualifies all other research groups not having direct access to these instruments. On the other hand we notice a lot of activities in European Union related eInfrastructure and equal chances for the entire scientific community.

The Virtual Laboratory (VLAB) project deployed a general architecture framework, which plays a crucial role in equalizing the chances of all research groups. It enables a remote usage of much different scientific instrumentation and focuses its activity on embedding labor equipments in grid environments (handling HPC and visualization). In general the issues concern the standardization of the labor equipment definition to treat it as a simple grid resource, supporting the end user under the term of the workflow definition and prioritizing jobs, which follow experiments on the equipments.

The VLAB in its current state is operational in a distributed computational environment. The physical layer includes the Polish national optical network PIONIER and the HPC and visualization infrastructure. The application, in fact the framework, can be used in all experimental disciplines, where access to physical equipments is crucial, e.g., chemistry (spectrometer), radio astronomy (radio telescope), or medicine (CAT scanner).

The scientific community will benefit from this project for several reasons. It will make scientific work easier. The infrastructure will provide remote access to laboratory devices. The users from smaller science institutions can use devices unavailable for them because of the cost or distance from the laboratory, which possesses it. VLAB delivers also additional functionality, like digital libraries (training courses for young researchers, data base of results with advanced visualization), tools for collaborative work and workflow systems, making the experiment as easy as possible ...

Selected Part of Solving Sparse System over Z^2 via Block Lanczos Algorithm

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Nowadays Lanczos algorithm belongs to mostly used methods solving large sparse linear systems. In our article we focus on solving systems over field Z^2. It has some advantages opposite to real case, because elements of this field can be represented as bits and therefore we can work with whole block of bits. But this needs effective implementation of matrix multiplication discussed below.

Supercomputers applications in quantum chemistry

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Quantum-chemical calculations are based on solving a great number of integro-differential equations. They demand multiple operations with huge matrices and additional space for the storage of huge number of the integrals evaluated in each step of the iterative SCF procedure to obtain the energy and electronic structure for the given geometry and electronic state of the molecular system under study. In the next steps, geometry optimization (based on energy gradients) and/or physic-chemical properties evaluation follows. Author's experience with large molecular systems calculated using various quantum-chemical software packages on some supercomputers is presented.

Latest advances in fully coupled thermal structural calculations using finite element method (FEM) with new energy conservation equation

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In this paper some latest advances in fully coupled thermal structural calculations are presented. The analysis is based on a new energy conservation equation, which the author believes represents the most complete formulation of the first principle of thermodynamics. The equation was implemented into a finite element code using large strain/ large deflection formulation utilizing the updated Lagrange method and the extended NoIHKH material model for cyclic plasticity of metals. If the new energy conservation equation proves to be experimentally correct, it will open new perspectives in the study of all coupled thermal-structural problems, mainly in the area of fast/ultra fast thermo-elasticity or thermo-plasticity.

Simulation of Data Flow Architecture in Parallel environment

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The paper describes simulation of the parallel data flow architecture DF KPI. This is designed on the department of computers and informatics FEI TU Košice. This contribution is divided to three parts. In the first part is described architecture of DF KPI. Next part describes some problems with programs writing (DFG) for data flow architecture. Third part describes simulation tool, which was developed for simulation of parallel architecture DF KPI. Additionally in this part is also described migration the simulator to the grid or cluster architecture.

CERN/LHC experimenty ATLAS, ALICE a ich výpočtové nároky na GRID

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The Large Hadron Collider (LHC) currently being built at CERN will produce enormous amount of data (nearly 15 Peta-bytes of data annually), which the community of high energy physics around the world will access and analyze. This paper describes the computing requirements and specifications of ALICE and ATLAS LHC experiments and discusses the contributions of Slovak institutes involved in these experiments from this point of view.

Job management in the LCG-type Grid

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Secure co-existence of many users' jobs in the Grid requires usage of certificates that allows also assigning different roles and priorities. Firstly, certificate management applicable in most of present-day Gird testbeds is introduced, and then a job preparation is described, with secure role transfer, job submission specifications and usage of MyProxy technique. Finally, a demo will show our FloodGrid application developed in the CrossGrid project using LCG middleware, now being ported into EGEE testbed that is operating in LCG but now starting to use its own gLite middleware.

Grid technológie v modelovaní dopravnej problematiky

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The content of this article summarizes the authors‘look from design the grid computing information systems in the transport. This is accomplished by some computers, which are able to create a grid computer system for solving. The grid computing system is needed for fulfiiel estimation and controls the large transport problems. Communication and modeling of this system is made by communication computer of the type knot. An important issue is the manner of methods using modeling stateful resources with web services in simulation and analytic approaches, sophisticated compute of simulating models. By modeling the real transport problems on the grid computers is supported the time saving.

