GRID TALK….

…by Vijay Sahota

Outline…

- What's the difference between Grids & Cluster

- Current trends in computing

- What relevant skill will I gain?

- What does MDX have?

- What is the NGS?

- Applications on the NGS

Definition…

"Grid computing is applying the resources of many computers in a network to solve 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."

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.

Grid…

Clusters daisy chained via the internet for HTC!
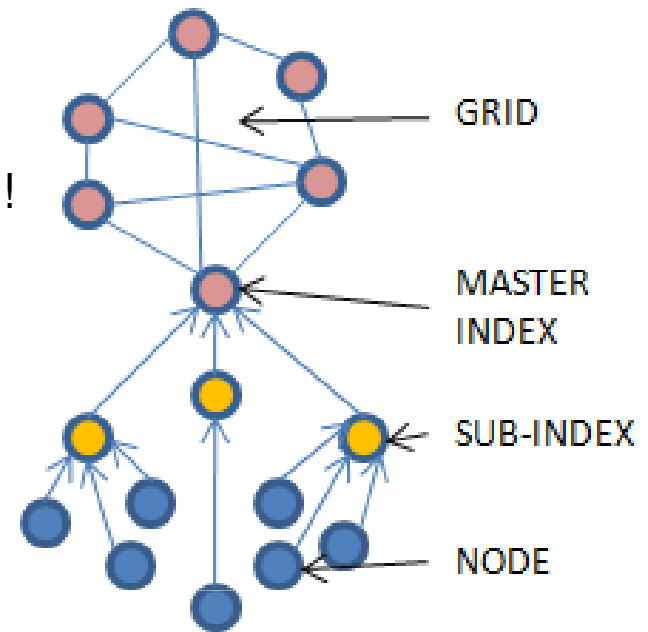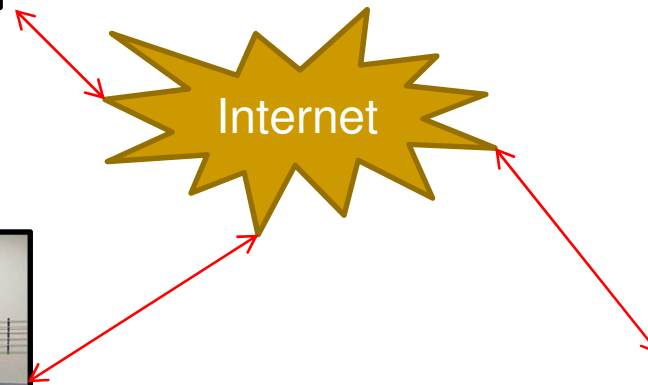
HPC/ Super Computer race...

•Super computers are super in every aspect

• Very expensive to run 2.5 + MW

• China has just recently won the CROWN

• SUPER COMPUTING IS MAINSTREAM

• YOU MAY BE USING ONE SOON!

