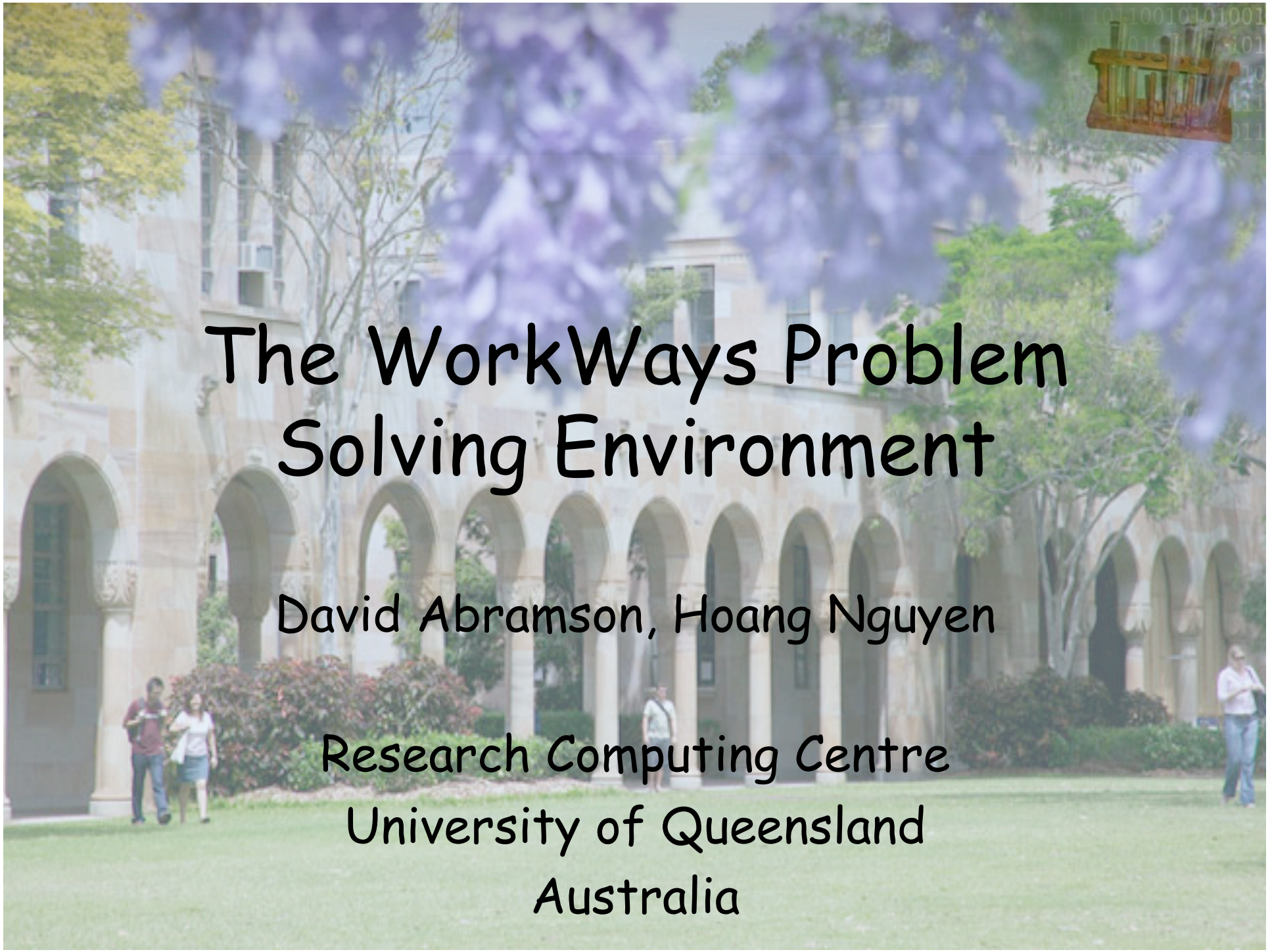
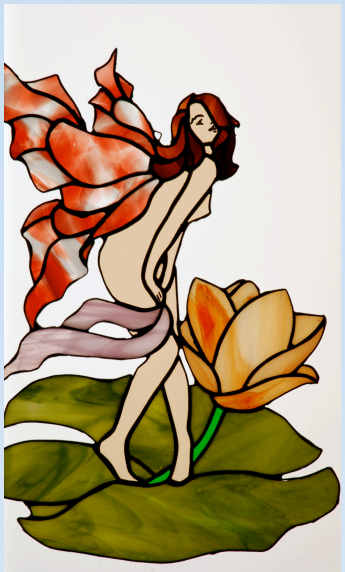
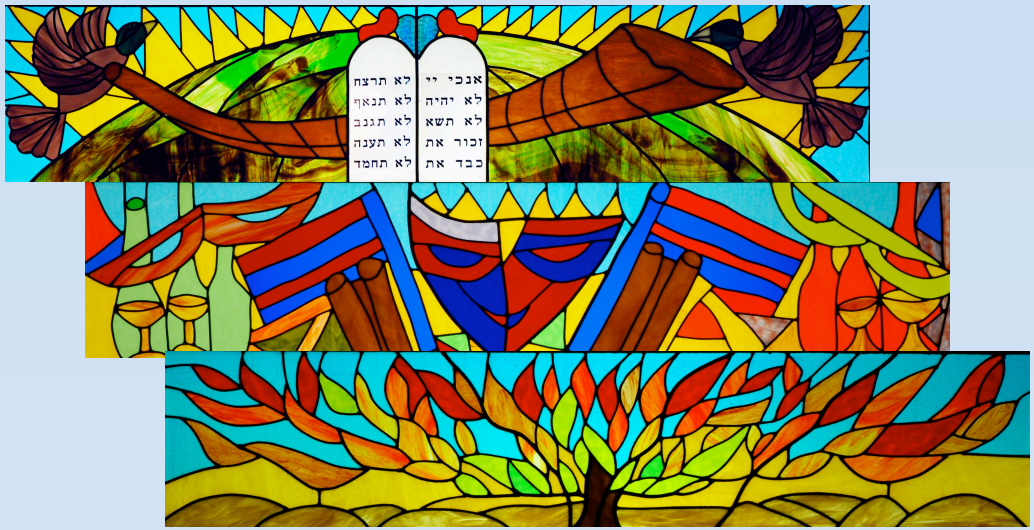


The WorkWays Problem Solving Environment

David Abramson, Hoang Nguyen

Research Computing Centre
University of Queensland
Australia




אנכי יי
לא יהיה
לא תשא
זכור את
כבד את
לא תרצח
לא תנאף
לא תגנב
לא תענה
לא תחמד

Outline

- Background
  - Science Gateways
  - Scientific Workflow
  - Kepler and Nimrod/K
- Motivation: Virtual microscopy and imaging
- Workways: Design and Implementation
- Case studies
- Conclusion & Future Work

Science Gateways

- A Web portal interfaced to a community-set of tools, applications, and data collection integrated
- Benefits
  - Accessibility
  - Usability
  - Sharing and collaborating
- LEAD, nanoHub, CAMERA, GridCHem

nanoHUB.org
an NCN project

GRID CHEM

CIPRES Cyberinfrastructure for Phylogenetic Research

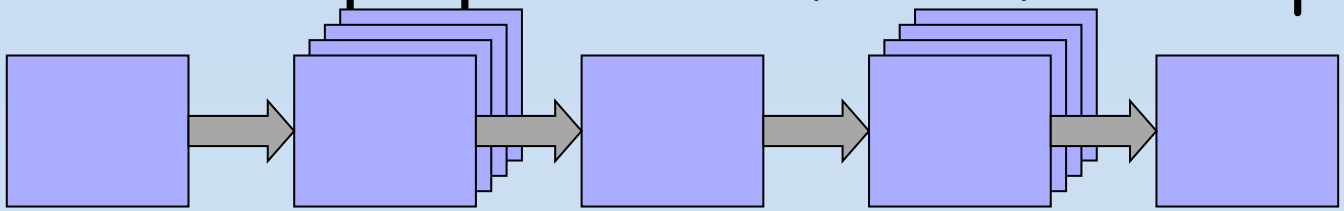
camera PORTAL

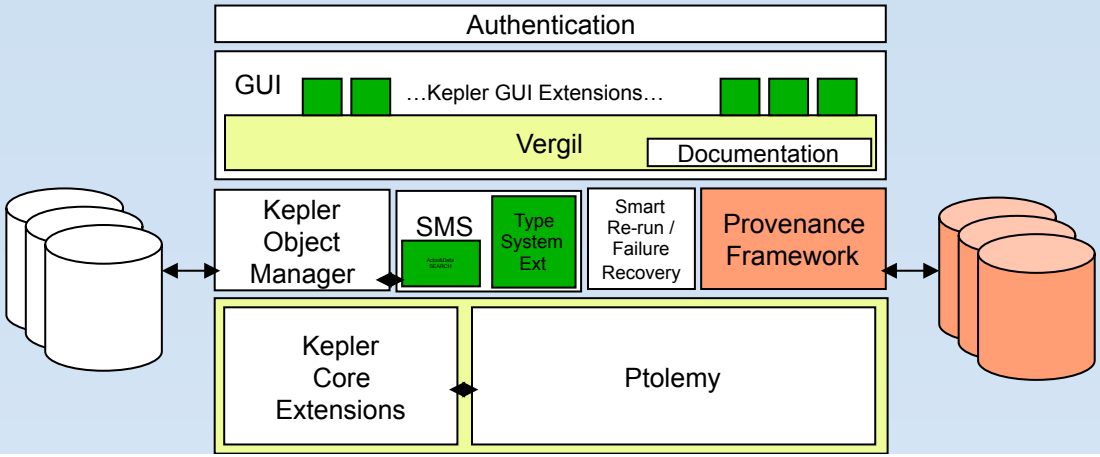
Scientific Workflows

- Automate, manage and execute various steps in scientific research
- Lots of "standards"
  - Pegasus, Kepler, Taverna, Triana, Vistrails, etc.
  - Applied in various science domains
- Unifying platform to build arbitrarily complicated computational applications by combining predefined components
- Typically not well integrated into portals

