Applied Workflows in Geodise

e-Science Workflow Services Workshop
Edinburgh (Dec 3rd – 5th 2003)

Dec 4th 2003

Prof Simon Cox

Computational Engineering & Design Group
School of Engineering Sciences
University of Southampton

Grid Enabled Optimisation and Design Search for Engineering (GEODISE)

Southampton, Oxford and Manchester

Simon Cox- *Grid/ W3C Technologies and High Performance Computing*
Global Grid Forum Apps Working Group

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*

University of Southampton

THE UNIVERSITY of MANCHESTER

GEODISE

The GEODISE Team ...

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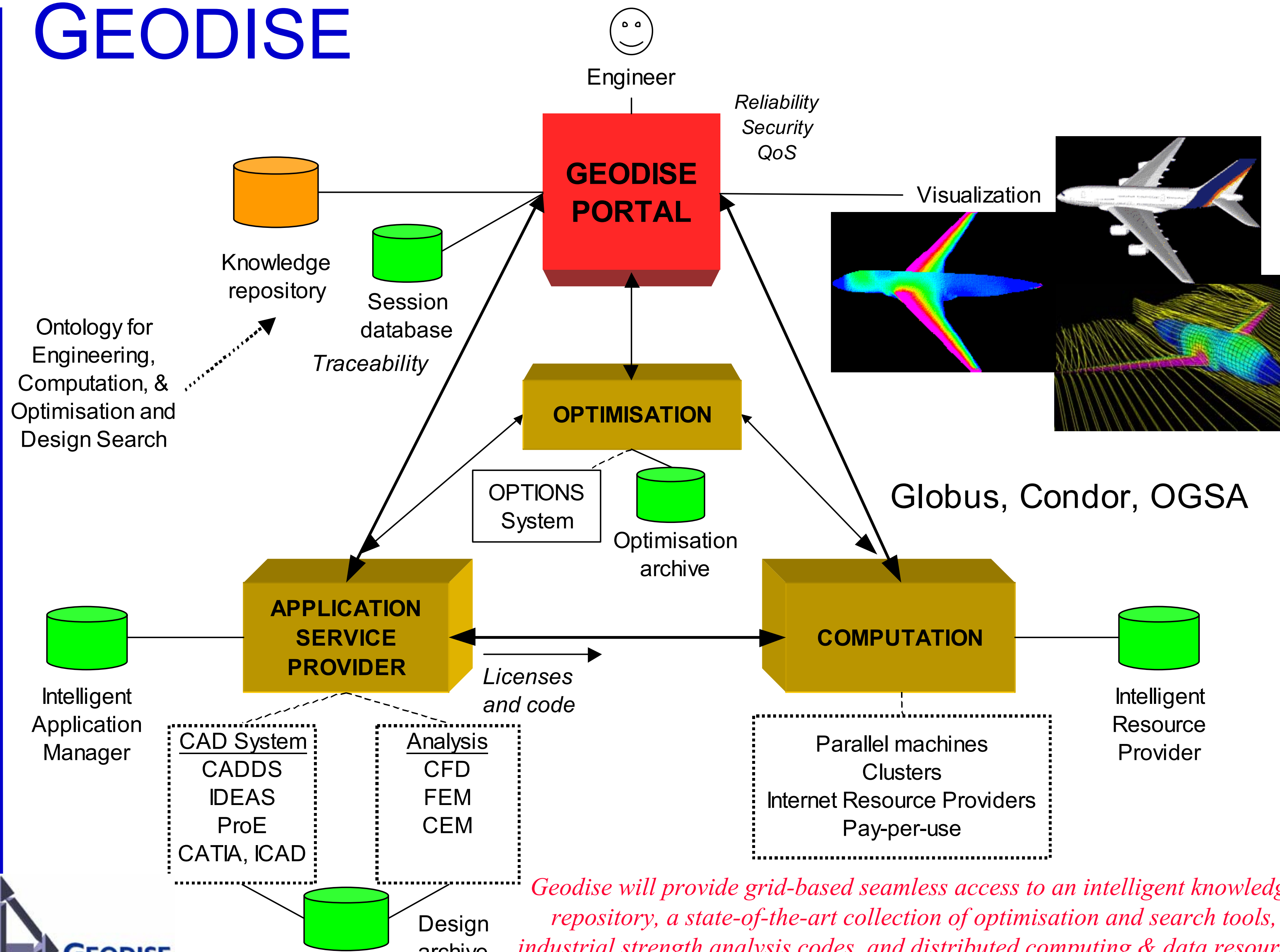
- Andy Keane
- Marc Molinari
- Graeme Pound
- Colin Puleston
- Nicola Reader
- Angus Roberts
- Mark Scott
- Nigel Shadbolt
- Wenbin Song
- Paul Smart
- Barry Tao
- Jasmin Wason
- Fenglian Xu
- Gang “Luke” Xue

GEODISE

GEODISE



Geodise will provide grid-based seamless access to an intelligent knowledge repository, a state-of-the-art collection of optimisation and search tools, industrial strength analysis codes, and distributed computing & data resources

A few of my favourite things to do with workflows

- Create
- Retrieve
- Cut ‘n’ Shut
- Configure
- Execute
- Monitor
- Share
- Steer
- Dynamically modify

GEODISE

When is a script not a script?

… when it’s a “workflow”

Scripting languages

Why use scripting languages?

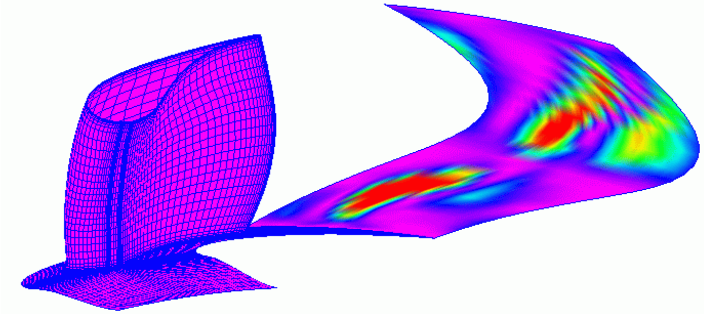
- Flexibility
- High-level functionality
- Quick application development
- Extend the user's existing PSE

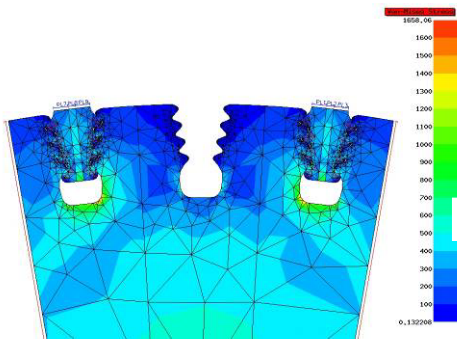
Example Script

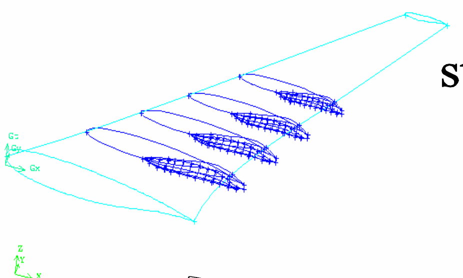
```
hostname = 'pacifica.iridis.soton.ac.uk'
jobmanager = [hostname,'/jobmanager-fork']
rsl = '&(executable="/bin/date")(stdout="remote.txt")'

%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')
```

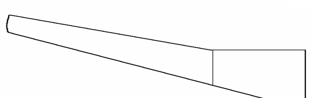
GEODISE

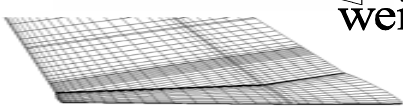
Design

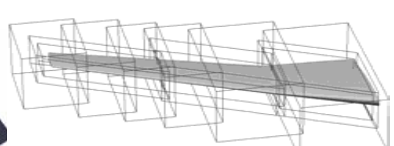


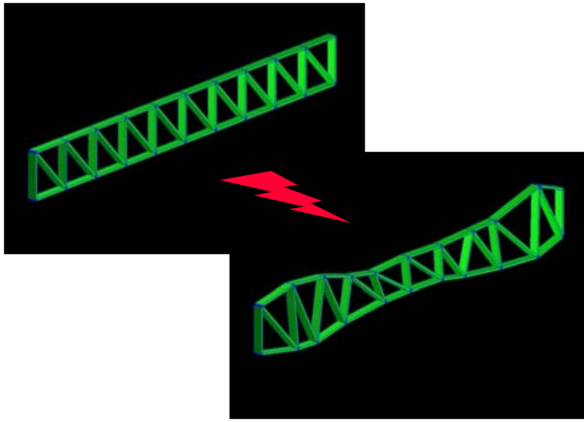


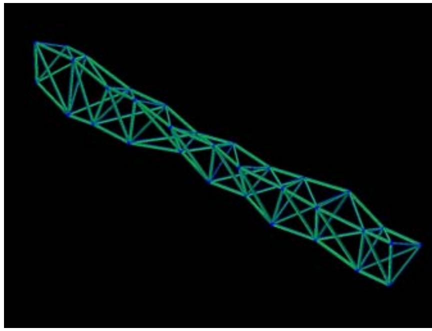


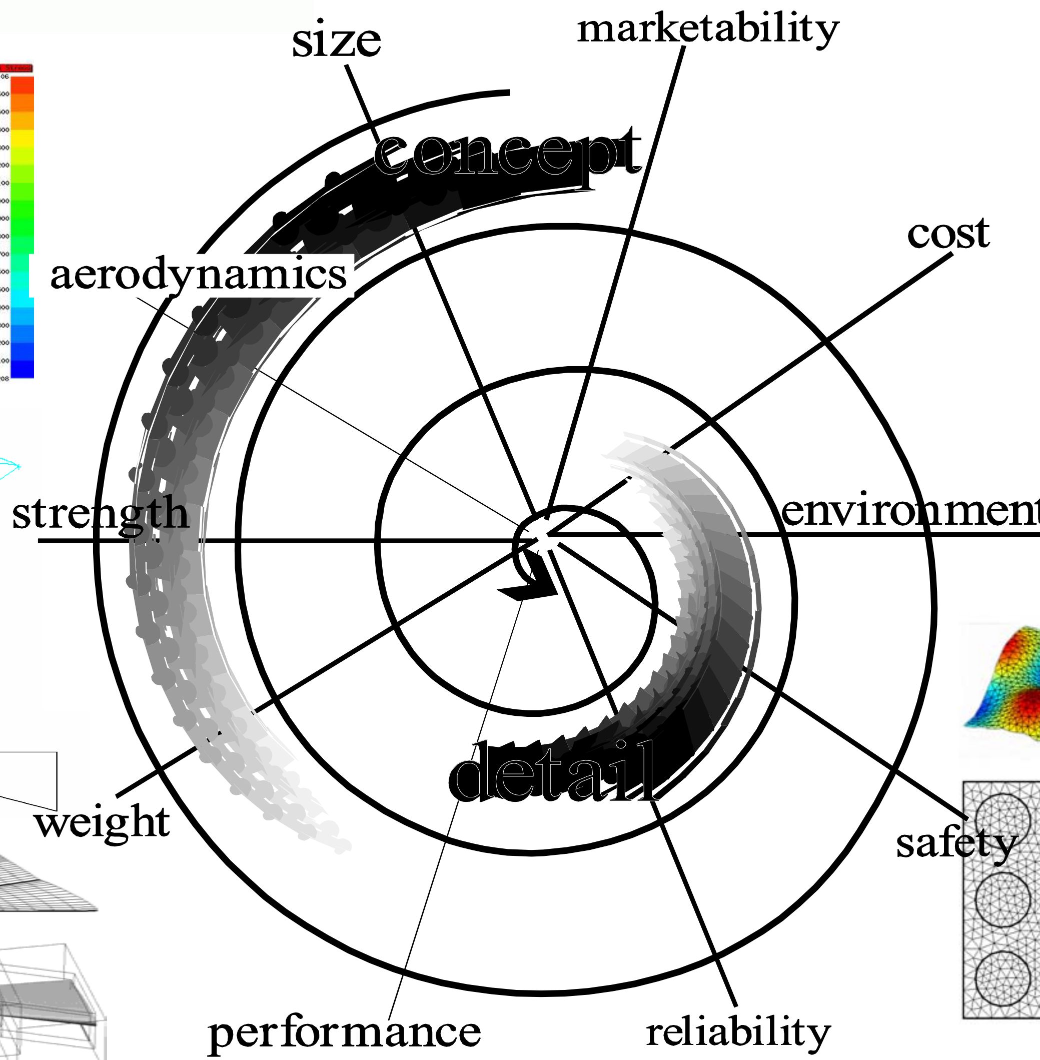


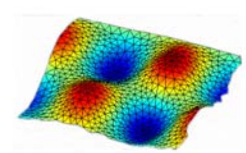


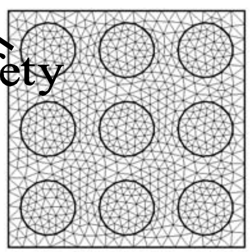


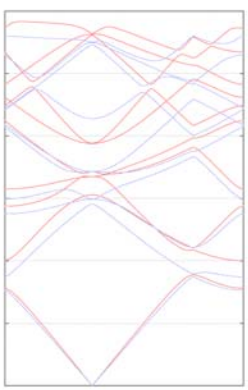





size
marketability
concept
cost
aerodynamics
strength
environment
weight
detail
safety
performance
reliability





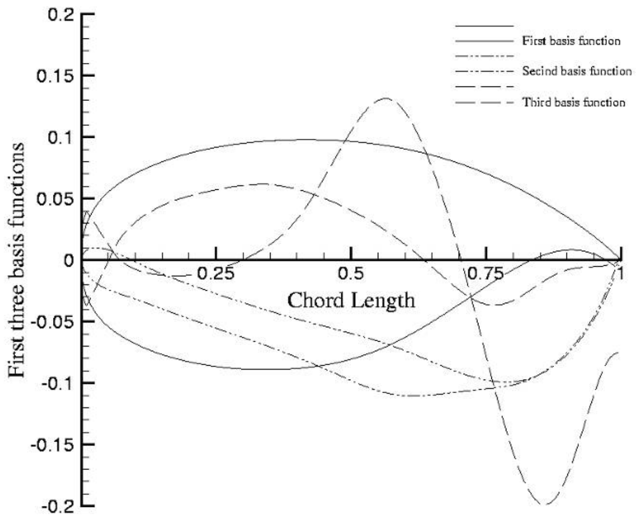


Aerodynamic Shape Optimisation using CFD

- Integration of CAD, mesh generation, and solver
  - Direct API access to CAD models
  - third-party standards based data exchange
- Robust mesh generation
  - Automatic mesh generation
  - Control over mesh properties
- Multi-fidelity models
  - Euler solver
  - Navier Stokes solver

Orthogonal Basis Function for Airfoil Design

- Parameterisation methods for airfoil:
  - mathematical functions
  - empirical basis functions
  - control points based curve fitting
- Orthogonal basis functions
  - unique mapping from parameter space to design space
  - for preliminary wing design
  - fewer number of design variables
  - different set of basis functions for different design task



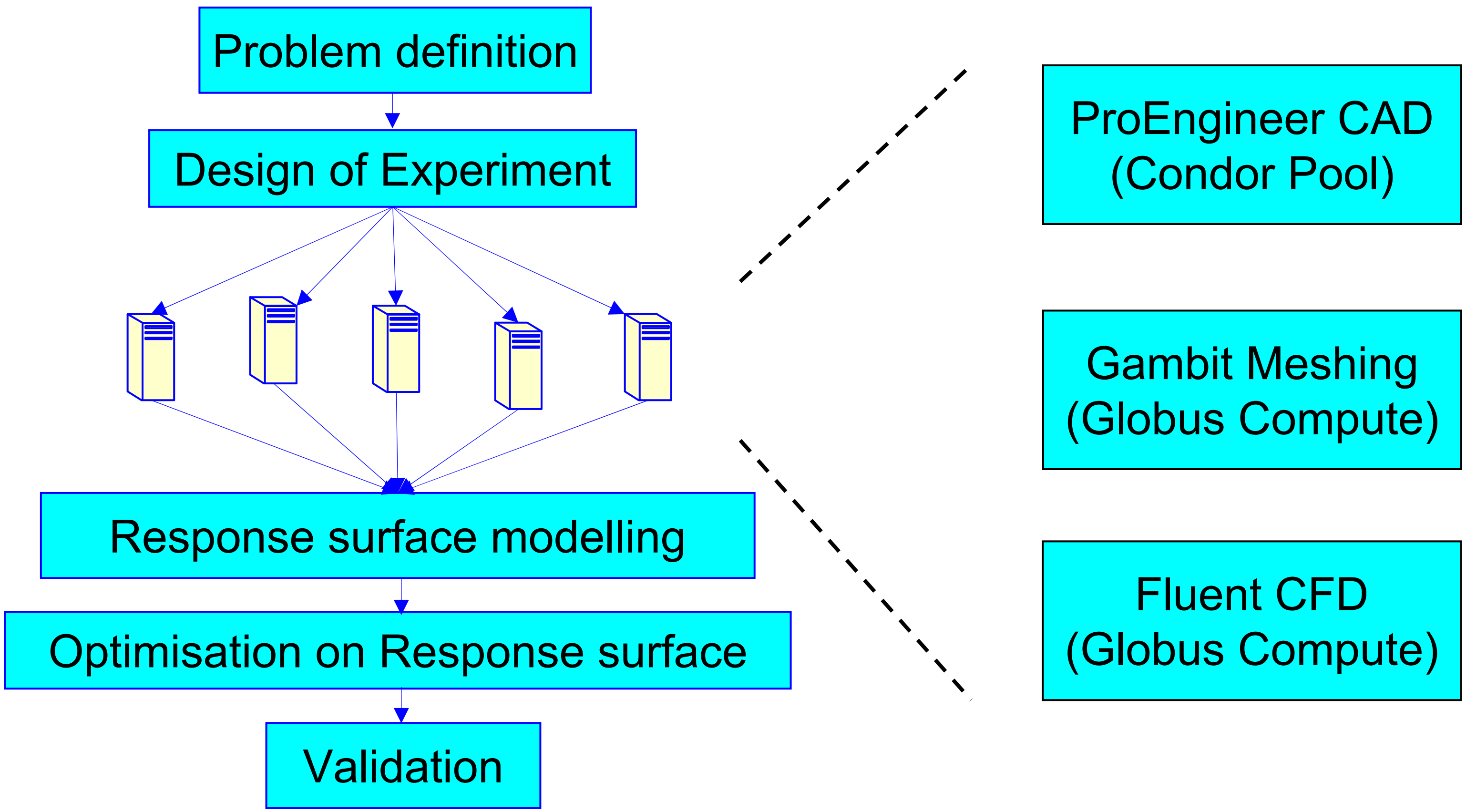
Robinson, G.M. and Keane, A.J., "Concise Orthogonal Representation of Supercritical Airfoils", Journal of Aircraft 38(3) (2001) 580-583.