A Real-Coded Genetic Algorithm for the Determination of Liquids Refraction Index

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Double exposure holographic method has been widely used to determine parameters of objects such as their refractive indices or sizes. However, there is a great disadvantage of this method – the refractive index of the used immerse liquid has to be known very accurate. This work schemes out a technique how to estimate the refractive index of immerse liquids for interferometric purposes and how to eliminate its refractive index change in dependence on the change of temperature and on shakes.

Ordered Fuzzy Decision Tree Building in Parallel

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Fuzzy decision tree (FDT) induction is an important problem of Machine learning and Fuzzy logic. There are several methods for Fuzzy Decision Trees (FDT) induction. One of the key points of these methods is choice an expanded attributes which associated with FDT node. Now we propose some heuristics for select such expanded attributes with differing costs. The basis of these heuristics is cumulative information estimation. Usage these heuristics allow us to build FDT with different properties: unordered, ordered FDT, etc.

e-Science: Experiences with utilization of the grid computational model based on using of the ARC middleware

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The aim of this contribution is to present the long term personal experiences with the grid computing obtained by using of the ARC middleware. The ARC middleware is provided by the open grid project: NorduGrid. In May 2002 NorduGrid built up a Grid infrastructure which has been suitable for production-level research tasks. Around this university project a multidisciplinary community of users grew up. We successfully applied the ARC middleware which is robust, reliable and user friendly, to solve the research tasks regarding to complex avalanche dynamics and image pattern recognition in microscopic video sequences. In the near future the computational tasks from other research areas such as biophysics, biochemistry, computational chemistry and high energy physics (CERN LHC experiments) are expected.

Authentication in Grid

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This document globally describes authentication methods and procedures, which are parts of the GSI component used in Grid environment. Document is specially addressed to authentication using standard X.509 certificates and out of it derived proxy certificates. In the last chapter, generation and usage of these certificates in Grid tool Globus Toolkit 4.0 are described. This paper contains concrete procedures of certificates generation, their security and usage during authentication. .

Analytical Modeling of Optimized Sparse Linear Code

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The high performance of nowadays programs (including numerical algebra packages) is achieved by explicit loop restructuring (mainly loop blocking). These transformations result in better temporal and spatial locality. In this paper, we introduce some basic techniques for improving the performance of programs. Then, we describe source code transformations based on loop reversal and loop for the SESOL (as an example of a mathematic modeling tool) code. We have concentrated on nowadays IBM processor's architecture with L1 and L2 caches. Our optimizations results in the significant performance improvement.

Environmental assessment of climate-change driven risks in landscape –decision support tool

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The data-knowledge infrastructure for environmental modeling in field of agriculture and forestry has been established as a framework for generating the environmental variables needed in process of environmental assessment. Nowadays, the data-knowledge infrastructure prototype developed is being tested within the scope of EC project INSEA (Integrated Sink Enhancement Assessment, www.iiasa.ac.at/Research/FOR/INSEA/). The primary aim of environmental modeling within the project is to produce reliable environmental data (NUTS2 level) consecutively realized in socio-economical assessment models (EUFASOM) on the NUTS0 and EU25 level. The EPIC model (www.brc.tamus.edu/epic/) is employed to set the environmental variables (greenhouse gases emission/sequestration, drought stress, crop production, soil erosion, etc.) with respect to climatic scenarios and management/land use alternatives firstly predefined. The data-knowledge infrastructure defined like a modeling framework becomes substantial when it is related to geographical areas. Data origin (mostly geo-referenced data in raster data representations) and modeling time step/period assumed requires sufficient computation facilities and capabilities, when the environmental variables being modeled have to be set up on the regional or higher administrative level (national, EU). The number of individual modeling elements (individual cell number, homogenous units) as well as the number of possible combinations of input variables and time step/period defined is rapidly increasing the number of model runs and results in huge amount of data need to be post-processed.

Grids and User Applications

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Collaborative science requires access to large, heterogeneous data collections, large-scale computing resources, high-performance networking and visualization. These environments combine aspects of traditional distributed and parallel computing systems - Grid systems. In this document we give a concise answer on the questions "What is the Grid and Grid computing?". First, the Grid concepts and technologies will be introduced. Most of the definitions are undertaken from the publications of the fathers of the Grid vision: Ian Foster and Carl Kesselman. In the second Section we describe brief the Grid architecture. The third Section is focused on the Globus Toolkit 4 (GT4) which supports the development of service oriented distributed applications and infrastructures. The Section 4 makes analysis of computational problems, and outlines some categories of them. The last Section presents how a computational task can be submitted to run on a Grid using the GT4 middleware.

E-Veda v EGEE - virtuálne organizácie

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This document gives a brief overview of the fields of research that uses the EGEE grid infrastructure. Description of the concept of virtual organization and the relationship between VO and its users is given. The method of creating new VOs by the EGAAP advisory board is explained. The special dteam VO is described. In the following a brief overview of existing virtual organizations covered by EGEE is given, with a description of the respective domains of research. Several proposed projects which are submitted to the EGAAP board are also described. Document is targeted towards researchers who consider using EGEE grid resources in their research by joining one of the existing VOs or by proposing a new one.