Nimrod/K Workflows

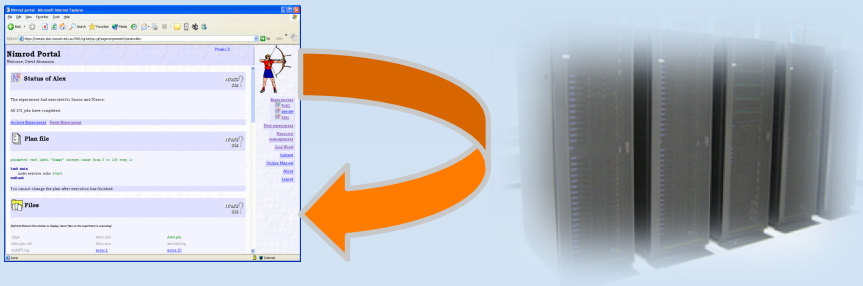
- Nimrod/K integrates Kepler with
  - Massively parallel execution mechanism
  - Special purpose function of Nimrod/G/O/E
  - General purpose workflows from Kepler



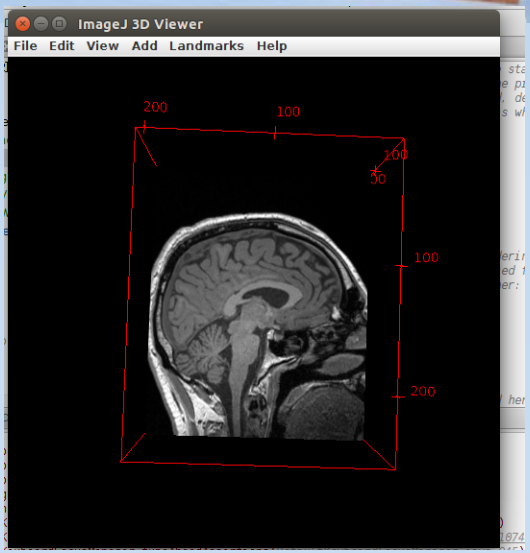


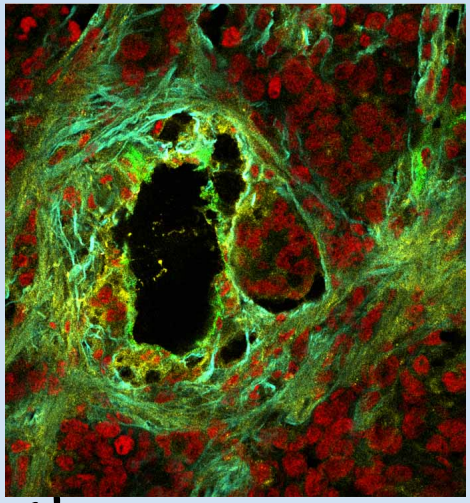
Motivation

- Support man-in-the-loop workflows
  - Ability to perform IO operations with a continuously running workflow
- Most existing workflow-based gateways
  - execute the workflow in batch mode
  - users provide inputs, execute, and collect outputs



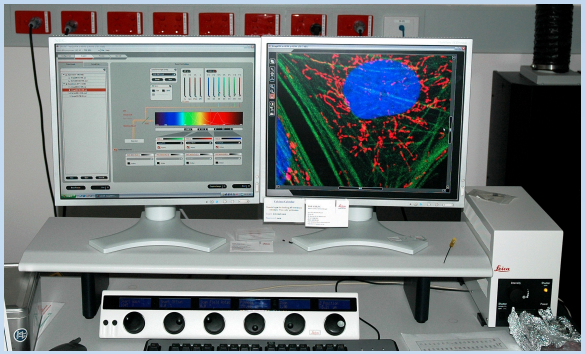
Motivation: Virtual Microscopy

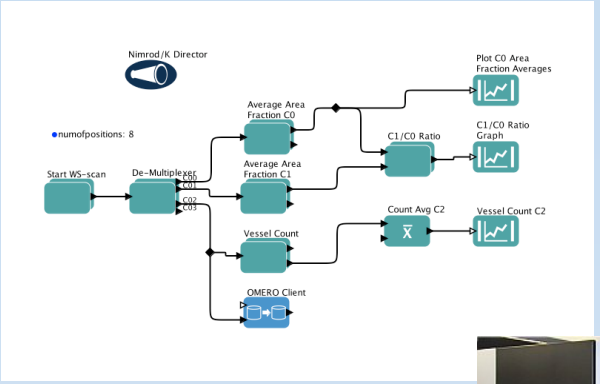


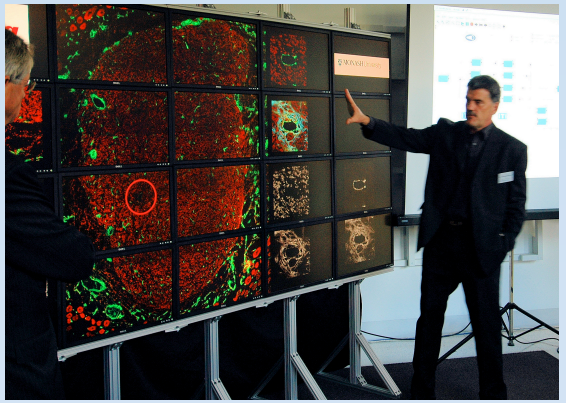


- Based on Kepler
  - Capture images from imaging device
  - Process images
  - Visualize and archive processed images
- Applications in
  - Cancer research
  - Neuroscience
- Typical interactions
  - Repeat scans to find regions of interest
  - Assist imaging processing algorithms

