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TBD

David Abramson

Director, Research Computing Centre

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Workflows for Science and Engineering

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Director, Research Computing Centre

Introduction

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- Some Science and Engineering Optimization Problems
- The Nimrod tool family
- Scientific Workflows
- Interacting with designs
- Towards data intensive workflows
- Conclusions

Some Science and Engineering Optimization Problems

Air pollution
Cope, Victorian EPA (in 1990)

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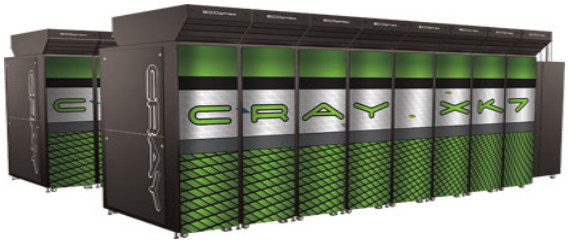

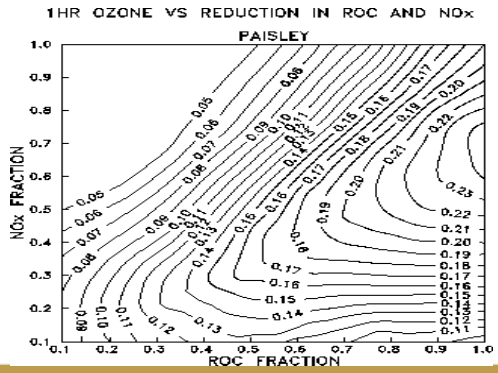

Wildfires
Lynch, Beringer, Uotila Monash U, AU

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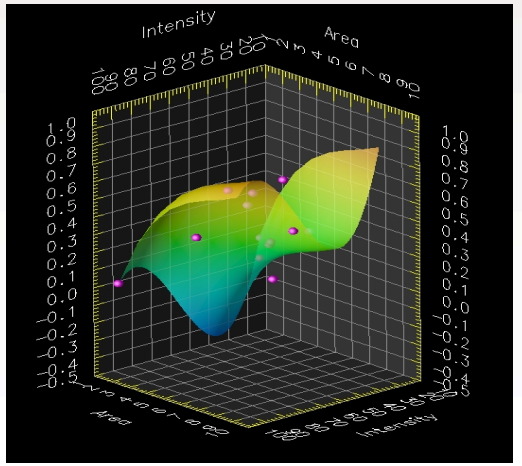

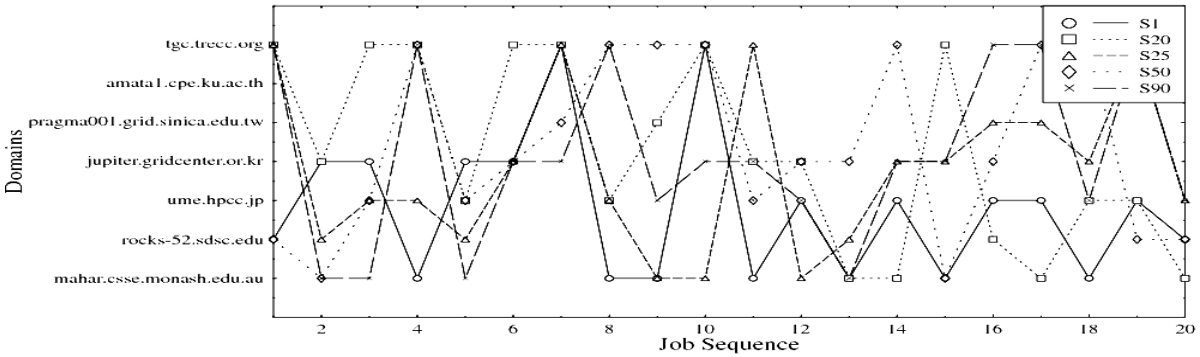

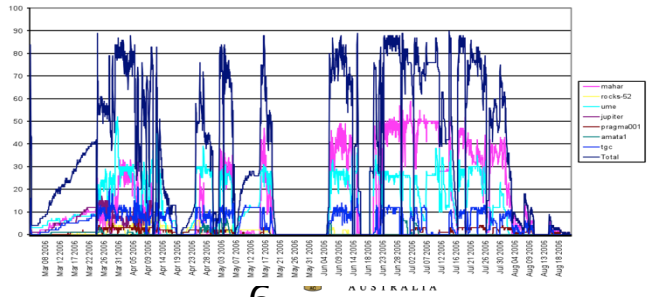

Aerofoil Design
Kipouros, Cambridge, UK

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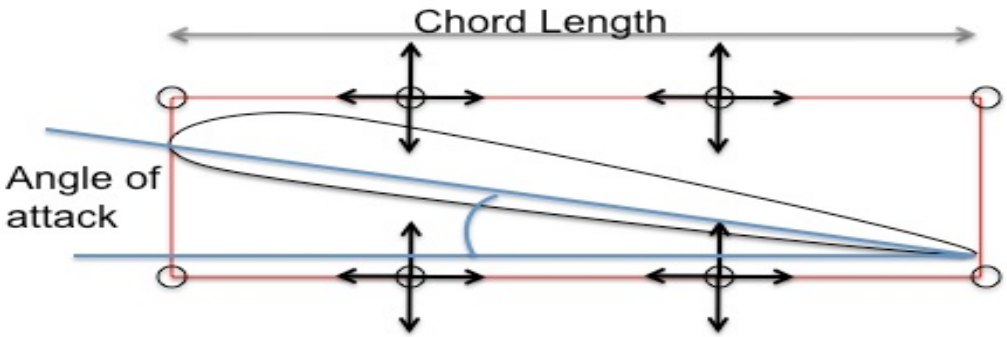
- Geometry management using Free Form Deformation – 8 design variables
- Evaluation of the aerodynamic characteristics, Cl, Cd, and Cm coefficients using Xfoil
- Investigation of the lift to drag trade-off subject to hard geometrical constraints to the thickness of the airfoil at 25% and 50% of the chord (in order to maintain practical significance



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Cardiac Science
Sher, Gavaghan, Rodriguez, Oxford
Mcculloch, Mihaylova, Kerckhoffs, UCSD

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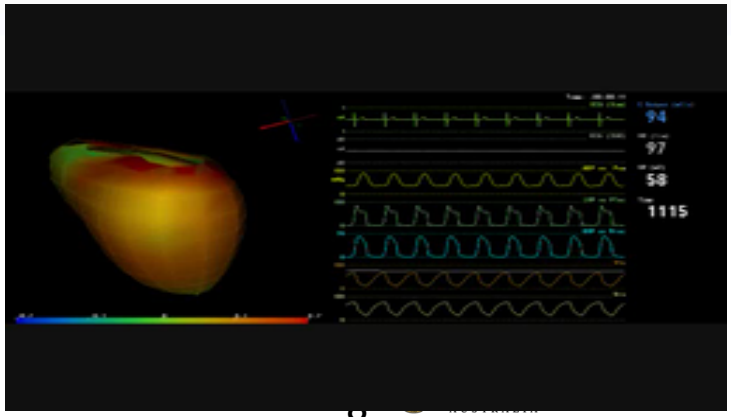
- Heart disease still leading cause of death
- Understanding the underlying physiological mechanisms is cheaper and faster when experimental studies are performed together with mathematical models & computer simulations
- Studying pathologies
- Developing & Testing drugs



Micromixer optimization
Kipouros, Cambridge, UK

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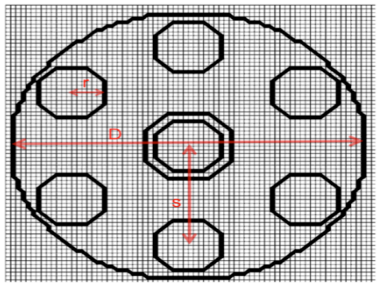
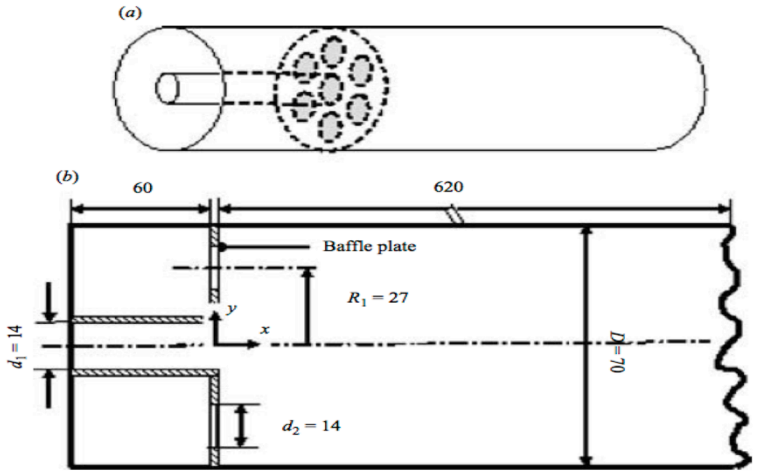
- Microfluidics
  - 10-9 to 10–18 litres amounts of fluids
  - Gaining importance in various fields
- Micromixer deals with mixing fluids in the smallest scale
- Active vs. passive



s >= 2*r + 1
s <= 34 - r



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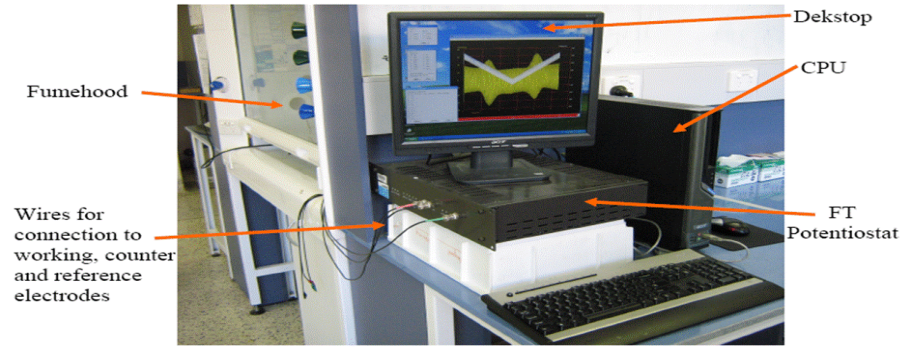
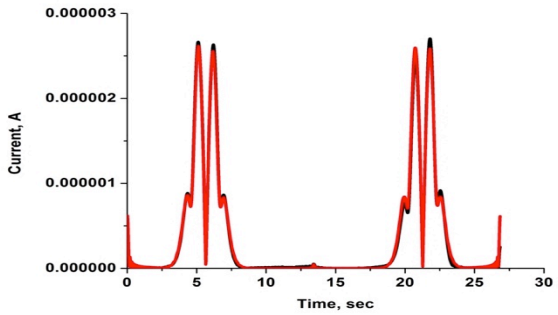
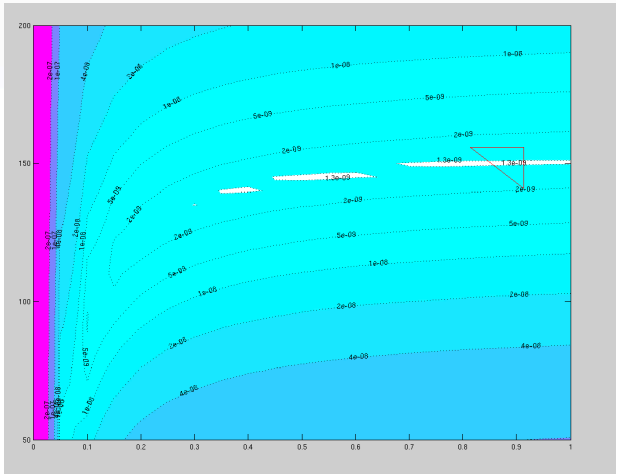
Electro-chemistry
Bond, Gavaghan: Monash, Oxford







