Grid middleware for engineering design search and optimisation

Graeme Pound

UK e-Science - All Hands Meeting
3rd September 2003

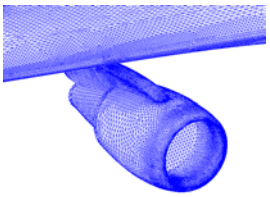
Grid Enabled Optimisation and Design Search for Engineering (GEODISE)

- Simon Cox- *Technical Director Southampton e-Science Centre. Grid/ W3C Technologies and High Performance Computing*
- Andy Keane- *Director of Rolls Royce/ BAE Systems University Technology Partnership in Design Search and Optimisation*
- Mike Giles- *Director of Rolls Royce University Technology Centre for Computational Fluid Dynamics*
- Carole Goble- *Ontologies and DARPA Agent Markup Language (DAML) / Ontology Inference Language (OIL)*
- Nigel Shadbolt- *Director of Advanced Knowledge Technologies (AKT) IRC*
- BAE Systems- *Engineering*
- Rolls-Royce- *Engineering*
- Fluent- *Computational Fluid Dynamics*
- Microsoft- *Software/ Web Services*
- Intel- *Hardware*
- Compusys- *Systems Integration*
- Epistemics- *Knowledge Technologies*
- Condor- *Grid Middleware*

The GEODISE Team

- Richard Boardman
- Sergio Campobasso
- Liming Chen
- Mike Chrystall
- Trevor Cooper-Chadwick
- Simon Cox
- Mihai Duta
- Clive Emberey
- Hakki Eres
- Matt Fairman
- Mike Giles
- Carole Goble
- Ian Hartney
- Tracey Hunt
- Zhuoan Jiao
- Andy Keane
- Marc Molinari
- Graeme Pound
- Colin Puleston
- Nicola Reader
- Angus Roberts
- Mark Scott
- Nigel Shadbolt
- Wenbin Song
- Paul Smart
- Barry Tao
- Jasmin Wason
- Fenglian Xu
- Gang Xue

Computational Fluid Dynamics



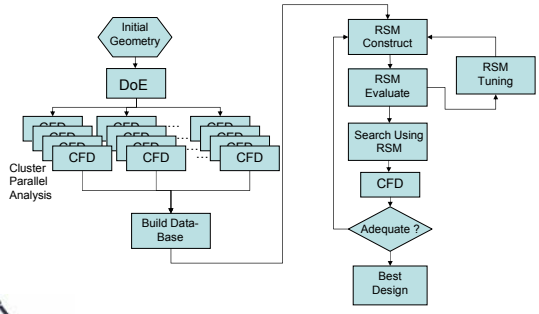
Design Challenges

Modern engineering firms are global and distributed

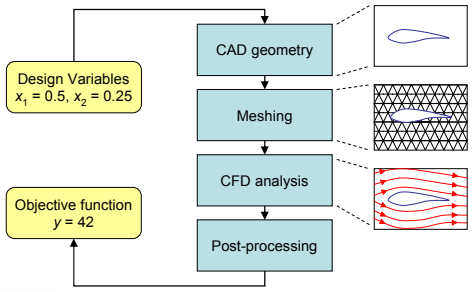
How to … ?

… improve design environments … cope with legacy code / systems	*CAD and analysis tools, user interfaces, PSEs, and Visualization*
… produce optimized designs	*Optimisation methods*
… integrate large-scale systems in a flexible way	*Management of distributed compute and data resources*
… archive and re-use design history	*Data archives (e.g. design/ system usage)*
… capture and re-use knowledge	*Knowledge repositories & knowledge capture and reuse tools.*

Design of Experiment & Response Surface Modelling



Defining the Objective Function



Scripting languages

Why use scripting languages?

- Flexibility
- High-level functionality
- Quick application development
- Extend the user's existing PSE
- Reduce the need for 'hacks'

Computational Toolbox

`gd_createproxy.m`	Creates a Globus proxy certificate for the user's credentials
`gd_destroyproxy.m`	Destroys the local copy of the user's Globus proxy certificate
`gd_certinfo.m`	Returns information about the user's certificate
`gd_proxyinfo.m`	Returns information about the user's proxy certificate
`gd_proxyquery.m`	Queries whether a valid proxy certificate exists
`gd_jobsubmit.m`	Submits a compute job to a Globus GRAM job manager
`gd_jobstatus.m`	Gets the status of a Globus GRAM job
`gd_jobpoll.m`	Queries the status of a Globus GRAM job until complete
`gd_jobkill.m`	Kills a Globus GRAM specified by job handle
`gd_putfile.m`	Puts a remote file using GridFtp
`gd_getfile.m`	Retrieves a remote file using GridFtp
`gd_rmfile.m`	Deletes a remote file using GridFtp
`gd_makedir.m`	Creates a remote directory using GridFtp
`gd_rmdir.m`	Deletes a remote directory using GridFtp

Example Script

```
hostname = 'pacifica.iridis.soton.ac.uk'
jobmanager = [hostname,'/jobmanager-fork']
rsl = '&(executable="/bin/date")(stdout="remote.txt")'

%Create a proxy certificate
gd_createproxy

%Submitting a globus job and returning handle
handle = gd_jobsubmit(rsl,jobmanager)

%Polling the job
gd_jobpoll(handle)

%Getting the standard output
gd_getfile(hostname,'remote.txt','local.txt');

%Print the output to screen
type('local.txt')
```

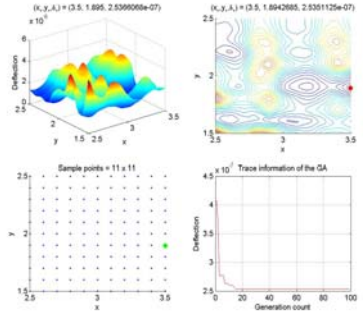

Job Submission Service Client

- Matlab client to job submission web service
- User detached from compute endpoint – Condor pool
- Machines publish available resources:
  - *HasProEngineer = TRUE*
  - *ProEngineerVersion = "2001400"*
  - *ProEngineerPath = "C:\Program Files\proe2001\bin*
- DIME file transfer over http
- MATLAB Client Functions:
  - **`grid_platform`** – Describes the platform requirements of the job
  - **`grid_submit`** – Submits the job to the web service, returns a job ID
  - **`grid_poll`** – Polls job ID
  - **`grid_status`** – Queries job status
  - **`grid_results`** – Retrieves the output files

Design Search & Optimisation Tools

- Objective Function Client
  - Grid-enabled objective function evaluation
  - Matlab functions provided:
    - gd_objsubmit – Transfers required files, submit jobs and returns handle
    - gd_objvalue – Retrieves function evaluation & cleans up files
    - gd_objcleanup – Removes remote files
- OptionsMatlab
  - Matlab interface to the Options design exploration system
  - *State of the art* design search and optimisation algorithms
  - Objective and constraint functions exposed as Matlab functions
  - Grid-enabled job brokers easily incorporated

Exploiting the UK e-Science Grid



Conclusions

- Open standards → Plug & Play resources
- Transparent access to Grid resources
- Components to high-level scripting languages
- Flexibility and scalability to meet engineer's requirements

Related Presentations

Thursday 4th September

CFD-based Shape Optimisation with GEODISE Toolkits
- Room: Conference Room 3
- Session Title: Applications 5
- Time: 0950 – 1010

Integrating Data Management into Engineering Applications
- Room: Conference Room 2
- Session Title: Databases and Data Access 2
- Time: 1015 – 1035