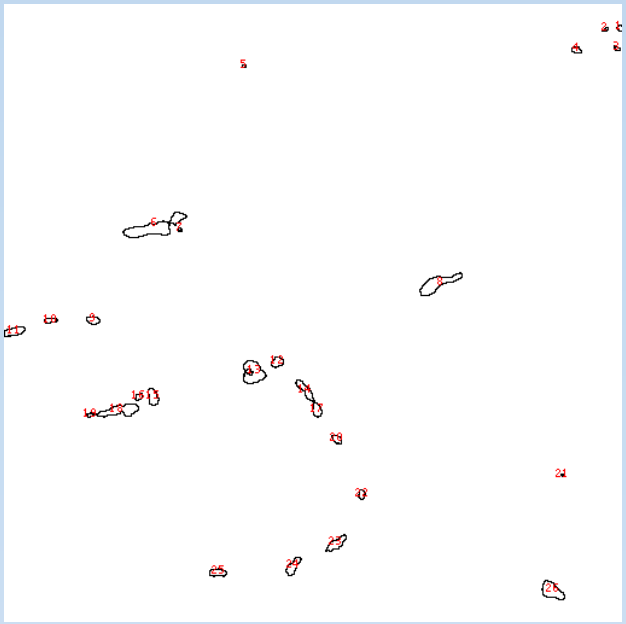
Cancer Imaging and Therapy

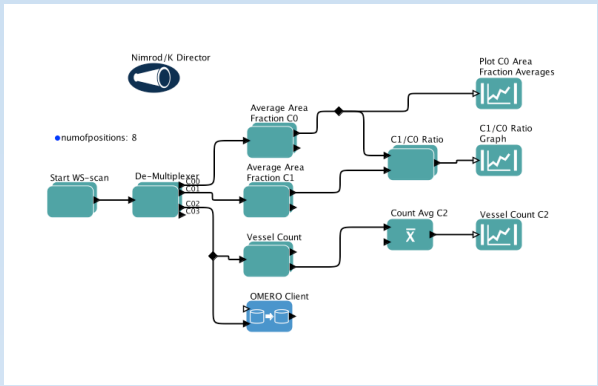


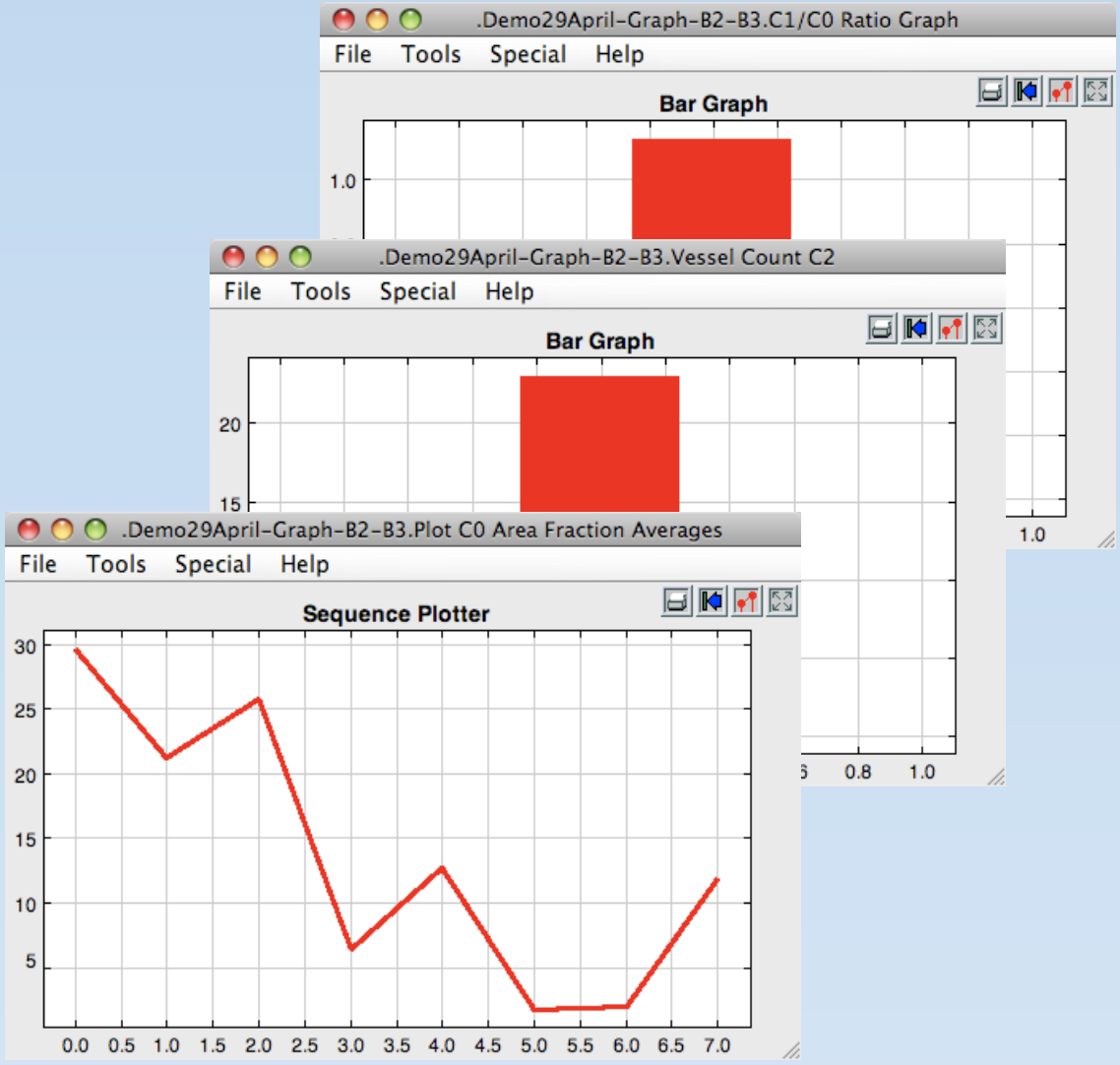




Cancer Imaging and Therapy

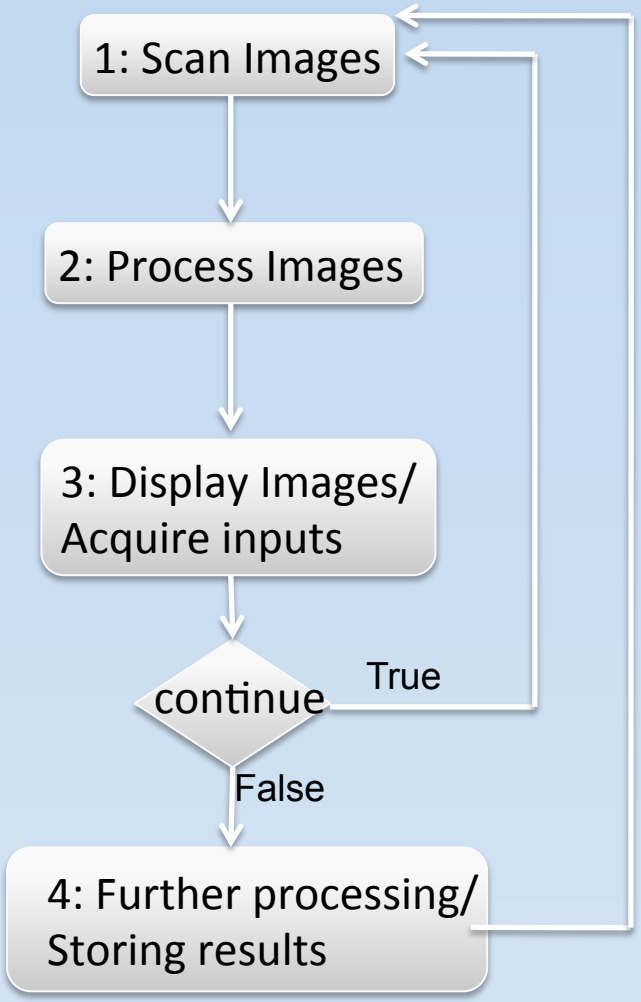




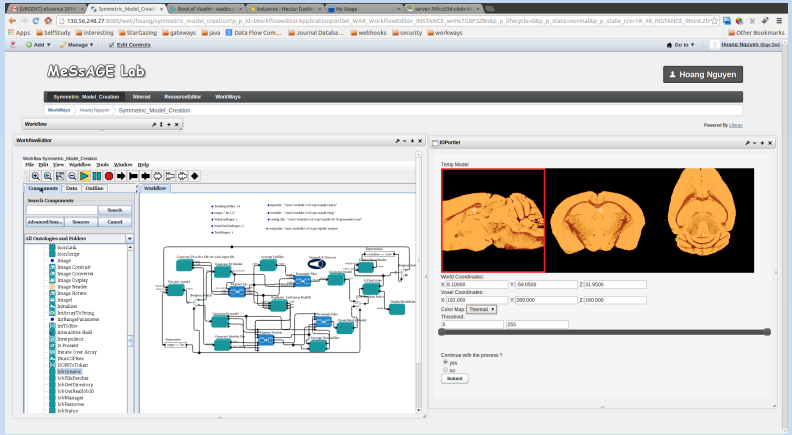


Motivation: Virtual Microscopy

- Consider a workflow as a continuously running service
- Once initiated, the workflow pauses itself waiting for inputs
- IO is performed while the workflow is running
- Can be achieved by introducing a feedback loop

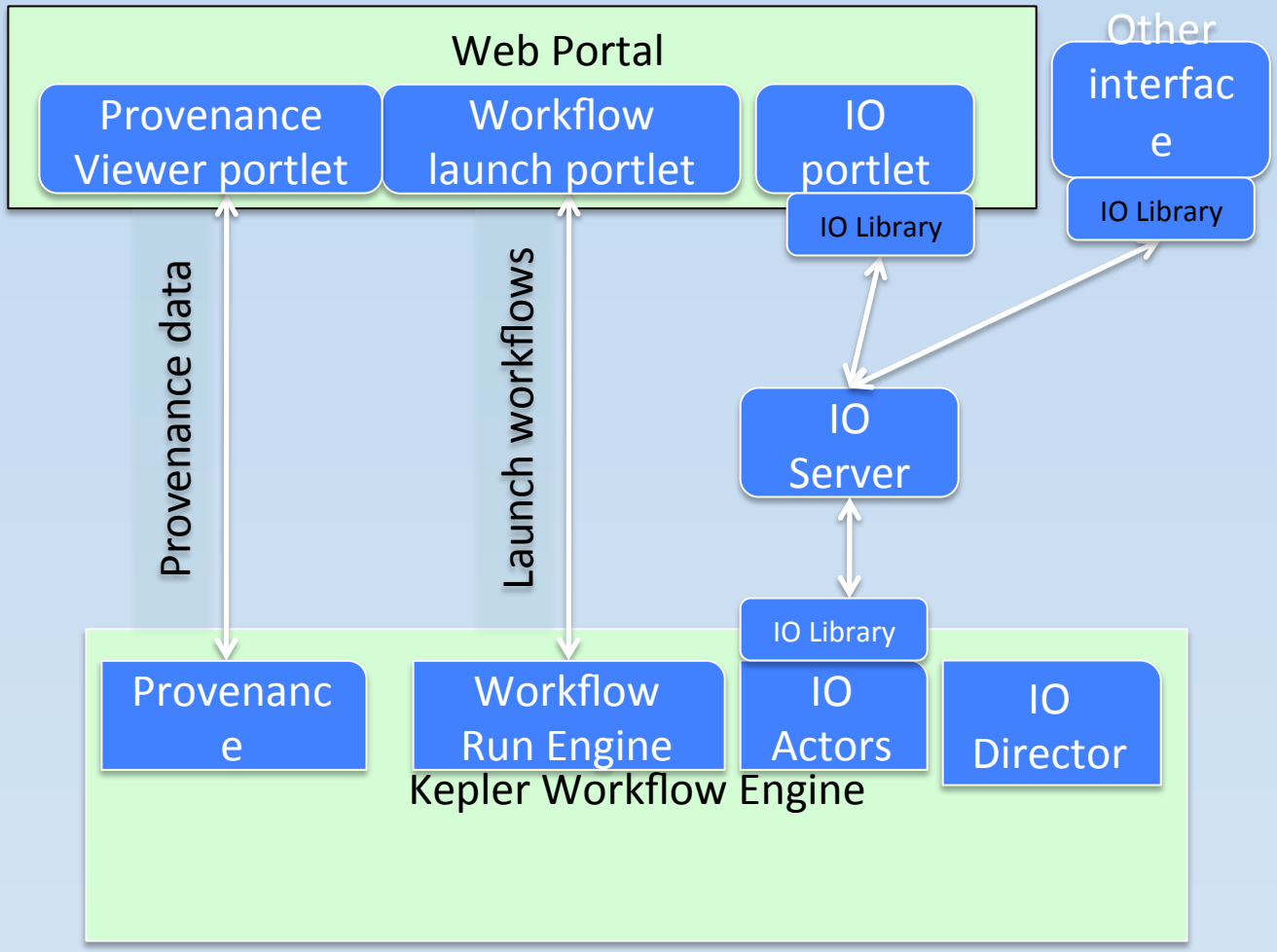


WorkWays



- 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


Web Portal
Provenance Viewer portlet
Workflow launch portlet
IO portlet
IO Library
Other interfac e
IO Library
Provenance data
Launch workflows
IO Server
IO Library
Provenanc e
Workflow Run Engine
IO Actors
IO Director
Kepler Workflow Engine