The Nimrod Tools Family

Nimrod supporting “real” science and engineering

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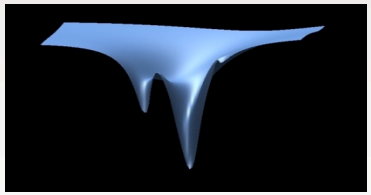
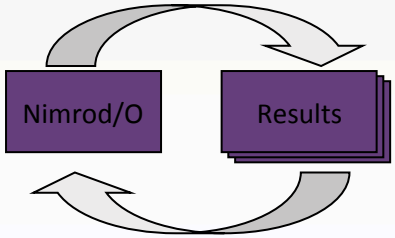
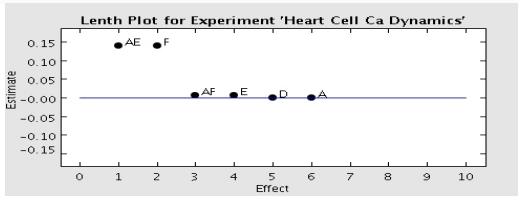
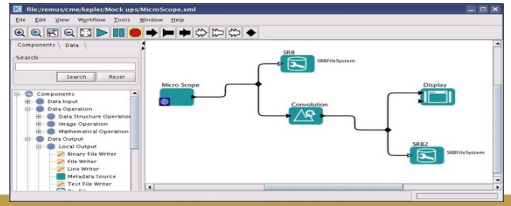
- A full parameter sweep is the cross product of all the parameters (Nimrod/G)
- An optimization run minimizes some output metric and returns parameter combinations that do this (Nimrod/O)
- Design of experiments limits number of combinations (Nimrod/E)
- Workflows (Nimrod/K)









