

Definition...

"Grid computing is applying the resources of many computers in a network to a single problem at the same time - usually to a scientific or technical problem that requires a great number of computer processing cycles or access to large amounts of data."

A well-known example of grid computing in the public domain is the ongoing SETI(Search for Extraterrestrial Intelligence) @Home project in which thousands of people are sharing the unused processor cycles of their PCs in the vast search for signs of "rational" signals from outer space.

-According to John Patrick, IBM's vice-president for Internet strategies, "the next big thing will be grid computing."

Outline...

- Introduction to Grid Computing
 - The Need for Grids
 - Concepts
 - Examples of real life use
 - Current status
- Future plans for Grid computing at Middlesex and Grids in general.

Why...

CPU Transistor Counts 1971-2008 & Moore's Law



Why not build/use a super computer...

AS OF JUNE 2008, IBM ROADRUNNER IS THE FASTEST...

- -12,960 IBM cell processors & 6,480 Opteron CPUs....
- -103.6 TB (103,600 GB) of Memory...
- -6,000 sq ft (0.5Km x 0.5Km)
- -With a Peak of 1.71 petaflops
- -Costing \$133 Million.

-Using **2.3MW** of energy!



Clustering...

-Basically a collection of cheap... standard computers networked together to perform a common task.

-There are basically 2 kind of computing....

- HPC & HTC!

-Respectively one mainly aims to solve problems as quickly as possible while the other aims to process as much data as possible.

-The latter being more relative to grid computing.



Bio HTC examples...



BLAST... Basic Local Alignment Search Tool Folding@Home... Similar to SETI but with protein folding



Grids, Grids, Grids.....Issues!

However Grids were created by the Physic dept who quiet often had to sieve through and process PBytes of data (1000 TB or 1mill GB).

-CERN a 27 Km particle accelerator.

-Designed to bash atoms to prove theoretical sub atomic.

-TEN YEARS IN THE MAKING!!!



Issues... The List!

It is easier said than done, just couple a few computers into clusters and then make them talk to each other via the internet...NO!

•How to store and distribute large amounts of data

•How to efficiently use the available CPUs

- •How to find what services are available
- •How to make this potential Hackers WMD Secure
- •How to make this environment reliable
- •Need a standard to communicate with each other

Data Storage and Processing...

There are mainly three things you need to do with data up/download it, store it to a standard and search/process the information.

The first two a standard format and uploading/ downloading has been more or less agreed on, and the favourite has been towards Grid FTP.

The third is an active field of research and one of the more famous names to be known are Data Mining and semantics.

"Data mining is the process of extracting patterns from data. Data mining is becoming an increasingly important tool to transform these data into information. It is commonly used in a wide range of profiling practices, such as marketing, surveillance, fraud detection and scientific discovery."

...wiki





CPU cycle scavenging...

Just to get you familiar with this concept, basically systems such as Condor & PBS Torque, there exists a master computer that monitors all the computers under its sub-domain.

This however is not a grid as it doesn't allow use over the internet, or communicate with others.

GRAM is a interface of the Globus project that enable users to locate, submit, monitor and cancel remote jobs on Grid-based compute resources. GRAM enables remote execution management in contexts for which reliable operation, stateful monitoring, credential management, and file staging are important. GRAM is not a job scheduler. Rather, it provides a single protocol for communicating with different batch/cluster job schedulers.



Services and reliability...

These two cases go hand in hand given that a reliable service depends on accurate information and knowing what is out there. In the case of Globus this is handled by the Monitoring and Discovery Services (MDS).

Similar to the CPU case, information like, CPU usage, Memory & Software Installed is traversed up a network tree to a master node in its domain which can be queried.

The overhead and delays involved will reflect on the accuracy of the data and is a limiting factor limiting the QoS a grid can give.

This information is also used in workflow managers to reliably execute more complex date flows. (note Taverna)



Security...



Given that possibly anyone can join or use a Grid (possible misuse), a management system was needed.

Trusted entities were established, mostly representing real organisations to issues certificates to uses; And so this is what Grid consist of to date,

A collections of Virtual Organisations that handle user identification and log all usage by users for liability.





Communications...

In order for grid to communicate with each other a common language must be defined and work over the internet.

The most preferred protocol has now become SOAP, and is the Bases for Web Services.

This basically is similar to HTML/XML, and is in more or less plain English and can be read with notepad.