Optimisation Workflow and Results

- Optimisation strategy:
  - Single optimisation method proved to be inefficient for practical problems, more complex strategies are required
  - Two-stage hybrid approach (Genetic algorithm + Gradient search)
- Surrogate modelling
  - CFD runs on complex configurations is too expensive (24hrs/run)
  - Surrogate modelling methods
    - Polynomial curve fitting
    - Stochastic method (DACE or Kriging)
    - Neural network
  - High-dimensional design space
- Combing response surface modelling (RSM) /two-stage approach

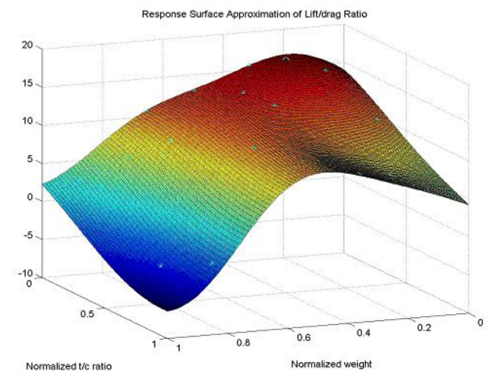
GEODISE

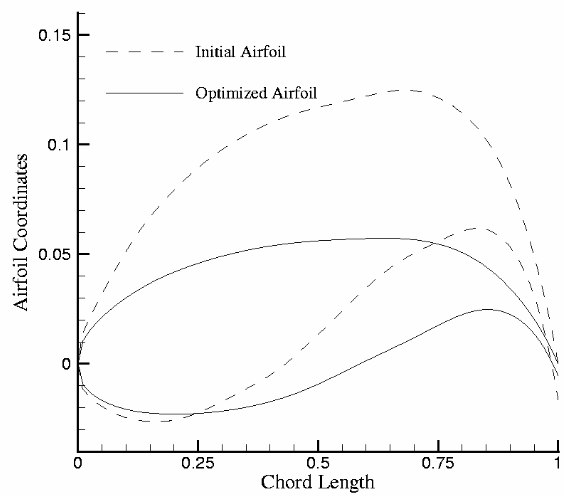
Workflow for aerodynamic shape optimisation using CAD, Gambit, and Fluent

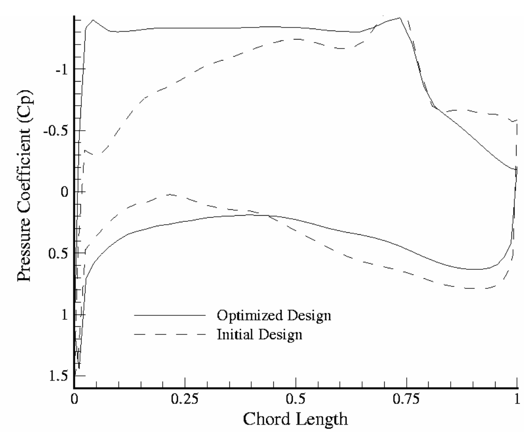


Response surface model and two-stage hybrid search using GA/Local tuning

- Response surface model
- two-stage hybrid search methods
- Comparison of Airfoil shape and pressure distribution



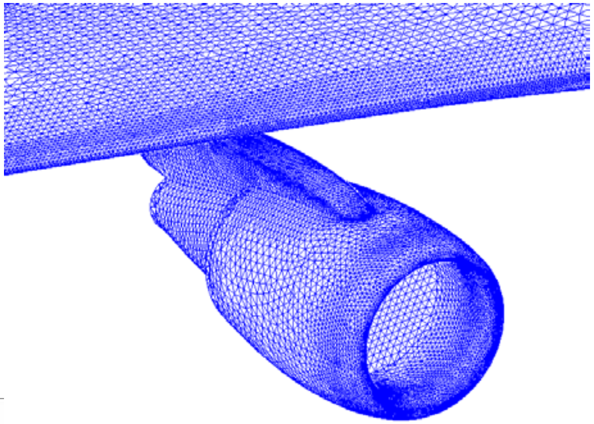




Engine Nacelle Optimisation

(problem definition)

Assumption: Noise radiated to ground reduces with increasing scarf angle



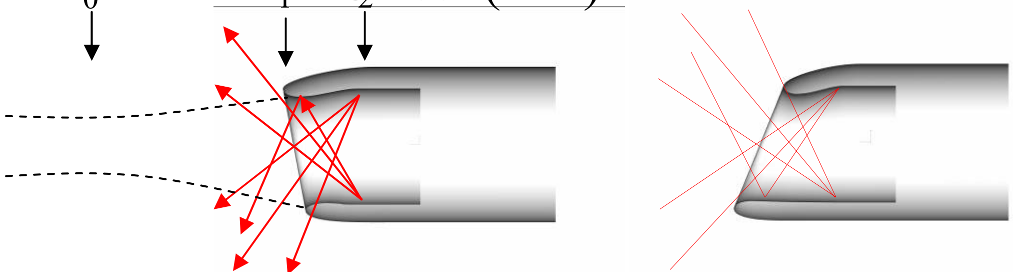
Objective function:

Total Pressure Recovery (pt_2/pt_1)

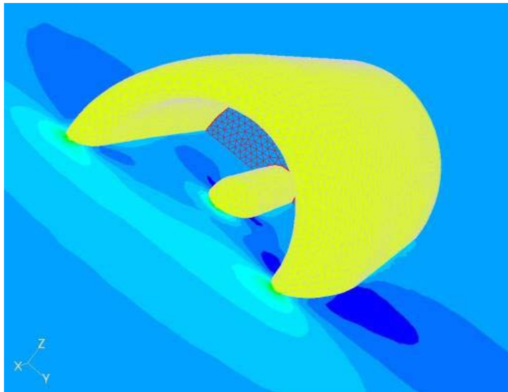
Design variables: Scarf Angle (degrees)

Axial Offset (mm)

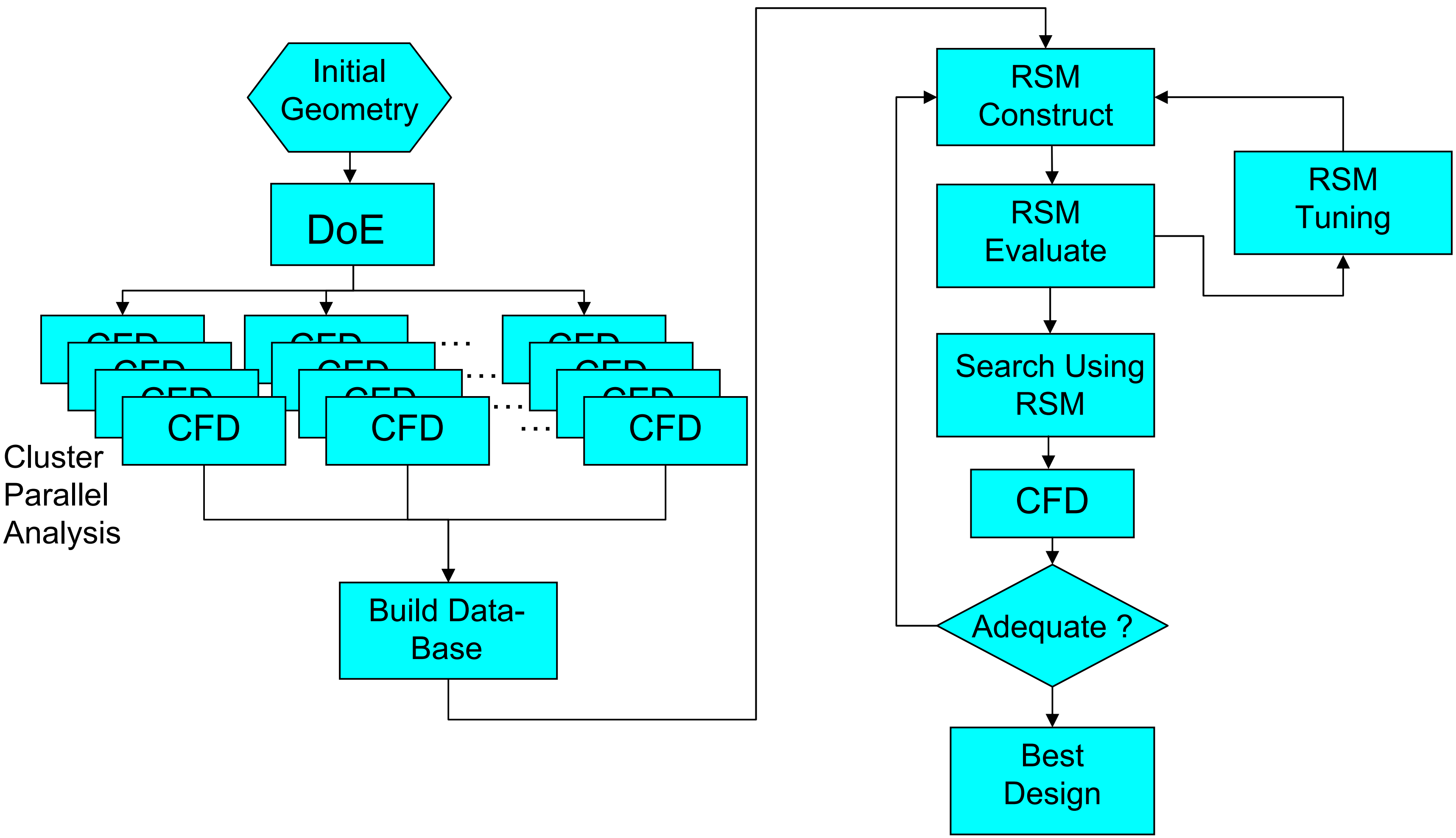
`



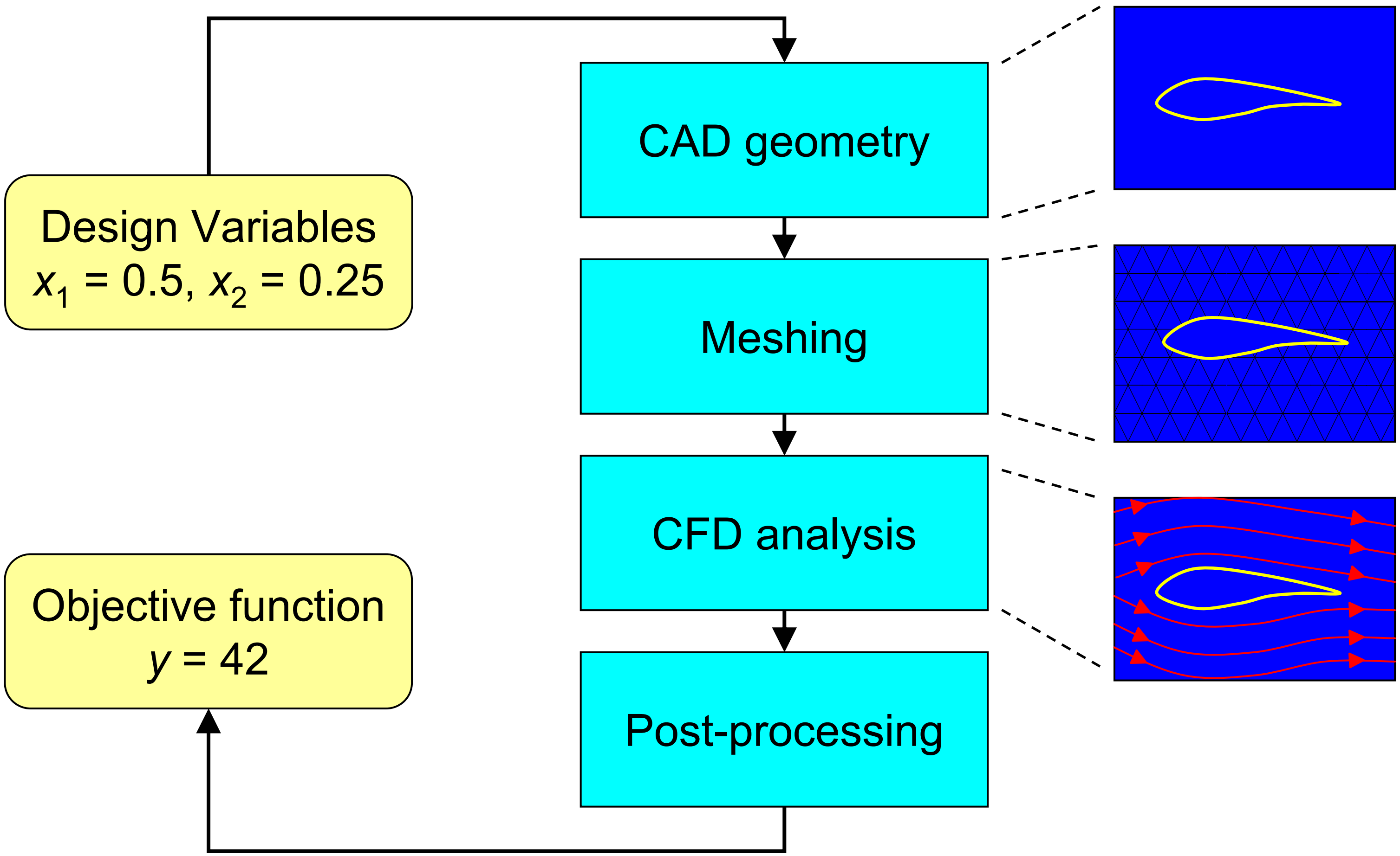
Total Pressure Recovery (TPR) = pt_2/pt_1