Implementation: IO framework

- CometD framework
  - Framework for asynchronous message passing using either HTTP or web socket
  - Messages are routed via different channels
  - Publish-subscribe is the default routing mechanisms
- IO Server
- IO Clients: IO actors & UI clients

Implementation: IO framework

- CometD framework
- IO Server
  - Assigns each (data) channel to an IO actor
  - Multiple UI clients may subscribe to a channel
  - Reserves two special (meta) channels
    - “/publishers”
    - “/subscribers”
- IO Clients

Implementation: IO framework

- CometD framework
- IO Server
- IO Clients
  - IO actors: publishers
  - UI clients (Web client): subscribers
  - Handshaking between IO actors and UI clients are done via the two meta channels
  - IOPortlet
  - IOActor

IOActor

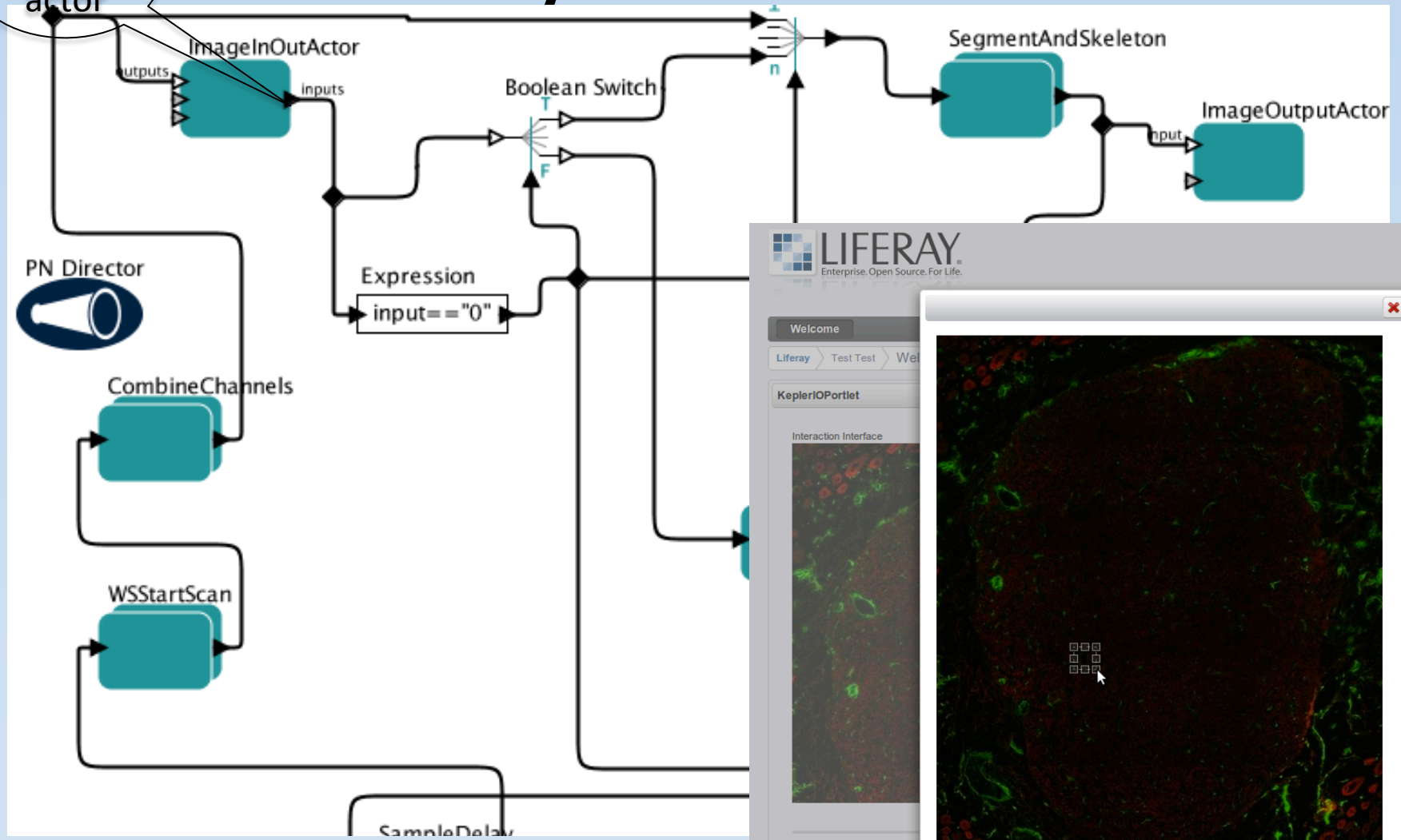
- Generic actor
  - Simplify the creation of (new) IO actors
  - Instantiate an IOActor & provide the actor definition
- IOActor definition
  - Actor name
  - Number of (supported) clients
  - Operation: input/output/inout
  - Additional information

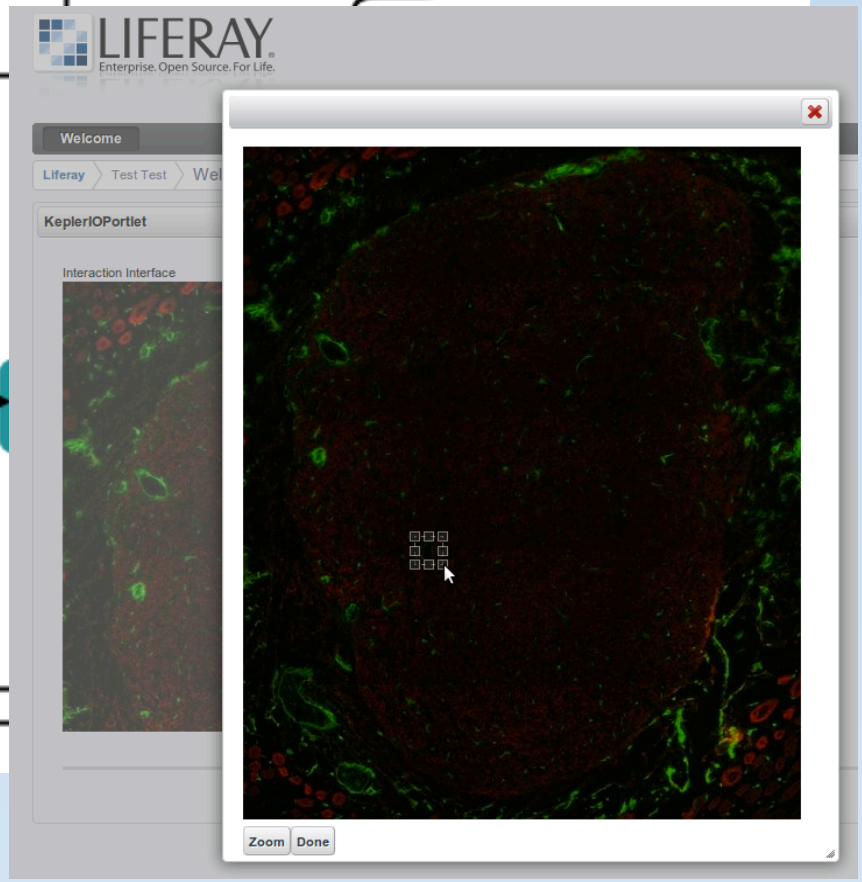
```
{
    actor: "ImageInOutActor"
    {
        operation: "inout"
        input_type: "text"
        prompt: "Choose an area in the image"
        output_type: "binary"
        display_type: "image"
        action: "subarea"
        wait_client: true
        wait_for_input: true
    }
}
```