NSCC-TJ

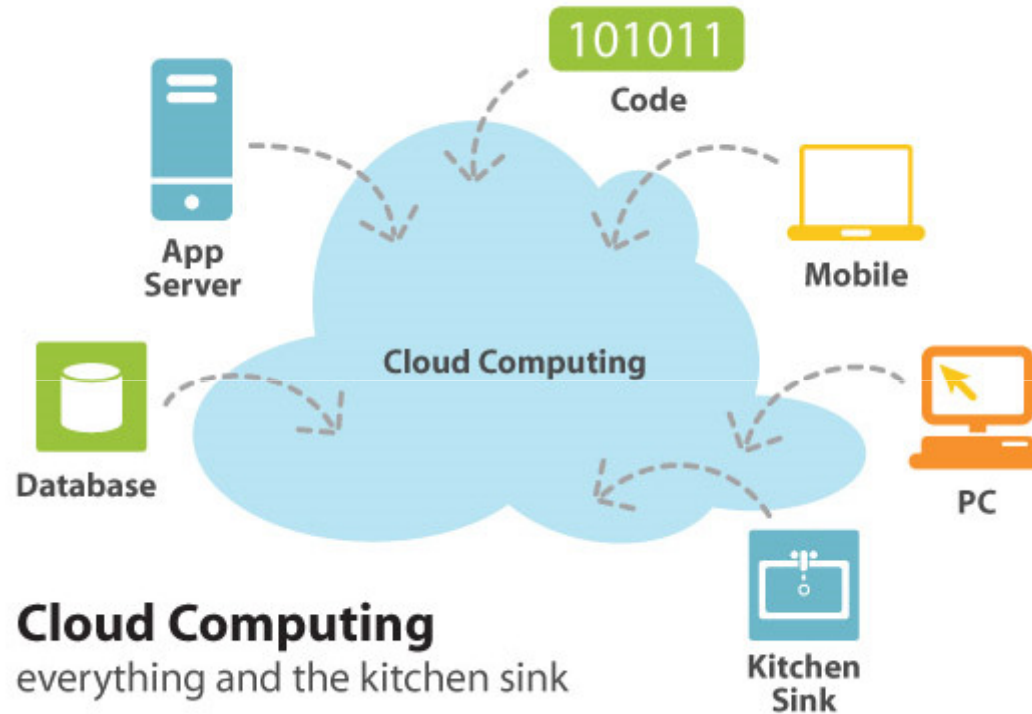¡¤Oil Exploration

¡¤Bioengineering and Drug

¡¤Construction Engineering

¡¤Meteorological

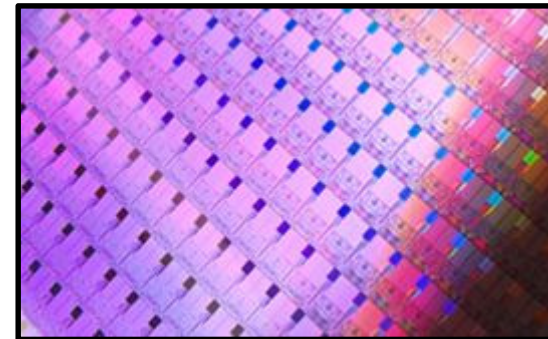# Cloud Computing...

Moore's Law…

CPU Transistor Counts 1971-2008 & Moore's Law
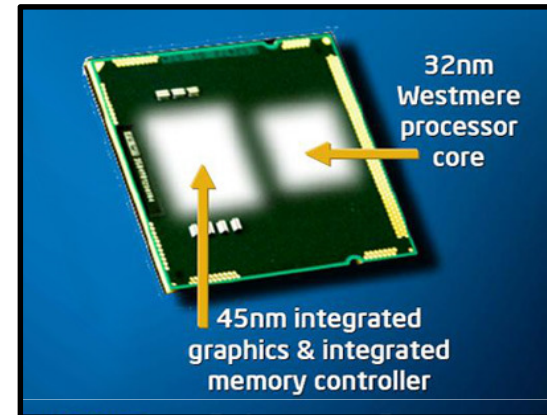
Parallelisation is Key part…

• we have reached maximum clock speeds
• we are increasing core counts
• we are integrating GPUs into CPUs
• we also have Intel MIC

•We will see a shift to exploit this tech
• GGPU and legacy x86 code will merge

• Any high performance software will be implemented in parallel code!

Skills to be gained…

If you start using any form of distributed computing, you will gain key skill in the areas of.....

- Computer hardware and computer networking skills
- Concepts of distributed systems
- Concepts of distributed software
- Handling & processing large data set
- Experience in running large simulations

This is standard what isn't is what follows!

Inherent skills …

Better Impact Factor!

- Better social/ networking skills
- Leader/ management skills
- Better **CV** outlook
- Willingness to learn
- Better equipped to answer interview questions.
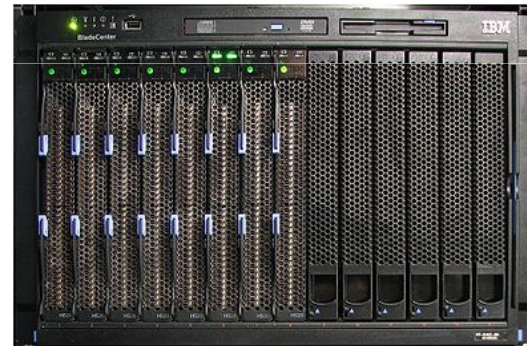
SAVING MONEY IS KING!

What do we have MDX…

Currently 2 resources, 1 Linux Condor pool cluster, and aces to the NGS.

Linux Cluster is actually a test bed to entice new user, currently it only have Matlab installed on it.

Just email me for a user account.

Tutorial will be online soon,

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.