Legacy Nimrod family

Plan File

Nimrod Portal

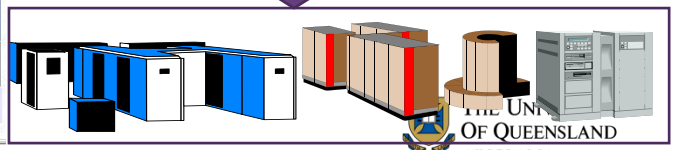
Nimrod/O

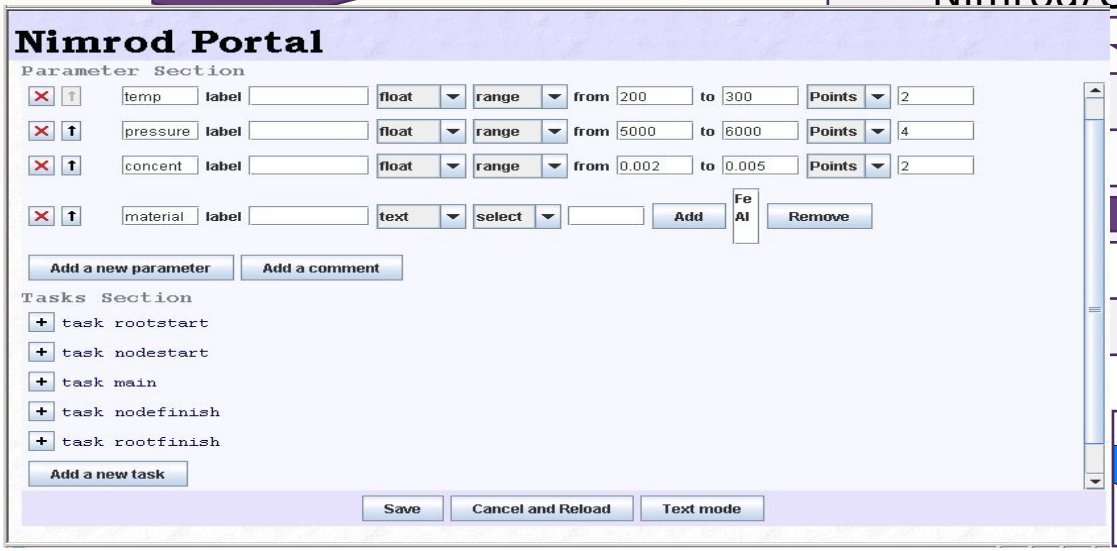
Nimrod/E

Nimrod/G

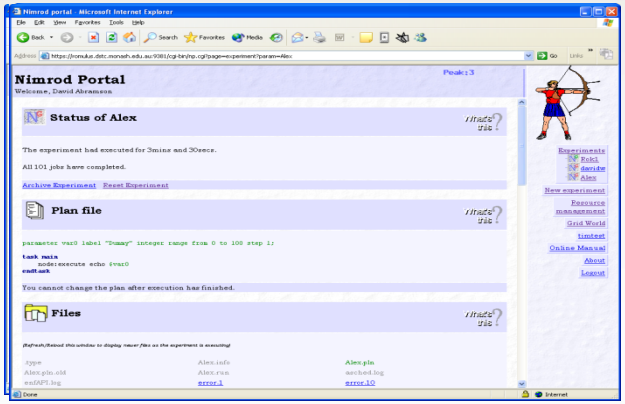
Actuators

Grid Middleware

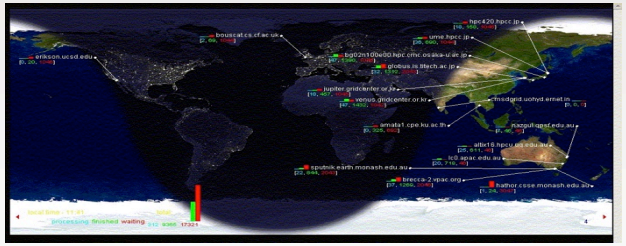




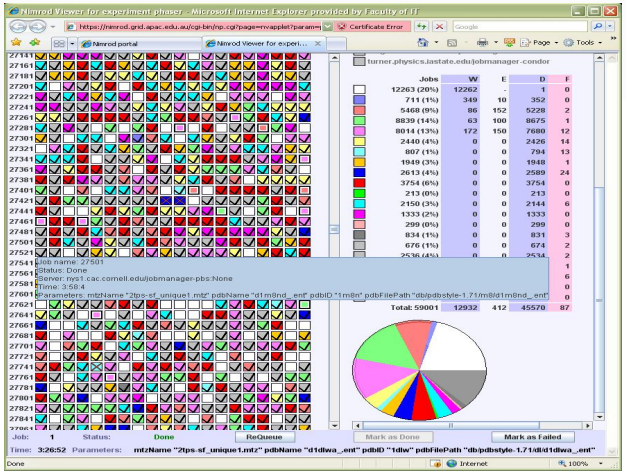
Nimrod Development Cycle



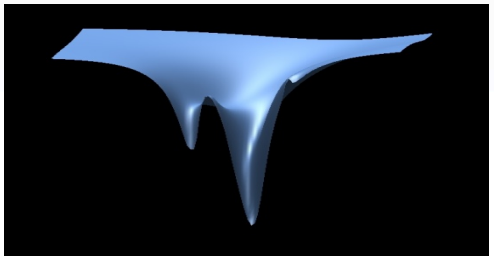
Prepare Jobs using Portal



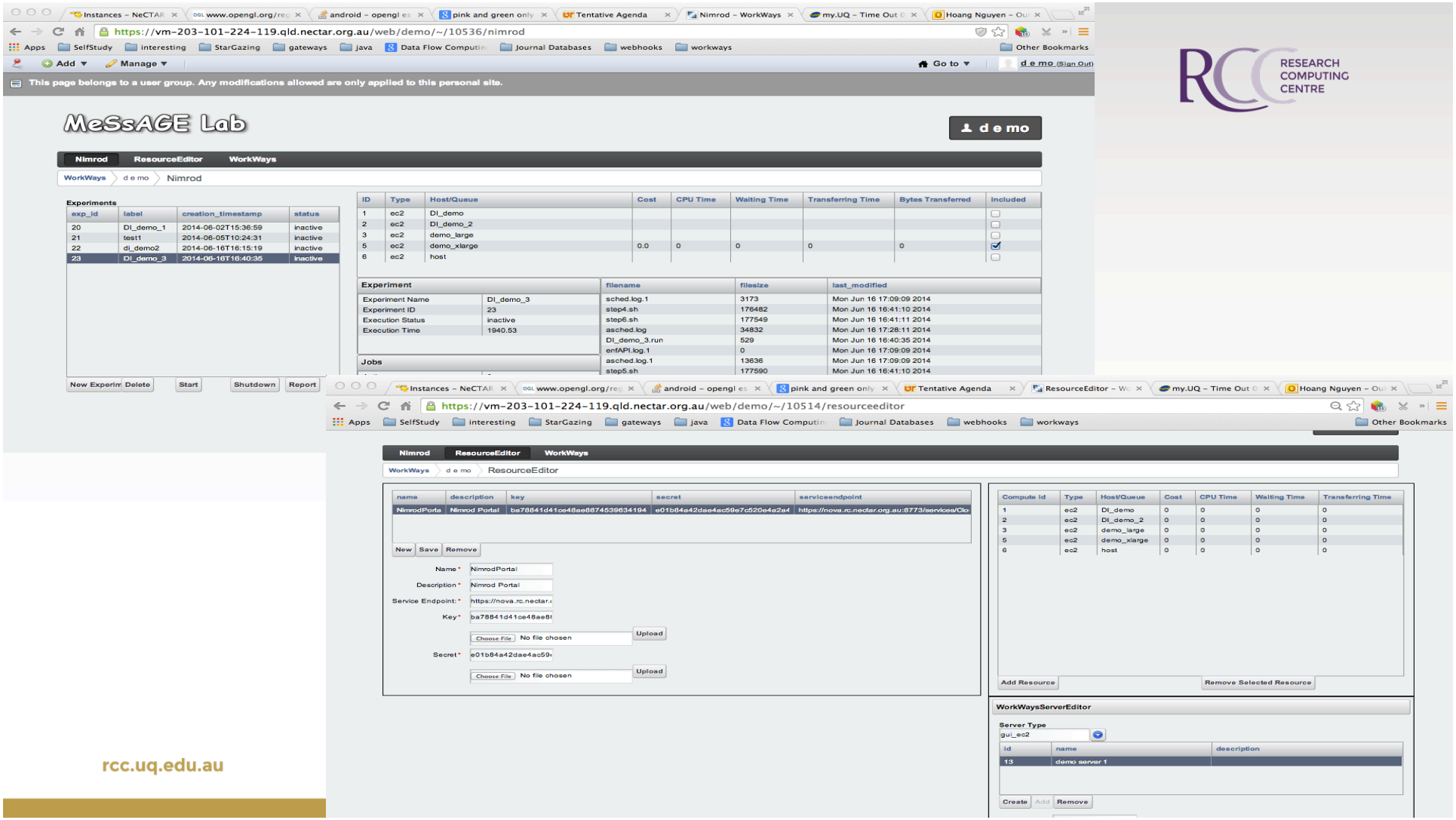
Sent to available machines



Jobs Scheduled Executed Dynamically



Results displayed & interpreted



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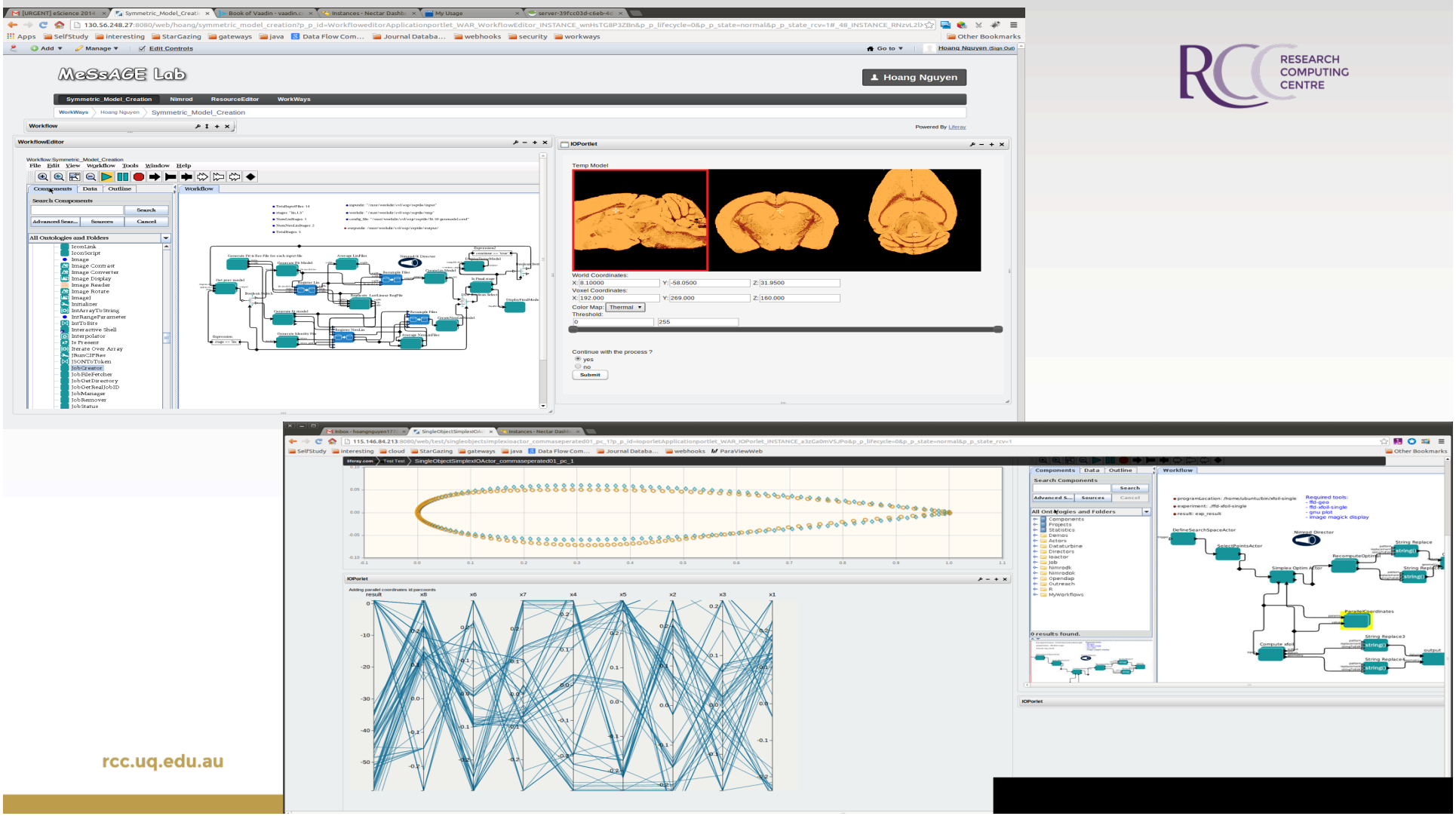
MeSsAGE Lab
Hoang Nguyen
Symmetric_Model_Creation
Nimrod
ResourceEditor
WorkWays
WorkflowEditor
IOPortlet
Temp Model
World Coordinates:
Voxel Coordinates:
Color Map: Thermal
Threshold:
Continue with the process ?
yes
no
Submit
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Scientific Workflows and Nimrod

Nimrod/K Workflows

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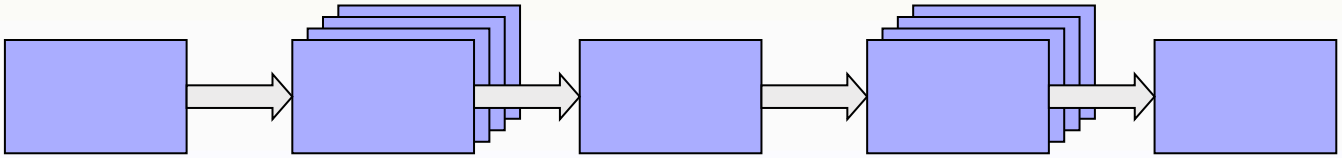
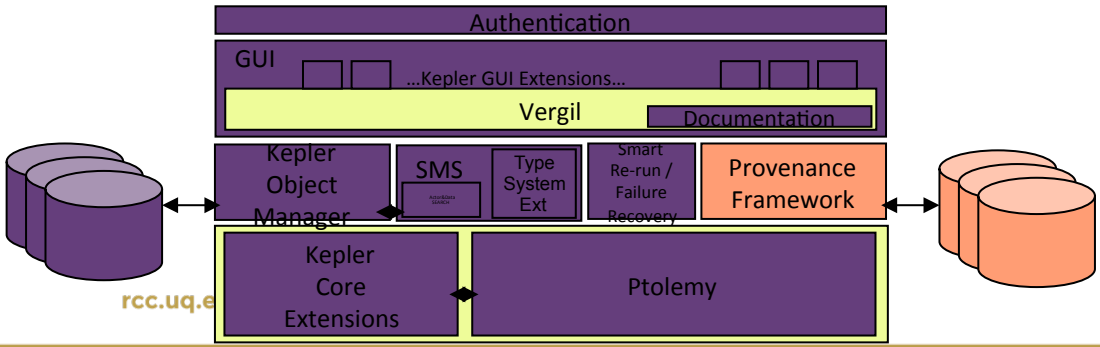
- Nimrod/K integrates Kepler with
  - Massively parallel execution mechanism
  - Special purpose function of Nimrod/G/O/E
  - General purpose workflows from Kepler

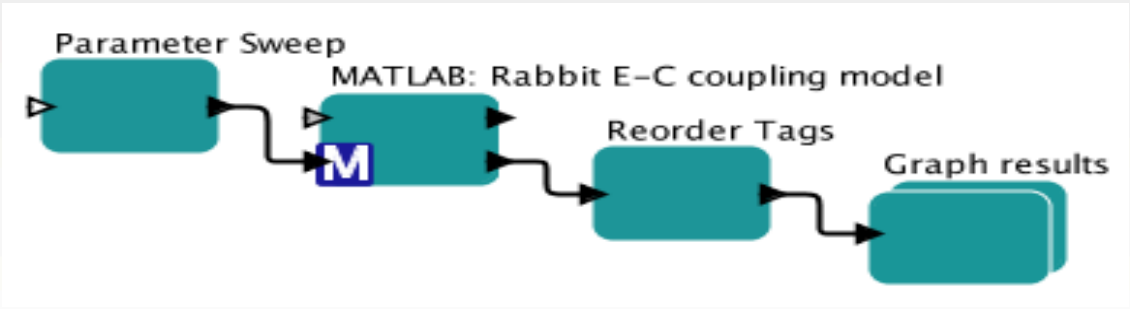


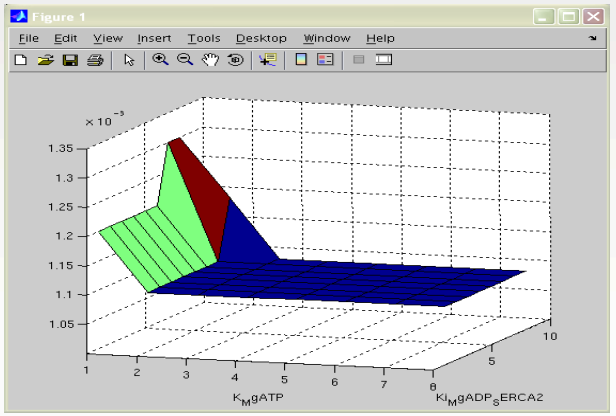


Workflow Threading

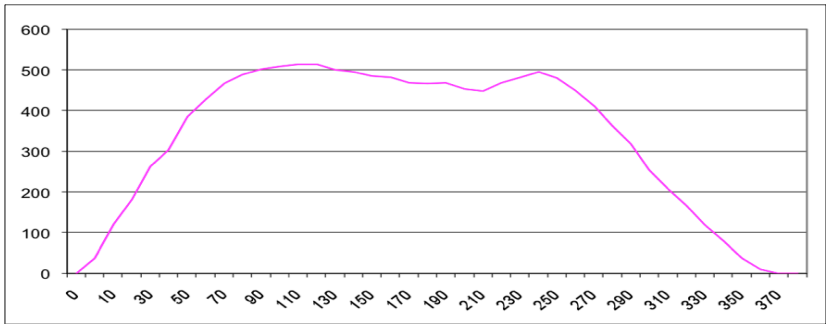
- Nimrod parameter combinations can be viewed as threads
- Multi-threaded workflows allow independent sequences in a workflow to run concurrently
  - This might be the whole workflow, or part of the workflow
- Tokens in different threads do not interact with each other in the workflow