IOPortlet

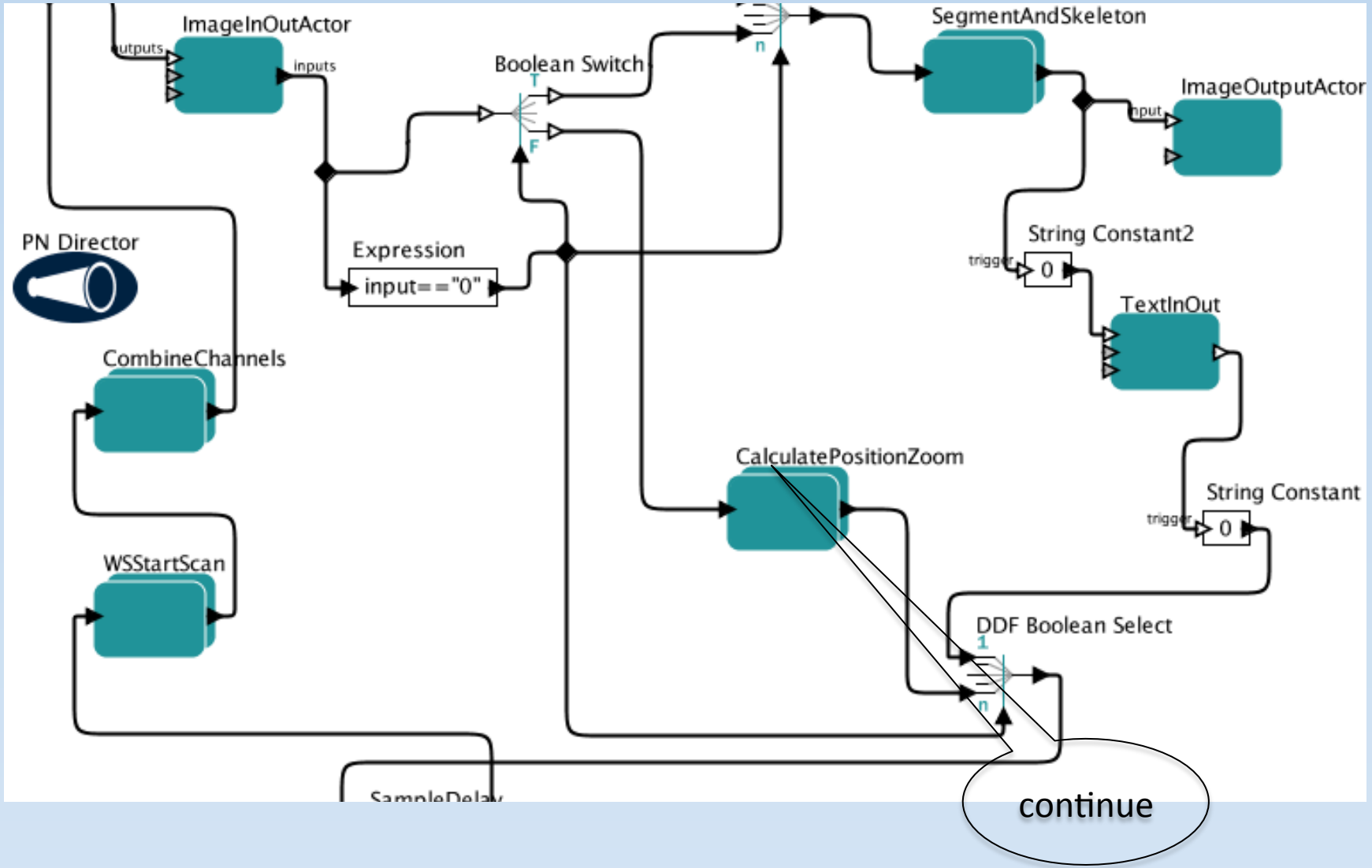
- Web UI client
- Vaadin framework
  - framework for building rich Web applications
- JSR-286 portlet
  - UI elements generated based on requests from connected IOActor
  - Limited UI elements

