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Scientific and Grid Workflow Management

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Abstract

Grid workflow management systems coordinate multiple job submissions over heterogeneous Grid resources.

They feature visual programming environments to give scientist a high-level view over distributed computations composed of Grid services.

This brief introduction to the field of scientific and Grid workflows includes a survey of selected workflow management tools and outlines current research trends.

Swiss Grid School SGS‘09 @ GPC’09, Geneva, Switzerland

Università
della
Svizzera
italiana

**Facoltà
di scienze
informatiche**

Cesare Pautasso

Ph.D. at ETH Zürich (2004)

Post-Doc at ETH Zürich in the Systems (IKS) Group

- Software: JOpera: Process Support for more than Web services

  http://www.jopera.org/

Researcher at IBM Zurich Research Lab (2007)

Assistant Professor at the new Faculty of Informatics, University of Lugano (USI), Switzerland (since September 2007)

- USI Representative in the SwiNG Assembly (since 2007)
- Grid Workflow Working Group Lead (since 2007)

More Information: http://www.pautasso.info/

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Outline

Why Workflow Management on the Grid?

Discussion: Scientific vs. Grid vs. Business Workflows

- Some Application Examples

Workflow Modeling Languages and Tools Overview

- Grid Workflow Language Patterns

Running Workflows on the Grid

- JOpera: Scientific Workflow for Eclipse
- Workflows and Provenance

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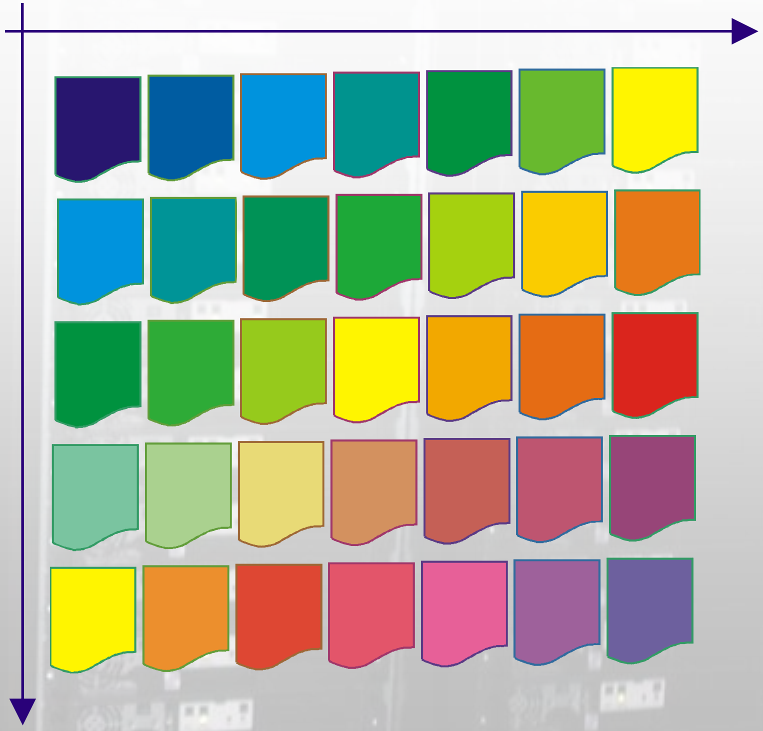
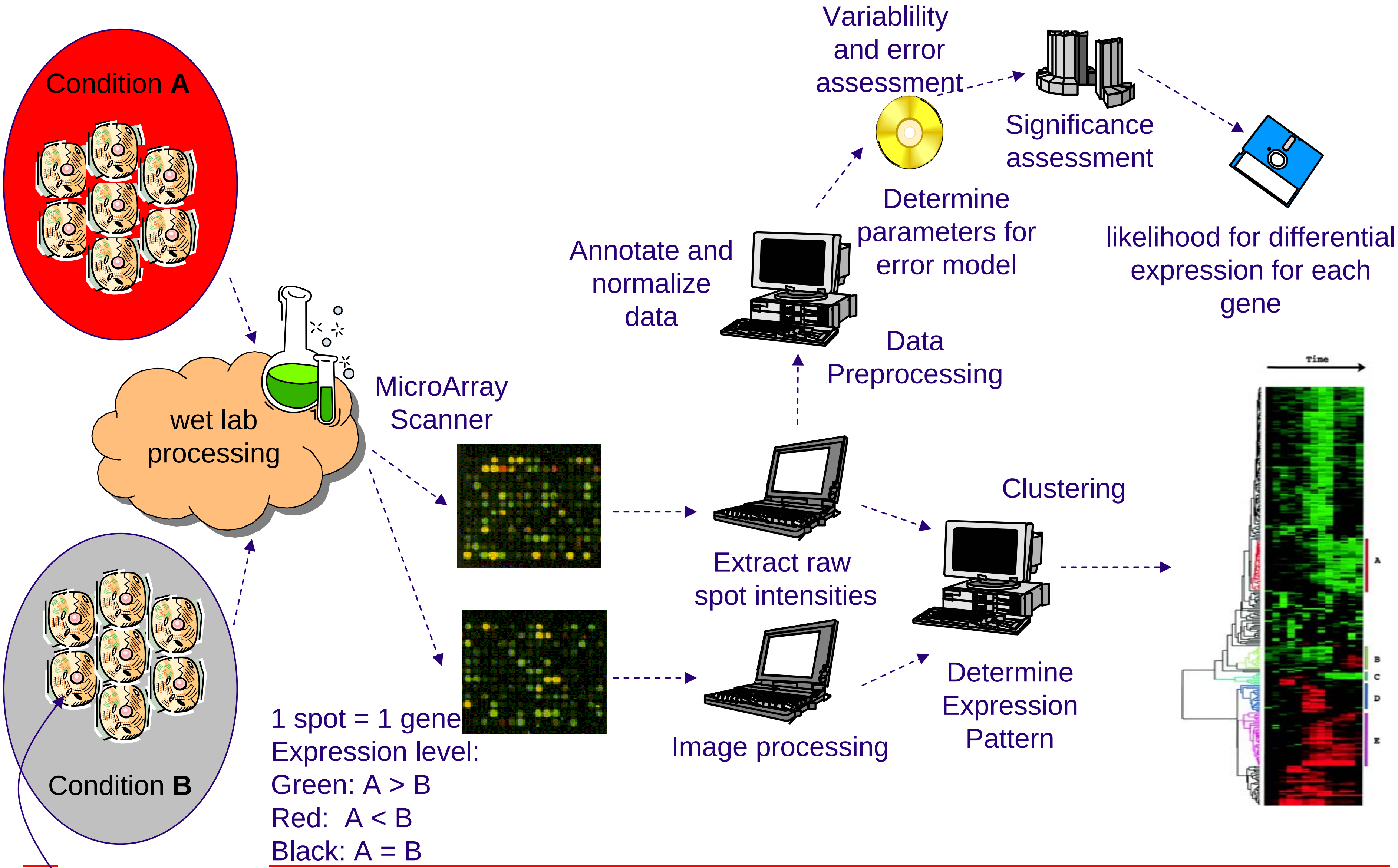
Why Workflow Management on the Grid?