Design of Experiment & Response Surface Modelling



Defining the Objective Function

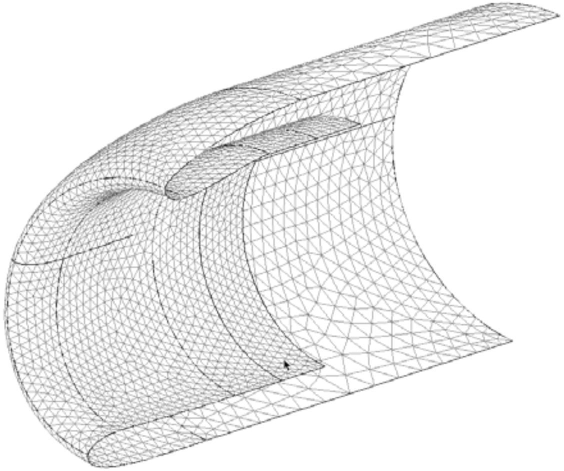


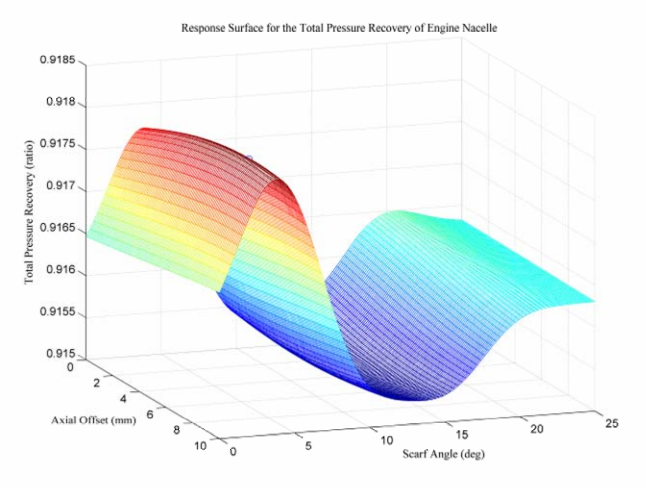
"Bigger workflows are made from little workflows,
Little workflows are made from littler workflows,
And so on…"

Engine Nacelle Optimisation (3D)

(some results)

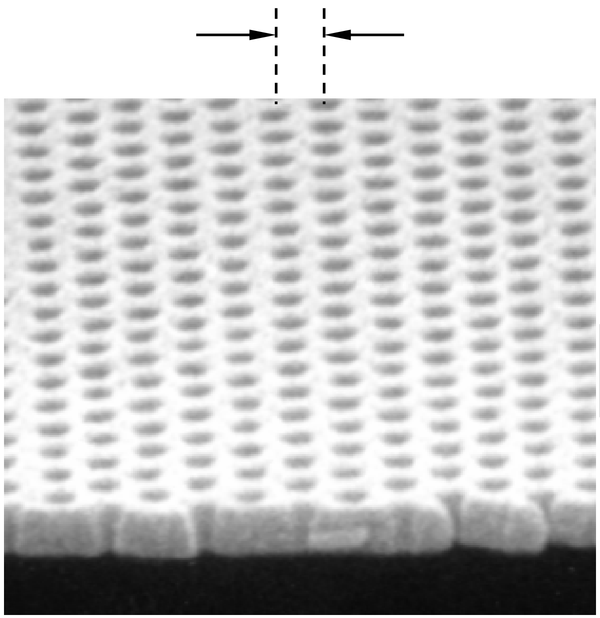
- Typical unstructured mesh used in the problem (left)
- Response surface model built for two design variables (right)
- The effect of other geometry parameters need to be investigated





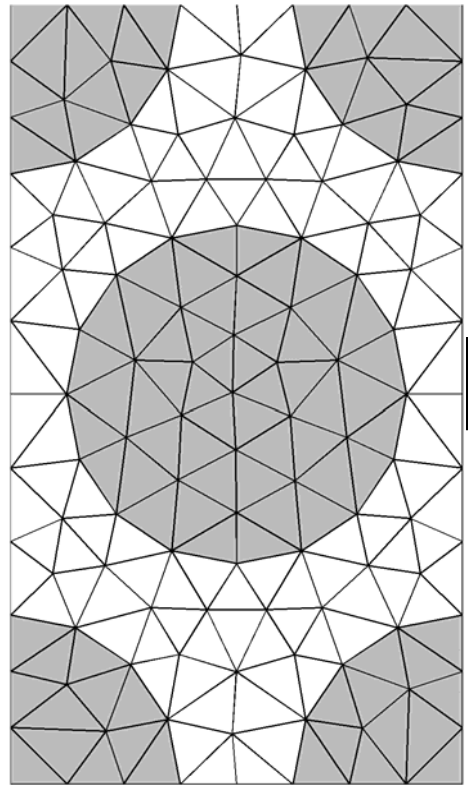
Photonic Device Modelling

pitch=300nm

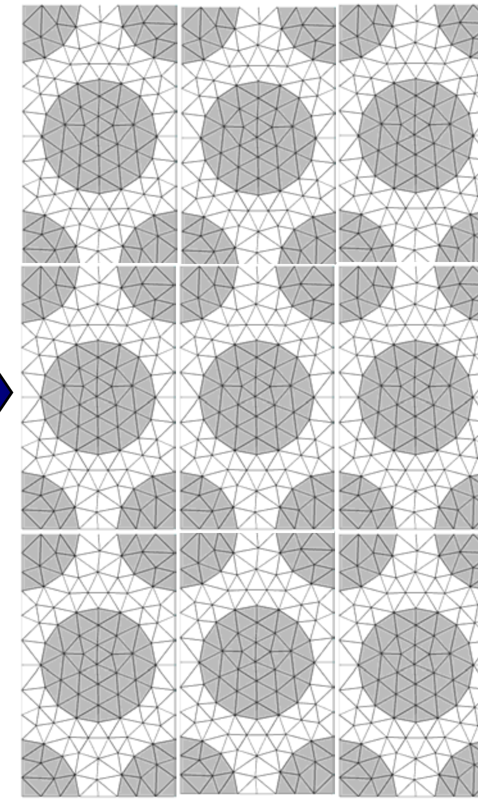


Bridge waveguide structure courtesy of Martin Charlton, Southampton Microelectronics Research Group.

REAL-THING (photo)



UNIT-CELL

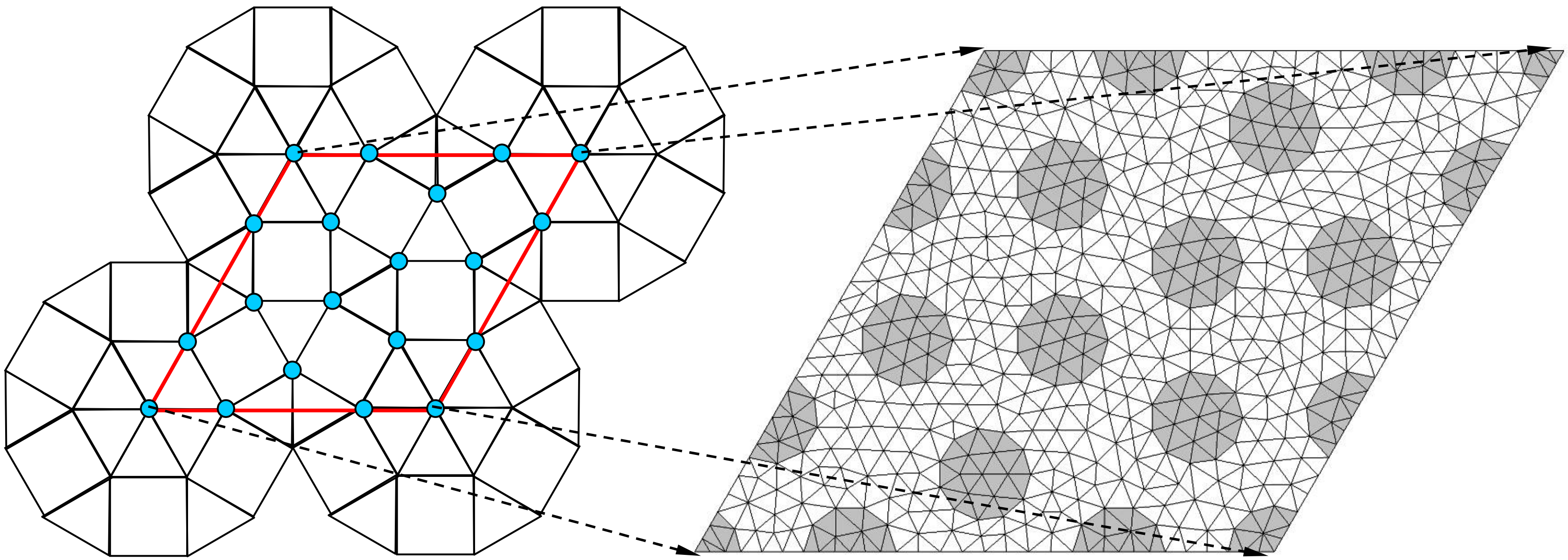


PERIODICALLY TILED UNIT-CELLS

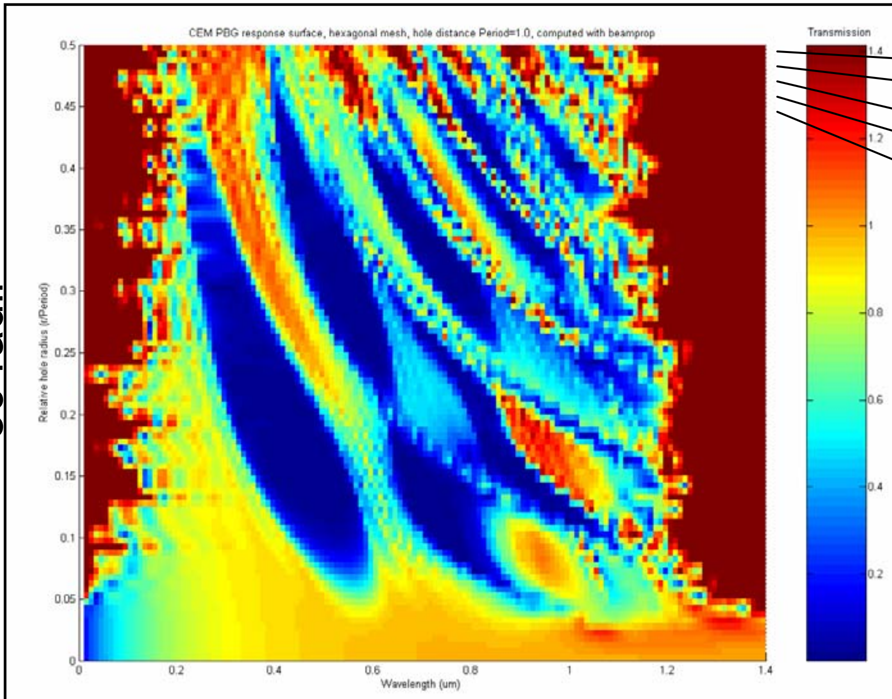
GEODISE

12-fold Symmetric Quasicrystals

- Based on tiling of dodecagons composed of squares and equilateral triangles
- Possesses 12 fold rotational symmetry
- Leads to a highly homogeneous band gap



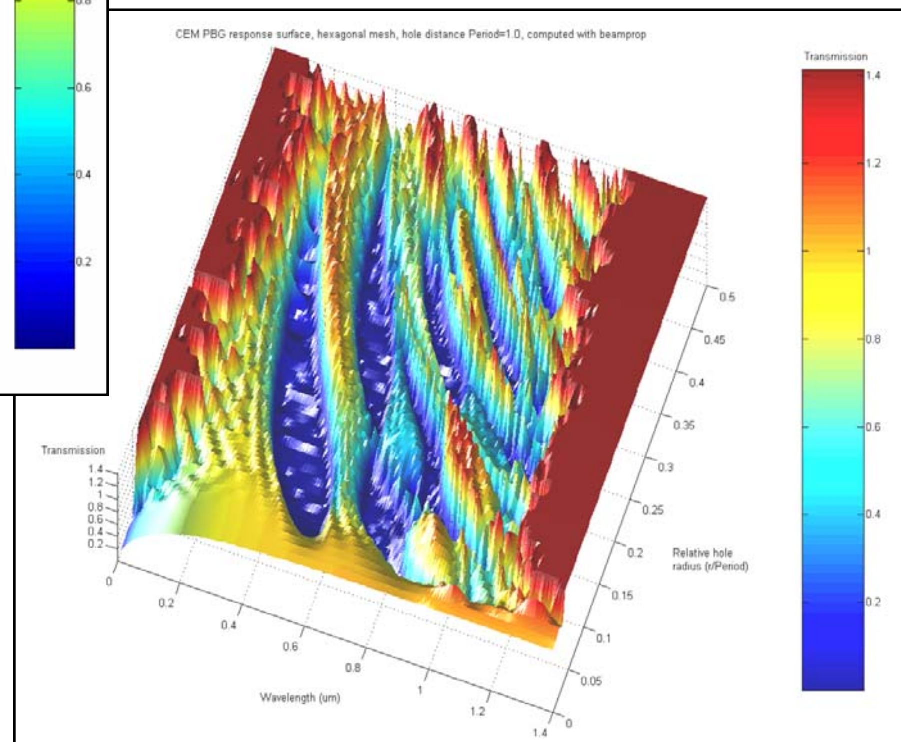
CEM Simulation Results



CompResource.1
CompResource.2
CompResource.3
CompResource.4
CompResource.1
…

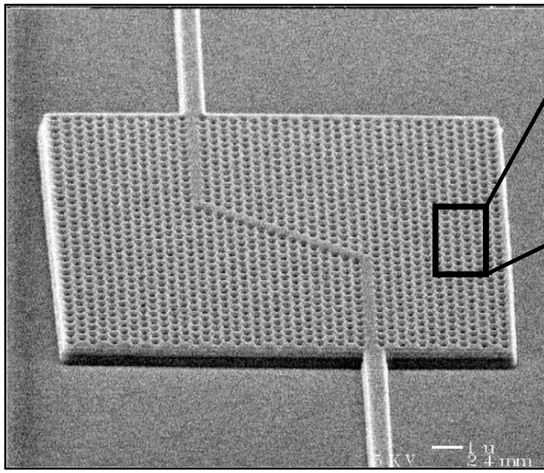
50 radii

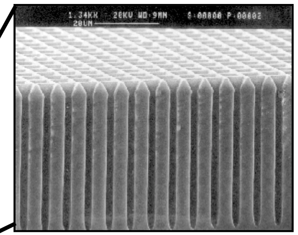
50 frequencies



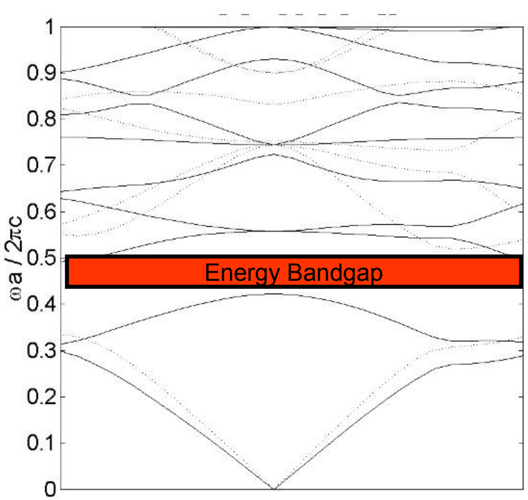
Photonic Crystal Response Surface / Photonic Band Gap Map