Complete Parameter Sweep

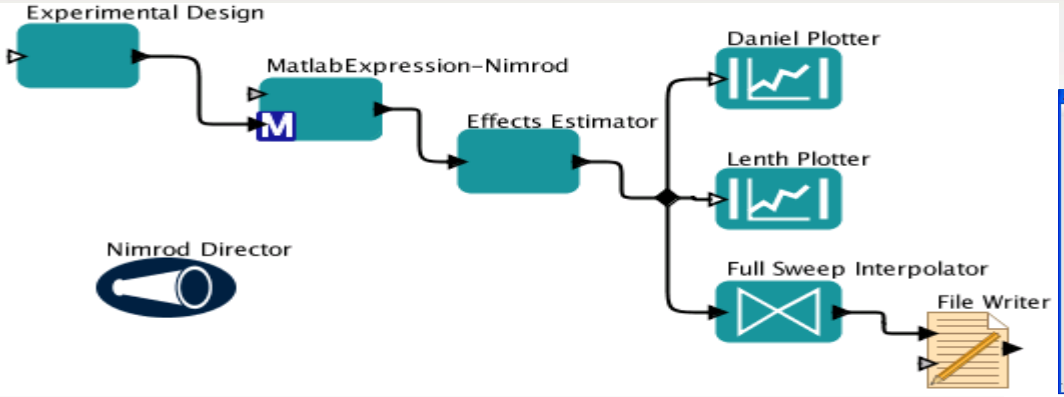


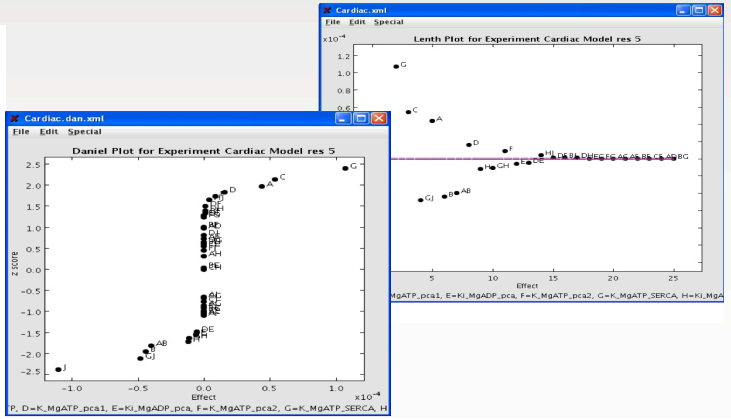


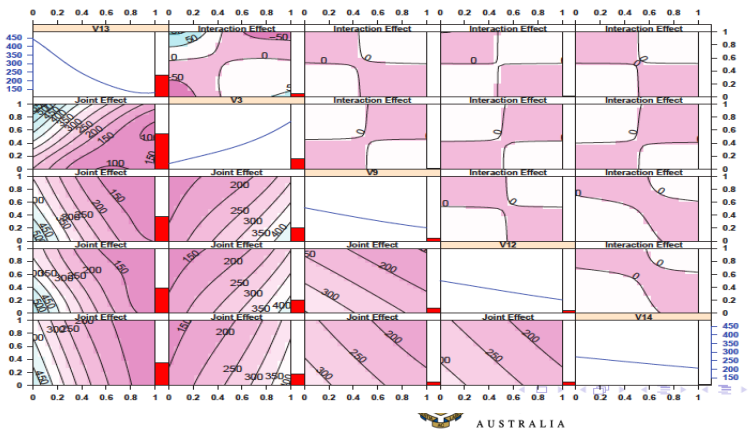
- Using a MATLAB actor provided by Kepler
- Local spawn
  - Multiple thread ran concurrently on a computer with 8 cores (2 x quads)
  - Workflow execution was just under 8 times faster
- Remote Spawn
  - 100's – 1000's of remote processes



Nimrod/EK Actors



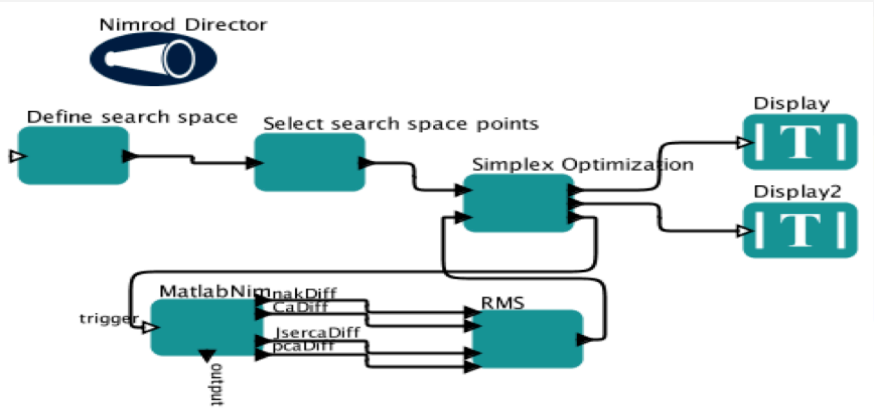




- Actors for generating and analyzing designs
- Leverage concurrent infrastructure

Nimrod/OK Workflows

- Nimrod/K supports parallel execution
- General template for search
  - Built from key components
- Can mix and match optimization algorithms



Interacting with Workflows

Workways (Hoang Nguyen)

WorkWays

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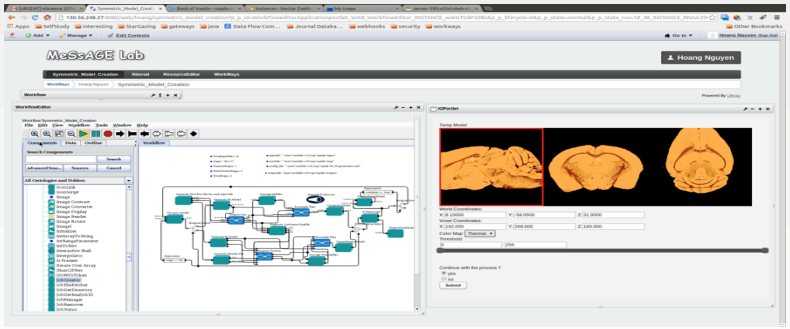
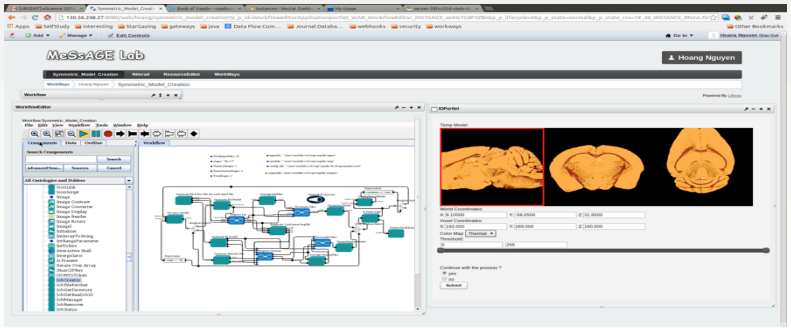
- Ease of use of Science Gateway
- Workflows as service
- IO through portlets
- Extensibility
  - Different IO mechanisms, protocols and topolgy
  - Different UI clients
- Currently Kepler as the workflow engine



WorkWays

- Leverage various existing technologies
  - Kepler workflow
  - Nimrod family toolkit
  - Liferay portal
- Virtual desktops
- AAF
- Various Web-based visualization tools
  - Parallel coordinates
  - Para-view Web



Micro-mixer design

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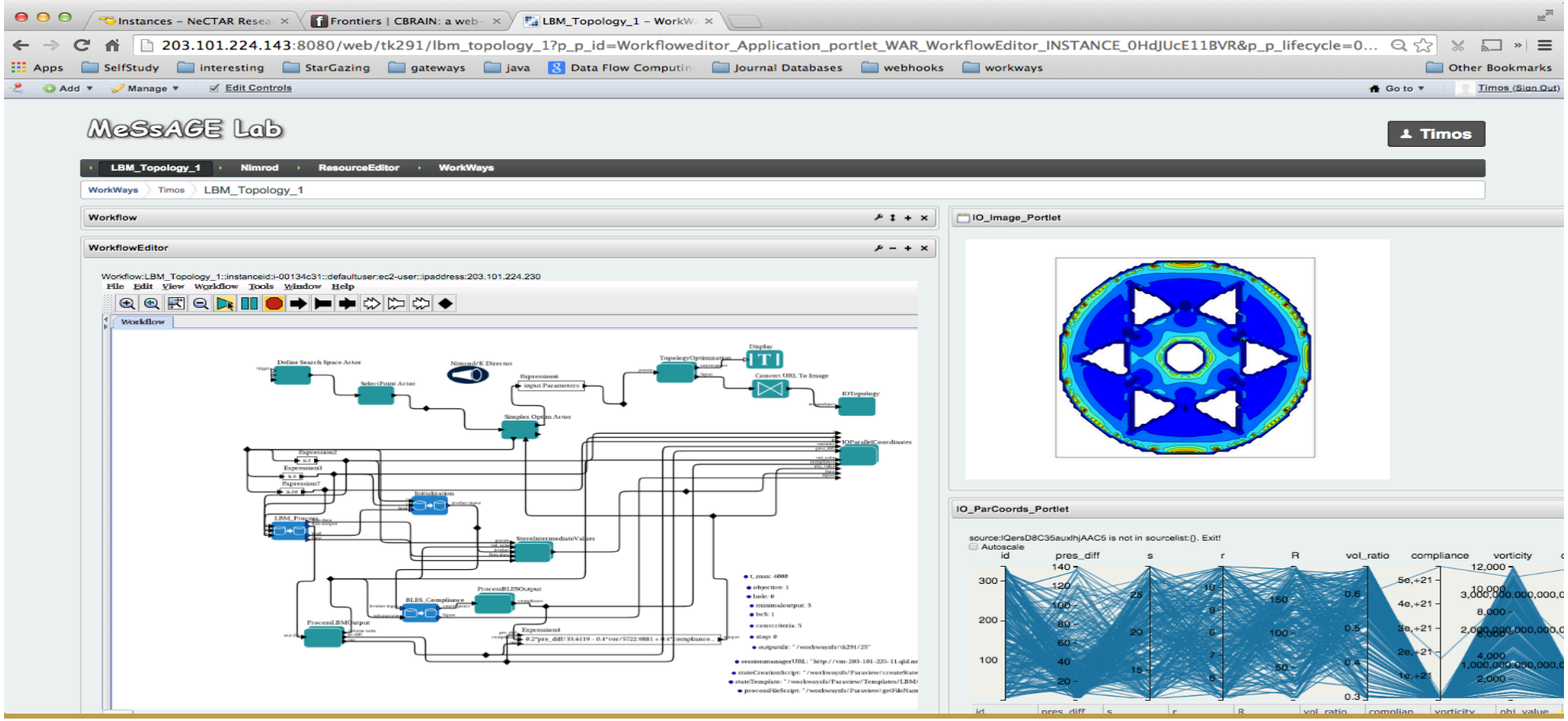

