

WEB PORTAL FOR SCIENTIFIC COMPUTING LIBRARY

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ABSTRACT

Scientific computing or computational science is a collection of tools, techniques and theories required to develop and solve mathematical models in science and engineering on a computer. There are many systems of scientific computing libraries developed nowadays, regardless of whether they are web-based or web application. However, the libraries are complex and not complete. In addition, most science teams collaborate across multiple geographically distributed institutions, therefore, it becomes more difficult to store, share and analyze the scientific data among the team members. By developing this Web Portal for Scientific Computing Library, good criteria of scientific computing library are identified. This project aims to provide sophisticated web portal to store codes, share results, and share knowledge on scientific computing. Furthermore, the scientific computing library focuses on multi-domain applications. The technologies used for this web portal development are ASP.Net as the scripting language with use of Microsoft Visual Studio 2008 and Microsoft SQL Server 2005 as the database application development software. The data set used is sequential algorithm in C and C++ programming language based on numerical simulation of partial differential equation. It is hoped that this project will give benefits to the scientists who utilize the scientific computing for their researches.

ABSTRAK

Komputeran saintifik atau komputasi sains ialah suatu koleksi alat-alat, teknik, dan teori yang diperlukan untuk membangunkan dan menyelesaikan model matematik dalam sains dan kejuruteraan menggunakan computer. Terdapat banyak sistem untuk perpustakaan komputeran saintifik yang dibangunkan hari ini, sama ada dalam bentuk web atau aplikasi web. Walau bagaimanapun, perpustakaan tersebut didapati complex dan tidak lengkap. Kebanyakan kumpulan sains berkolaborasi dengan institusi sehingga merentas sempadan geografi. Oleh itu, ia menjadi sukar untuk menyimpan, berkongsi, dan menganalisa data saintifik antara ahli kumpulan. Dengan membangunkan Portal Web untuk Perpustakaan Komputeran Saintifik ini, kriteria yang bagus untuk perpustakaan komputeran saintifik dikenalpasti. Projek ini menyasarkan untuk menyediakan portal web yang sofistikated untuk menyimpan kod, berkongsi hasil keputusan, dan berkongsi pengetahuan mengenai komputeran saintifik. Tambahan pula, perpustakaan komputeran saintifik ini memfokus kepada pelbagai bidang aplikasi. Teknologi yang digunakan untuk membangunkan portal web ini adalah *ASP.Net* sebagai bahasa pengaturcaraan dengan penggunaan *Microsoft Visual Studio 2008* dan *Microsoft SQL Server 2005* sebagai perisian pembangunan aplikasi pangkalan data. Set data yang digunakan adalah algoritma turutan dalam bahasa pengaturcaraan C dan C++ berdasarkan simulasi numerik persamaan pembezaan separa. Projek ini diharap dapat memberi faedah kepada saintis yang menggunakan komputeran saintifik untuk kajian.

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CHAPTER I

INTRODUCTION

1.8 Introduction

People nowadays are unquestionably dependent on computers and the Internet that connect them. The emergence of Internet has affected the way people live. The growth of Internet exceeds according to recent statistics reported in Internet World Stats for year 2008 on world Internet users, there is more than 1.596 billion people use Internet. From that number, Asia region users rank highest with 650.4 million of Internet users (refer to Figure 1.1). Malaysian Communications and Multimedia Commission (MCMC) published statistics on Malaysia's internet penetration in their report on year 2008 that 14.9 million people which are equivalent to 59% of the Malaysia population are Internet users.

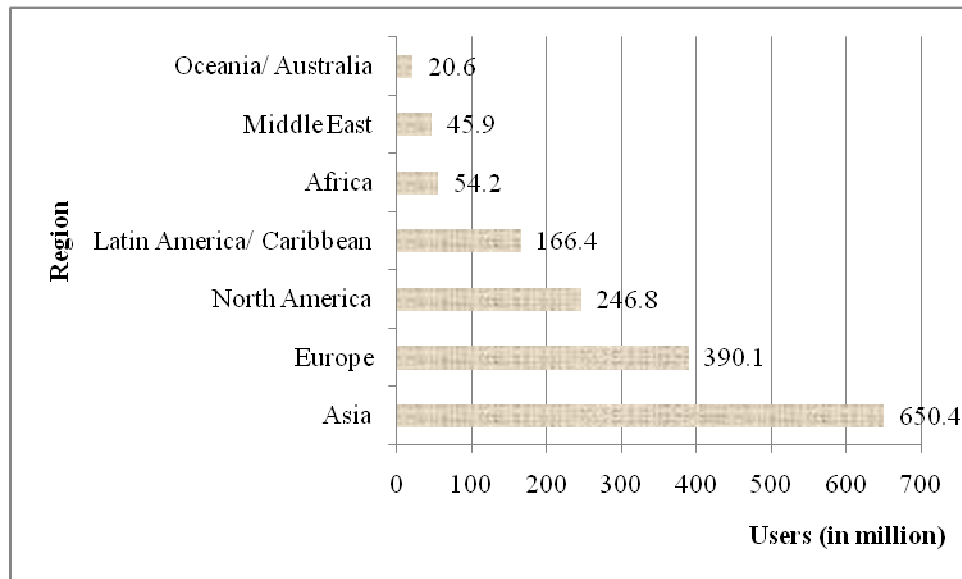


Figure 1.1 World Internet users by world region (Internet World Stats, 2009)

Advances in new information technologies and development of the Internet and World Wide Web (WWW) in the 1990s have changed the computing environment for both individuals and businesses. Since its birth in the 1990s, people have been witnessed to widespread use of the WWW for commercial purposes (Li and Dasgupta, 2005). Variety of web applications are also includes scientific applications.