Case Study: Scan Workflow

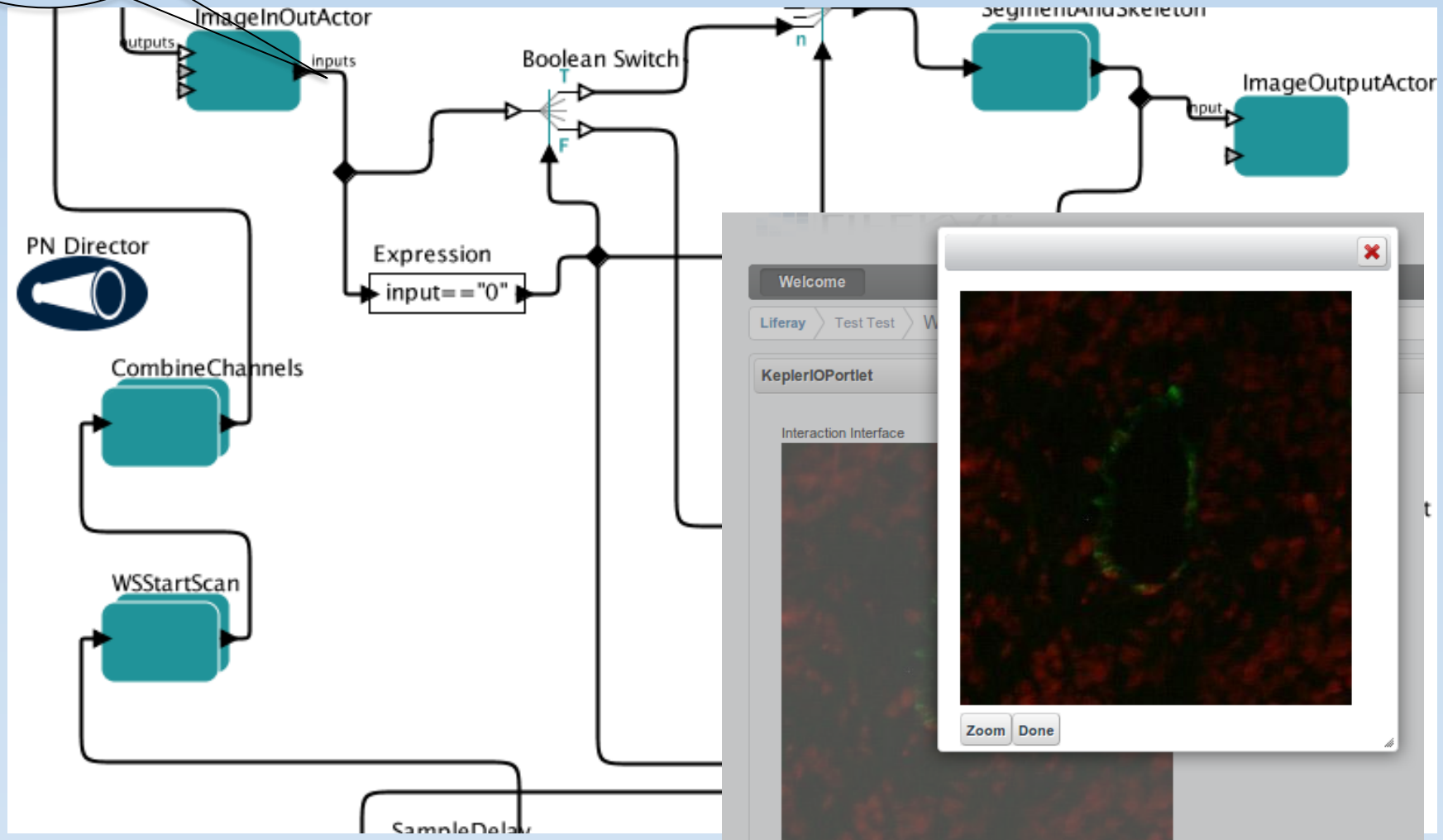




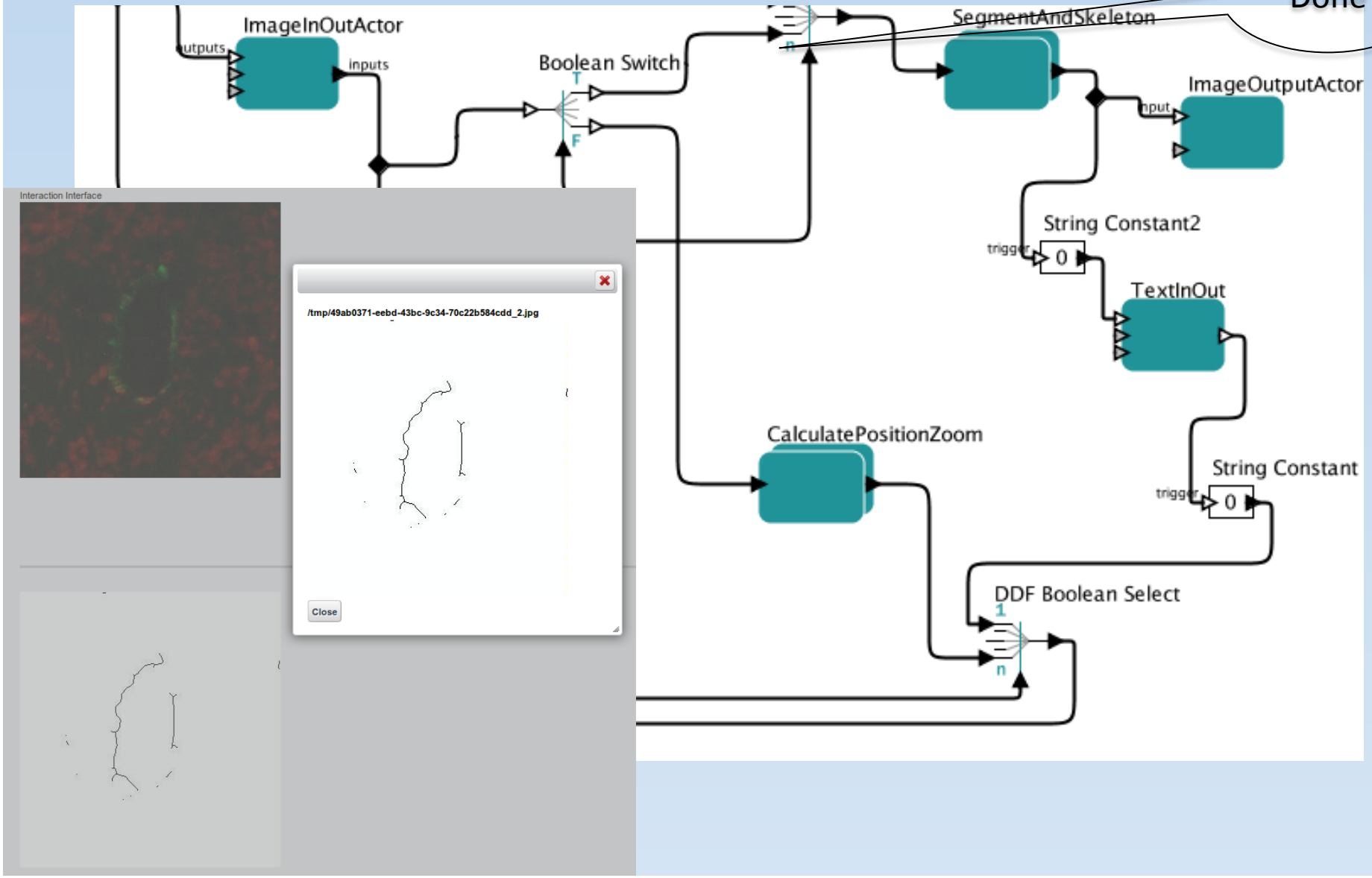
Case Study: Scan Workflow



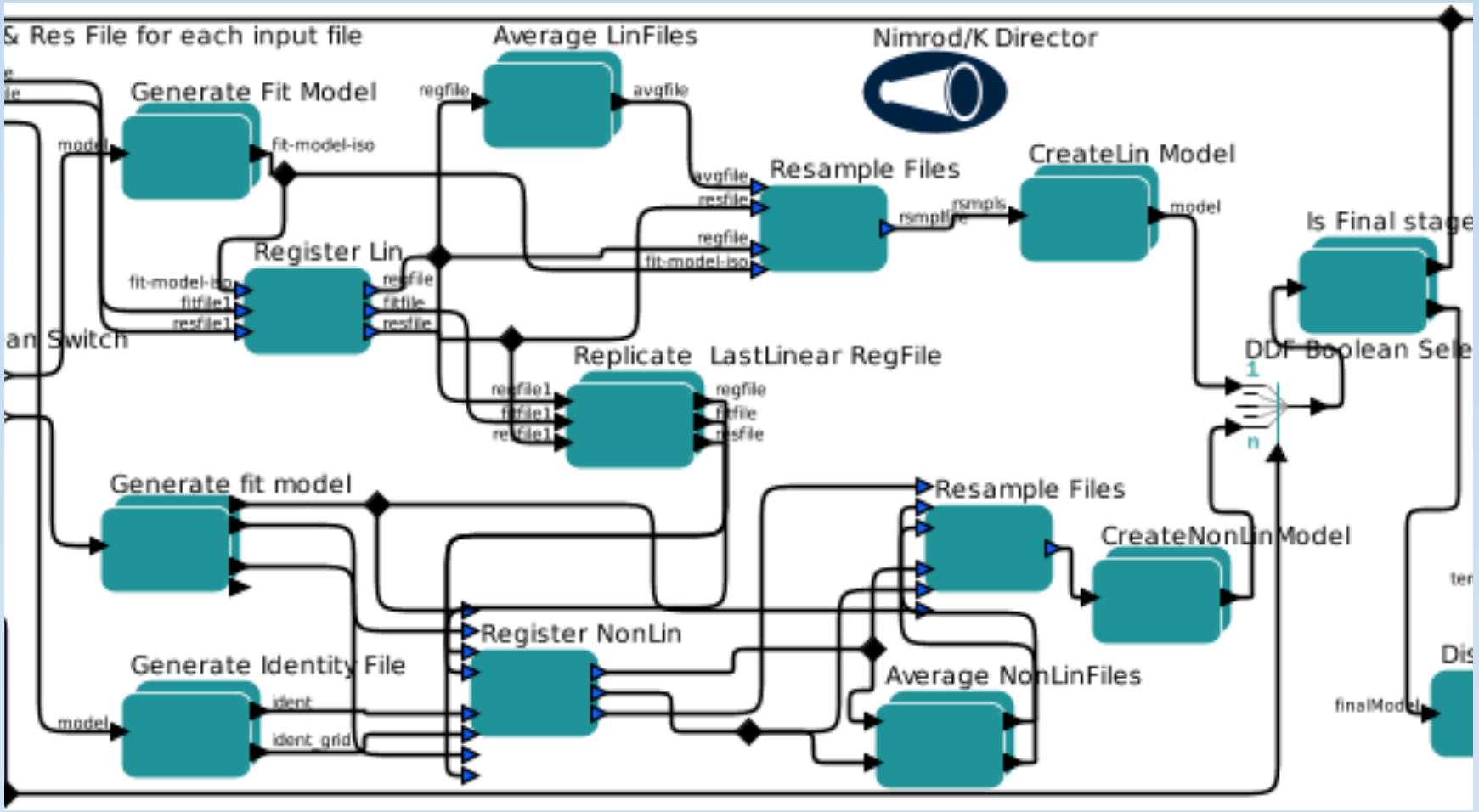
Case Study: Scan Workflow

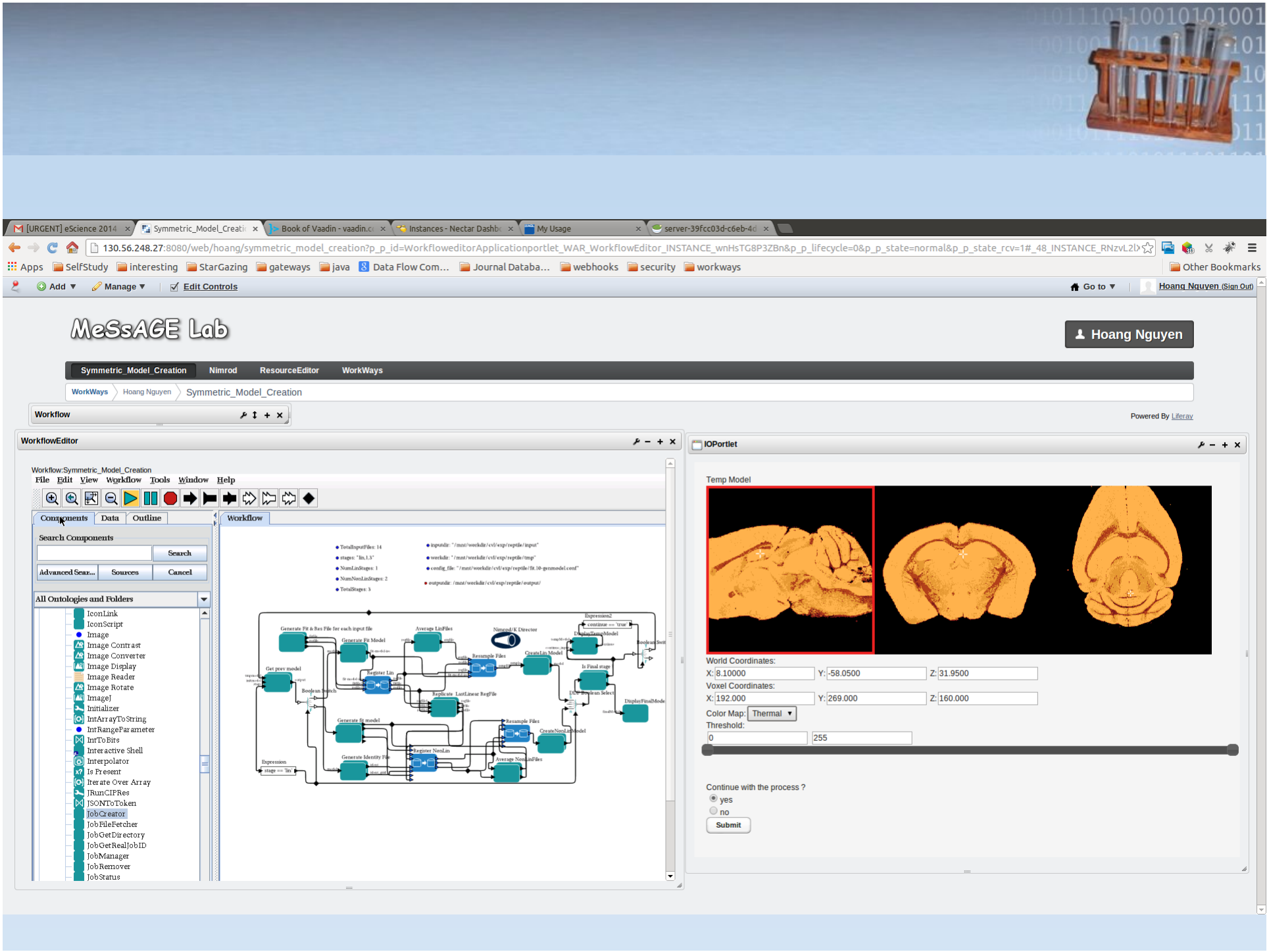


Case Study: Scan Workflow

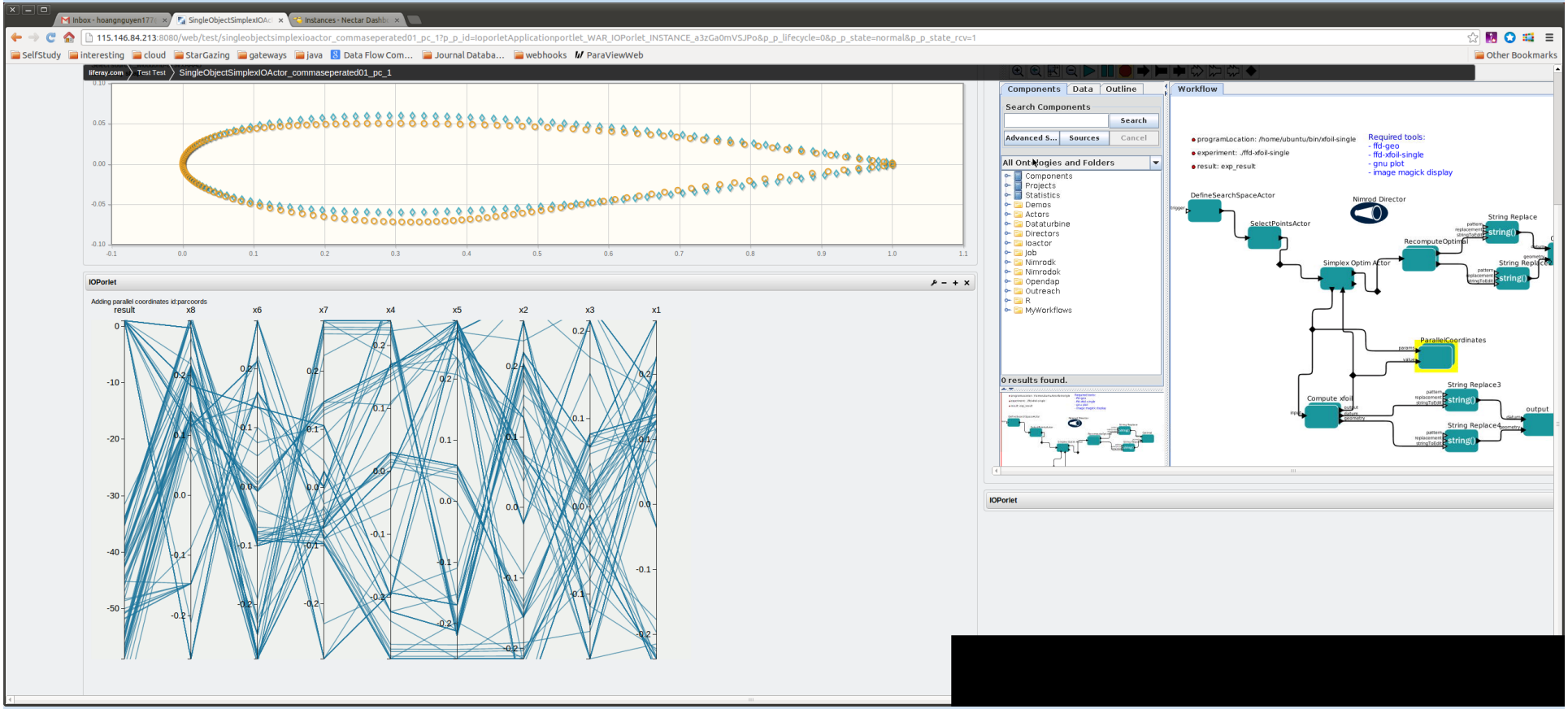


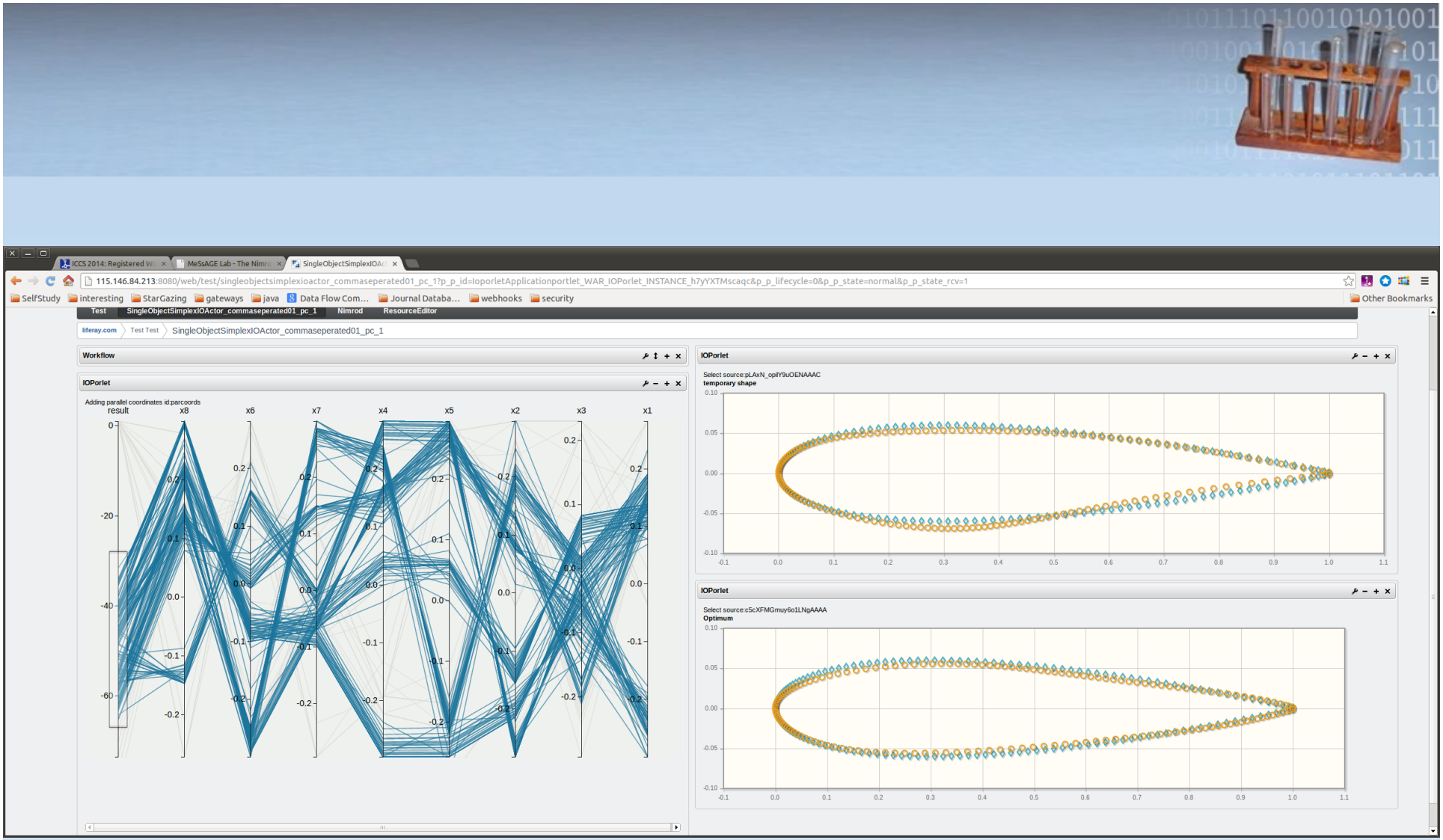
MRI Image segmentation

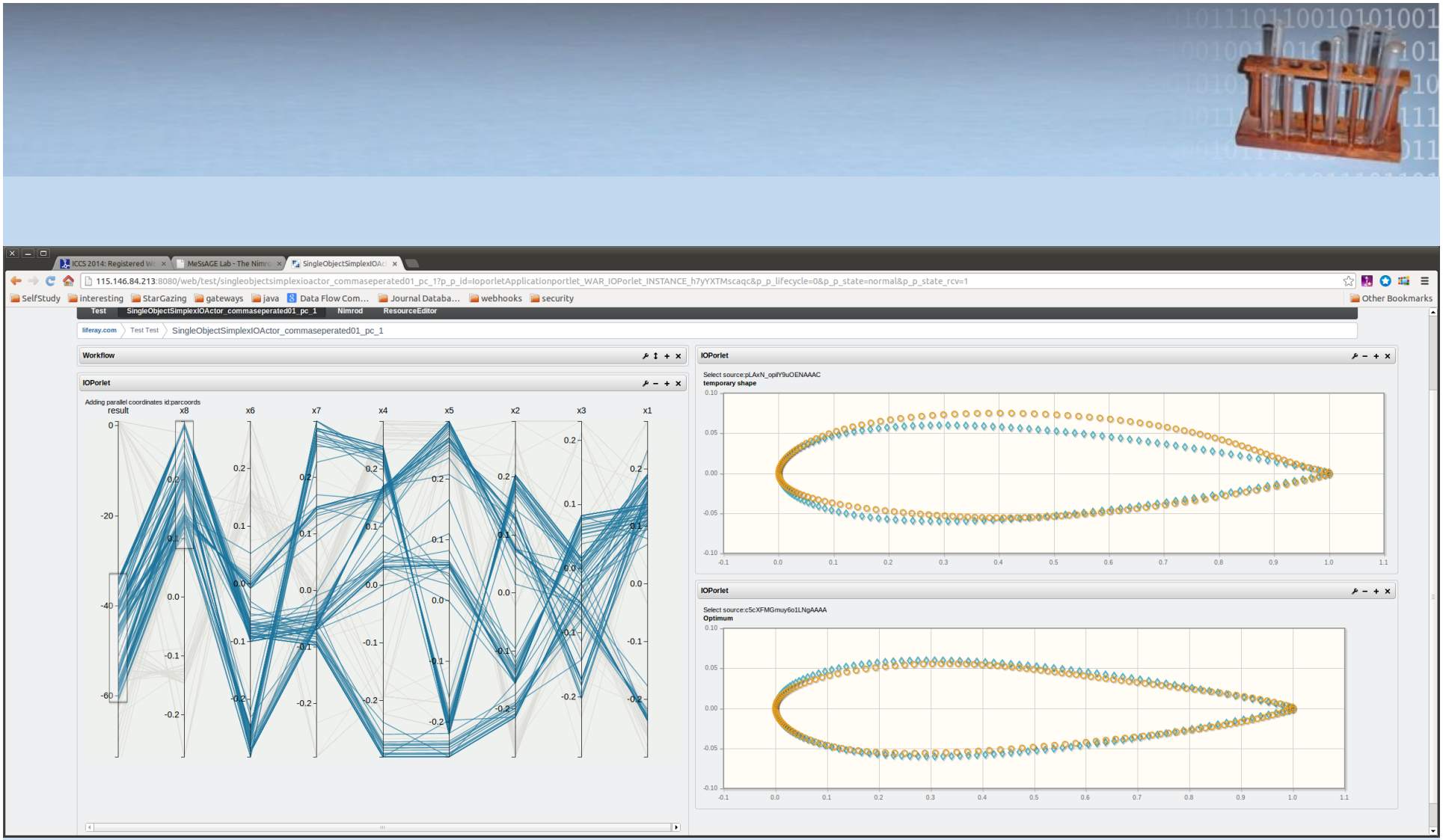



[URGENT] eScience 2014
Symmetric_Model_Creati
Book of Vaadin - vaadin.c
Instances - Nectar Dashb
My Usage
server-39fcc03d-c6eb-4d
130.56.248.27:8080/web/hoang/symmetric_model_creation?p_p_id=WorkfloweditorApplicationportlet_WAR_WorkflowEditor_INSTANCE_wnHsTG8P3ZBn&p_p_lifecycle=0&p_p_state=normal&p_p_state_rcv=1#_48_INSTANCE_RNzvL2lX
Apps
SelfStudy
interesting
StarGazing
gateways
java
Data Flow Com...
Journal Databa...
webhooks
security
workways
Other Bookmarks
Add
Manage
Edit Controls
Go to
Hoang Nguyen (Sign Out)
MeSsAGE Lab
Hoang Nguyen
Symmetric_Model_Creation
Nimrod
ResourceEditor
WorkWays
WorkWays
Hoang Nguyen
Symmetric_Model_Creation
Workflow
Powered By Liferay
WorkflowEditor
Workflow:Symmetric_Model_Creation
File
Edit
View
Workflow
Tools
Window
Help
Components
Data
Outline
Search Components
Search
Advanced Sear...
Sources
Cancel
All Ontologies and Folders
IconLink
IconScript
Image
Image Contrast
Image Converter
Image Display
Image Reader
Image Rotate
ImageJ
Initializer
IntArrayToString
