GRID computing in Drug Development, Dispensing Using MEMS and NEMS

Prof. Shonal A Vaz
Lecturer Vidyalankar Polytechnic,Wadala,Mumbai

Prof. Chetashri S.Bhusari
Lecturer ,Vidyalankar Polytechnic,Wadala,Mumbai

Prof. Bhagyshri Kulkarni
Lecturer, Vidyalankar Polytechnic,wadala,Mumbai

Abstract

In this paper we will discusses how grid computing can be used to design and implementation the process of drug discovery and dispensing by continuously monitoring the person with the helps of MEMS and NEMS. With the development if Grid computing it is possible because Grid computing allows users to share computer power and data storage capacity over the internet on any zone or locale. Today grids computing enhanced work done in many fields of healthcare and MEMS/NEMS have scaled this feature, also taken the initiatives to design HealthGrid which is working for both clinicians and researchers to create and promote awareness of the advantages associated with the grid technologies.

Keywords : Grid Computing, MEMS, NEMS, Drug Dispensing

INTRODUCTION

Grid computing connects many individual computers, creating a large system with massive computational power and with no barrier of the distance between the two systems. Since the job is divided into many small pieces that can be processed simultaneously, research time is drastically reduced from years to months or even days as on today. Importance is the cost effectiveness of the technology because we can make better use of resources which are geographically distributed[1].

Drug discovery is a process that can take as many as years from the day first drug discovered in the laboratory until the actual drug which can be used, is brought to market. The challenge for pharmaceutical companies, researchers now is reducing the research timeline between the discoveries till usage. Many such companies, researchers, technology developers are trying to achieve this goal through the application and integration of advanced technologies such as grid computing, chemistry, computer graphics and high performance computing (HPC). Molecular modeling has facilitated as a popular methodology for drug design, it is nothing but combination of computational chemistry and computer graphics. Molecular modeling can be implemented as a master–worker parallel application, which can take advantage of HPC technologies such as clusters and Grids for large-scale data exploration[2].

MEMS, or Micro-Electro-Mechanical Systems, are tiny chips that can be produced by semiconductor processes to combine mechanical sensing, control and motion to solid state electronics to deliver extraordinary functionality and versatility. Essentially all of the mechanical and electromechanical machines from the macro-world can now be crafted into a tiny chip that can enter the micro-world and

interact with life systems. MEMS can sense pressure, detect motion, measure forces, identify bio-agents, pump and control fluids, and perform other actions that have great value to the medical and biological fields[8].

Automated dispensing systems uses electronic and controlled dispensing of the drug stored in the storage devices. Tracking can be done for the amount of drug to be dispensed the drug and more important is when to dispense the drug. The main here is it help nurses to obtain medications at the point of use for the person[11].

As the a summary of above discussion,MEMS and NEMS are used to track the medical parameter of the person, which can be submitted to grid computing system, Grid will help in development of the drug with the help of stored data of previous researcher and also with the help researcher using grid, and finally patient can be given medication at appropriate time even if he forgets.

How Grid Technology is used by different actors in health care

- Researchers can use grid computing's processing power to hunt for new viruses, search and discover for new drugs, model disease outbreaks, image the body's organs and determine treatments for patients
- Doctors can power of grid computing to access the relevant health data irrespective of where and how the data is used it is stored.
- Patients can be made aware by giving a more individualised form of healthcare
- Healthcare workers can be in better position to collaborate and even share large amounts of information between all of them [11].

How MEMS/NEMS can be used for Drug Dispensing

MEMS/NEMS act as transducer which convert physical parameter into electrical quantity like voltage, current and uses communication system to communicated them. Today variety of MEMs systems are available, MEMS system consist of

- Micro-pump – used to pump small amounts of drug (about pico-liters)
- Micro-gear – this is a SEM (Scanning Electron Micrograph) of a Sandia Gear, each tooth is about 8um or the size of a human red blood cell
- Micro-mirror – used in telecommunications.
- Fluid Channel – for micro pump
- Heads Up display – the reason this is a MEMs device is because it utilizes micro mirrors.