Photonic Crystal - Optimisation

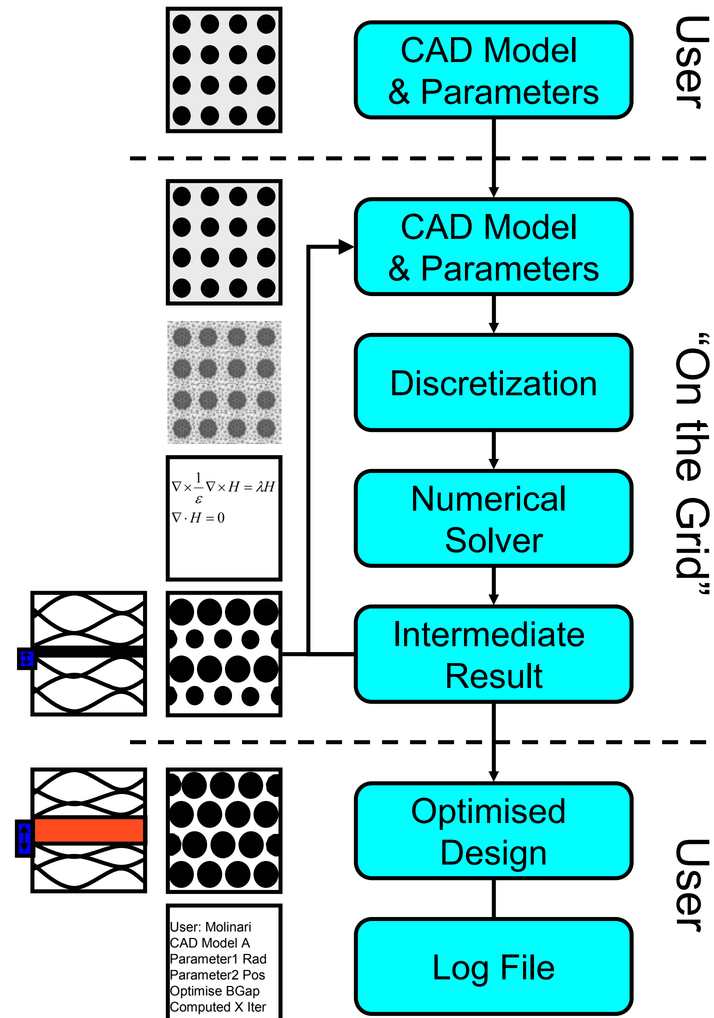




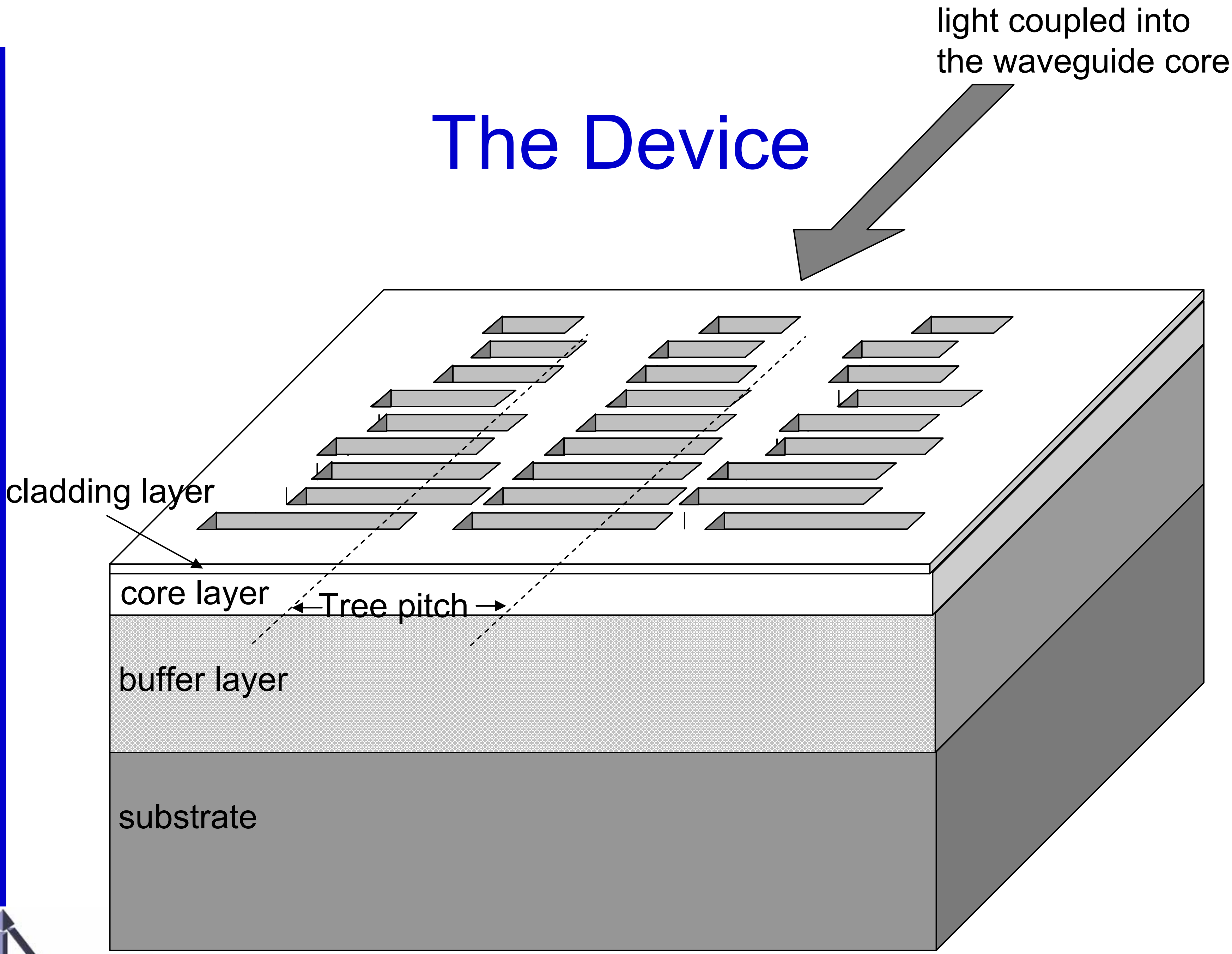
Location, size & density of holes determine the optical bandgap.



The aim of this design optimisation process is to find a configuration which maximises this bandgap and minimizes energy loss.



The Device



light coupled into
the waveguide core
cladding layer
core layer
Tree pitch
buffer layer
substrate

The Script

geometry_optimise_EDIT.m

Scripting languages

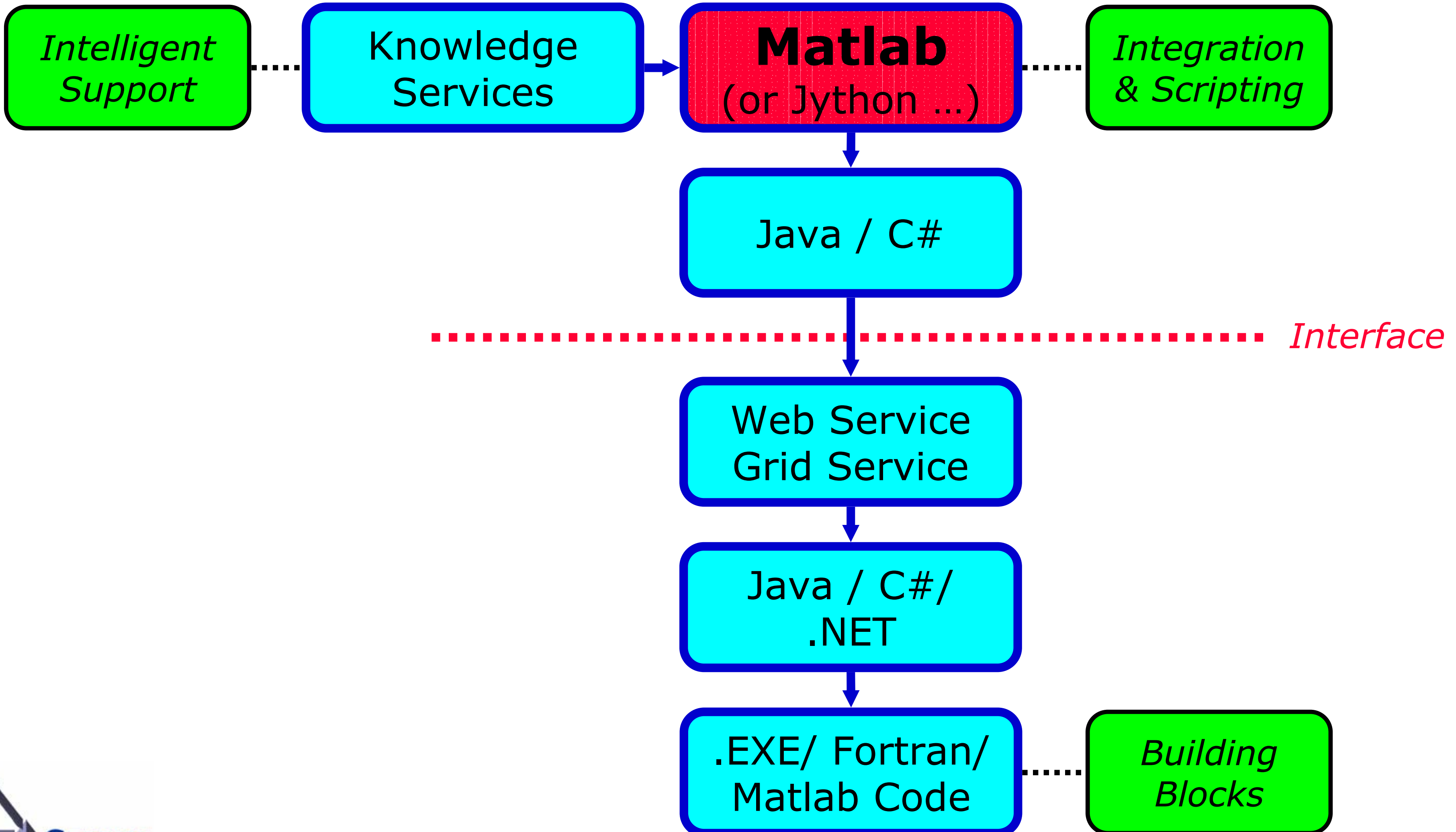
Why use scripting languages?

- Flexibility
- High-level functionality
- Quick application development
- Extend the user's existing PSE

Grid-Enabled Matlab Scripting Environment

- Motivations:
  - Flexible, transparent access to computational resources
  - Easy to use for engineers (and in widespread use)
- Our Approach
  - Matlab chosen as the hosting environment
    - Extend the user's existing PSE
    - High-level functionality
    - Quick application development
    - … is our execution/ enactment engine too
  - Computational resources exposed in the form of Matlab functions
    - Job submission to Globus server using Java Cog
    - Job submission to Condor pool via Web services interface
  - Integration of CAD, Mesh generation, and Fluent solver via the use of intermediate data format, often standard-based, or package-neutral
  - Hybrid search strategies to make the best use of different search methods
- Can also use Python, Jython, etc.

Geodise Architecture



Grid-Enabled Toolkits in Matlab

	Function Name	Descriptions
Proxy management	`gd_createproxy`	Creates a Globus proxy certificate from the user's credentials
	`gd_proxyinfo`	Returns information about the user's proxy certificate
	`gd_proxyquery`	Queries whether a valid proxy certificate exists
	`gd_certinfo`	Returns information about the user's certificate
	`gd_destroyproxy`	Destroys the local copy of the user's Globus proxy certificate
Job submission	`gd_jobkill`	Terminates the GRAM job specified by a job handle
	`gd_jobstatus`	Returns the status of the GRAM job specified a job handle
	`gd_jobpoll`	Queries the status of a Globus GRAM job until complete
	`gd_jobsubmit`	Submits a GRAM job to a Globus server
Data archive	`gd_getfile`	Retrieves a file from a remote host using GridFTP
	`gd_putfile`	Transfers a file to a remote host using GridFTP
	`gd_archive`	Stores a file in repository with associated metadata
	`gd_query`	Retrieves metadata about a file based on certain criteria
	`gd_retrieve`	Retrieves a file from the repository to the local machine
	`gd_sendtext`	Sends a SMS text message to the specified mobile phone number

Pound, G.E., Eres, M.H., Wason, J.L., Jiao, Z., Cox, S.J., and Keane, A. J., "A Grid –enabled Problem Solving Environment (PSE) for Design Optimisation within Matlab", 17th International Parallel and Distributed Processing Symposium (IPDPS 2003) 22-26 April 2003, Nice, France, 2003

GEODISE

Scripting the optimisation workflow within Matlab

MATLAB

File Edit View Web Window Help

Current Directory: D:\geodise2\orthfoil

```
>> % import java class
import org.geodise.optimisation.*;
% problem definition
nvars = 2;
lvars =[-1, 0.06];
uvars =[1,0.18];
vars = [0.3, 0.12];
% Options data structure for orthfoil problem
orthfoilRSM = JavaOptData(nvars, vars, lvars, uvars);
% JavaOptions
opt = JavaOptions;
opt.Load(orthfoilRSM);
niters =15;
ncons = 1;
vars =[0.154185145,0.146553658,-0.251986064,0.134932023,0.538988307,0.177126053,0.044716965,0.062852334,-0.541704384,0.122527654,0.941380805,0.165200035,-0.455053
objs =[9.736681192,10.74828461,1.096400541,12.85513197,10.61839788,5.582960856,12.07712295,8.01420247,3.852191454,13.66563896,8.578822294,5.875477296,12.71259167,
cons=zeros(1,15);
lcons=-1*ones(1,15);
ucons=ones(1,15);

% fill in the data
opt.optfill(niters, nvars, ncons, vars, cons, objs, lcons, ucons);
% find hyperparameters
orthfoilRSM.objmod=4.1;
orthfoilRSM.conmod=2.1;
opt.optrss(orthfoilRSM);
% plot the response surface
npoints=100;
orthfoilRSM.update=0;
orthfoilRSM.omethd=0;
orthfoilRSM.niters=1;
x1=[orthfoilRSM.lvars(1):(orthfoilRSM.uvars(1)-orthfoilRSM.lvars(1))/(npoints-1):orthfoilRSM.uvars(1)];
x2=[orthfoilRSM.lvars(2):(orthfoilRSM.uvars(2)-orthfoilRSM.lvars(2))/(npoints-1):orthfoilRSM.uvars(2)];
for i=1:npoints
    orthfoilRSM.vars(1)=x1(i);
    for j=1:npoints
        orthfoilRSM.vars(2)=x2(j);
        opt.Search(orthfoilRSM);
        obj(j,i)=orthfoilRSM.objfn;
    end
end
mesh(x1,x2,obj);
orthfoilRSM.niters=100;
orthfoilRSM.omethd=4.0;
opt.Search(orthfoilRSM);
```

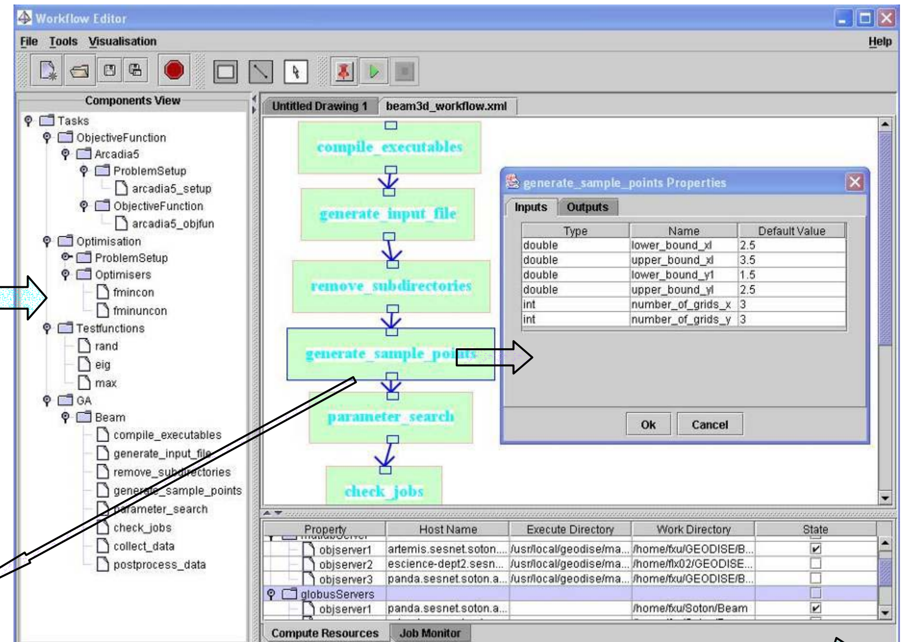
Start

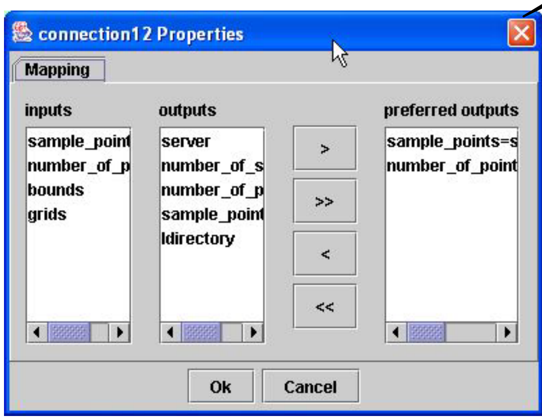
GEODISE

Workflow

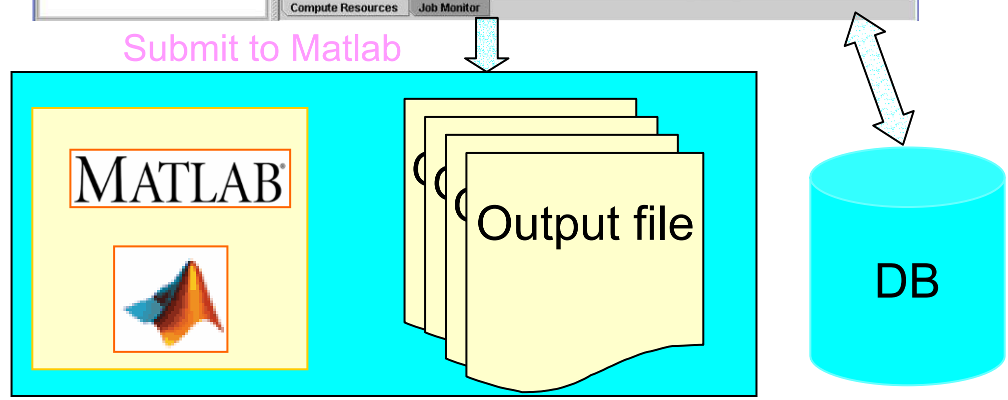
Workflow Editor

```xml
<?xml version="1.0" encoding="UTF-8"?>
…
<Functions>
   <Testfunctions>
       <rand type="Instance">
          <inputs>
             <input1 type="int" name="n" value=" 5 "/>
          </inputs>
          <outputs>
             <output type="matrix" name="A"
value=""/>
          </outputs>
       </rand>
   </Testfunctions>
</Functions>
```