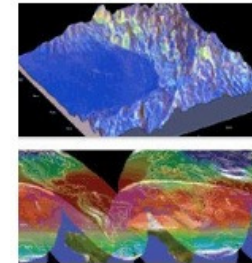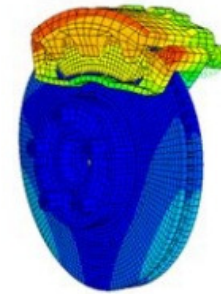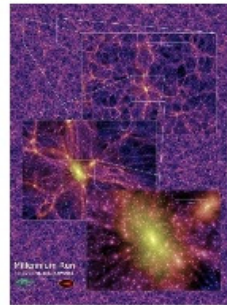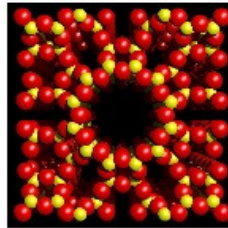This means that there is **always some one to support** your queries.

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

Applications...

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

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."
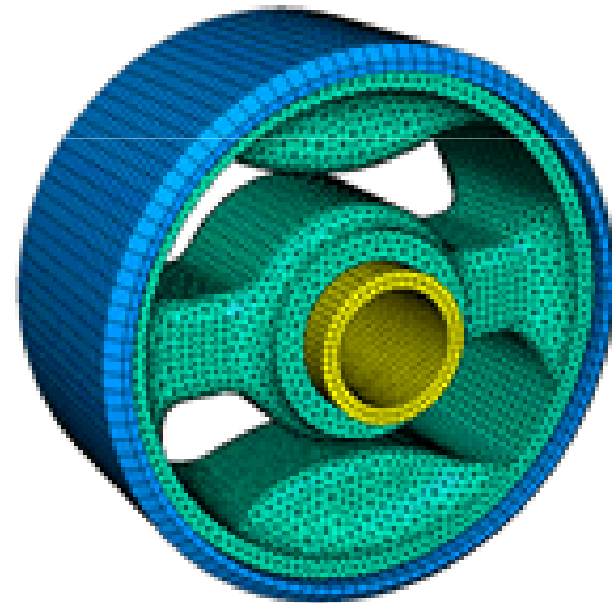
Fluent...

