XRAY Grid

TO BE OR NOT TO BE ?

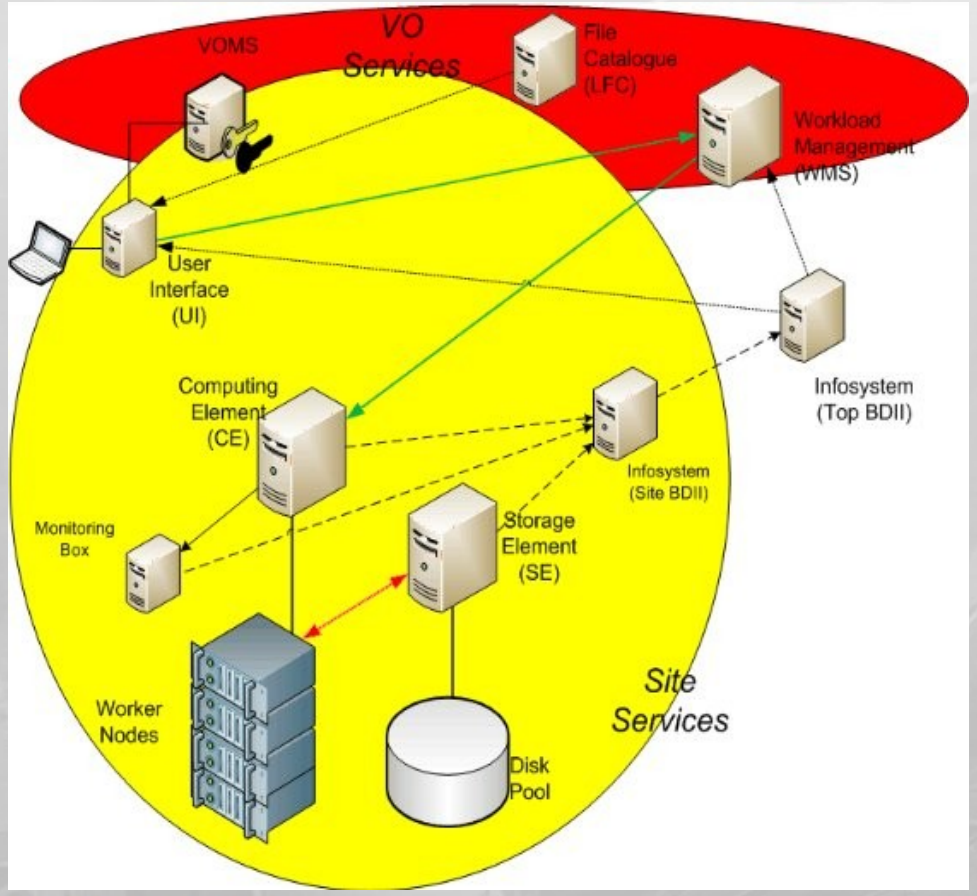
I was not always a Grid sceptic !

- I started off as a grid enthusiast e.g. by insisting that Grid be part of the ESRF Upgrade Program outlined in the Purple Book :

- In this talk I will try to explain why nowadays I oscillate between being a Grid sceptic and Devils' advocate

Which Grid are we talking about ?

- ***EGEE / gLite grid*** :