Submit to Matlab



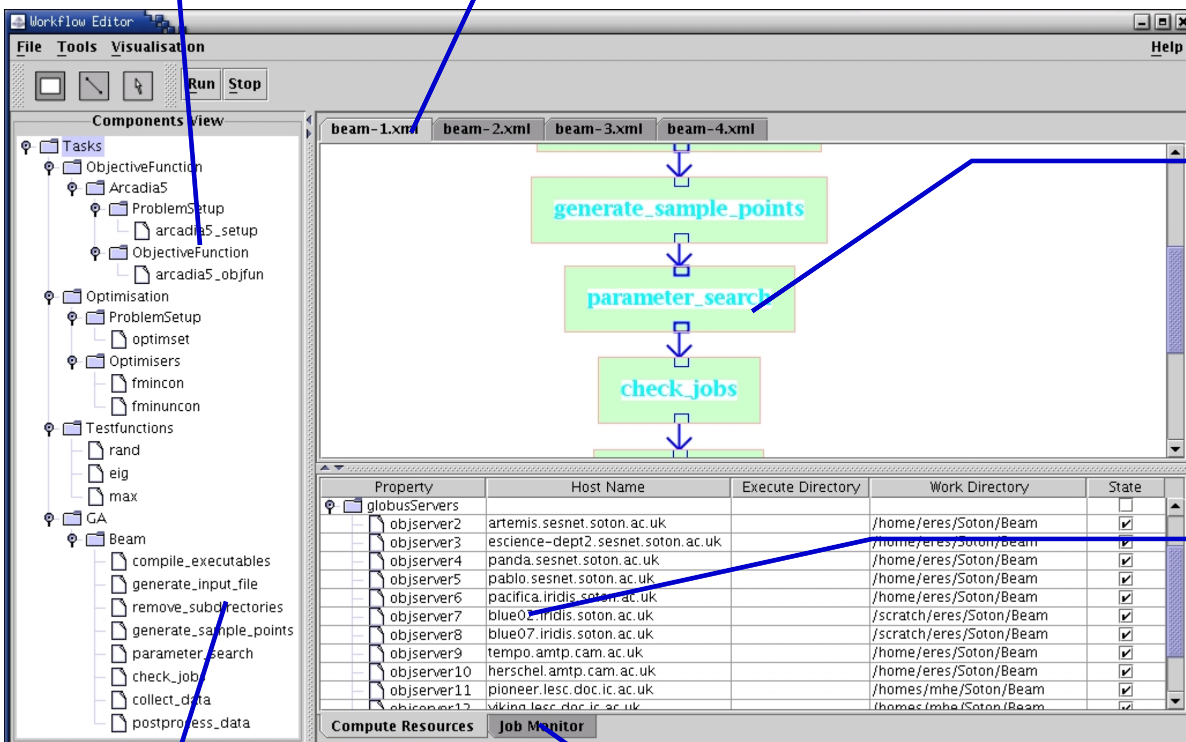
Workflow Tool (Part i)

Retrieve

Projects

Composition Area

Execution - Mapping to Resources



Functions

Monitoring and Steering

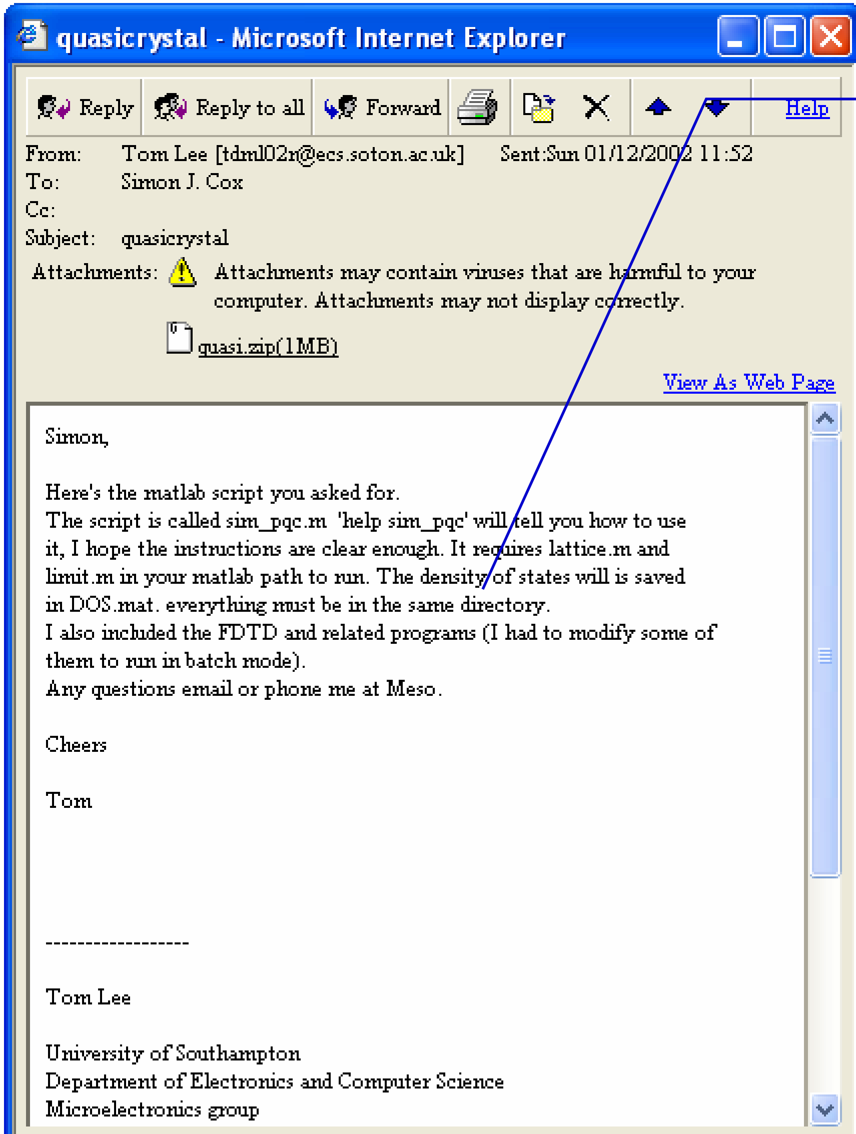
GEODISE

A few of my favourite things to do with workflows- review

- ✓ Create
- ✓ Retrieve
- ✓ Cut ‘n’ Shut
- ✓ Configure
- ✓ Execute
- ✓ Monitor
- Share
- Steer
- Dynamically modify

GEODISE

Sharing (i)


quasicrystal - Microsoft Internet Explorer

Reply | Reply to all | Forward | Help

From: Tom Lee [tdml02r@ecs.soton.ac.uk] Sent:Sun 01/12/2002 11:52
To: Simon J. Cox
Cc:
Subject: quasicrystal
Attachments: Attachments may contain viruses that are harmful to your computer. Attachments may not display correctly.
quasi.zip(1MB)

View As Web Page

Simon,

Here's the matlab script you asked for.
The script is called sim_pqc.m 'help sim_pqc' will tell you how to use
it, I hope the instructions are clear enough. It requires lattice.m and
limit.m in your matlab path to run. The density of states will is saved
in DOS.mat. everything must be in the same directory.
I also included the FDTD and related programs (I had to modify some of
them to run in batch mode).
Any questions email or phone me at Meso.

Cheers

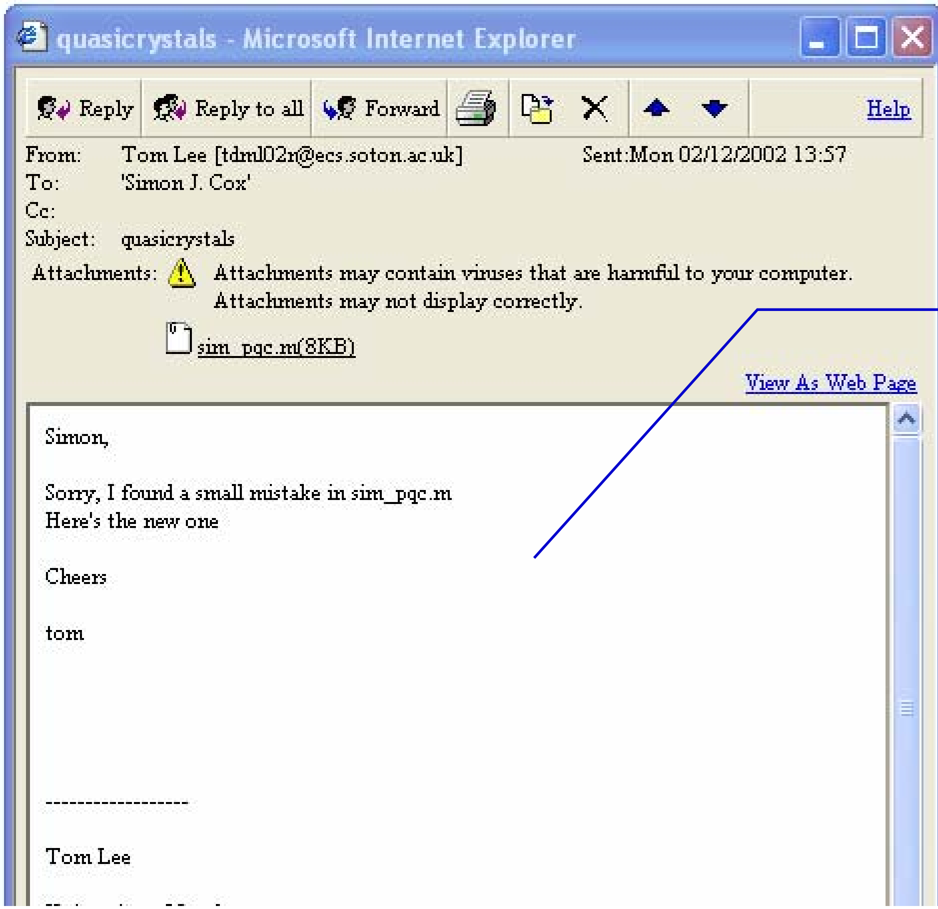
Tom

Tom Lee

University of Southampton
Department of Electronics and Computer Science
Microelectronics group

Here's the matlab script you asked for.
The script is called sim_pqc.m 'help sim_pqc' will tell you how to use it, I hope the instructions are clear enough. It requires lattice.m and limit.m in your matlab path to run. The density of states will is saved in DOS.mat. everything must be in the same directory.
I also included the FDTD and related programs (I had to modify some of them to run in batch mode).
Any questions email or phone me at Meso.

Sharing (ii)




```
Simon,

Sorry, I found a small mistake
in sim_pqc.m
Here's the new one

Cheers

tom
```

P.S. "Provenance" too

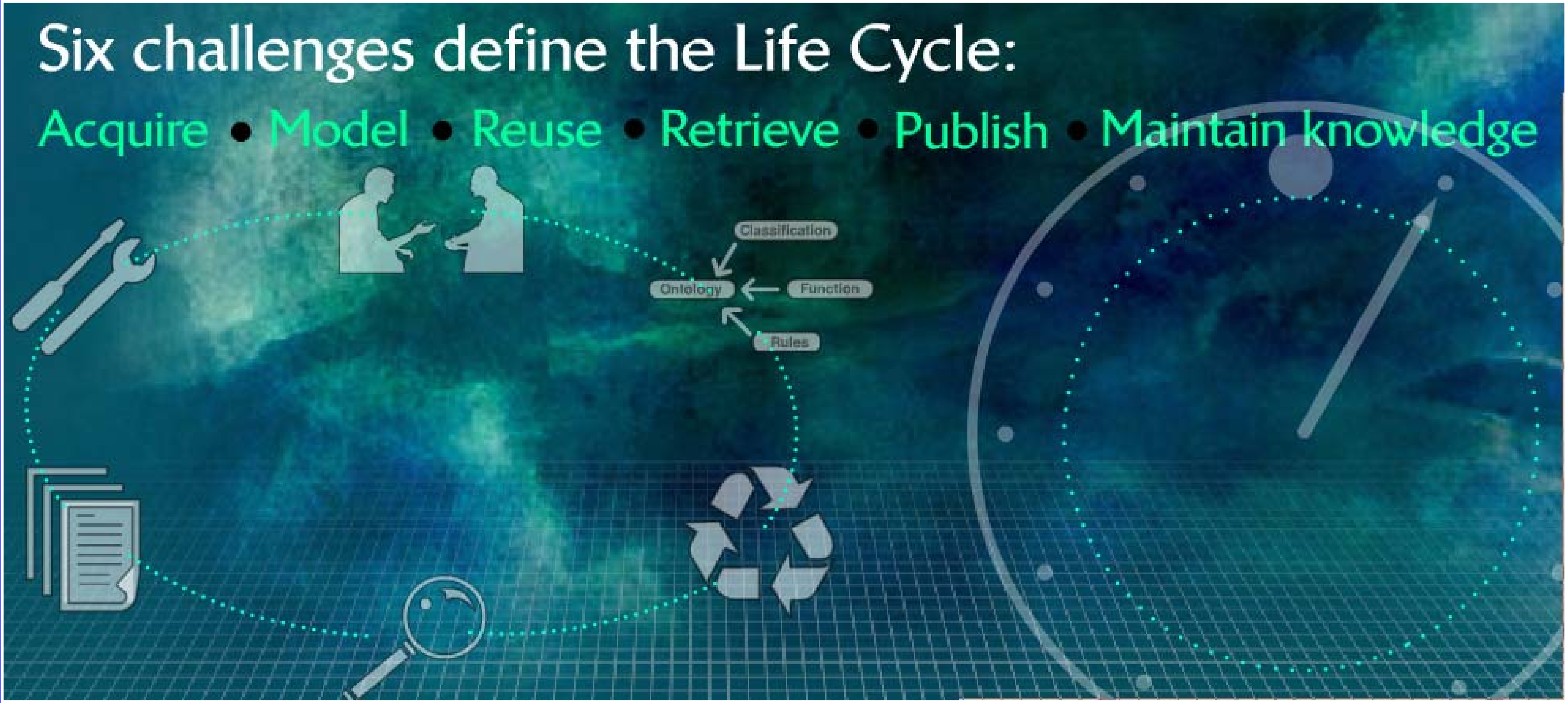
GEODISE

Semantics & Knowledge

Semantic Grid in e-Science

- Bridging the gap:
  - Grid: seamless access to distributed computation and data resources
  - e-Science: distributed collaboration and reuse of knowledge and resources
  - Semantic Grid: Semantic Web technology applied on Grid application
- Building ontology and semantically enrich resource for reuse and management
  - Resource is semantically meaningful
  - Expressed using a standard conceptualization
  - Which is well recognized within a specific community of practice.

Knowledge Technologies



Knowledge Acquisition (KA)

Knowledge sources

Domain experts, software manuals & textbooks.

KA techniques

Interview, protocol analysis, concept sorting etc.