Fluent is a commercial Fluid Dynamics Program produced by Ansys. You need a license server (FlexNet) to take full advantage of this software. Acts like an extension to your workbench.
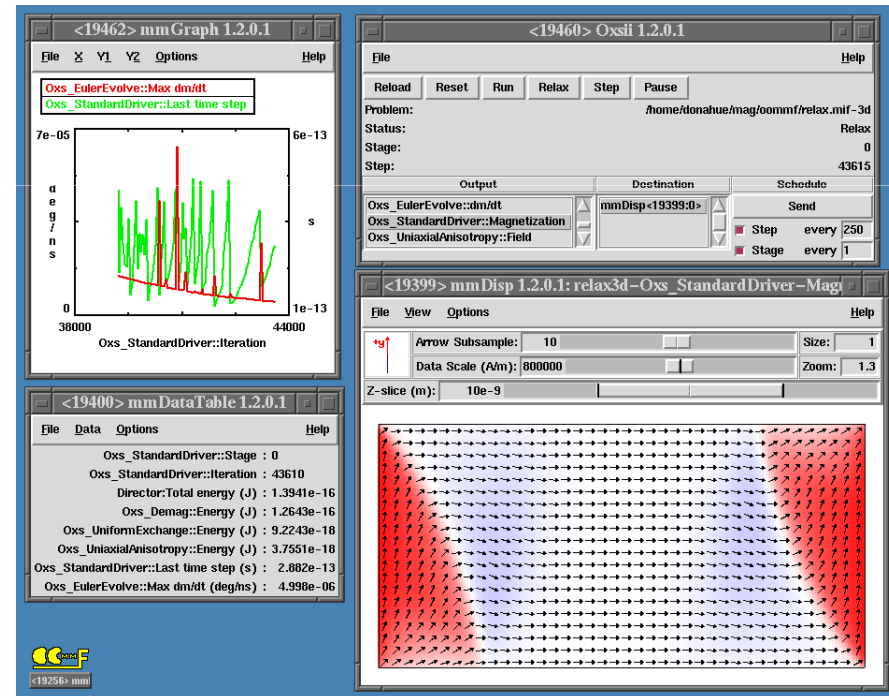
ANSYS FLUENT's interactive solver set-up, solution, and post-processing make it easy to pause a calculation, examine results with integrated post-processing, change any setting, and then continue the calculation within a single application. Case and data files can also be read into ANSYS CFD-Post for further analysis with advanced post-processing tools and to compare results from different cases side-by-side.
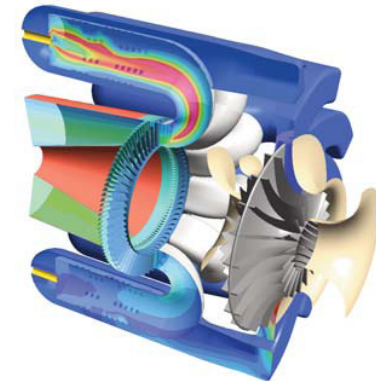
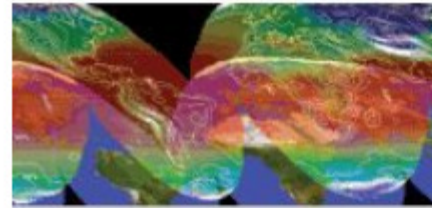# The Object Oriented Micro Magnetic Framework ...
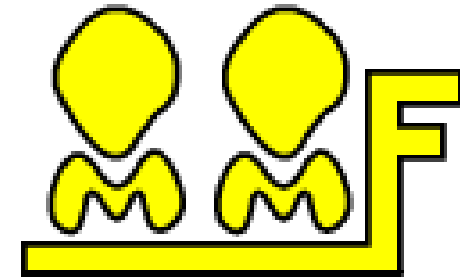
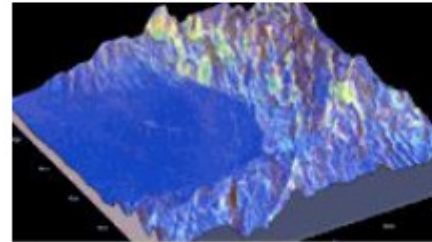**OOMMF - The Object Oriented Micro Magnetic Framework** is a portable, extensible public domain micro magnetic program and associated tools that are intended to form a completely functional micro magnetic package
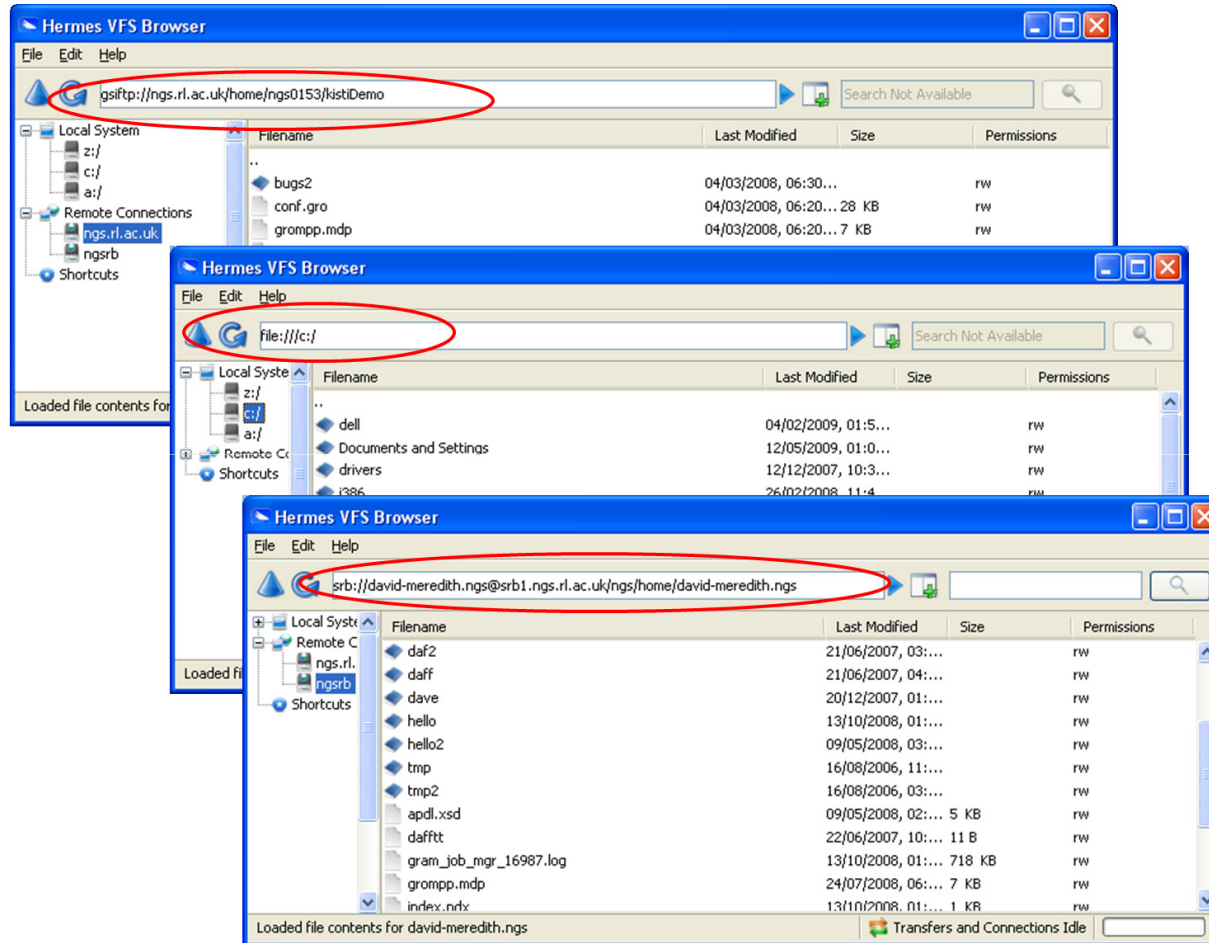
Others...