According to Borgman *et al.* (2004), few repositories offer the tools and services that scientists appear to desire, such as the ability to store data for personal analysis and use, and tools to monitor and interpret data in the field so that changes can be made to experiments in progress. The majority of scientific researchers save all of their data and they reuse those data when applicable to future research. However, their available tools support analysis of data much better than they do preservation and sharing. As a result, scientists often store data with minimal documentation and do little toward preservation other than to back up files. These approaches are largely local and do not adequately support future access and use. Therefore, an approach of Web Portal for Scientific Computing Library (PSCL) will be developed to overcome the current problem.

A few studies have investigated and surveyed web-based scientific computing library research in the recent past. These studies include proposing collaboration tool to support and facilitate data sharing (Chin and Lansing, 2004; Drummond and Marques, 2005), discuss on management of computing services and resources, and also building

and executing complex application (Dozsa *et al.*, 2006; Suzumura *et al.*, 2001), aims on repository concept for scientific computing (Lazar *et al.*, 2007; Brezany and Winslett, 1999; Mitra *et al.*, 2007), discuss of sharing scientific data (Chin and Lansing, 2004; Mitra *et al.*, 2007), and discuss on user environment for problem solving (Akzhalova and Aizhulov, 2007; Vazhkudai *et al.*, 2007).

1.9 Problem Background

Scientific computing library is a collection of tools, techniques and theories required to develop and solve mathematical models in science and engineering on a computer (Steeb *et al.*, 2004). Usually, it is used as predictive analysis tools. Among organizations or people that use or need this scientific computing are programmers at corporations, research laboratories and academic institutions. The core of scientific computing is designing, writing, testing, debugging and modifying numerical software for application to a vast range of areas, from graphics, meteorology and chemistry to engineering, biology and finance (Oliveira and Stewart, 2006).

From the observation that has been done on existing scientific computing libraries, it is found that the libraries are quite complex to use for the beginners and the libraries content is not complete (refer to subtopic 2.5.3). Knowledge resources are not centralized and the amount of distributed knowledge sources available can constitute an obstacle for finding and retrieving the relevant knowledge. Moreover, this critical mass of scientific computing is also a factor which contributes to the storage problem. As a result, the users waste time searching for the necessary scientific computing to perform work task efficiently (Razmerita, 2004).

According to Vazhkudai (2007), traditionally, scientists have conducted their experiments or raw data collection at various facilities, and then leave their data sets in

hand for analysis back at their home institutions. Most science teams collaborate across multiple geographically distributed institutions. Therefore, it becomes difficult for each user to store and analyze a given experiment's data storage and management infrastructure is imperative for the full production scale of experiments to ensure flexible and efficient accessibility and the proper integrity of metadata management and tracking. Even the majority of users, especially at academic institutions are given an integrated software analysis infrastructure; they would often be confined to run analyses just on local desktop computers. Therefore, access to computational resources is required to properly conduct more sophisticated data analyses, or any associated simulation / modeling of experimental samples.

1.10 Problem Statement

This research focuses on developing a PSCL based on four domains which are chemistry, biology, mathematics, and computer science. Comparison of existing system on scientific computing library in market and comparison of previous studies on scientific computing library were done.

The following research question is addressed to solve the problem: Could PSCL stores and manages data in multiple formats and multi-domain applications?.

This research is conducted to address the issues by utilizing content management system using web portal technology. The system proposed allows solving different scientific problems at any time through the internet technologies. It offers an attractive alternative to expensive supercomputers and parallel computer systems for high-performance computing.

1.11 Objectives

This project aims to achieve the following objectives:

- a) To investigate scientific computing library as a content management system and the way it can be managed online.
- b) To study the criteria of existing scientific computing library in market.
- c) To gather and analyze scientific computing material for the repository.
- d) To design and develop a prototype web-based application to support scientific computing library that can manage scientific algorithm.

1.12 Scope

The scopes of this project are:

- a) The study focuses on scientific computing for real case problem in Institute of Ibnu Sina (IIS), Universiti Teknologi Malaysia (UTM).
- b) The data set focuses on sequential algorithm in C and C++ programming language which is based on numerical simulation of Partial Differential Equation (PDE) for any physical problem statement.
- c) The prototype is done for UTM and focuses on the proposed model.
- d) The project develops a prototype web-based application for managing scientific algorithm with three modules which are users, scientific algorithm providers, and scientific librarian.