Tools used

PC-PACK integrated knowledge engineering toolkit

Knowledge acquired

EDSO domain knowledge, EDSO processes and problem definition

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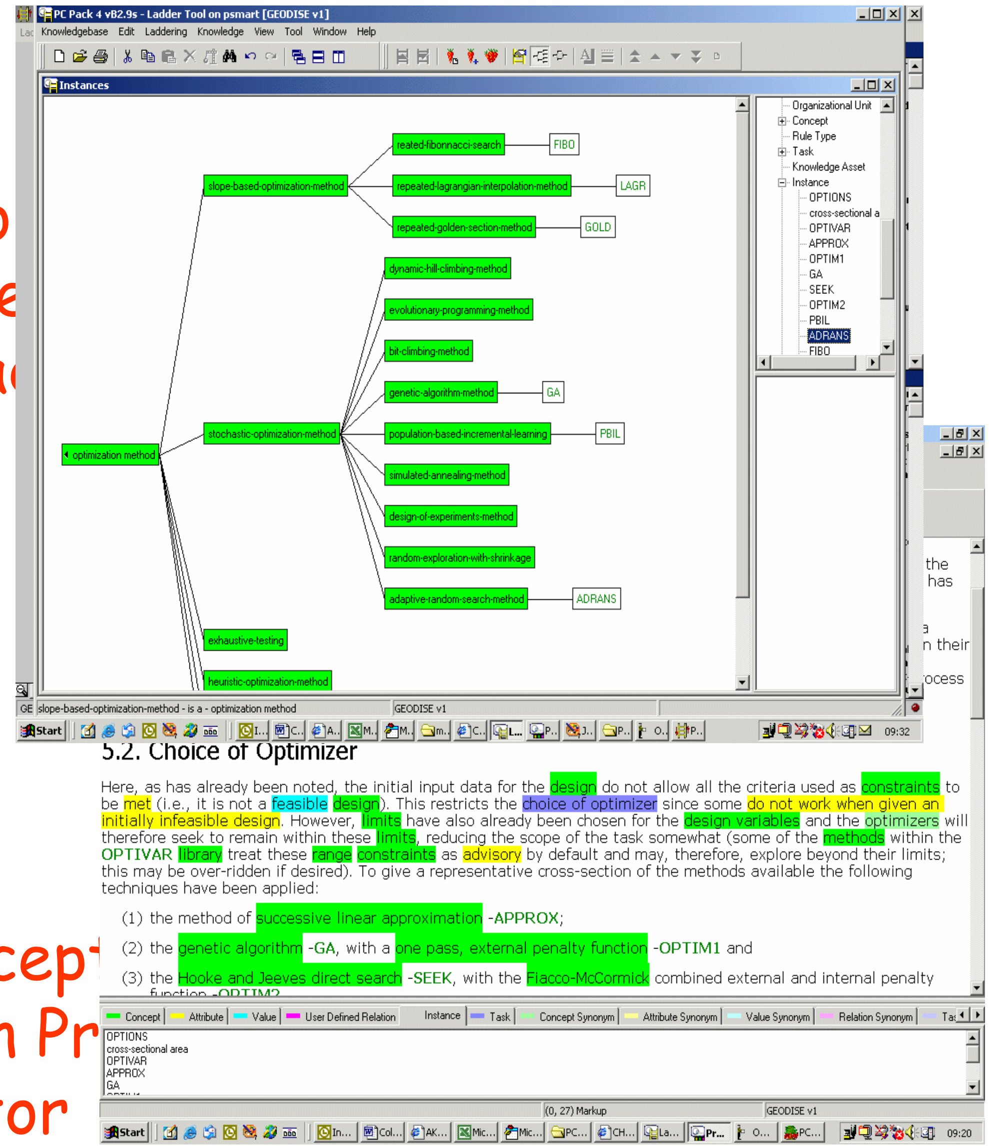
Editor



GEODISE

Knowledge Modelling

Techniques

CommonKADS knowledge engineering methodologies.

Knowledge models

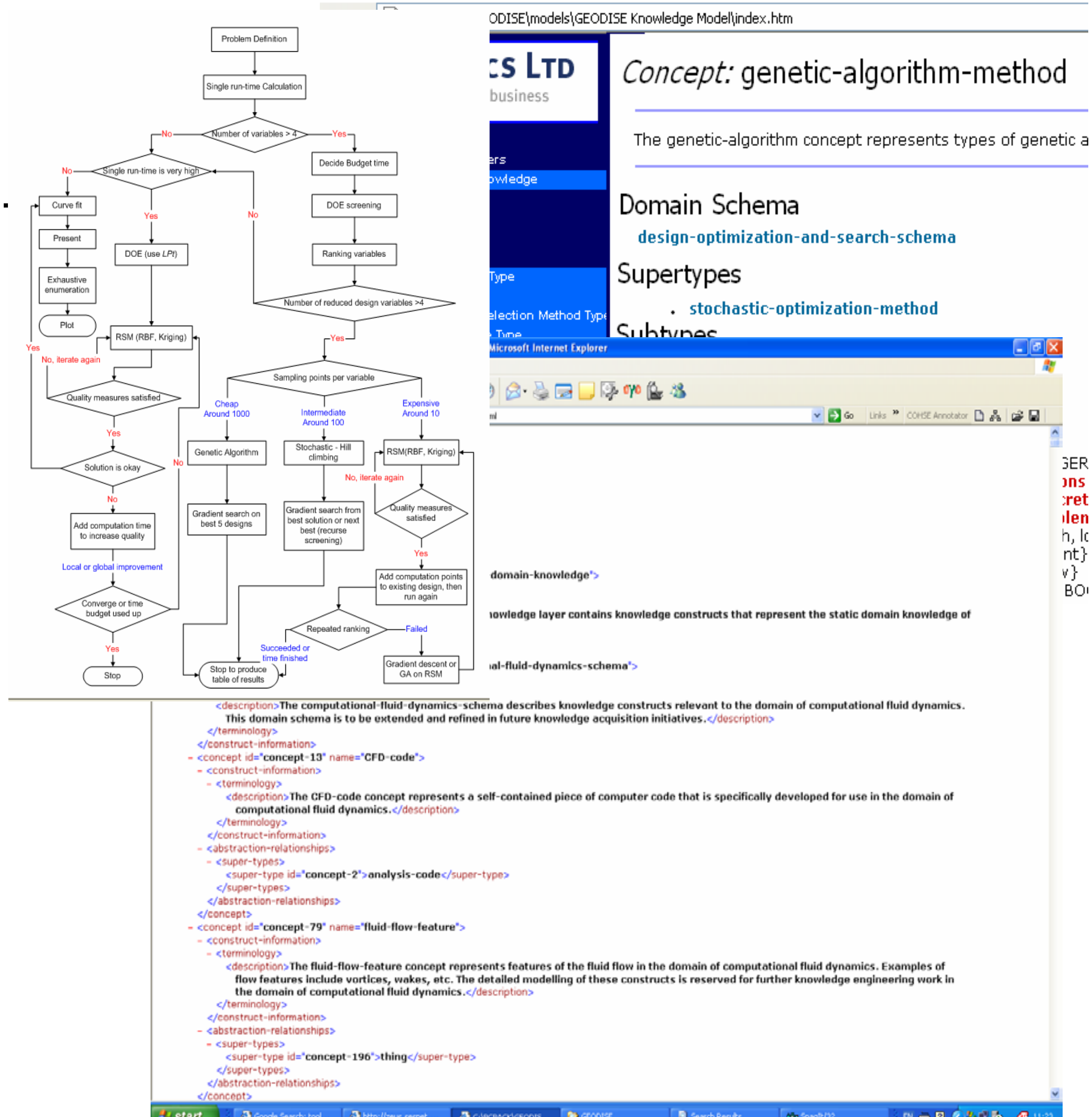
Organization, agent & task templates, domain schema inference rules.

Tools used

PC-PACK integrated knowledge engineering toolkit

Deliverables

Knowledge web in HTML, XML and UML, Conceptual task model, EDSO process flowchart



Ontologies

- common conceptualisation of a domain -

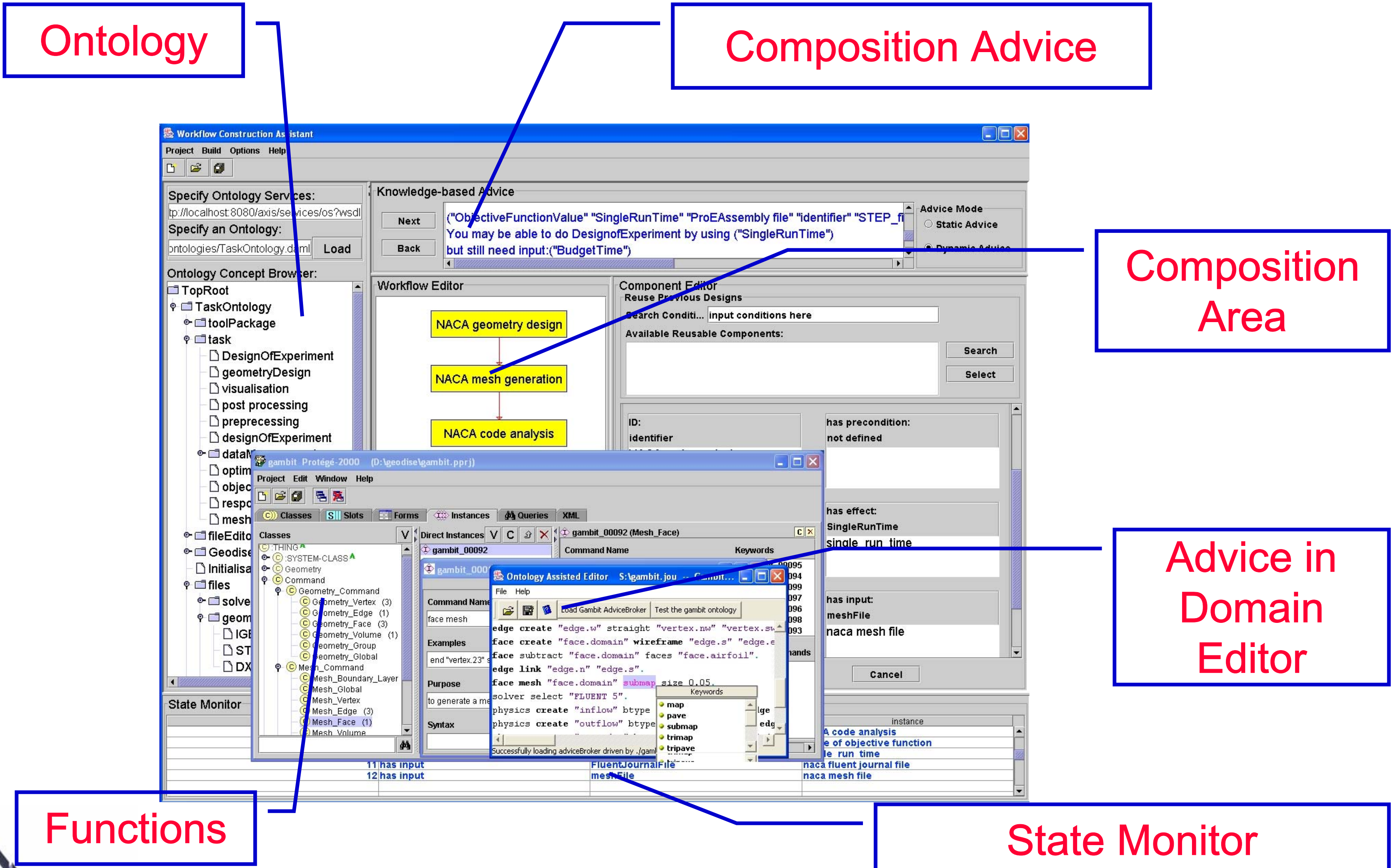
Semantic Workflow support in Geodise

- Ontology modelling
  - Definition: Domain conceptualisation that collect a controlled set of vocabulary and their relationship through hierarchy and explicitly expressed properties.
  - Examples: User profile ontology, Problem profile ontology, Task ontology, etc.
- Instance generation
  - Definition: Semantic enriching instances by referencing to ontology files
  - Methods: annotation content with ontology, populating ontology with content
- Semantic consumption
  - Ontology driven instance querying
  - Ontology driven from generation
    - task configuration
    - Problem setup
  - Ontology assisted domain script editing
  - Service oriented workflow composing – querying semantic enriched service component.

GEODISE

Workflow Tool

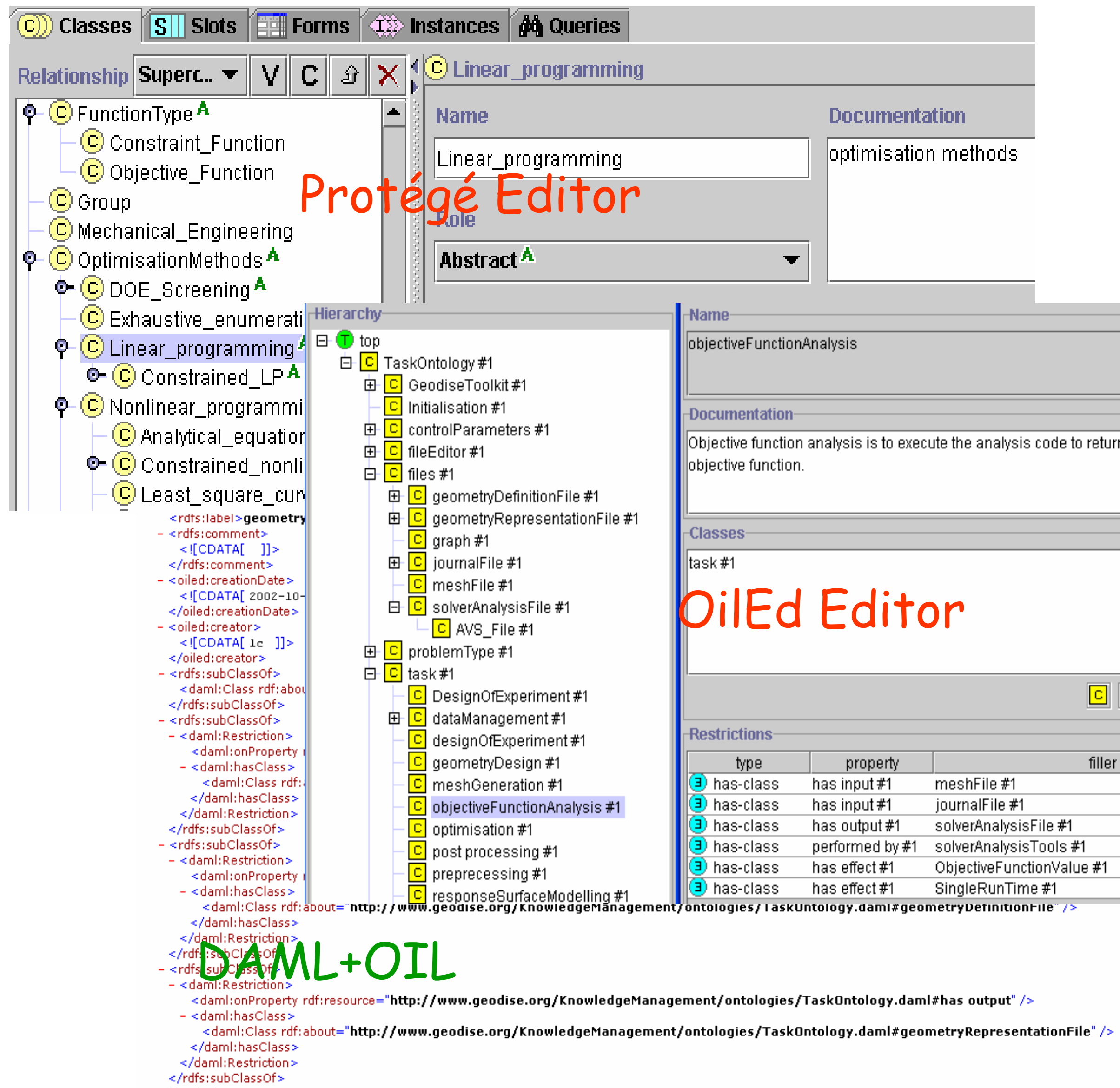
(… with added semantics)



GEODISE

Ontology Development (1)

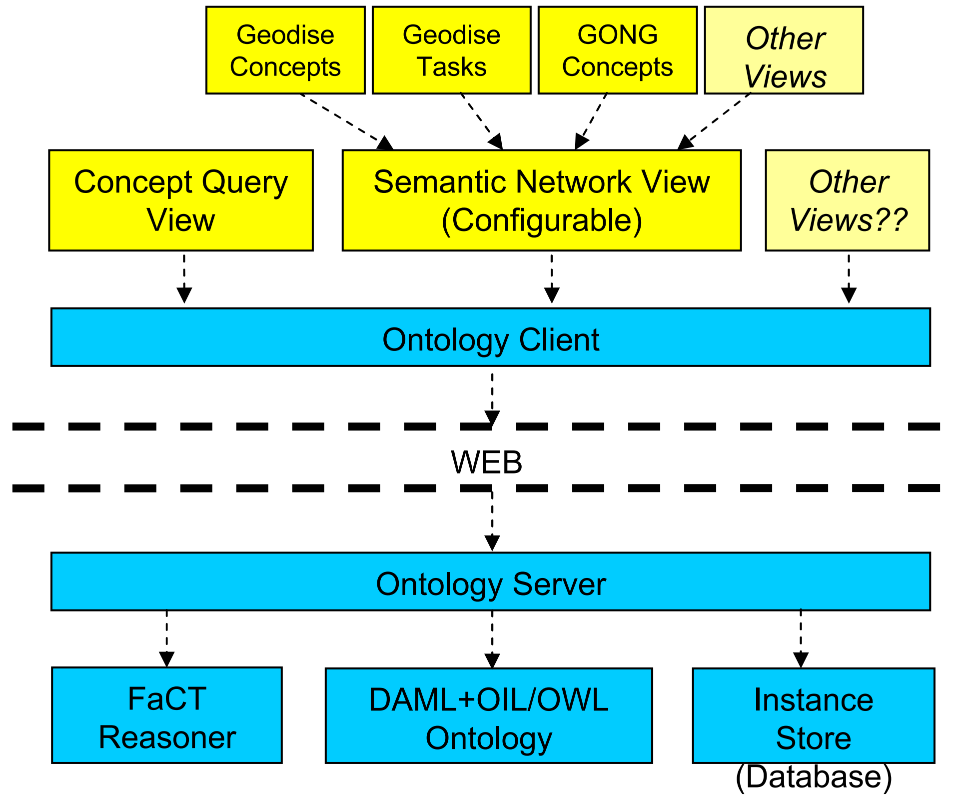
- Tools
  – Protégé & OilEd Editor
- Representation
  – DAML+OIL & CLIPS
- Deliverables
  – EDSO domain ontology
  – EDSO task ontology
  – Mesh generation tool (Gambit software) ontology
  – User-profile ontology