- **GNU Plot**
- **IDL**
- **Octave** - (a Matlab-alike language)
- **Matlab Compiler Runtime**
- **MGL Tools**
- **POV-Ray**
- **R**
- **Root**
- **Sabre**
- **SciPy**
- **Weka**

Hermes…

NGS Portal…

Submit My Job

My Job : *Abaqus Flexing wire*   Save SaveAsNew New

▸ Review and submit My Job (the active job) to the selected candidate host.

My Job Summary

Application Name: (Browse / Select New Application)		Abaqus	Edit
Application Version:		6.6-1	Edit
Job Name:		Abaqus Flexing wire	Edit
Job Category:		Engineering	Edit
Selected Execute / Submission Endpoint:		ngs.rl.ac.uk:2119/lsf	Edit
Candidates:	\<Candidate Hosts\> Update		Edit
Port:		2119	Edit
Path (JobManager):		/lsf	Edit
Executable:		/usr/ngs/ABAQUS_6_6_1	Edit
Standard Input File:			Edit
Standard Output File:		StdOut.txt	Edit
Standard Error File:		StdErr.txt	Edit
Working Directory:			Edit
Job Status:		UNSUBMITTED	**<Check Job Status**
JobHandle:			**<Kill Job Process** **<Force Kill Job**
Process Count:		1	Edit
Job Type:		single	Edit
Node Count:			Edit
Min Mem (MB):			Edit
Max Mem (MB):			Edit
Arguments:		"job=flexwire" "input=std_inst"	Edit

Job Description: Edit

Abaqus v6.6-1
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template configured by A.Maniopoulou (HPCSG,RAL,STFC)

This is an simple example-job of a flexing 1D wire. It is a serial job, although Abaqus has MPI like capabilities.

The input files required for this examaple can be retrieved and staged into your home (or working) directory from ngs.rl.ac.uk:/apps/abaqus/examples/std_inst.inp This template is setup to stage the example input files from this directory. Before running this example, change and/or create the working directory on the "Detail" page.

To now run this example job (or another job based on this template) go to the "Submit/Run" page and check the box next to "Ok to overwrite the job status when re-submitting the job" and "Stage all data when submitting job" then click the "Submit My Job" button. The status of the job should appear in red. First it will say submitted. To update the status, click on "Check Job Status". When completed, go to the "Data Transfer" or "Browse Host" page and download your output.

For more information about Abaqus on the NGS (RAL node) refer to:

Authenticate
Applications
Job Categories
Browse Host
Data Transfer
SrbMdasEnv
Admin
Info

My Job:
○ PageLayout
○ JsdlLayout

Detail
Candidate Hosts
Description
Executable
Arguments
Environment
File Systems
DataStaging
Files/Links
<JSDL/>
Submit/Run

Some still need CMD…

```
Type = "Job";
JobType = "normal";
Executable = "/usr/ngs/FLUENT";
Environment = { "FLUENT_LICENSE_FILE=license-server-info" };
Arguments = "solver solver-options";
CpuNumber = 1;
StdOutput = "std.out";
StdError = "std.err";
Myproxyserver= "myproxy.ngs.ac.uk";
InputSandbox = {"input"};
InputSandboxBaseURI = "gsiftp://ngsui03.ngs.ac.uk:2811/home/ngsxxxx/fluent";
OutputSandbox = {"std.err","output","std.out"};
OutputSandboxBaseDestURI = "gsiftp://ngsui03.ngs.ac.uk:2811/home/ngsxxxx/fluent";
Requirements = (
    member("NGS-UEE-FLUENT", other.GlueHostApplicationSoftwareRunTimeEnvironment) #
);
ShallowRetryCount = -1;
```

Will be e-Science website update…

Some time in the new year...!

Thank you for your time!