Kinds of Grid Computation

One Job Submission

Parameter Sweep





Condition A

Condition B

wet lab processing

MicroArray Scanner

1 spot = 1 gene
Expression level:
Green: A > B
Red: A < B
Black: A = B

Image processing

Extract raw spot intensities

Data Preprocessing

Annotate and normalize data

Determine parameters for error model

Variablility and error assessment

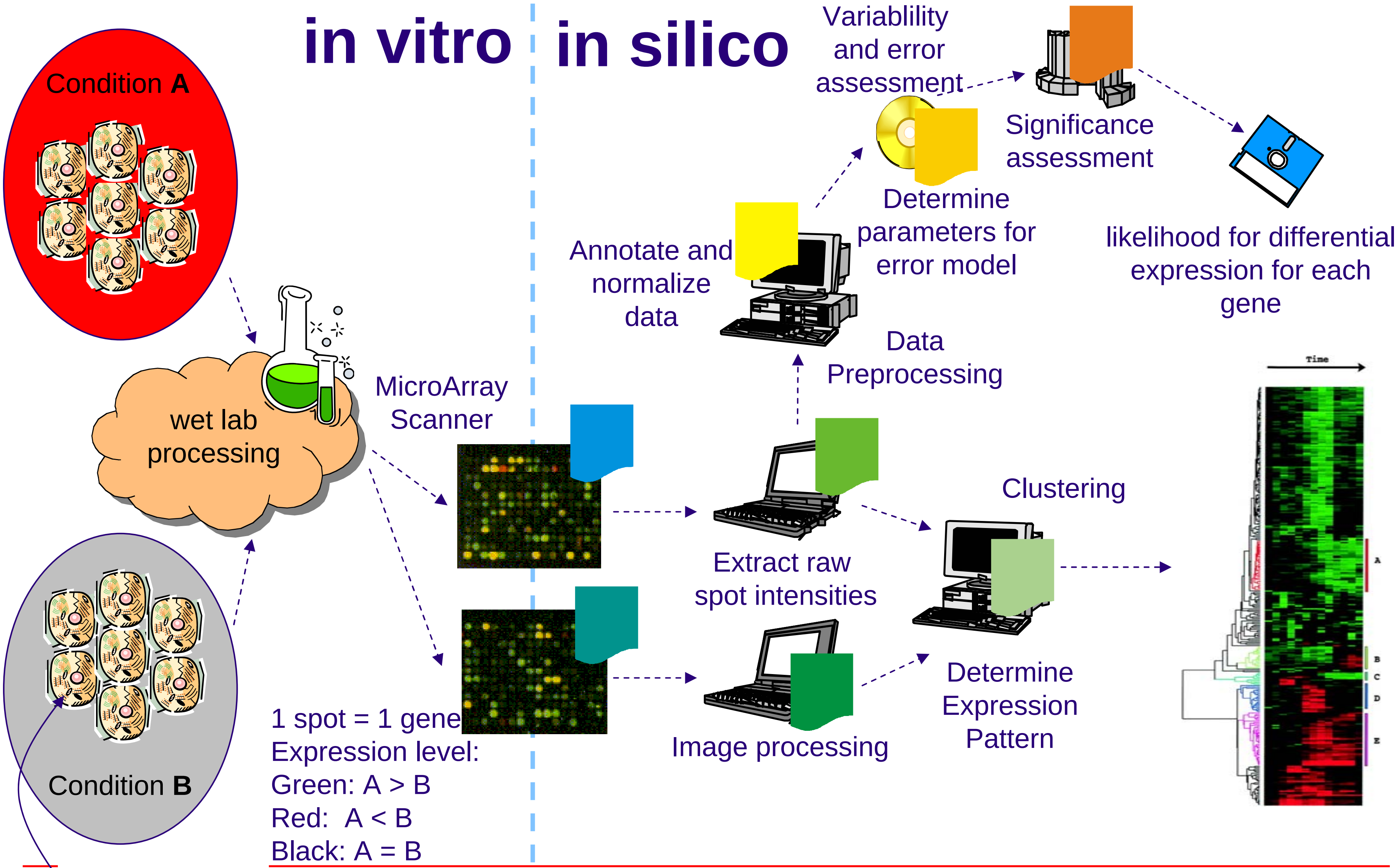
Significance assessment

likelihood for differential expression for each gene

Clustering

