


# Grid middleware for engineering design search and optimisation

Graeme Pound


UK e-Science - All Hands Meeting  
3<sup>rd</sup> September 2003



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## Grid Enabled Optimisation and Design Search for Engineering (GEODISE)

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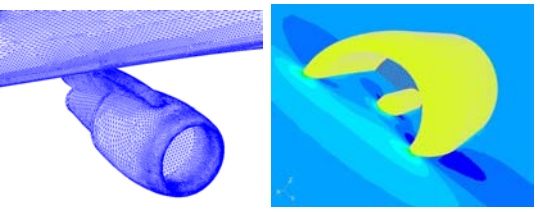

## The GEODISE Team

<ul style="list-style-type: none"> <li>• Richard Boardman</li> <li>• Sergio Campobasso</li> <li>• Liming Chen</li> <li>• Mike Chrystall</li> <li>• Trevor Cooper-Chadwick</li> <li>• Simon Cox</li> <li>• Mihai Duta</li> <li>• Clive Emberey</li> <li>• Hakki Eres</li> <li>• Matt Fairman</li> <li>• Mike Giles</li> <li>• Carole Goble</li> <li>• Ian Hartney</li> <li>• Tracey Hunt</li> <li>• Zhuoan Jiao</li> </ul>	<ul style="list-style-type: none"> <li>• Andy Keane</li> <li>• Marc Molinari</li> <li>• Graeme Pound</li> <li>• Colin Puleston</li> <li>• Nicola Reader</li> <li>• Angus Roberts</li> <li>• Mark Scott</li> <li>• Nigel Shadbolt</li> <li>• Wenbin Song</li> <li>• Paul Smart</li> <li>• Barry Tao</li> <li>• Jasmin Wason</li> <li>• Fenglian Xu</li> <li>• Gang Xue</li> </ul>
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## Computational Fluid Dynamics


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## Design Challenges

*Modern engineering firms are global and distributed*

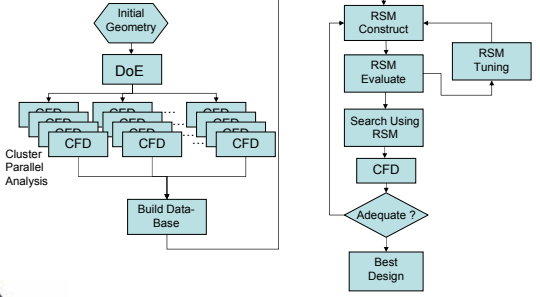
How to ... ?

... 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.




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## Design of Experiment & Response Surface Modelling

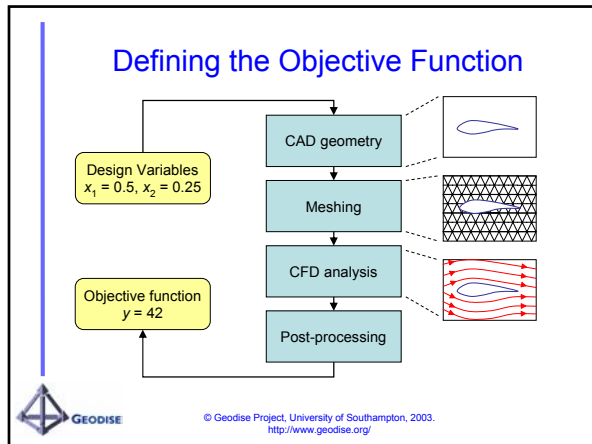


```

graph TD
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    BuildDB --> RSMConstruct[RSM Construct]
    RSMConstruct --> RSMEvaluate[RSM Evaluate]
    RSMEvaluate --> SearchRSM[Search Using RSM]
    SearchRSM --> CFD[CFD]
    CFD --> Adequate{Adequate?}
    Adequate --> BestDesign[Best Design]
    Adequate --> RSMConstruct
    RSMEvaluate --> RSMConstruct
    RSMEvaluate --> RSM_Tuning[RSM Tuning]
    RSM_Tuning --> RSMConstruct
  
```



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## Scripting languages

Why use scripting languages?

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

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## Computational Toolbox

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

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## Example Script

```

hostname = 'pacific.iris.soton.ac.uk'
jobmanager = [hostname, '/jobmanager-fork']
rsi = '%(executable)bin/date')(stdout='remote.txt')

%Create a proxy certificate
gd_createproxy

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

```

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## 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

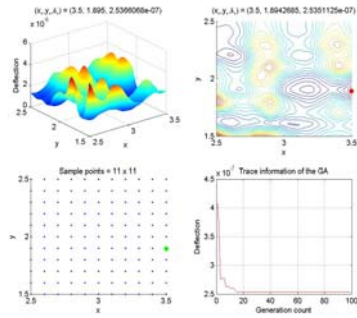
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## Design Search & Optimisation Tools

- 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

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## Exploiting the UK e-Science Grid



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## 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



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## Related Presentations

Thursday 4<sup>th</sup> 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



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