How Grid Computing and MEMS technology can be Integrated Architecture

Aim of Drug Discovery Grid is to build a collaboration platform using which drug discovery can be implemented. The main purpose of project is to use large-scale computation and data intensive scientific applications in the fields of medicine chemistry and molecular biology with the help of grid middleware.

Grid platform

Since its Grid computing, it involves supercomputers, clusters, and PCs owned by universities, research labs, and companies. These resources are centrally managed by IT professionals, are powered on most of the time, and are connected by full-time, high-bandwidth network links. But these resources usually are underutilized. In order make the full usage of this systems increase the throughput these systems can be used when they are idle. One such application Drug Discovery Grid. We only use the idle time of the cluster and supercomputing system.

Software and Resources of the drug development Grid

Drug Development Grid is build on the existing Grid technologies and tools for performing compute and data intensive computing on distributed resources. Therefore there is necessity of a layered architecture and the software. This are essential for performing molecular modeling on distributed resources. The components of the **Drug Development Grid** software and resources used are:

1) The Dock and gsDock software for molecular modeling.
2) Toolkits for Drug Discovery such as CDB maintain software, preprocess and security-related tools.
3) Web portal for grid administrator, resources provider and consumer.
4) Grid middleware based on BOINC .

Module in which Drug Development Grid is implemented

Drug Development Grid mainly contains four major components of Modules:

- Front End
- Access Node
- Compute Client and
- Applications

Front End : It is global main server, consists of the following modules:

- Job management module (scheduling, task generator, Distribution of task, result accumulation and result evaluation etc.),
- User Management module,
- Resources Management module,
- Data Service and
- Web Portal.

Access Node: It is similar to front end. It consists of the following modules:

- local job management module,
- local resources management module and
- local data service.

The default implementation of the local job management module is OS-based fork process on every

Computer Client:

The resource management plug-in for LSF is also deployed on some sites with LSF(Load Sharing Facility) faculty. Other plug-in for PBS(public broadcasting Service), Condor and GE(Grid Engine) is also considered.

The Compute Client software installed on every node of site. When idle, a request for the data on a specific illness from slave server. Then it perform computations on this data, stores the results back to the slave server, once the present task is completed demand for a new task is generated. The slave server maintains local resources. It will request more work from global resource on demand[11][12].

Implementation and Application of Drug Development Grid

Drug Development Grid uses a simple but rich set of abstractions for files, applications, and data. A project defines application versions for various platforms (Alpha, Linux/x86, Linux/AMD64, intel Param etc.).

An application can consist of an many set of files. A task represents the inputs to a computation: the application contains a set of references files as input, and sets of argument and variable carrying information. Each task has parameters such as compute, memory and storage requirements and a even deadline for completion. A result represents the result of a computation: it consists of a reference to a task and a list of references to output files.

Files (associated with application versions, task, or results) have project-wide unique names and are non editable. Files can be replicated, uploaded and Download: It consists file includes a list of URLs from which it may be downloaded or uploaded. These files have information about where they should resident in the host or the server, to prove authentication of the file and how they may be transferred on the network that is in compressed or uncompressed format.

When the compute client communicates with a scheduling server it reports completed work, and receives an document describing a collection of the above entities. The client then downloads and uploads files and runs applications; it maximizes concurrency, using multiple CPUs when possible and overlapping communication and computation.

The server complex of a project is centered around a relational database that stores descriptions of Drug Development Grid applications, platforms, versions, task, results, accounts, teams, and so on. Server functions are performed by a set of web services and daemon processes: Scheduling servers handles RPCs(Remote Processes calls) from clients; it issues work and handles reports of completed results.

Data server's handles file uploads using a certificate-based mechanism to ensure that only legitimate files, with prescribed size limits, can be uploaded. File downloads are handled by plain HTTP[11].

MEMS and Network of Computer

Micromirrors: photonic/Optical communications

Micromirros are responsible for development of network of MEMS. Micromirrors are the fundamental micro-mechanical component for optical cross connect switches that switch light frequencies from one set of fibers to another. This process includes an input/output port, an actuator, and a mirrored surface. When voltage is applied to the actuator, it causes the mirror to move and direct the light to a specific output port. The mirror then remains static until the light path needs to be redirected.