EGEE middleware for grid application developers

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The EU EGEE projects aims to build the largest general purpose Grid in a world. While primarily driven by the requirements from High energy physics community, the EGEE middleware -- gLite -- provides a solid basic Grid working environment. The lecture will provide a short gLite middleware overview, followed by more specific information about the key features of the gLite workload management and data management concepts.

More detailed explanation will be given to services developed by the CESNET (Czech Republic) groups, that target the difficult task of job tracking in a distributed Grid environment. The overview and details of use of the Logging and Bookkeeping service, which keeps up to date information about live jobs on the Grid, will provide enough details for its advanced use and for understanding of information that it provides. The newly introduced Job Provenance is a job information repository, that keeps data about all the jobs run on an EGEE Grid (currently provided they were submitted via the gLite workload management system). This data could be used for any statistical purposes (including the evaluation of Grid performance), but they can also be used to re-run jobs in the same or modified conditions.

The EGEE users are organized in Virtual Organizations (VOs), that are also responsible for allocation of resources and VO specific user support. Most EGEE VOs are application oriented, we will present a VOCE, the Virtual Organization for Central Europe. This VO is application neutral, providing international Grid environment for people with serious grid needs but not (yet) associated with any application oriented VO. The way how to register and use VOCE, and how to access information related to it will be presented.

In the last part, high level API for grid applications (GAT), outcome of a GridLab project, will be introduced. This API, which is currently furtherly developed within the Simple Application Grid API (SAGA) activity in GGF, targets application developers needs for a simple uniform development environment for otherwise complex and heterogeneous Grids.

Collaboration and Knowledge Sharing in Grid Applications

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In this paper we describe a solution for collaboration and knowledge sharing based on text notes entered by a user. Theory, implementation and use of such system – EMBET is described. The key idea is that a user enters notes in a particular situation/context, which can be detected by the computer. Such notes are later displayed to other or the same users in a similar situation/context. The context of user is detected from computerized tasks performed by user.

In the K-Wf Grid, grid services are semi-automatically composed to workflows, which should solve a user problem. It was identified that even when services and input and output data are well semantically described, there is often no possibility to compose an appropriate workflow e.g. because of missing specific input data or fulfillment of a user and application specific requirements. To help user in workflow construction it is appropriate to display notes and suggestions entered by the same or different users. Thus experts can collaborate and fill up application specific knowledge base with useful knowledge, which is shown to users in the right time.

The solution was used and evaluated in the Pellucid IST project and it is further developed in the K-Wf Grid IST project.

K-Wf Grid project demo

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The K-Wf Grid project aims at developing a system, which would enable even unskilled users to access the facilities of Grid computing. It allows users to create workflows of grid and web services, execute these workflows and view their results. Moreover, it employs comprehensive monitoring system and knowledge management facilities in order to learn from each service execution. The learned facts are then examined and later used for better composition of new workflows. The project middleware is accessible through a collaboration-enabled web portal. The project uses three different applications to test the developed middleware suite. Two of these applications deal with modeling - one of weather, the other of traffic and pollution. Third application is a business ERP system.

FloodGrid demo (CrossGrid project)

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CrossGrid project has developed, implemented and exploited new grid components for interactive computation- and data intensive applications like simulation and visualization for surgical procedures, flooding crisis team decision support system, distributed data analysis in high-energy physics, and air pollution combined with weather forecasting. This presentation will show our FloodGrid application developed in the CrossGrid project that consist of cascade of three simulations (meteorological, hydrological and hydraulic). Application configuration (preparation of parameters) and interactive steering of the FloodGrid application is done via our web portal, through which also visualization of simulation results can be shown.

Grid infrastructures in Central Europe

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The paper presents current state of Grid infrastructures in Central European countries. It aims to provide information for discussion about future of Grids in Slovakia, by presenting how are the national Grid initiatives organized in surrounding countries. After brief introduction to different types of Grid infrastructures, national Grid infrastructures are presented in more detail with focus on type of coordination at national level. While some countries have Grids initiatives established as projects funded at national level, others have Grid centers coordinating Grid related national activities. At the end, the current state of Grid infrastructure in Slovakia is presented.

IEPSAS-Kosice: experiences in running LCG site

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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 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 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.

Mediterranean Grid of Multi-Risk Data and Models

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The paper presents the MEDIGRID project that aims at creating a distributed framework for multi-risk assessment of natural disasters and it will integrate models of forest fire behavior and effects, flash floods and landslides. These models will be upgraded to web applications in order to be able to run remotely as web services over the internet. A distributed repository with EO data combined with field measurements will be created. In the paper the MEDIGRID system architecture and simulation models are described, with conclusions towards the project's future.

Knowledge Assimilation for Performance Prediction of Grid Services

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As the Grid 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 workflow scheduling. A service is needed which is able to estimate the behaviors of each web service deployment in the Grid. Herein we present the design of such service capable of estimating WS behaviors 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.