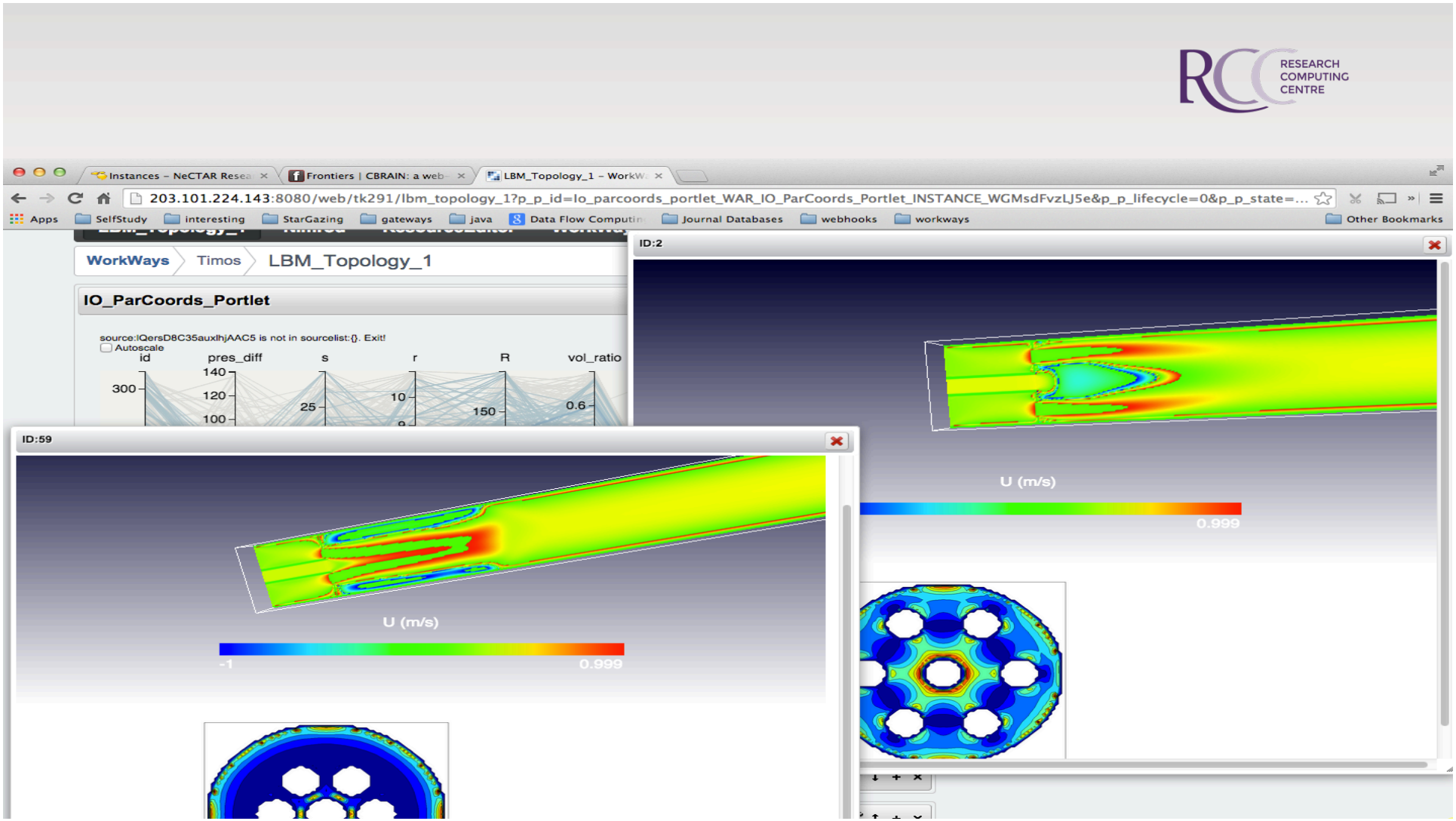
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interesting
StarGazing
gateways
java
Data Flow Computin
Journal Databases
webhooks
workways
Other Bookmarks
WorkWays
Timos
LBM_Topology_1
IO_ParCoords_Portlet
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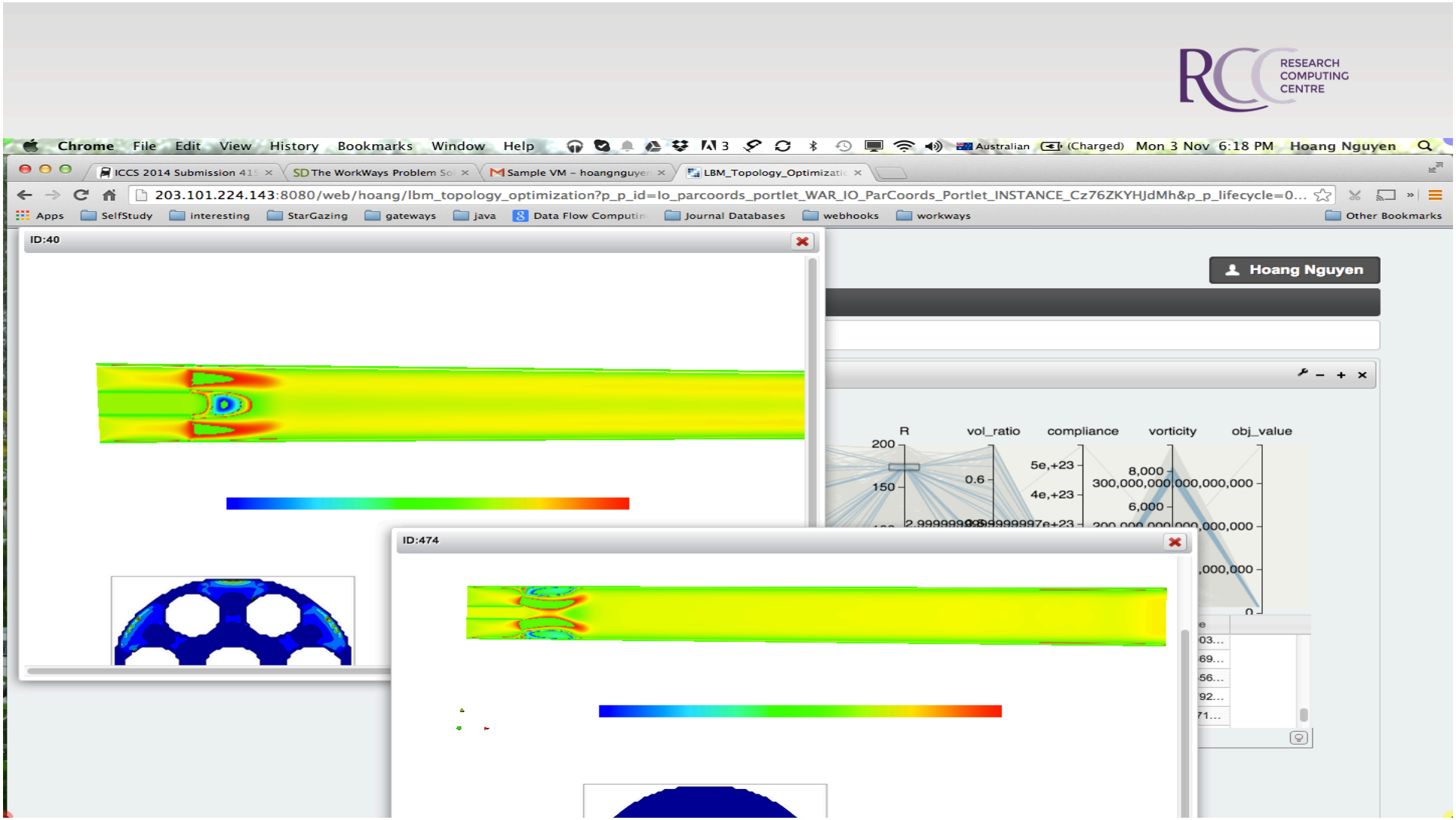
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Chrome File Edit View History Bookmarks Window Help
Australian (Charged) Mon 3 Nov 6:18 PM Hoang Nguyen
ICCS 2014 Submission 41
The WorkWays Problem
Sample VM – hoangnguyen
LBM_Topology_Optimizatic
203.101.224.143:8080/web/hoang/lbm_topology_optimization?p_p_id=lo_parcoords_portlet_WAR_IO_ParCoords_Portlet_INSTANCE_Cz76ZKYHJdMh&p_p_lifecycle=0...
Apps SelfStudy interesting StarGazing gateways java Data Flow Computin Journal Databases webhooks workways Other Bookmarks
ID:40
Hoang Nguyen
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4e,+23
8,000
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ID:474

Optimal Topology

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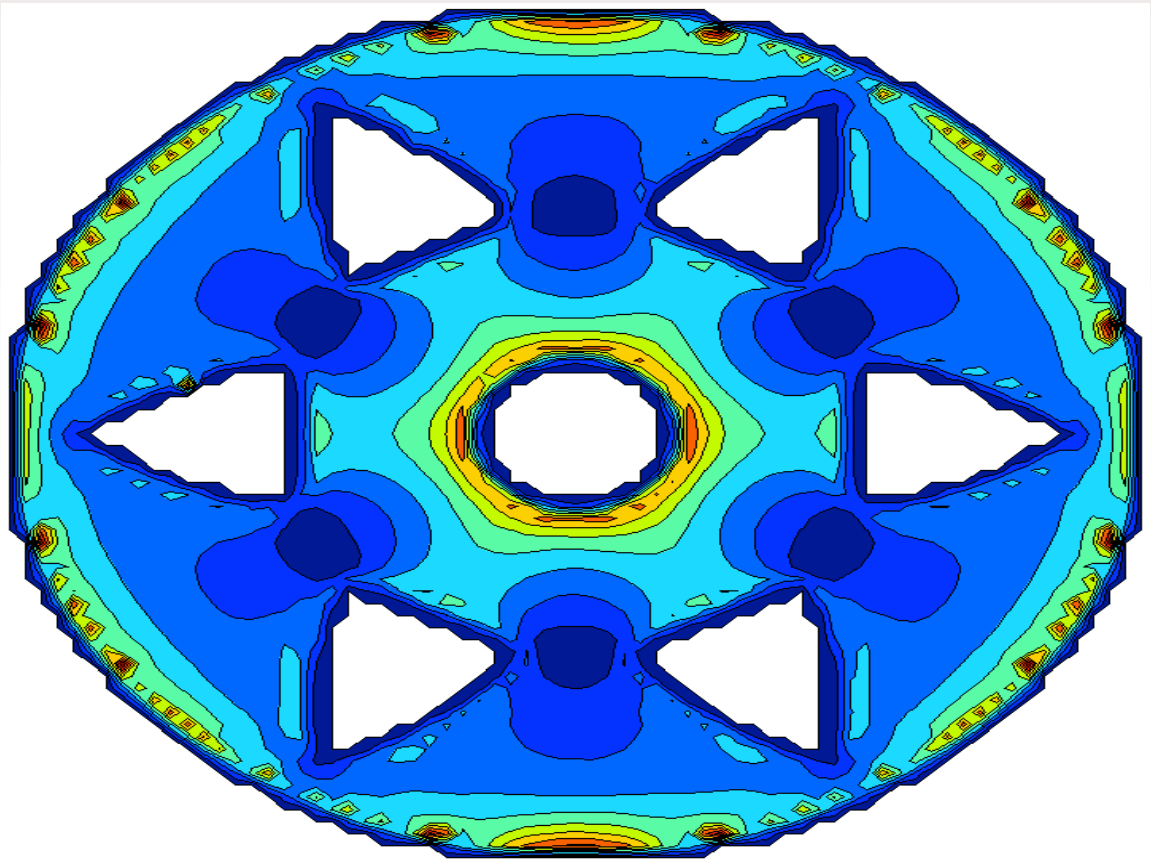
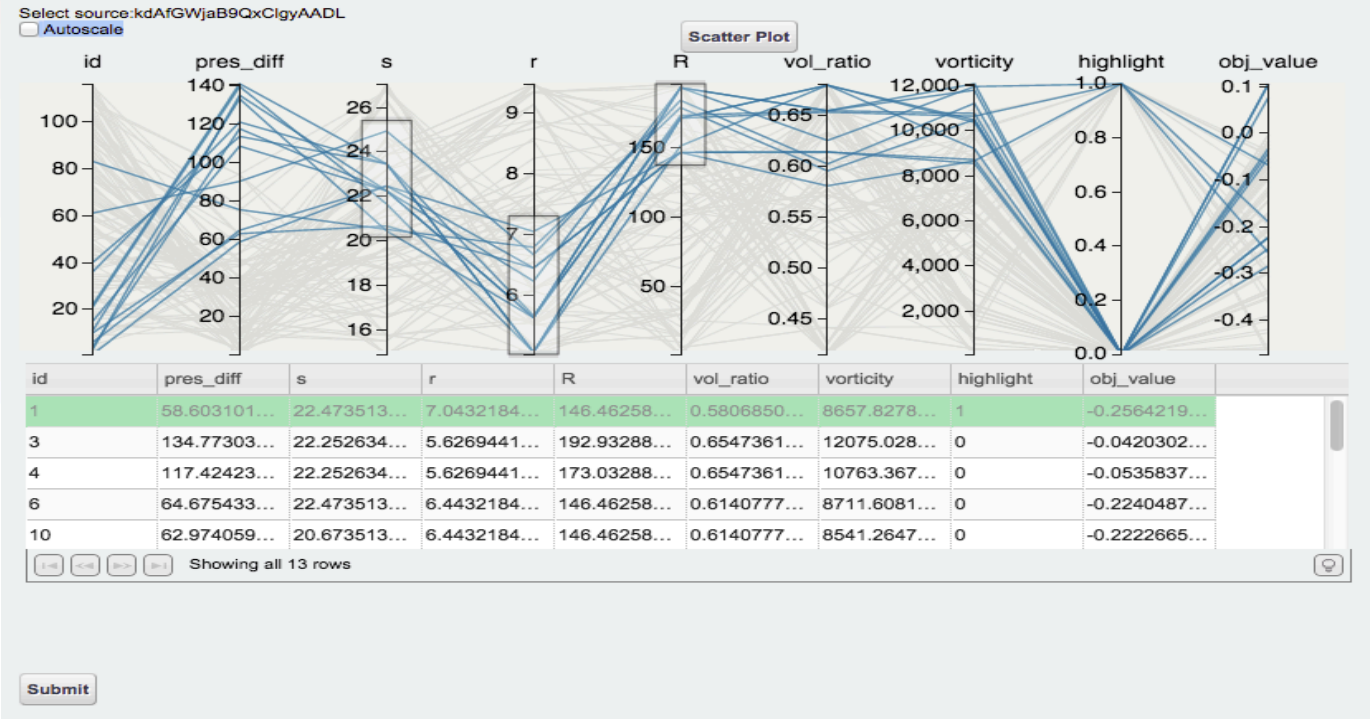
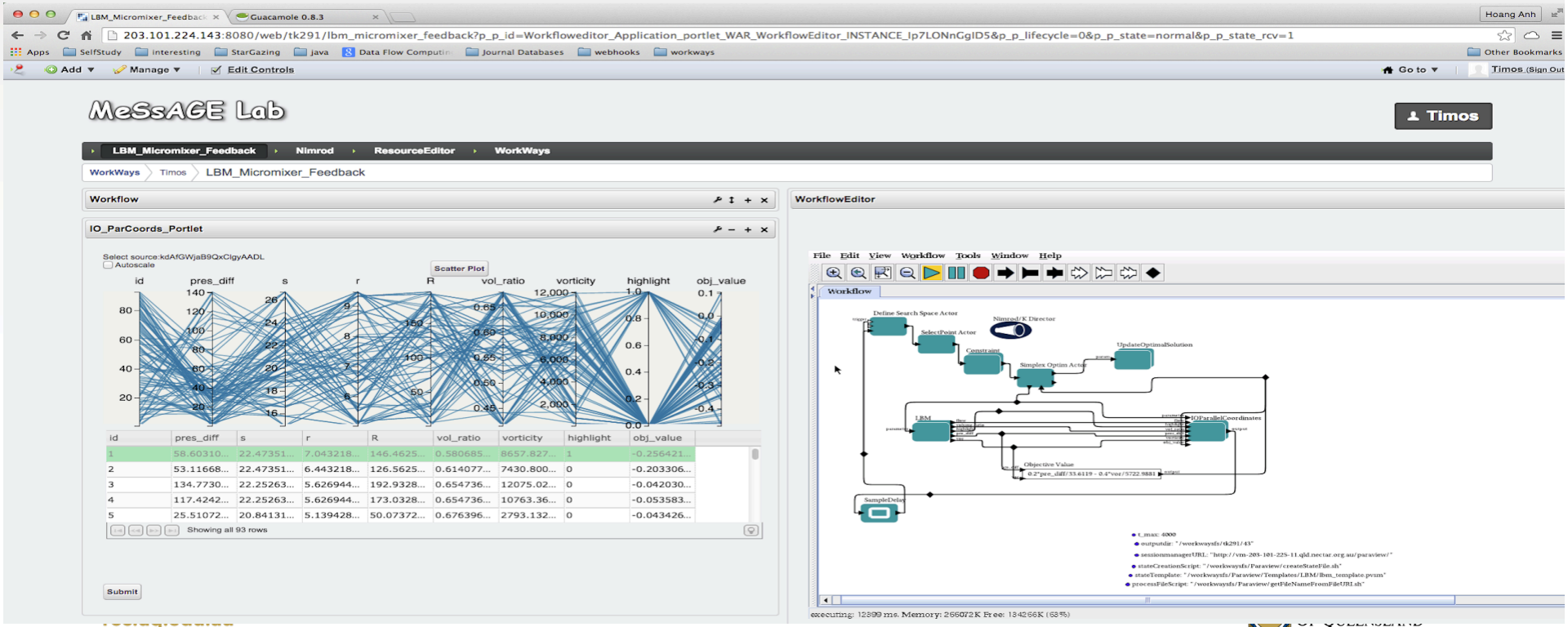