Determine Expression Pattern

Cell population



in vitro

in silico

Condition A

wet lab processing

Condition B

Cell population

MicroArray Scanner

1 spot = 1 gene
Expression level:
Green: A > B
Red: A < B
Black: A = B

Extract raw spot intensities

Image processing

Data Preprocessing

Annotate and normalize data

Determine parameters for error model

Variablility and error assessment

Significance assessment

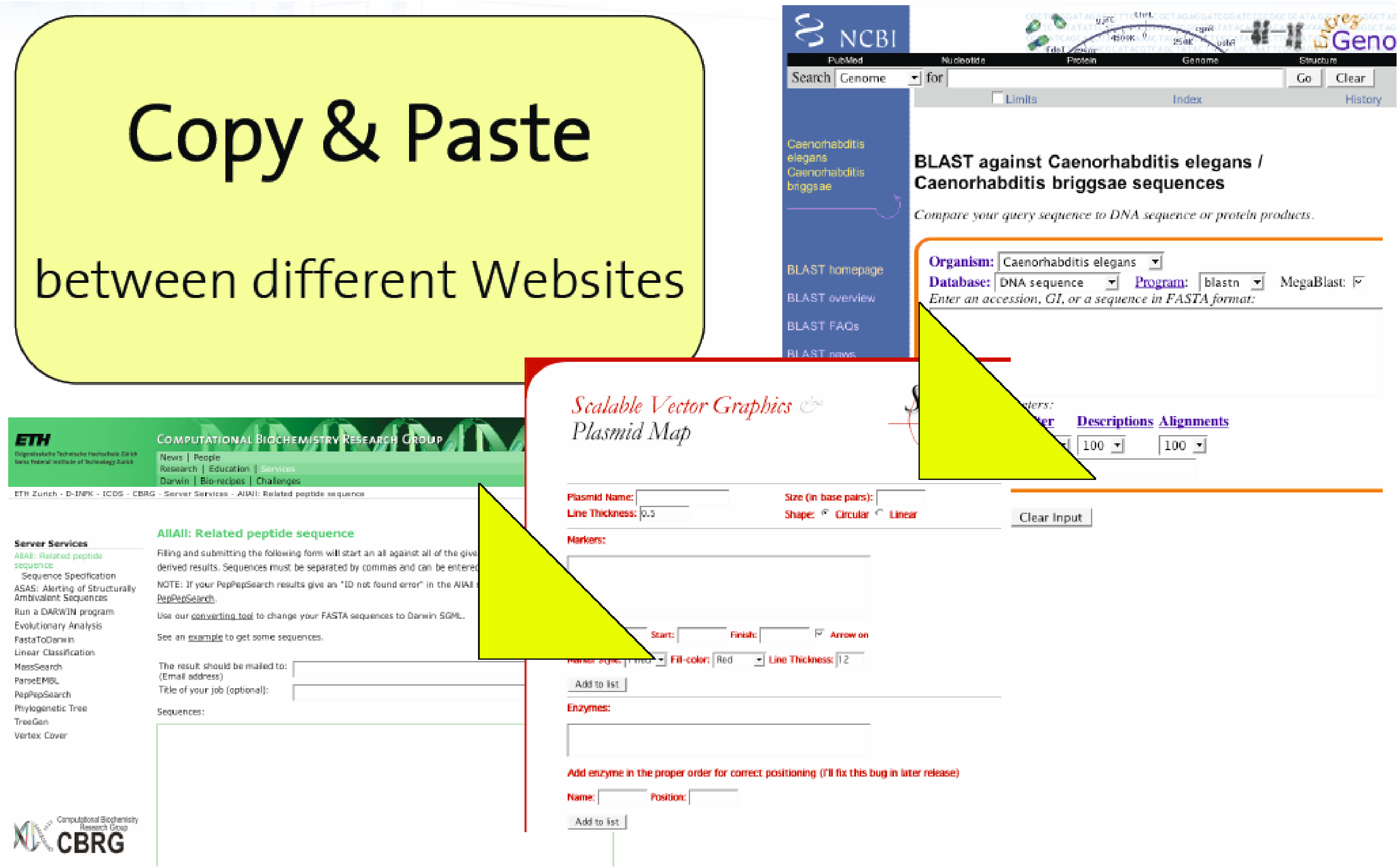
likelihood for differential expression for each gene