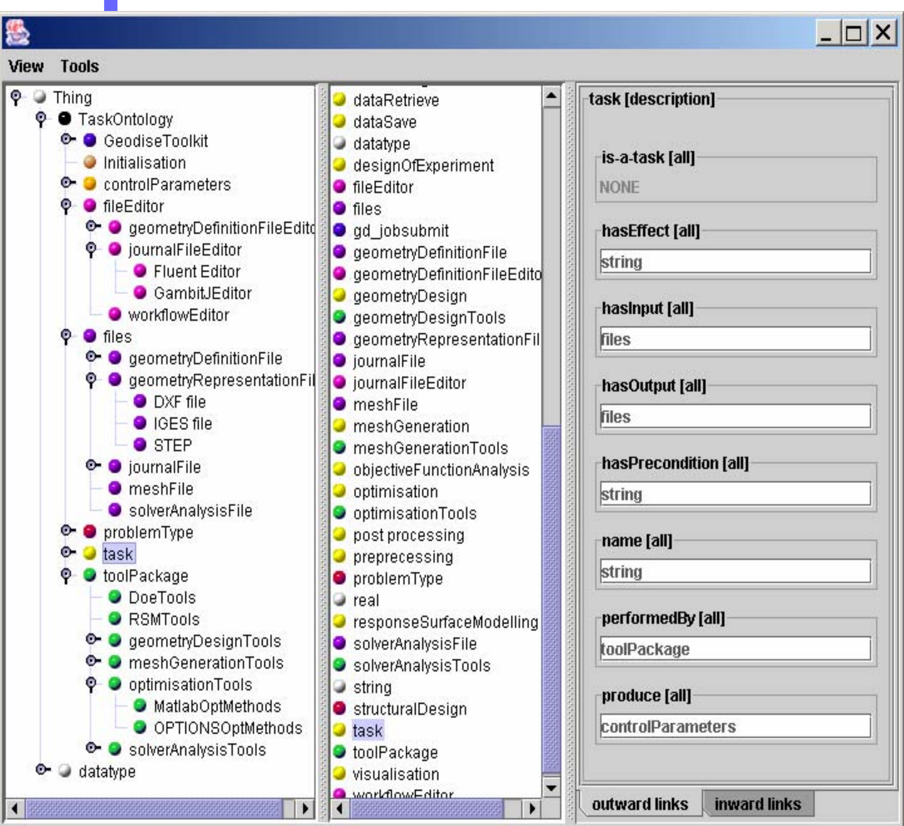


GEODISE

Ontology Development (2)

- Ontology Views
  - DL ontologies (DAML/OWL)
  - Simplified views
  - Tailored to specific domains

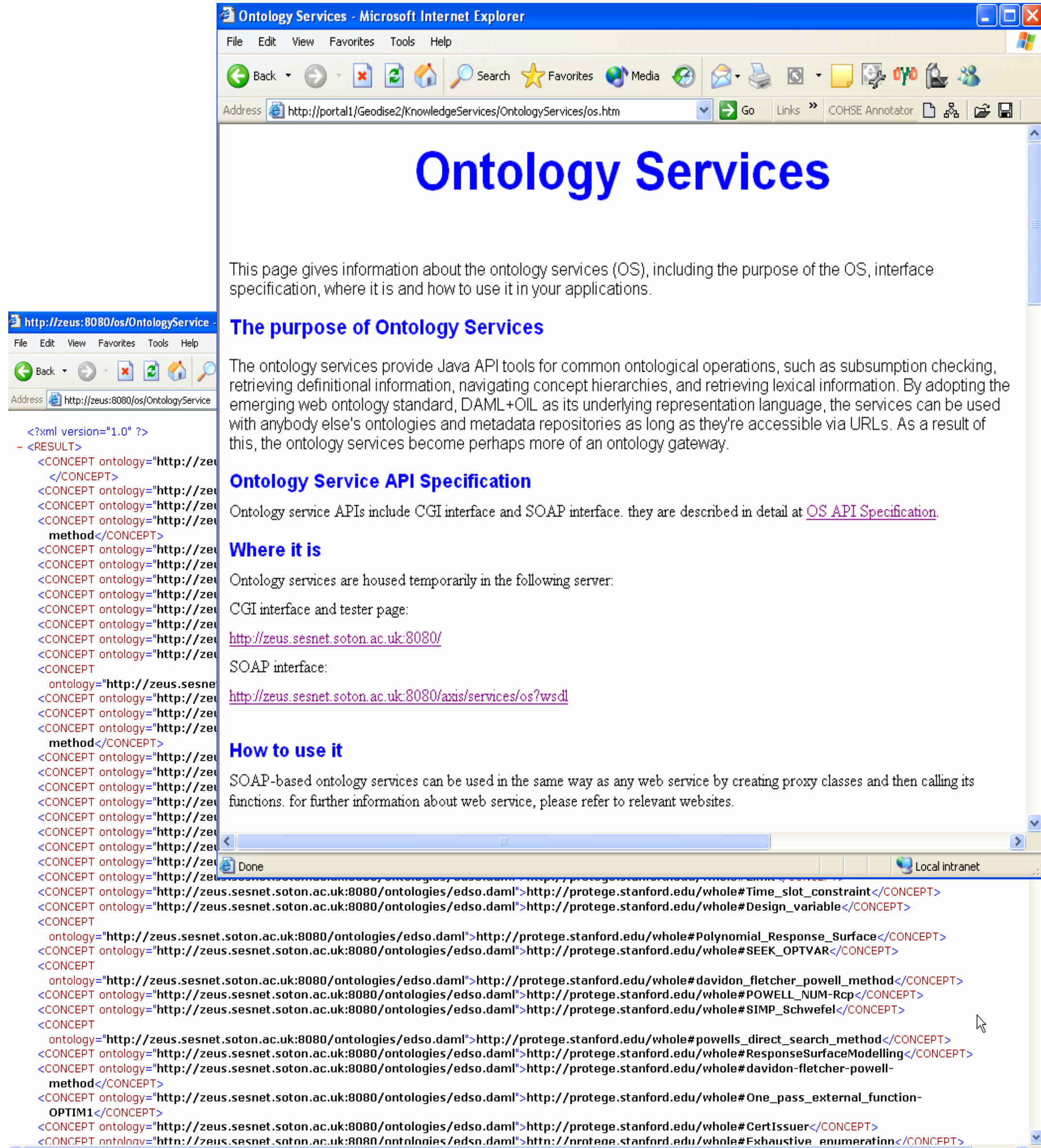




- Ontology Views
  - Underlying complexity hidden
- Ontology editing by…
  - Knowledge engineers
  - Domain experts

Ontology Services

- Facilitating ontology sharing & reuse
  - Ontology service APIs
- Domain independence
  - DAML+OIL/OWL standards
- Soap-based web services -WSDL
- Java, Apache Tomcat & Axis technologies



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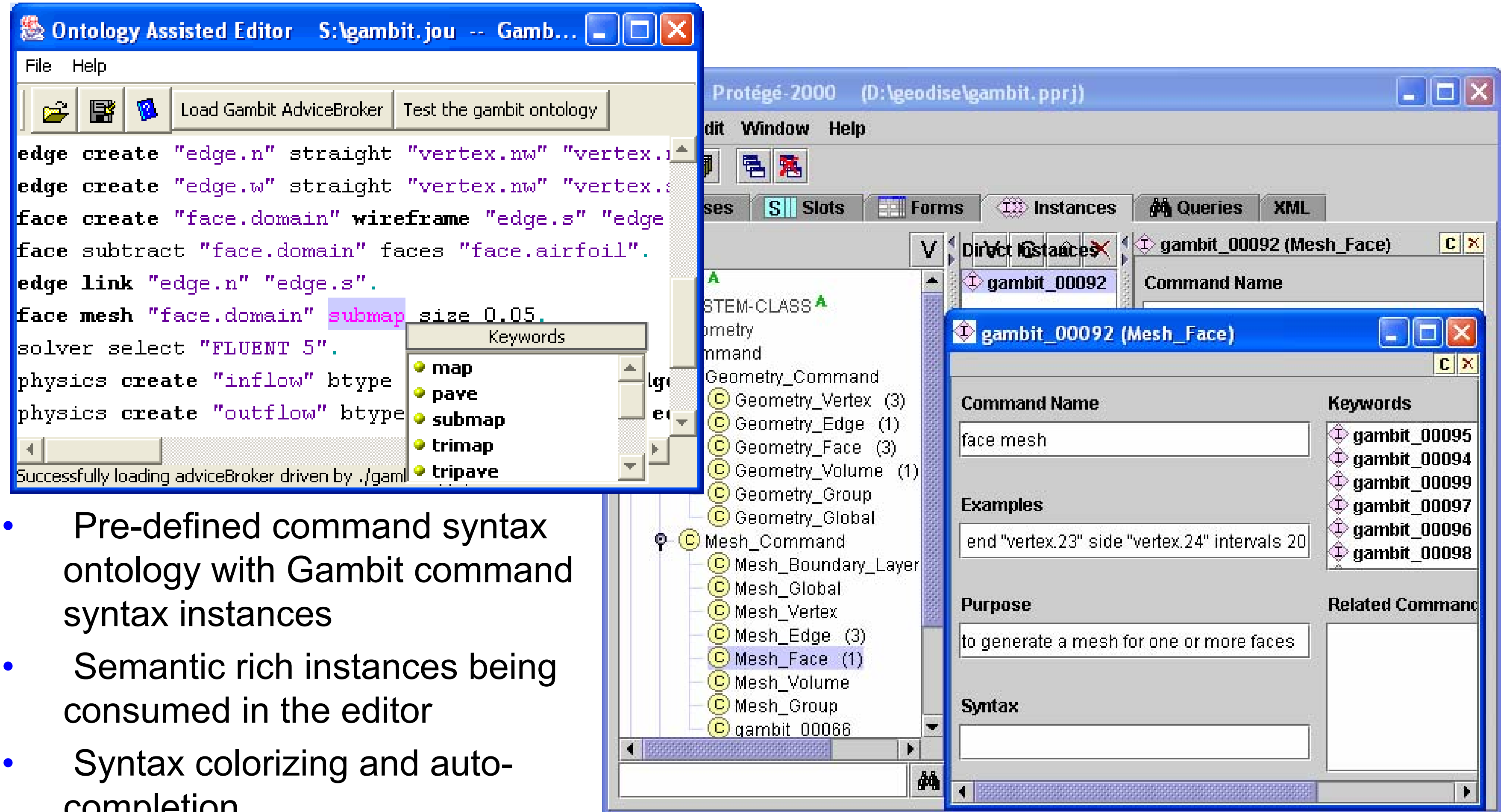
Ontology Assisted Domain Script Editor

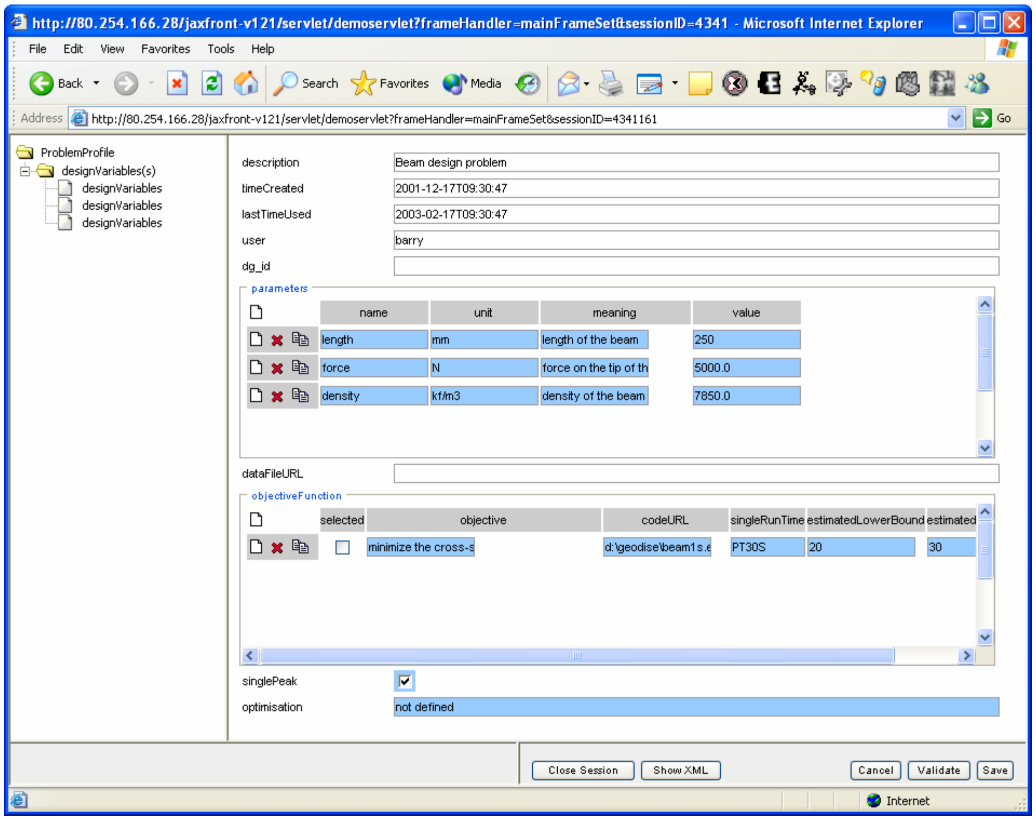


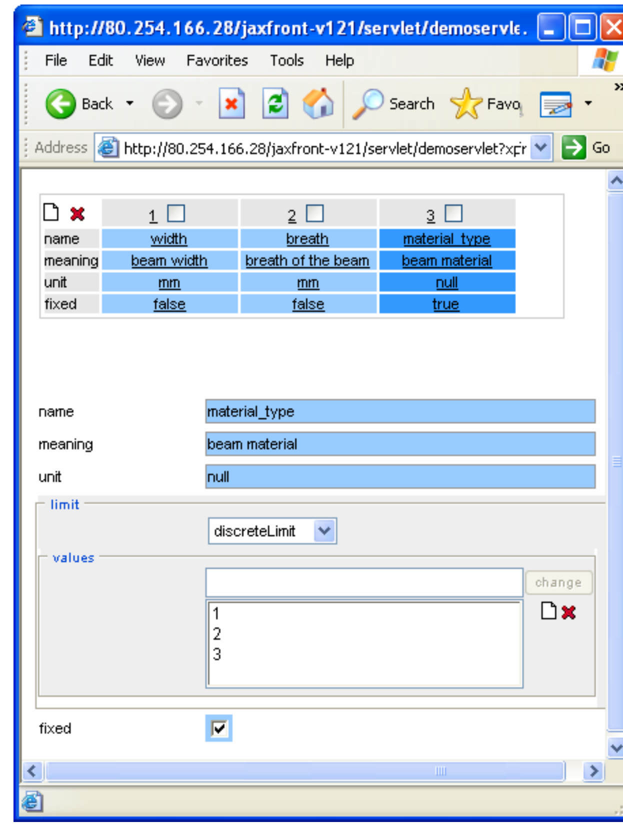
- Pre-defined command syntax ontology with Gambit command syntax instances
- Semantic rich instances being consumed in the editor
- Syntax colorizing and auto-completion

GEODISE

Ontology Driven Forms in Geodise -1

- Setting up problems (a scenario using JaxFront)