Parallel Coordinates

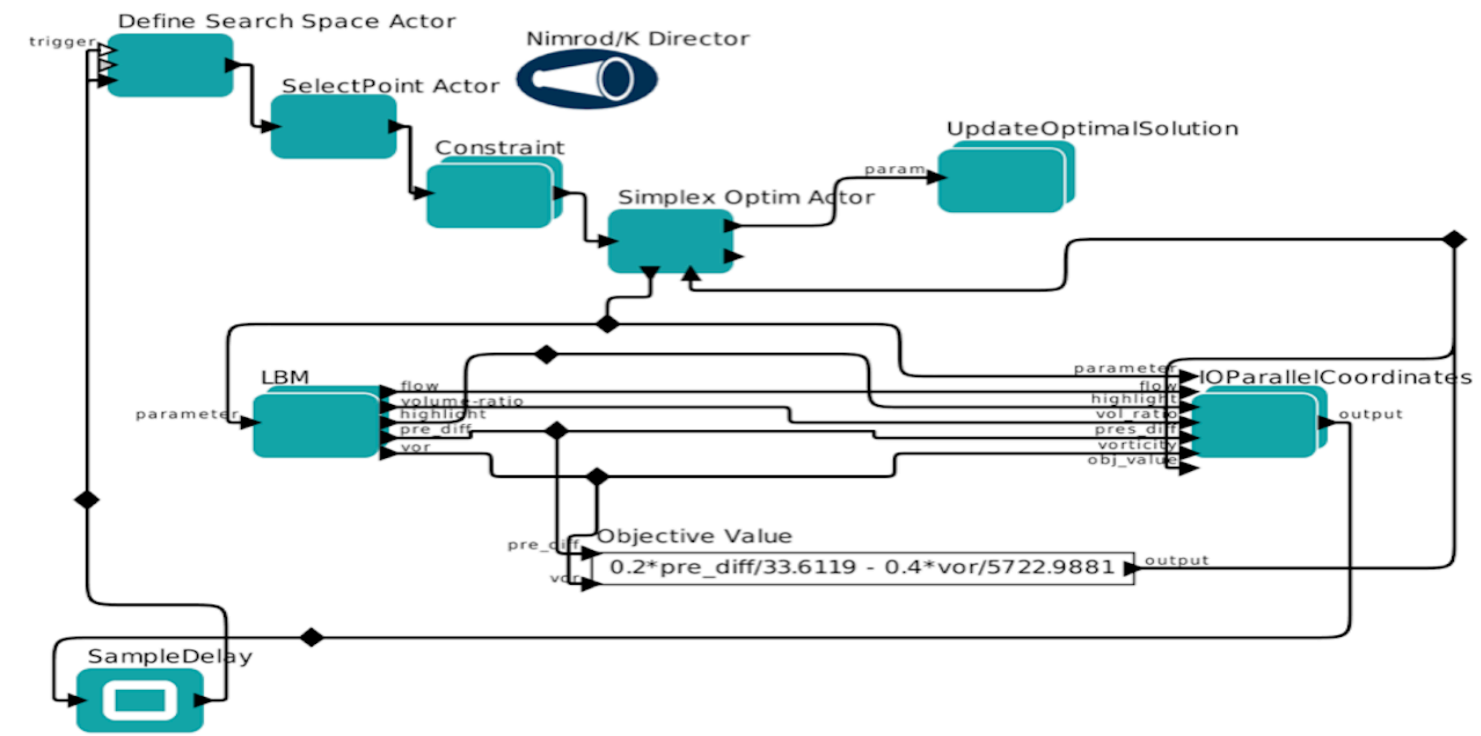


id	pres_diff	s	r	R	vol_ratio	vorticity	highlight	obj_value
1	58.603101...	22.473513...	7.0432184...	146.46258...	0.5806850...	8657.8278...	1	-0.2564219...
3	134.77303...	22.252634...	5.6269441...	192.93288...	0.6547361...	12075.028...	0	-0.0420302...
4	117.42423...	22.252634...	5.6269441...	173.03288...	0.6547361...	10763.367...	0	-0.0535837...
6	64.675433...	22.473513...	6.4432184...	146.46258...	0.6140777...	8711.6081...	0	-0.2240487...
10	62.974059...	20.673513...	6.4432184...	146.46258...	0.6140777...	8541.2647...	0	-0.2222665...