Two main things...

- 1) Services can be used using a web page
- 2) Jobs that are submitted are also in this format.

Still some people still like to use the command line.

Figure 1 <wsdl:message name="TitleInquirySoapIn"> <wsdl:part name="parameters" element="tns:TitleInquiry" /> </wsdl:message> ... <wsdl:types> <s:schema elementFormDefault="qualified" targetNamespace="http://mycounty.com/"> </s:schema elementFormDefault="qualified" targetNamespace="http://mycounty.com/"> <s:schema elementFormDefault="qualified" targetNamespace="http://mycounty.com/"> </s:schema elementFormDefault="qualified" targetNamespace="http://mycounty.com/"> </s:schema elementFormDefault="qualified" targetNamespace="http://mycounty.com/"> </schematraction="http://mycounty.com/"> </schematraction="ht

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The NGS used to stand for the National Grid Services, but are undergoing a rebranding and can't shake of this term!

It is a free Grid for academic use consisting of many institutes....





Because the NGS is an existing professional, entity – an executive decision has been made to off load all the management side of Grid computing at Middlesex to them.

This means that there is **always some one to support** your queries.

Also while we are formulating our resources at Middlesex, **We can use the existing facilities** already up an running provided by the NGS members.

Why should we even bother with providing our resources? Why not leech!

Who Uses The NGS...

There are many applications in use, I however will go thorough just a few, one in each field.

NGS Scientific Software Applications



CosmoMC...



CosmoMC is a Markov-Chain Monte-Carlo (MCMC) engine for exploring cosmological parameter space, together with code for analysing Monte-Carlo samples and importance sampling. The code does brute force (but accurate) theoretical matter power spectrum and Cl calculations with CAMB.



EMBOSS is a suite of bioinformatics applications i.e. sequence analysis programs and other assorted programs like enzyme kinetics.

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Emission tomography and especially Positron Emission Tomography (PET) has a fast growing importance in modern medicine for both diagnostic and treatment purposes. At the same time there is a demand for higher imaging quality, accuracy and speed. Enhanced by the wider availability of powerful computer clusters, Monte Carlo simulations are an essential tool for current and future emission tomography developments. Examples for such developments are the design of new medical imaging devices, the optimization of acquisition protocols and the development and assessment of image reconstruction algorithms and correction techniques.



That's a MOUSE!

LAMMPS

LAMMPS has potentials for soft materials (biomolecules, polymers) and solid-state materials (metals, semiconductors) and coarse-grained or meso-scopic systems. It can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale.

LAMMPS runs on single processors or in parallel using message-passing techniques and a spatialdecomposition of the simulation domain. The code is designed to be easy to modify or extend with new functionality.

LAMMPS is distributed by Sandia National Laboratories, a US Department of Energy laboratory.





Weka is a collection of machine learning algorithms for data mining tasks. The algorithms can either be applied directly to a dataset or called from your own Java code.

Weka contains tools for data pre-processing, classification, regression, clustering, association rules, and visualization. It is also wellsuited for developing new machine learning schemes.



Abaqus...

Abaqus is a commercial Finite Element Analysis Program produced by Simulia. According to the code authors "It allows the detailed behaviour of a complex assembly to be studied to: refine concepts for a new design, understand the behaviour of new materials, or simulate a discrete manufacturing process. The software suite delivers solutions for nonlinear problems and large-scale linear dynamics applications."





Blender

Blender is the free open source 3D content creation suite, available for all major operating systems under the GNU General Public License.

It can be used for modelling, UV unwrapping, texturing, rigging, water simulations, skinning, animating, rendering, particle, and other simulations, non-linear editing, compositing, and creating interactive 3D applications, including games.



Not what you want???

The above were only a few real examples, unfortunately what services that are on the Grid are dictated by its user. And as you may have notices it was mostly modelling and simulations.

In reality, the grid should be as versatile as your normal desktop computer, so long as it can run on a computer, it can run on a grid.

Also if it is repetitive than you can almost certainly increase performance too.



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Your Registration Authority operator(s): Vijay Sahota

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Please don't forget to install the new CA certificates! As of December 2007, we have taken the precaution to generate

new certificates, following a security incident:

http://www.grid-support.ac.uk/content/view/182/184/

For more information see the CA user documentation at: <u>http://www.grid-support.ac.uk/content/category/5/25/42/</u>