The transmission fibers used are simple, unamplified, single-channel 2.5-Gb/s pipes to optically amplified, Tb/s systems transporting hundreds of wavelength-division-multiplexed (WDM) light signals.

The result is an end-to-end photonic network which is more reliable and cost-effective, and which has minimal performance drop-off. However the development of an all-optical network has been complex and challenging due to the integration of optics, mechanics and electronics[7].

Privacy and consent

Grid technology can offer the field of medicine numerous benefits, but its application to healthcare is not straightforward.

Major issues with such wide spreading of data on the grid are

1. Issues concerning security, data protection and privacy
2. Will the researchers share the data
3. Whether patient is willing so share his bio-logical data
4. Whether the one suing the data will give proper results
5. Anit MEMs committees will allow to follow such process.

Many grid-based eHealth initiatives involve the storage of large amounts of patient data that must be kept in an accessible but secure manner, and must abide by data protection laws. eHealth initiatives must be designed with this in mind, and services provided to anonymise data.

However with care, healthgrids can overcome these issues.

RadiotherapyGrid,used in the treatment of cancer patients, ensures the data is fully secure by using security tools built into EGEE that only authenticated users have access to. Patient consent will also be of vital importance when dealing with data about identifiable individuals in healthgrids, as in other areas of healthcare.

Patients should be fully informed about who will have access to their records and how they will be used. Well-defined research can cope with these restrictions and initiatives such as @neurIST and Health-e-Child successfully use patient data to improve treatments[5].

Medical and Health care with help of grid computing in India

GARUDA is India's first national grid initiative bringing together academic, scientific and research communities for developing their data and compute intensive applications with guaranteed QoS. GARUDA grid is an aggregation of resources comprising of computational nodes, mass storage and scientific instruments distributed across the country.

GARUDA is a SOA based cyber infrastructure connecting computational nodes, mass storage and scientific instruments distributed across the country.

The Department of Information Technology (DIT), Government of India, has funded Centre for Development of Advanced Computing (C-DAC) to deploy the nation-wide computational grid "GARUDA" spanning across 17 cities and 45 institutions with an aim to bring Distributed/Grid networked infrastructure to academic labs, research labs and industries in India.

The Proof of Concept (PoC) phase, initiated along with ERNET (Indian Education & Research Network), ended on March 2008, accomplished its deliverables by connecting 17 cities across 45 academic and research institutes country wide along with the required softwares for managing grid computing applications.

The establishment of Indian Grid Certification Authority (IGCA) for the first time in India by CDAC in November 2008 has allowed full access to worldwide grids for Indian Researchers and represented a landmark in this domain[10].

What Next for MEM/NEMS

BioMEMS can be interconnect micro-mechanics, silicon chip semiconductor electronics, and the basic living molecular processes and future results and discoveries and inventions will be phenomenal and sometimes unexpected.

There are Visionaries whoa re thinking blend molecular biology with computational systems at the atomic scale to create bio-nano-electro-mechanical systems (BioNEMS) that could become a major factor in nanotechnology.

But in the simple term, many small biotech concerns and some major semiconductor makers will continue to commercialize products based on BioMEMS. In some areas, BioMEMS has improved existing medical technologies. But brand new medical health care devices never before seen in the medical sector will be developed and launched for the general public[8].

CONCLUSION

Grid computing are emerging field for sharing and accumulating data which are distributed geographically. This resource can be for solving large-scale compute and data intensive problems in,medical fields like drug development, dispensing and even can be used for research of the new illness and to provide remedy for the same.

Several supercomputers and computer clusters located in different location of India as the initiative taken by GARUDA project.

To add to scalability MEMS and NEMS can be used to monitor the health of patient and by making photonic/optical network.

And Finally proper doses to be dispensed to the person under treatment. This integration of technology will improve the health status of the person due to which nation, country will be benefited since it has healthy man power.

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