IntRangeParameter
IntToBits
Interactive Shell
Interpolator
Is Present
Iterate Over Array
JRunCIFRes
JSONToToken
JobCreator
JobFileFetcher
JobGetDirectory
JobGetRealJobID
JobManager
JobRemover
JobStatus
Workflow
IOPortlet
Temp Model
World Coordinates:
X: 8.10000
Y: -58.0500
Z: 31.9500
Voxel Coordinates:
X: 192.000
Y: 269.000
Z: 160.000
Color Map:
Thermal
Threshold:
0
255
Continue with the process ?
yes
no
Submit

Airfoil Design

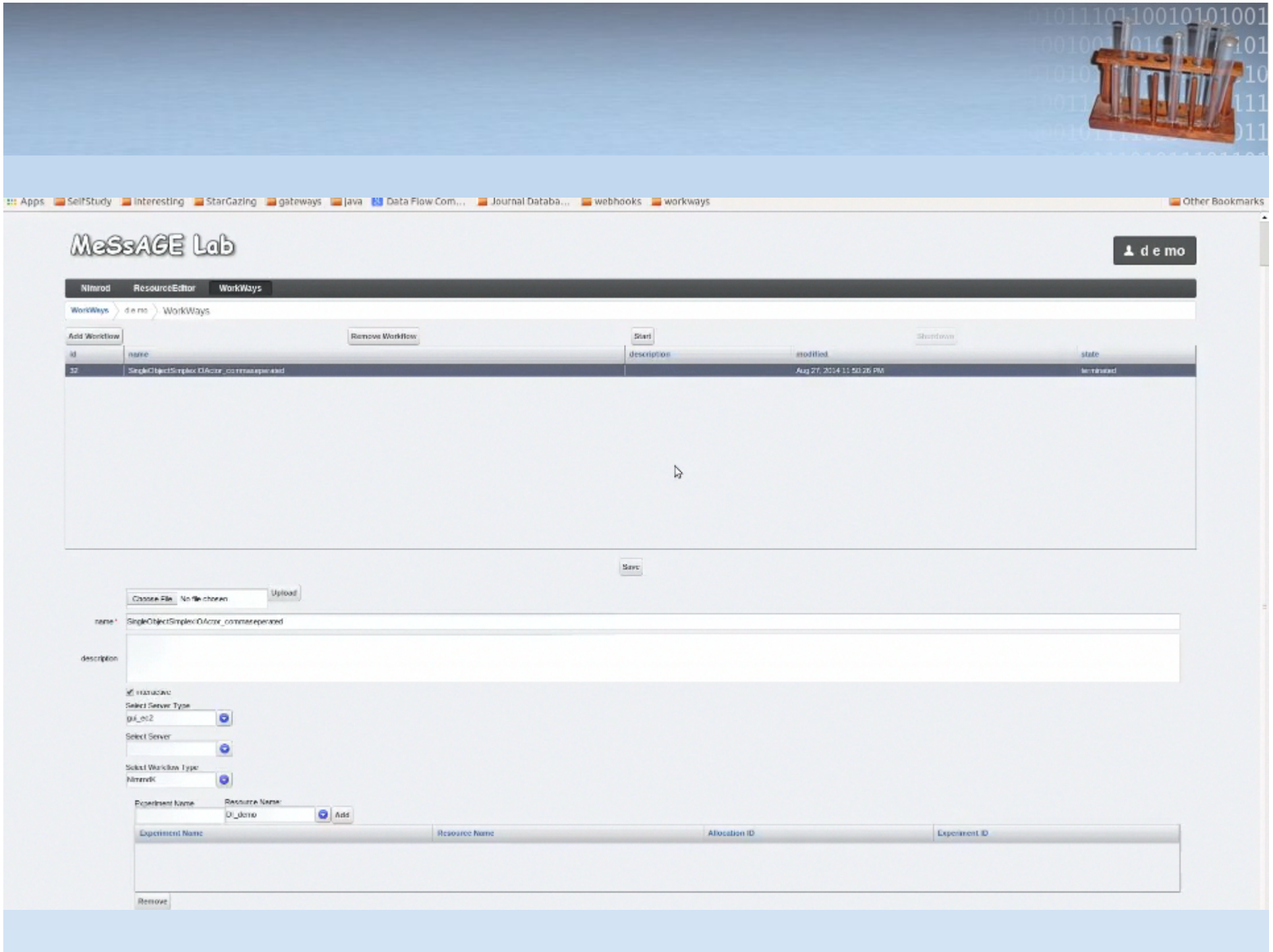



ICCS 2014: Registered
MeSsAGE Lab - The Nimr
SingleObjectSimplexIOAc
115.146.84.213:8080/web/test/singleobjectsimplexioactor_commaseperated01_pc_1?p_p_id=IoporletApplicationportlet_WAR_IOPorlet_INSTANCE_h7yYXTMscaqc&p_p_lifecycle=0&p_p_state=normal&p_p_state_rcv=1
SelfStudy
interesting
StarGazing
gateways
java
Data Flow Com...
Journal Databa...
webhooks
security
Other Bookmarks
Test
SingleObjectSimplexIOActor_commaseperated01_pc_1
Nimrod
ResourceEditor
liferay.com
Test Test
SingleObjectSimplexIOActor_commaseperated01_pc_1
Workflow
IOPorlet
Adding parallel coordinates id:parcoords
result
x8
x6
x7
x4
x5
x2
x3
x1
IOPorlet
Select source:pLAxN_opilY9uOENAAAC
temporary shape
IOPorlet
Select source:c5cXFMGmuy6o1LNgAAAA
Optimum


ICCS 2014: Registered
MeSsAGE Lab - The Nimr
SingleObjectSimplexIOAc
115.146.84.213:8080/web/test/singleobjectsimplexioactor_commaseperated01_pc_1?p_p_id=ioporletApplicationportlet_WAR_IOPorlet_INSTANCE_h7yYXTMscaqc&p_p_lifecycle=0&p_p_state=normal&p_p_state_rcv=1