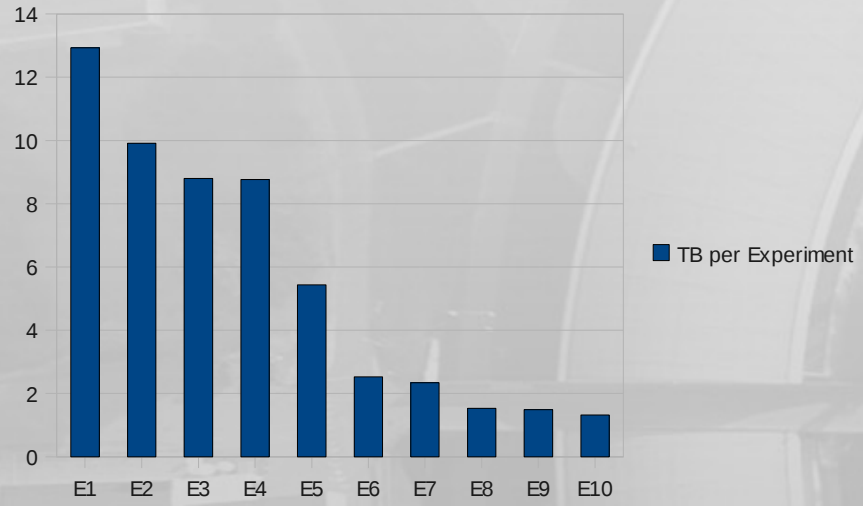
Synchrotron Requirements

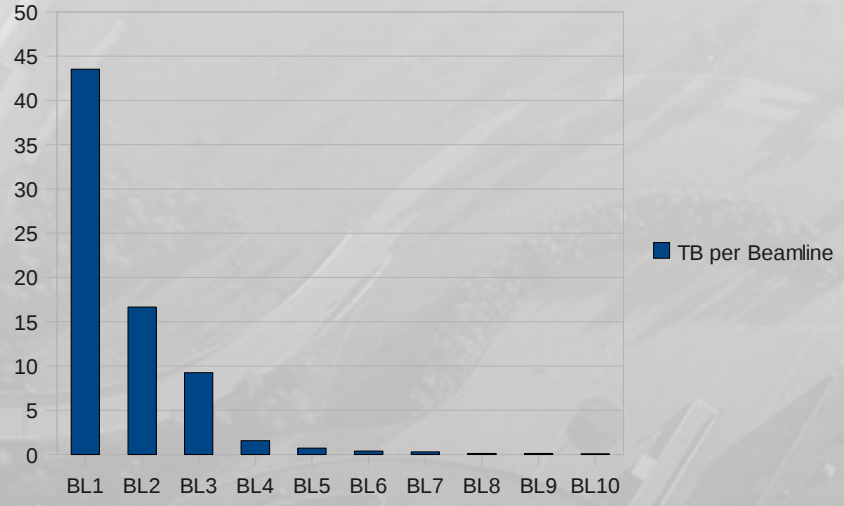
- Lots of small jobs – 100000's running for minutes
- Jobs often read and write images – 100's images / job
- Experiments generate lots of data – up to Tera Bytes / day
- Large number of small users groups – 100's /year
- Many diverse experiments – 1000's / year

XRAY Science is DATA INTENSIVE !

- ESRF has currently 400 TB,
  end of 2009 800 TB, in the future Petabytes ...

- Data per Experiment and per Beamline
  since January 2009 :

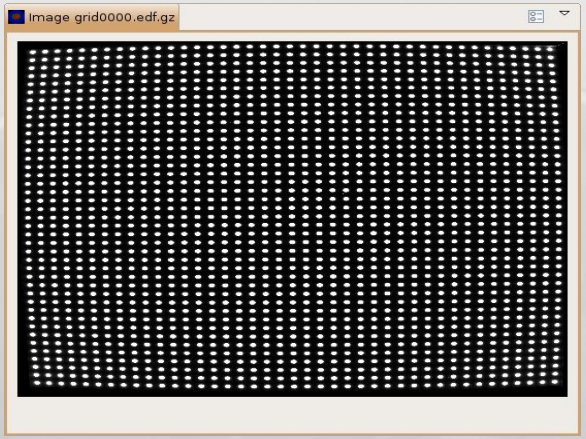




European Synchrotron Radiation Facility

Test program - spd

- ***Spd is a program to correct 2D images for*** :
  - Spatial distortion : 2d spline curve
  - Flood field : image division
  - Background field : image subtraction



  - One image takes about 17 seconds
  - Additional images take a fraction of a second

  - Simple but typical of many programs used on 2d images :
    - Low on CPU, High in I/O