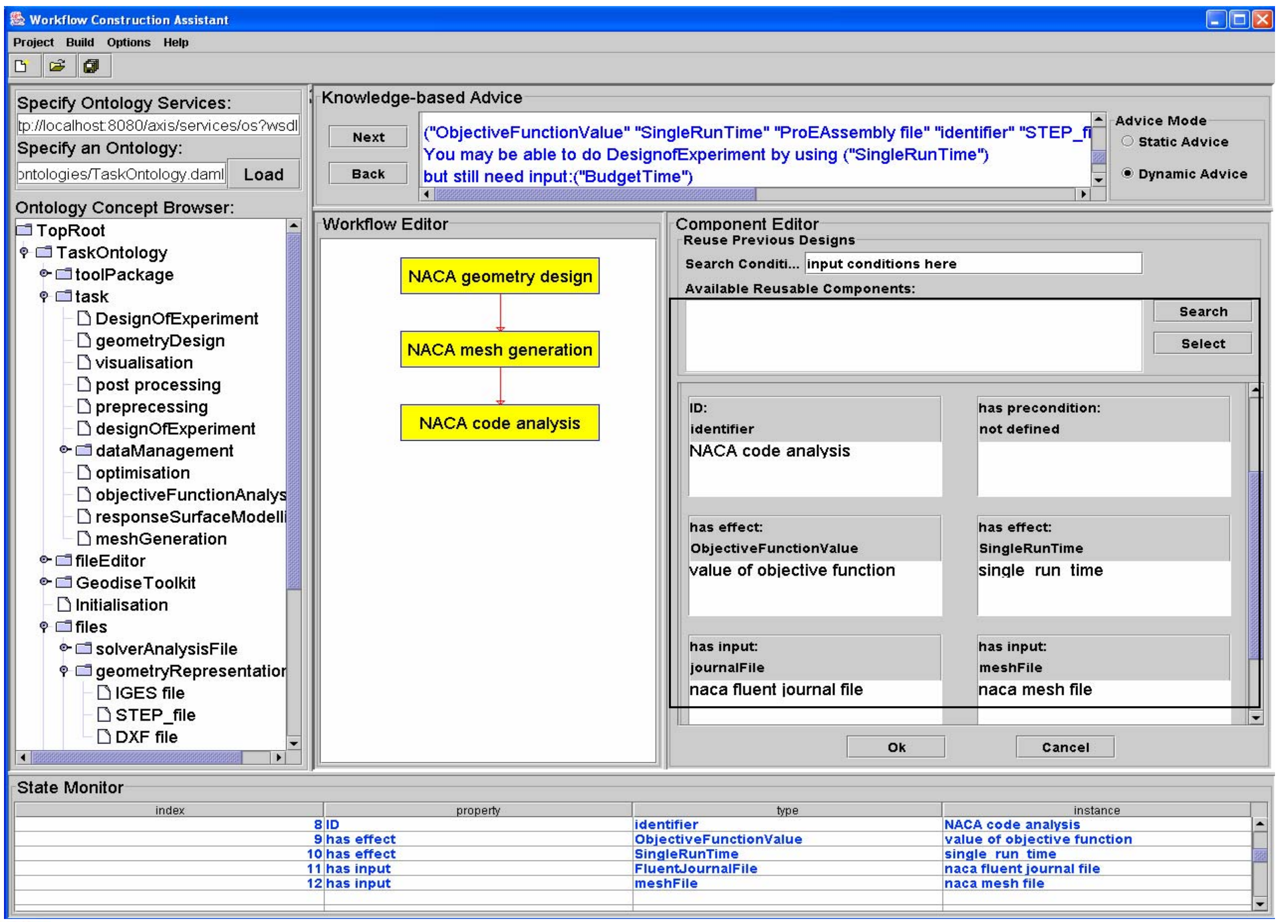




GEODISE

Ontology Driven Forms in Geodise -2

- Configuring tasks in Workflow Composing Environment

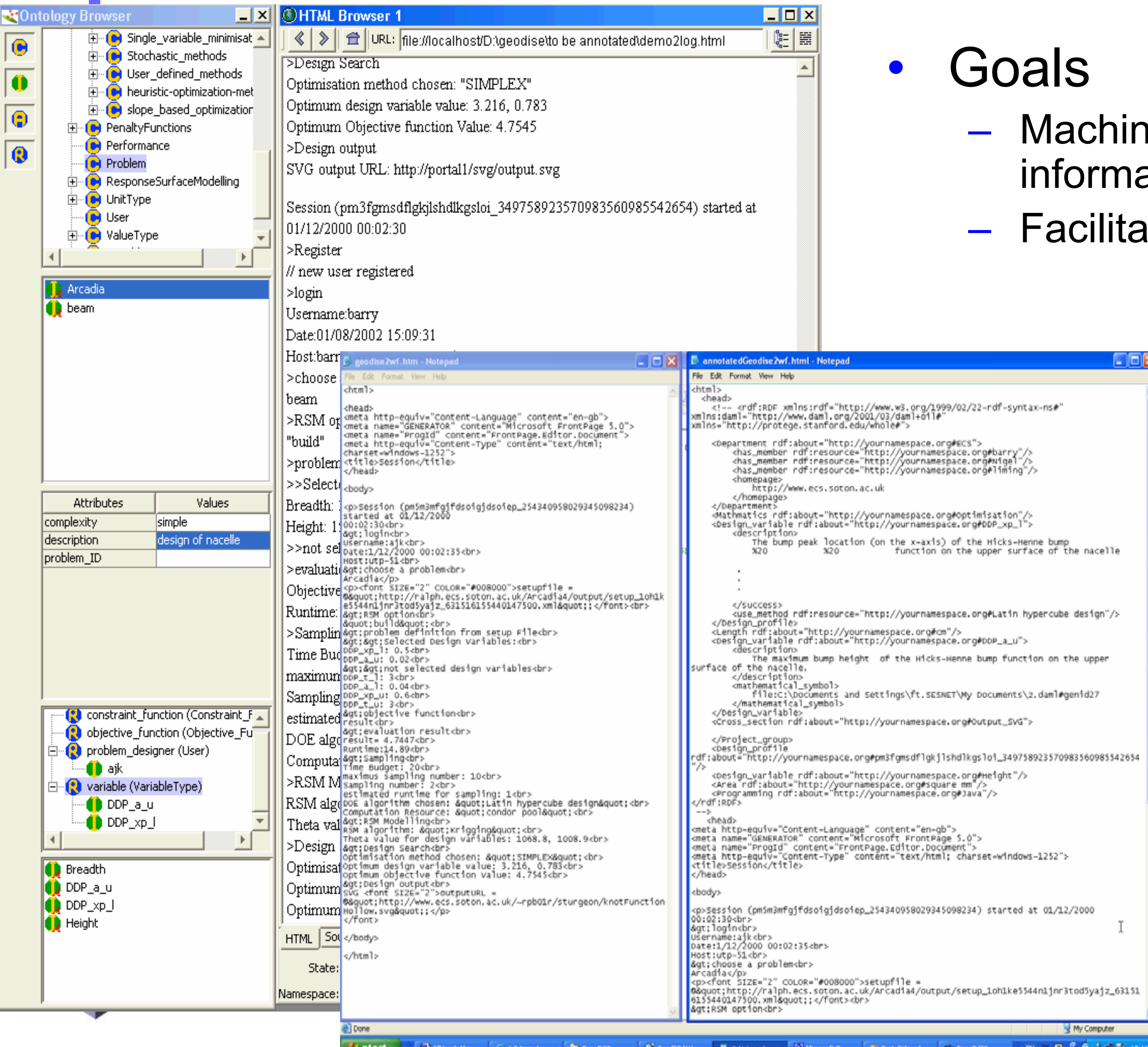


GEODISE

Exploiting Knowledge in Geodise

Knowledge Application 1:

Create Semantic Content

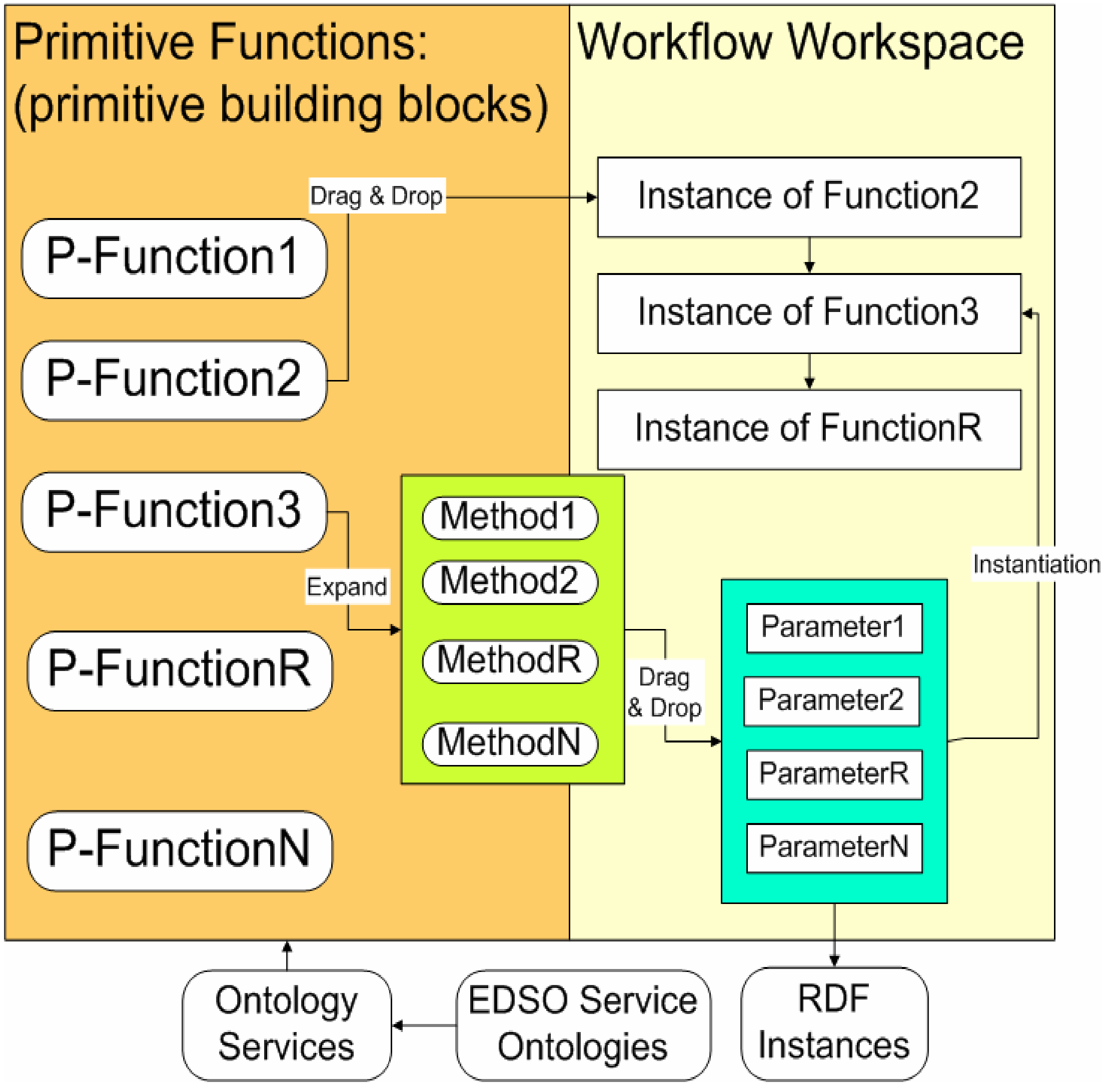


- Goals
  - Machine understandable information
  - Facilitate sharing & reuse
- Techniques & tools
  - OntMat-annotizer
  - Geodise Ontologies
- Example
  - OPTIONS log-files annotation

Knowledge Application 2:

Ontology-assisted Workflow Management

- Features:
  - Function selection
  - Function instantiation
  - Database schema
  - Semantic instances
  - Semantic workflow
- Technologies:
  - EDSO ontologies & ontology services
  - Java JAX-RPC, DOM/SAX

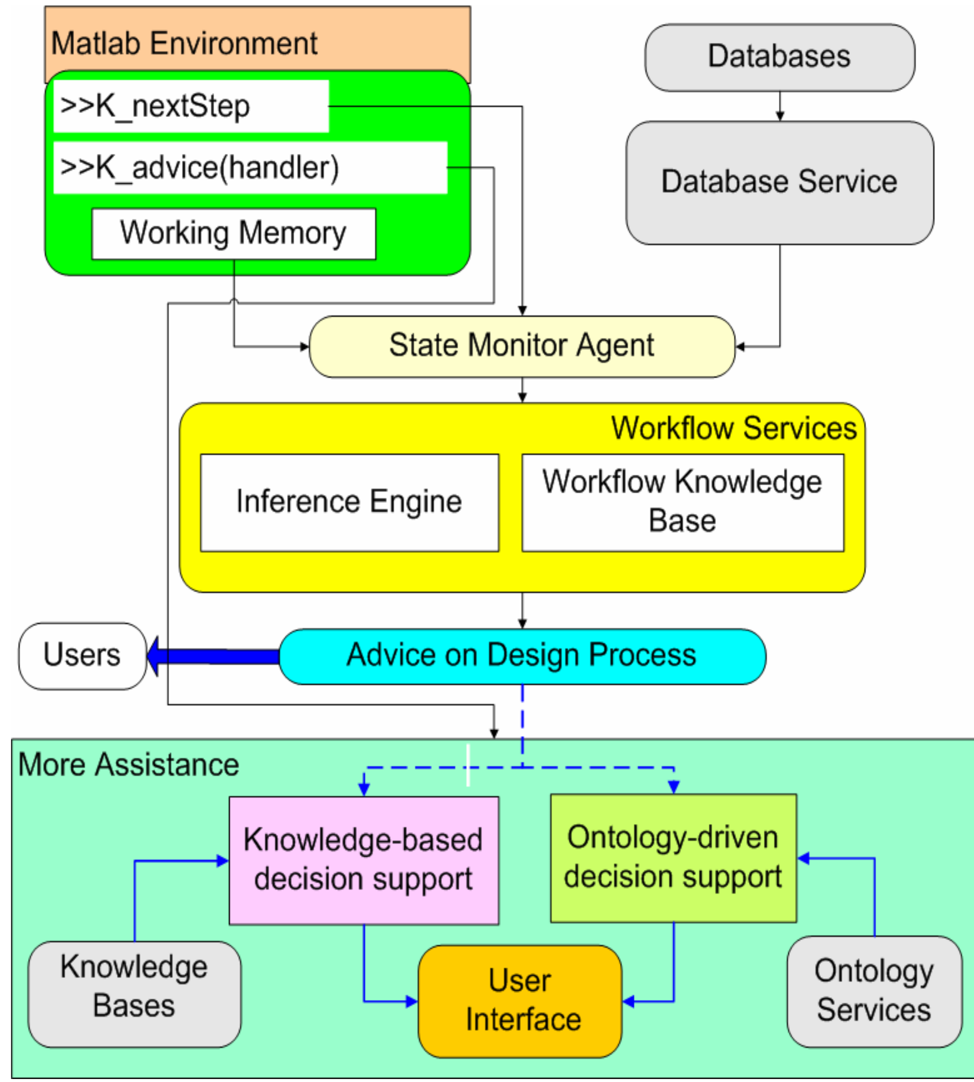


GEODISE

Knowledge Application 3:

Knowledge-based Design Advisor

- Features
  - Context-sensitive advice
  - Advice at multi-levels of granularity (process, task …)
  - KBSs as knowledge services
- Technologies
  - Knowledge engineering
  - EDSO ontologies
  - Rule-based reasoning techniques



GEODISE

Intelligent Workflow Monitoring and Advice
(“rule-based to case-based in real-time”)

- Updating constructed workflow using rule-base
  - At run-time:
    - find ‘similar’ workflows to the one constructed
    - is this one performing ‘as expected’? Might a different workflow outperform current one?
  - Resolution: Perhaps problem is anomalous?
    - Change method/ modify workflow?
    - Feedback to expert … update rule-base?
- Exploiting new components in workflows
  - Example
    - New optimisation method added in semantically consistent way
    - Workflows constructed (by expert) with new method, … and then:
  - ‘*similar workflow*’ search above will find workflows with new method in:
    - Might they outperform the currently constructed workflow?
    - Substitute new method into constructed workflow?
    - Feedback to expert … update rule-base?

GEODISE

A few of my favourite things to do with workflows- review (ii)

- ✓ Create
- ✓ Retrieve
- ✓ Cut ‘n’ Shut
- ✓ Configure
- ✓ Execute
- ✓ Monitor
- ✓ Share
- ✓ Steer
- ✓ Dynamically modify

GEODISE

Questions

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')
```