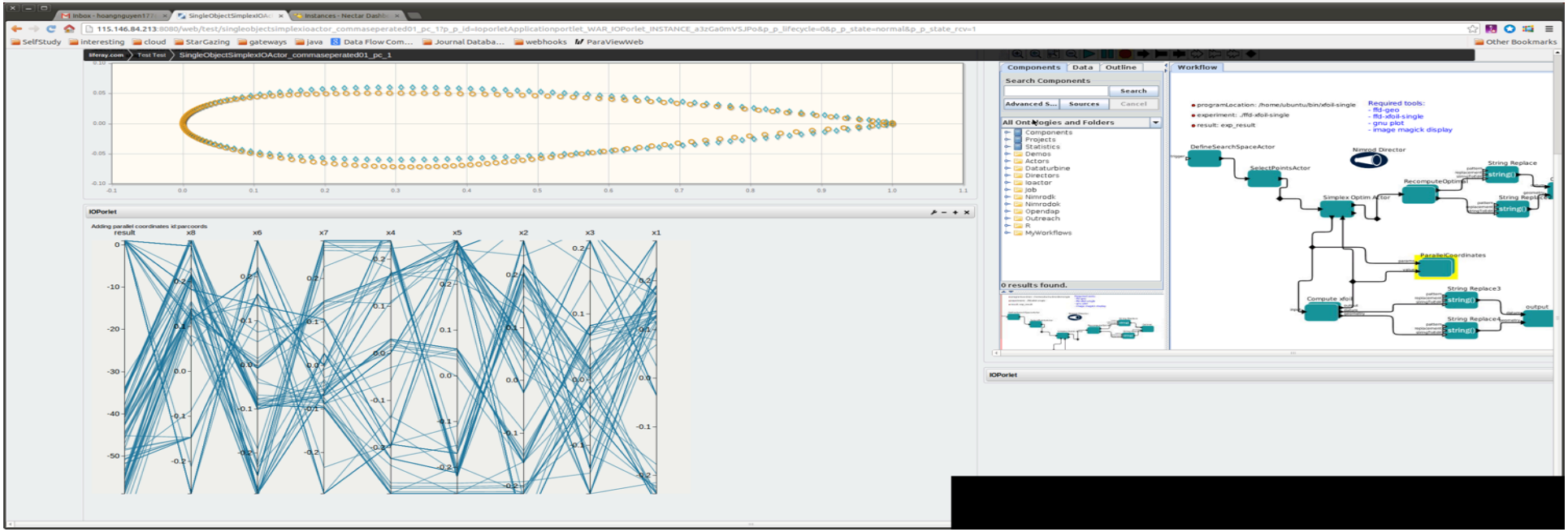
Micromixer Optimization



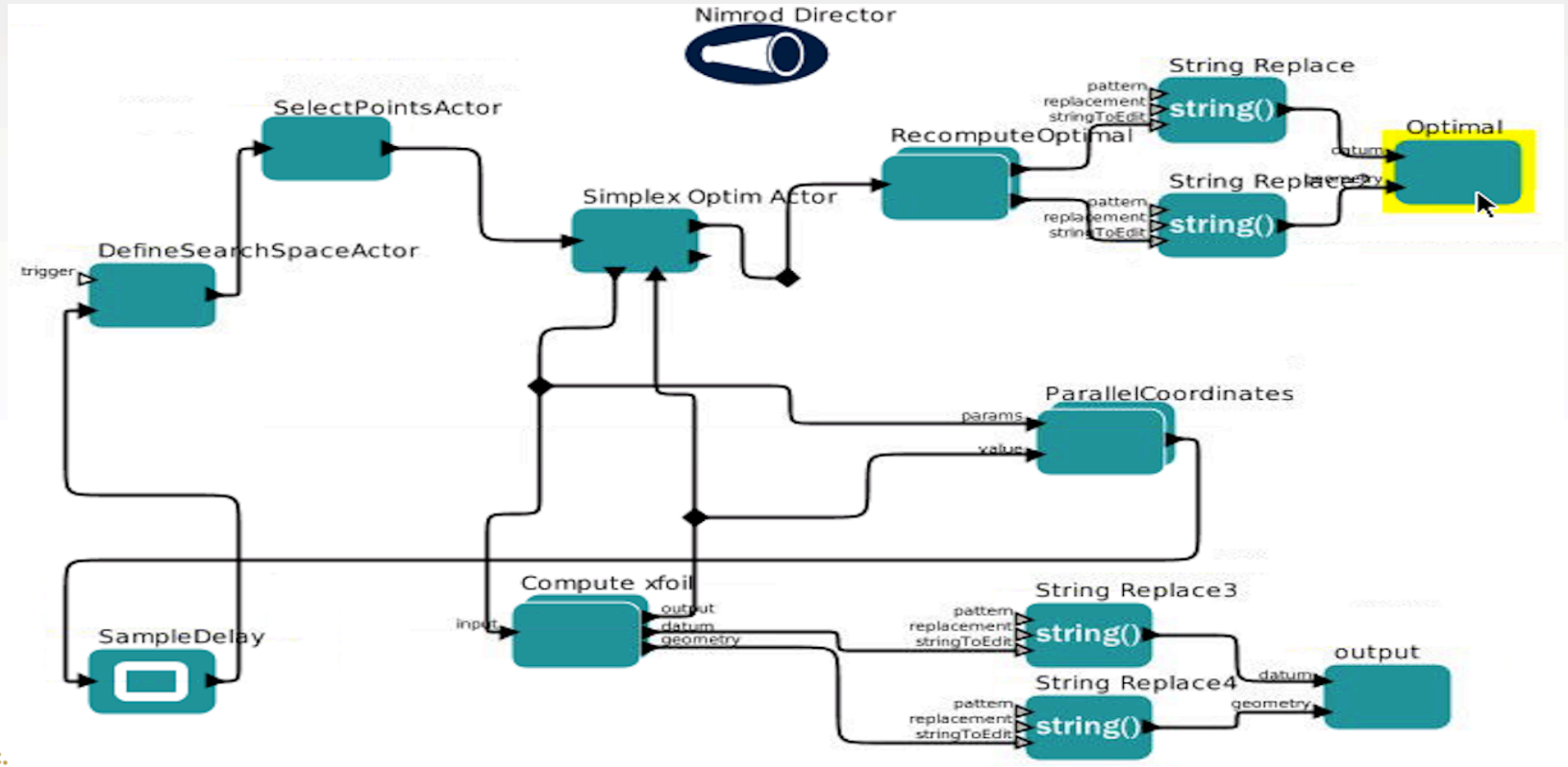
Micromixer optimization Workflow



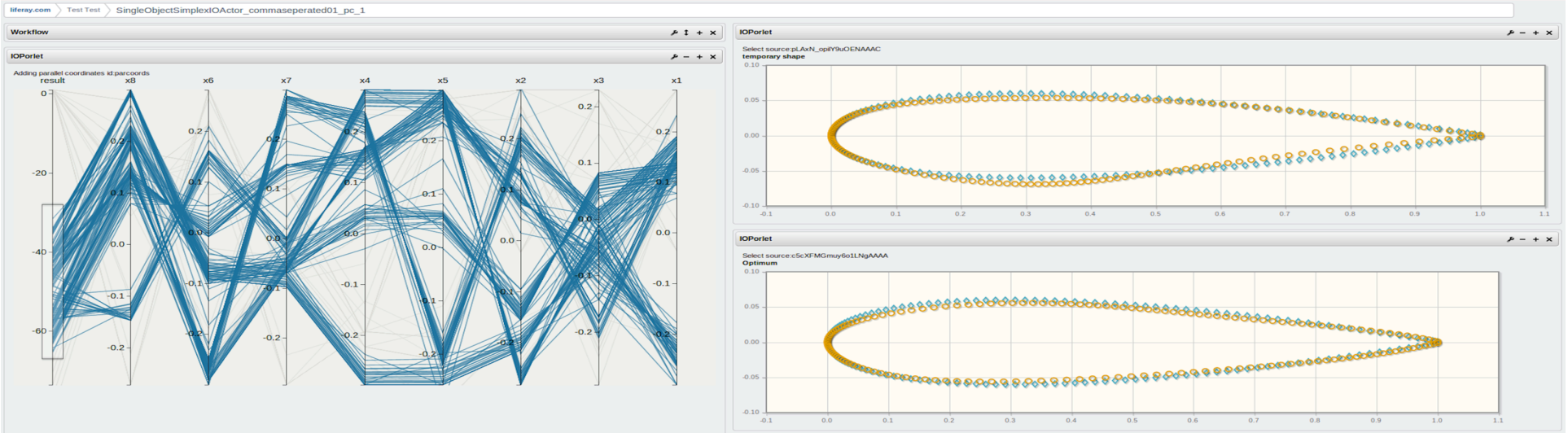
Airfoil Design



2D airfoil optimization



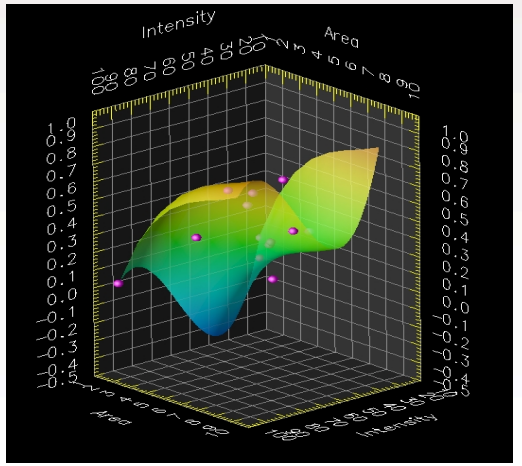
2D airfoil optimization

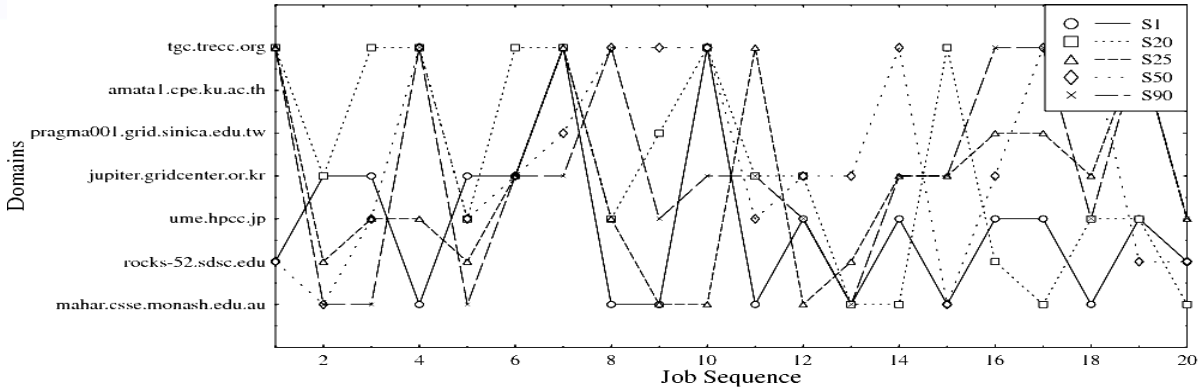


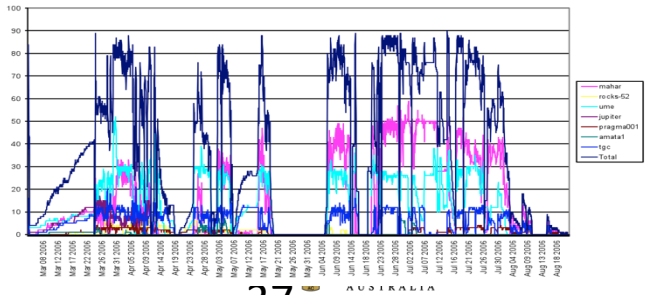
Data Intensive Workflows

Wildfires
Lynch, Beringer, Uotila Monash U, AU

RESEARCH COMPUTING CENTRE







Use Case: Microscopy

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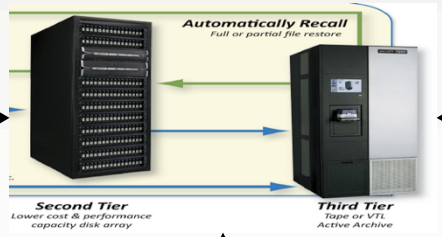
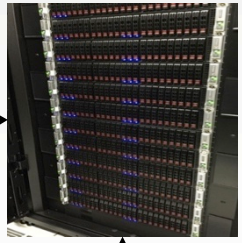
Capture