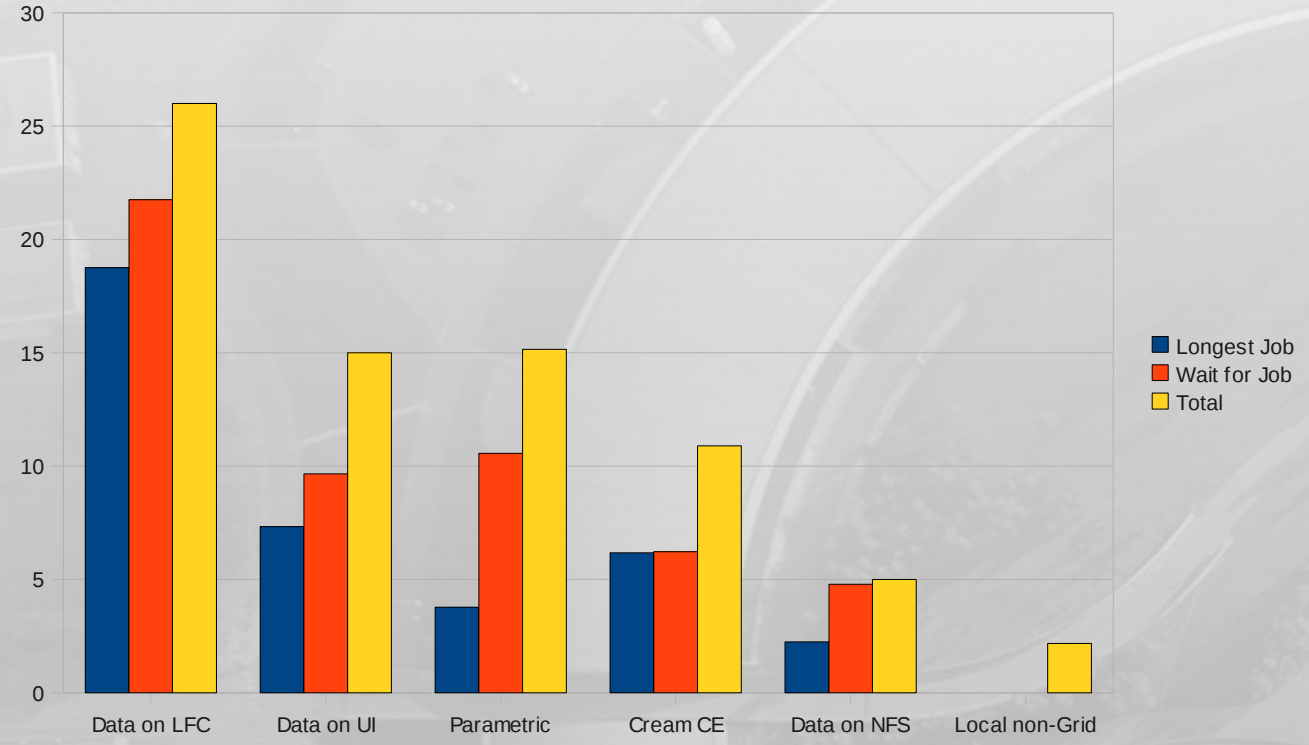
  - Typical data set is 180 images x 8 i.e. 1.44 GB
  - Typical experiment measures HUNDREDS of data sets

grid_spd

- ***grid_spd*** is a script written by ***Emmanuel Taurel*** to test running spd on the XRAY grid setup by ***Clemens Koerdt*** and ***Fernando Calvelo***

- Test scenarios :
  - Data on User Interface, submit Jobs to WMS
  - Data on LFC, submit Jobs to WMS
  - Data on LFC, submit jobs directly to CREAM-CE
  - Data on LFC, submit Parametric jobs
  - Data on NFS, submit jobs to CREAM-CE
  - Data on NFS, run job from command line

grid_spd results



XRAY Grid

TO BE ?

- We could assume :
  - Grid is OK for synchrotron science
  - Programs will run slower but still run
  - External users will be able to use the grid resources
  - Data can be exported and accessed from UI
  - Middleware (gLite) will get better (and faster) with time
  - National Grid Initiatives will provide free resources

XRAY Grid

OR *NOT TO BE ?*

- We could assume :
  - Grid is NOT OK for synchrotron science
  - Data intensive applications are not adapted to Grid
  - LFC and WMS are too slow
  - SE does not provide fast, direct access to data
  - Exporting data is not adapted to occasional intense usage
  - Middleware (gLite) will not change drastically
  - Future of gLite is uncertain, funding stops in 2010

XRAY issues with EGEE/Glite

- LFC :
  - Very slow for many files
- WMS :
  - Very slow, optimised for long jobs
- SE :
  - dcache + DPM are slow, not directly mountable
- WN :
  - Users cannot run with their UID/GID
  - Not adapted for MPI intensive applications
- GridFTP :
  - Needs tuning by guru's, not reliable, no/poor Windows support
- Grid certificates :
  - Not clear that they scale to 1000's of XRAY users

Why is (EGEE) Grid not adapted ?

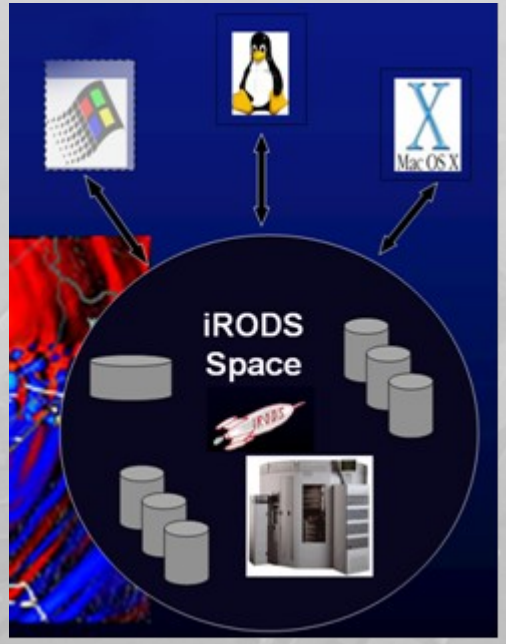
- Grid assumes each node is independent
- File systems are not mounted locally on WN's
- Grid file I/O is much slower than locally mounted files
- Grid does not provide any improvement over clusters
- Why would you want to use the Grid in this case ?