The shaded area in Figure 1.2 shows scope of research that is done in this project. This research framework acts as a guideline for the author to do the research. This scope will be discussed in detail for the later chapters.

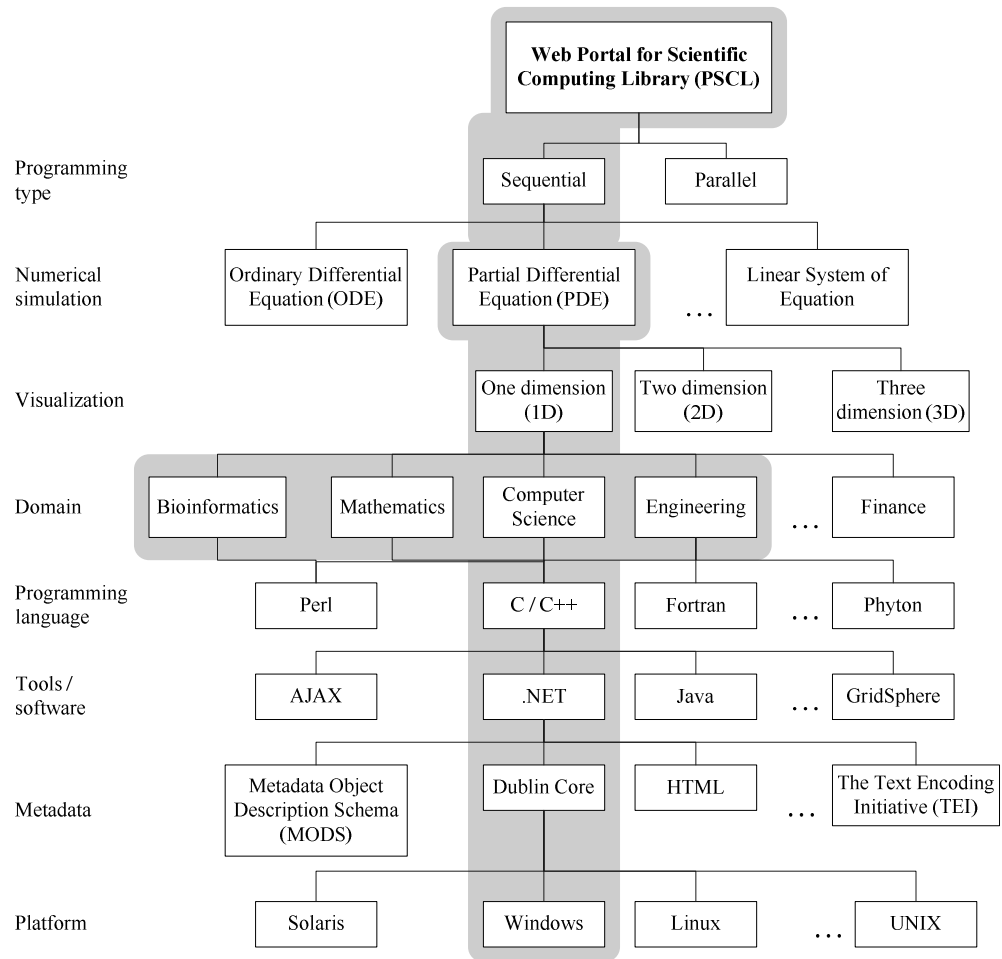


Figure 1.2 Research framework

1.13 Project Importance

Ideally, users would like all resources to be virtualized and not to have to deal with storage or transfer components and issues. Therefore, the importance of the PSCL is to enable widely accessible scientific computing, anytime and anywhere, without worrying about the physical storage or data transfer. It is hope to shorten time for researchers to search a huge amount of scientific computing and thus, can improve their experiments. PSCL also enables:

- a) Scientists to easily store, archive, and publish data to the community.
- b) Data and basic knowledge sharing among scientists.
- c) Scientists to search and retrieve information that they require.
- d) Scientists to share their insights with others without geographically constrained.
- e) Utilization of mathematical simulation to support the target market and target user.

Due to the growing complexity of the web, portals have become essential to the Internet users. Portals allow easy access to information by integrating heterogeneous applications or data sources in consistent way. It gives users a personalized and restricted view of domain information (Rovan, 2008).

This scientific computing library will be developed in order to:

- a) Achieve accuracy, reliability, and stability towards the exact solution in multi-discipline industry.
- b) Help the target market.
- c) Minimize the absolute error between approximation solution and exact solution.
- d) Solve actual problem in industry.

The PSCL will be developed with hope to give better understanding about sharing of scientific data among users. It also hopes to give general knowledge on simulation of the scientific data in order to get the result.

1.14 Chapter Summary

This chapter gives general idea on the project of PSCL based on research of repository of scientific data. Problem background describes current problem in managing scientific computing. Problem statement is the main question that needs to be addressed. Objectives are elements that need to be achieved at the end of this project, while scope is the project boundary that has been identified. Project importance explains on the benefits gained by the parties involved in this project. It is hoped that this project will be very beneficial to everyone and can contributes to the future of research and development.

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