SelfStudy
interesting
StarGazing
gateways
java
Data Flow Com...
Journal Databa...
webhooks
security
Other Bookmarks
Test
SingleObjectSimplexIOActor_commaseperated01_pc_1
Nimrod
ResourceEditor
liferay.com
Test Test
SingleObjectSimplexIOActor_commaseperated01_pc_1
Workflow
IOPorlet
Adding parallel coordinates id:parcoords
result
x8
x6
x7
x4
x5
x2
x3
x1
IOPorlet
Select source:pLAxN_opilY9uOENAAAC
temporary shape
IOPorlet
Select source:c5cXFMGmuy6o1LNgAAAA
Optimum

Future Work

- Support more objects
- Support asynchronous IO
  - Enhancement of Kepler directors
- Support different UI client(s)
  - Tiled display wall
- Multi-clients interacting with one workflow


Apps
SelfStudy
Interesting
StarGazing
gateways
java
Data Flow Com...
Journal Databa...
webhooks
workways
Other Bookmarks
MeSsAGE Lab
demo
Nimrod
ResourceEditor
WorkWays
WorkWays
demo
WorkWays
Add Workflow
Remove Workflow
Start
Shutdown
id
name
description
modified
state
32
Aug 27, 2014 11:50:26 PM
terminated
Save
Choose File
No file chosen
Upload
name*
description
Interactive
Select Server Type
gui_ec2
Select Server
Select Workflow Type
NimrodK
Experiment Name
Resource Name:
UI_demo
Add
Experiment Name
Resource Name
Allocation ID
Experiment ID
Remove

Questions

To work with such truly gifted scientists has been a blessing.

Vale Professor Martin Lackmann,
Monash University
May 22nd 2014

Vale Dr. Anouchka Mihaylova
UCSD
May 17th 2014