Pre-process

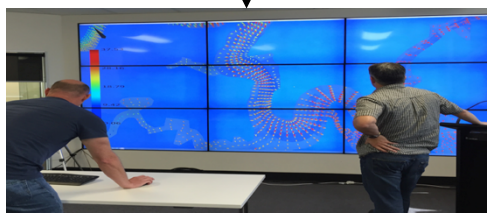
Store



Analyze



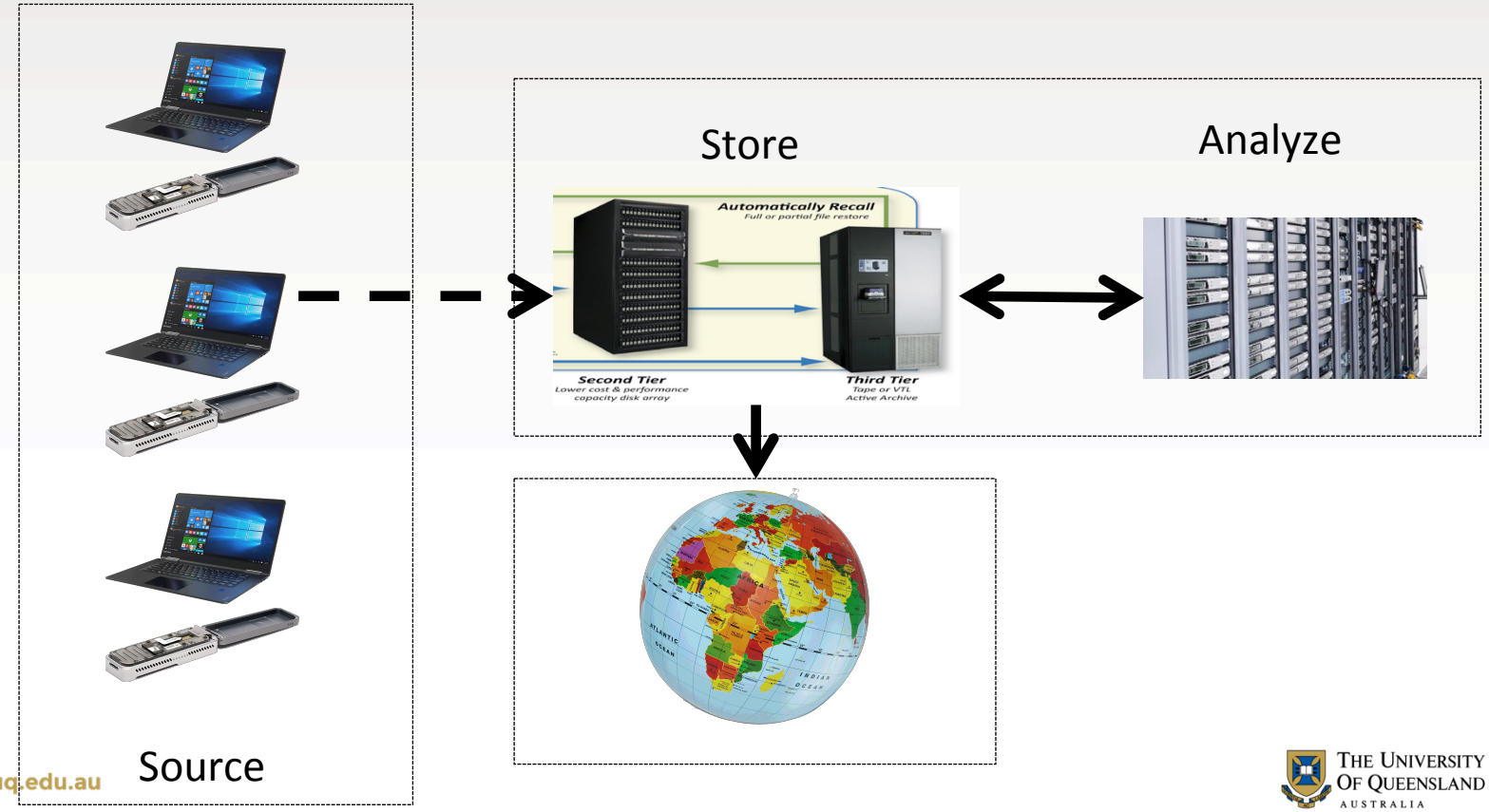
Publish & Share



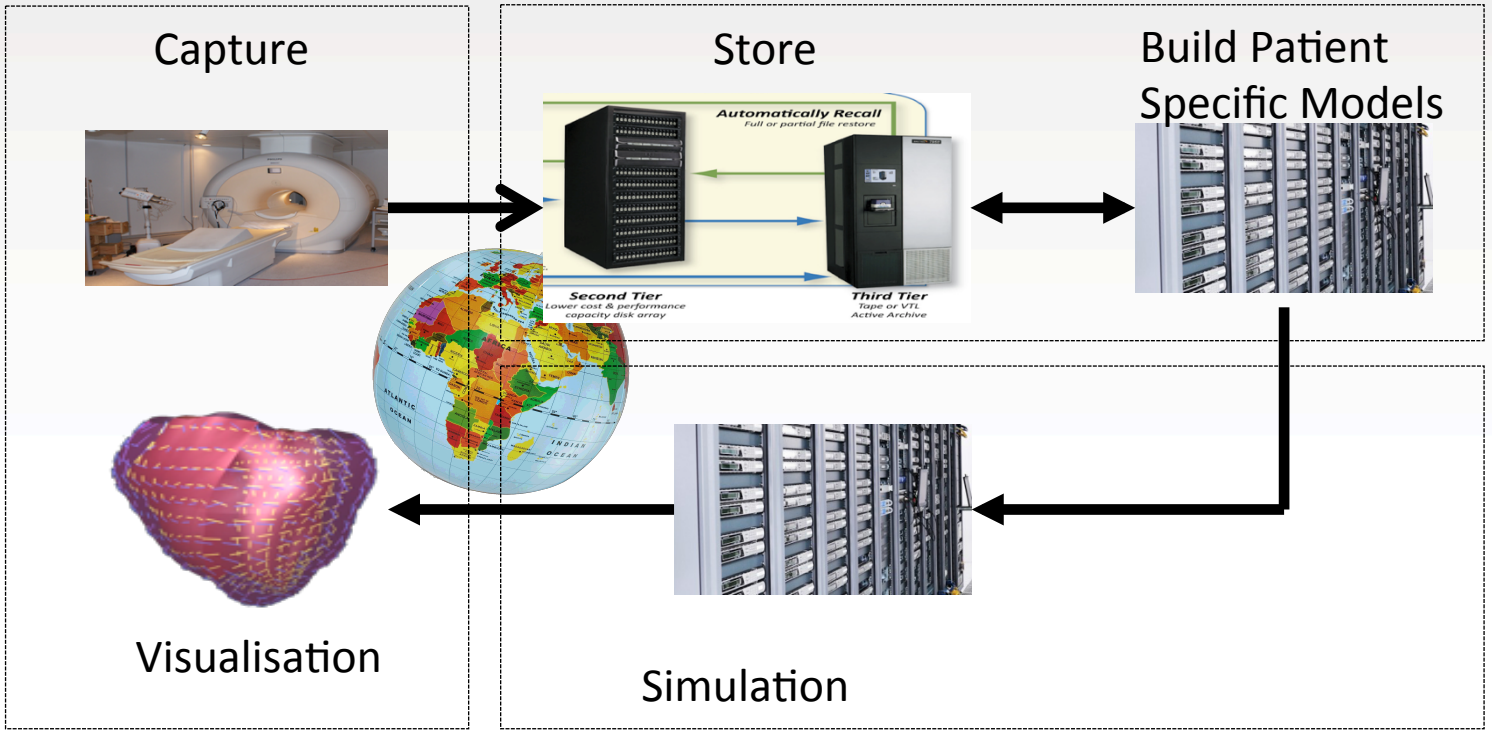
Interpret

THE UNIVERSITY OF QUEENSLAND AUSTRALIA

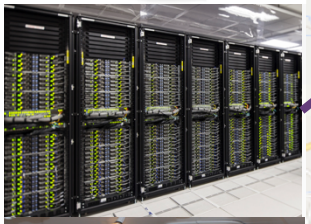
Use Case: Personal Genomics

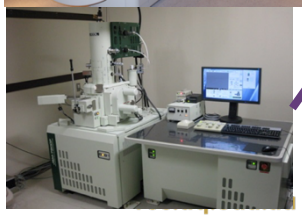


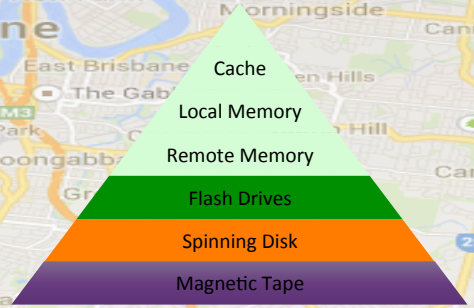
Use Case: Cardiac Science



The MeDiCI landscape

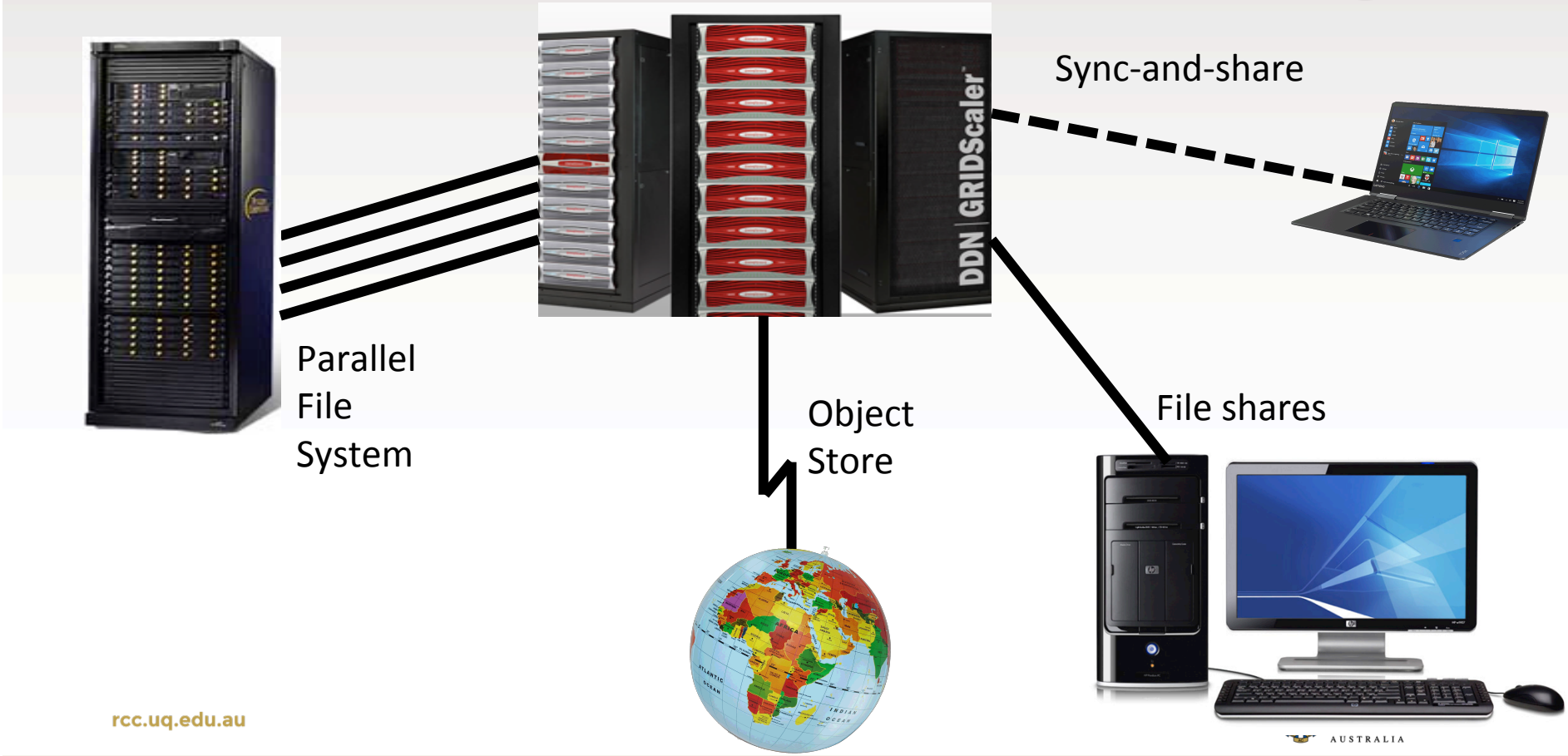






Remote Data Centre

MeDiCI unifies data access



Conclusions

RESEARCH COMPUTING CENTRE

- Workflows are useful for scripting complex computational science and engineering problems
- Conceptually easy to add optimization
- User interaction requires new workflow actors
- Integration to a Science Gateway allows very powerful workflows to be exposed to wider communities.
- Placing a common file system under the workflow engine seems to be promising