XRAY grid next steps

- Gridify and benchmark more applications :
  - Penelope – a radiation dose monte-carlo simulation
  - Peaksearch – a 2D and 3D peaksearching code
  - Laminography – a tomography technique
  - FDMNES – an xray spectra calculation MPI code
  - Fit2dCake – a radial integration program
  - XDS – a protein structure refinement program
- Try to use GridFTP for transferring real data, test iRods
- Install a faster scheduler e.g. Condor, and connect to ESRF local batch system

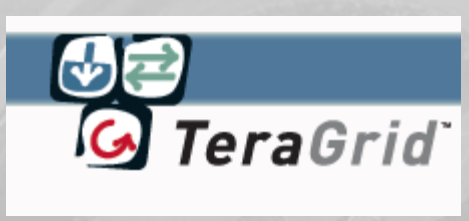
XRAY – A Hybrid Grid

- Setup local optimised clusters with high performance local file systems and batch submission systems
- Provide Grid access via direct login and grid certificates
- Export data via gridFTP and iRods :
- Use gLite for long jobs or remote batch submission
- Preinstall common xray software

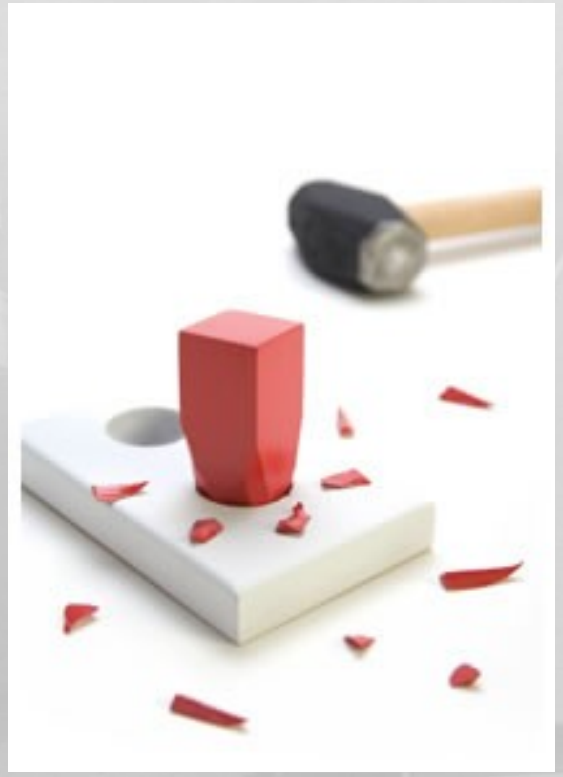


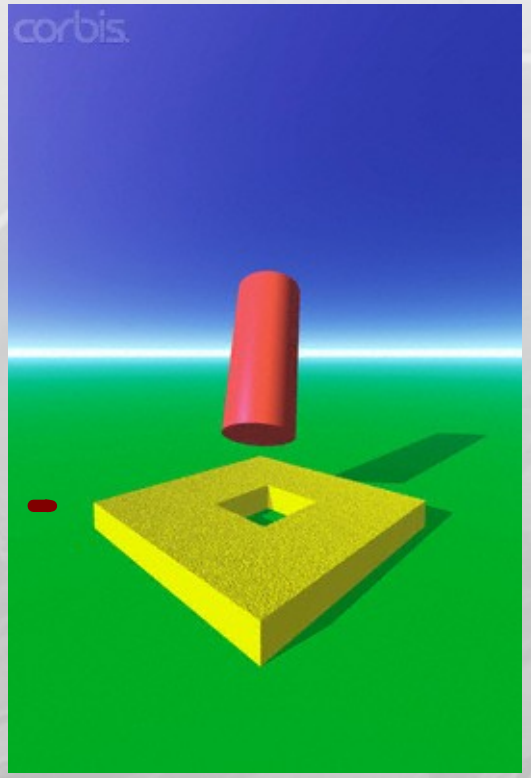
HPC-grid versus HEP Grid

- High Performance Computing refers to optimised clusters for running cpu + data intensive and mpi applications
- Users have an account on the worker nodes
- File systems and network is optimised
- Computation is done on :
  - Multi-core CPU's
  - GPU's
- Hardware and software is installed and managed locally



XRAY Science and Grid ?





Conclusions*

- EGEE/Glite based Grid has a steep learning curve, is not user friendly however it does seem to work for certain applications
- First impression of EGEE/gLite based Grid is that it is not suited to XRAY science
- A big thanks to DESY for help so far but we need more if we want to run data intensive applications on the grid
- A better return on investment for data intensive applications seems to be to invest in HPC e.g. GPU's, multi-core CPU's

* we reserve the right to change these conclusions in the future 8-)