Clustering

Determine Expression Pattern

Copy & Paste

between different Websites



NCBI

PubMed Nucleotide Protein Genome Structure

Search Genome for Go Clear

□ Limits Index History

Caenorhabditis elegans Caenorhabditis briggsae

BLAST homepage

BLAST overview

BLAST FAQs

BLAST news

BLAST against Caenorhabditis elegans / Caenorhabditis briggsae sequences

Compare your query sequence to DNA sequence or protein products.

Organism: Caenorhabditis elegans

Database: DNA sequence **Program:** blastn MegaBlast: ☑

Enter an accession, GI, or a sequence in FASTA format:

...ters:

...ter **Descriptions** **Alignments**

100 100

Clear Input

ETH Eidgenössische Technische Hochschule Zürich Swiss Federal Institute of Technology Zurich

COMPUTATIONAL BIOCHEMISTRY RESEARCH GROUP

News | People
Research | Education | Services
Darwin | Bio-recipes | Challenges

ETH Zurich - D-INFK - ICOS - CBRG - Server Services - AllAll: Related peptide sequence

Server Services

AllAll: Related peptide sequence
Sequence Specification
ASAS: Alerting of Structurally Ambivalent Sequences
Run a DARWIN program
Evolutionary Analysis
FastaToDarwin
Linear Classification
MassSearch
ParseEMBL
PepPepSearch
Phylogenetic Tree
TreeGen
Vertex Cover

Computational Biochemistry Research Group CBRG

AllAll: Related peptide sequence

Filling and submitting the following form will start an all against all of the give derived results. Sequences must be separated by commas and can be entered

NOTE: If your PepPepSearch results give an "ID not found error" in the AllAll PepPepSearch.

Use our converting tool to change your FASTA sequences to Darwin SGML.

See an example to get some sequences.

The result should be mailed to: (Email address)

Title of your job (optional):

Sequences:

Scalable Vector Graphics & Plasmid Map

Plasmid Name: Size (in base pairs):

Line Thickness: 0.5 Shape: ● Circular ○ Linear

Markers:

Start: Finish: ☑ Arrow on

Marker style: Filled Fill-color: Red Line Thickness: 12

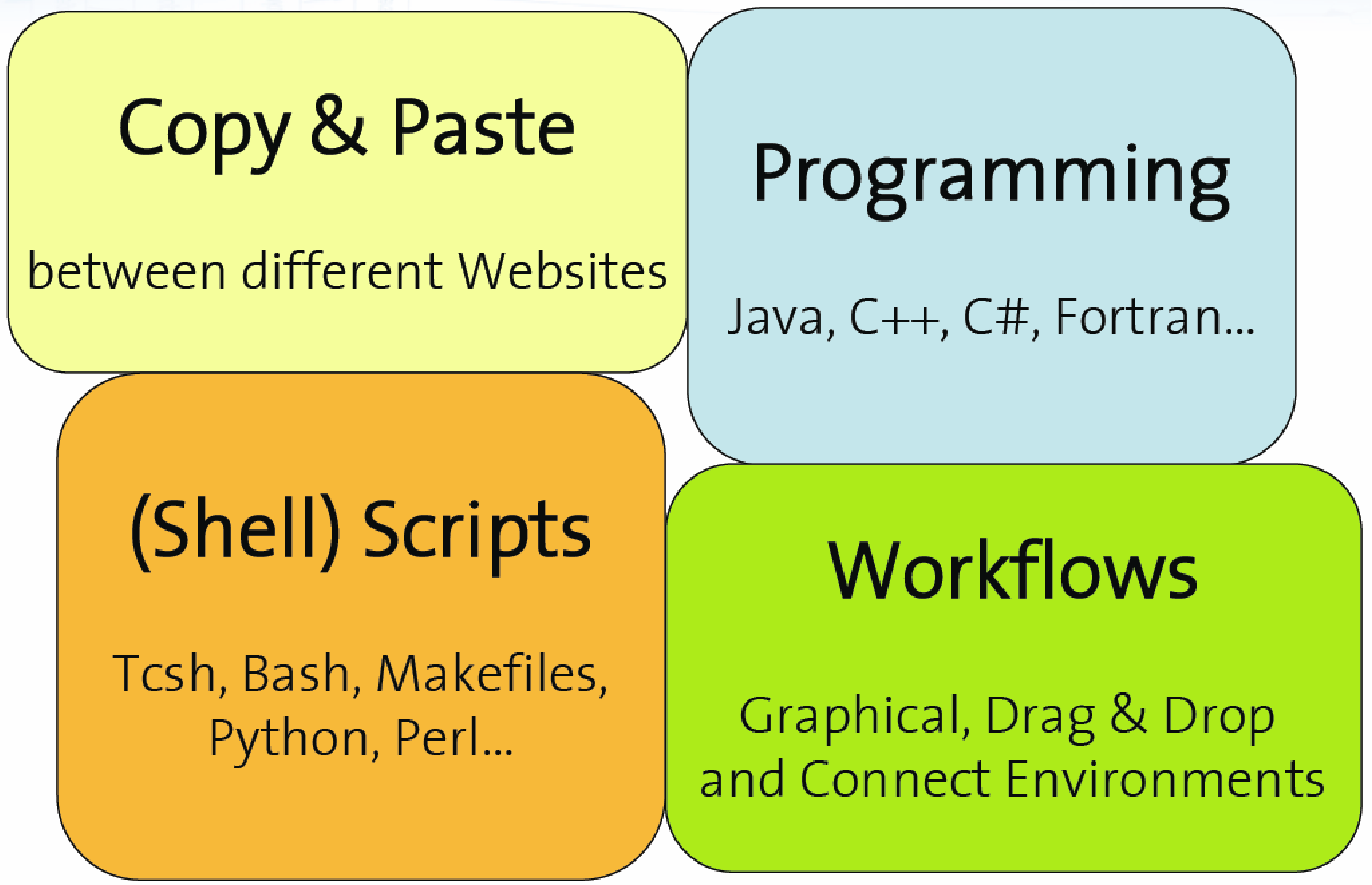
Add to list

Enzymes:

Add enzyme in the proper order for correct positioning (I'll fix this bug in later release)

Name: Position:

Add to list



Copy & Paste

between different Websites

Programming

Java, C++, C#, Fortran…

(Shell) Scripts

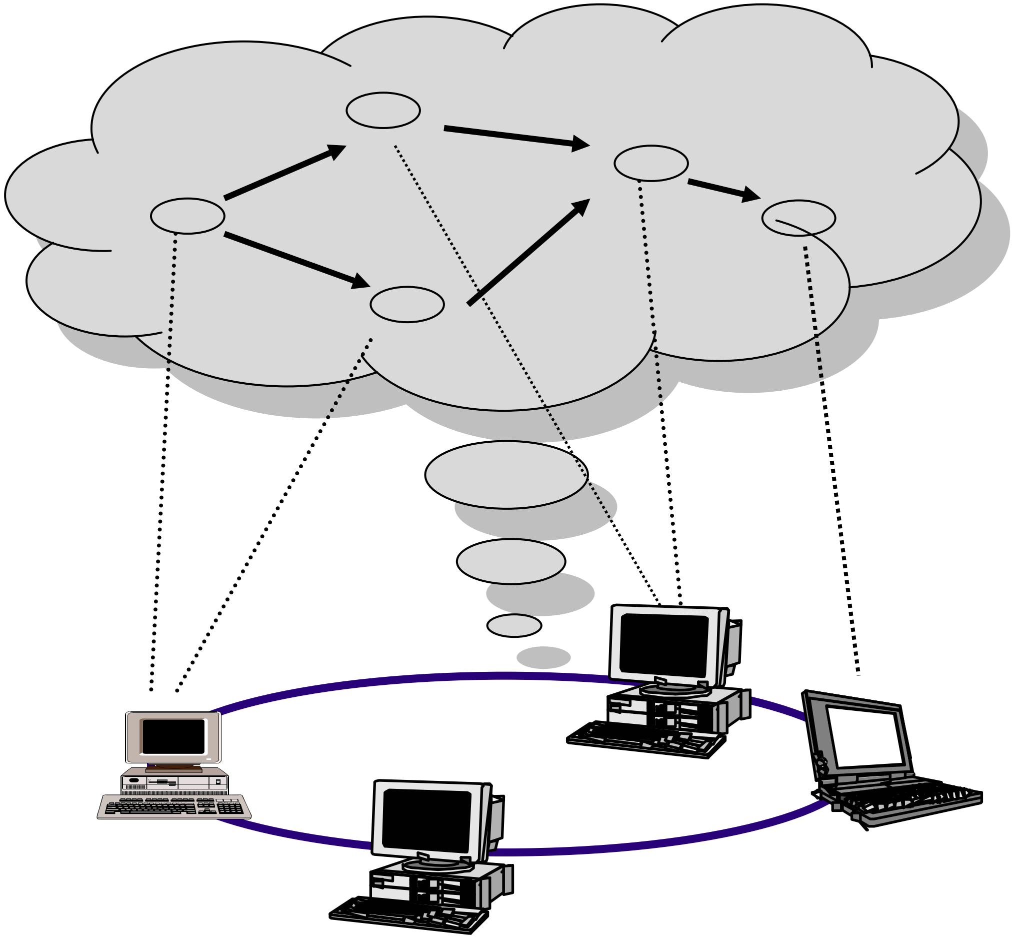
Tcsh, Bash, Makefiles, Python, Perl…

Workflows

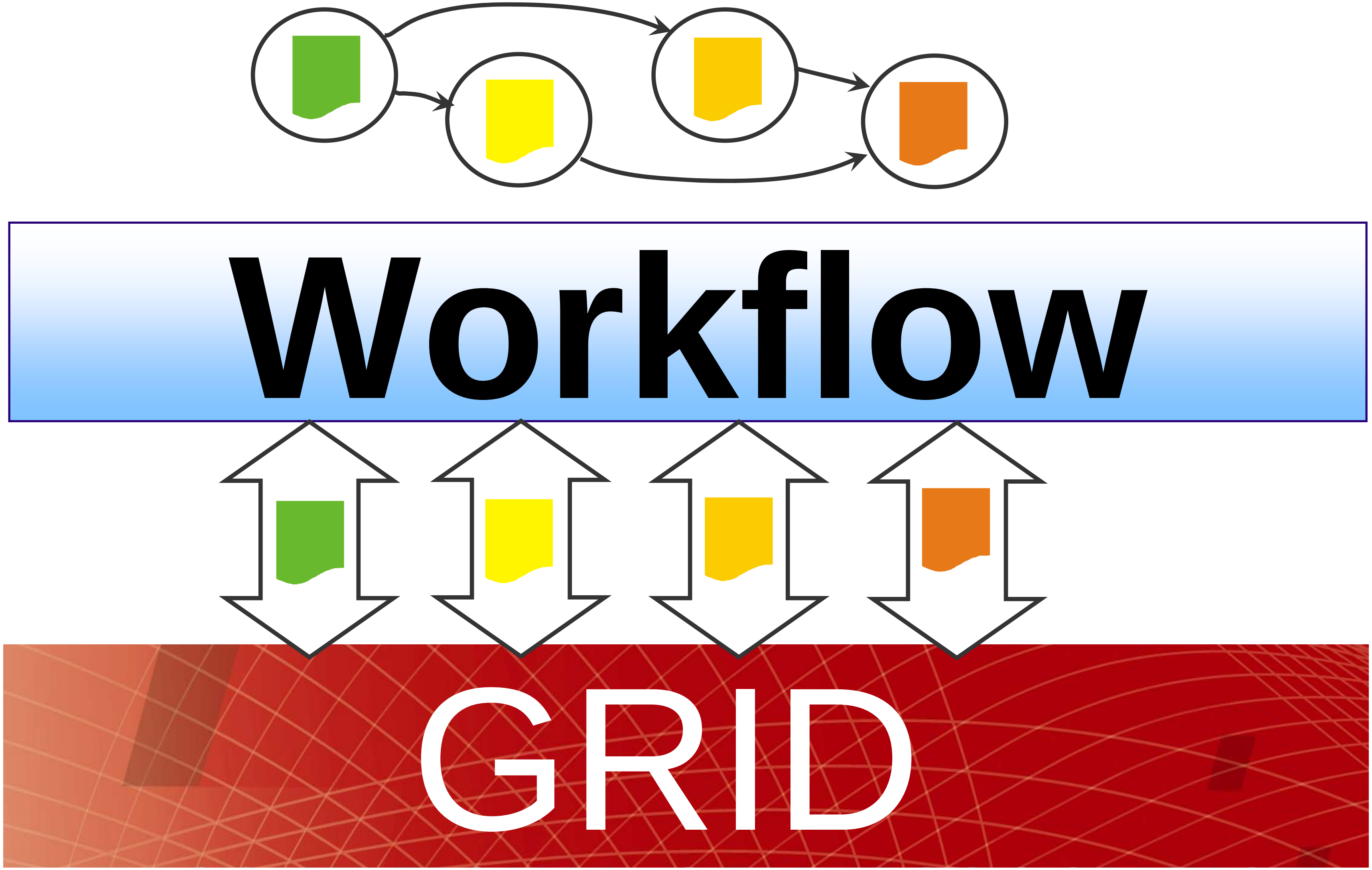
Graphical, Drag & Drop and Connect Environments

Vision for Scientific and Grid Workflows

Make it easy to build Grid applications composed of **multiple jobs**



> “Provide the scientist with a platform that takes care of all data handling and record keeping chores so that the user can concentrate on the *science* and not *computer science*”



Workflow

GRID

Some (Scientific) Workflow Management Systems

- Askalon
- Bigbross Bossa
- BioPipe
- BPMN
- Breeze
- Carnot
- Con:cern
- DAGMan
- DiscoveryNet
- Dralasoft
- GEL
- GridAnt
- Grid Job Handler
- GWFE
- GWES
- ICENI
- Inforsense
- JIGSA
- JOpera
- Kepler
- Karajan
- Oakgrove's reactor
- OSIRIS
- OSWorkflow
- OpenWFE
- Pegasus
- Pipeline Pilot
- P-GRADE
- PowerFolder
- Ptolemy II
- Savvion
- Seebeyond
- SCIRun
- ScyFLOW
- SDSC Matrix
- SHOP2
- Taverna
- Teuta (UML)
- Triana
- Trident
- Twister
- Ultimus
- Versata
- Viztrails
- wftk
- XFlow
- YAWL
- Wildfire
- WFEE
- WS-BPEL
- ZBuilder

Scientific vs. Grid vs. Business Workflows

The Origins: Business Process Management

<u>who</u> has to do <u>what</u>, <u>when</u>

The Origins: Business Process Management

- A business process describes key procedures within an organization. They involve:
  - multiple steps
  - numerous people
  - large amounts of resources
- In large business organizations there are many factors that increase the complexity of the business processes:
  - processes are not well documented
  - conformance to rules not guaranteed
  - people lack information about context
  - company lacks monitoring tools
  - steps, people and resources are not properly coordinated
- Workflow Management Systems try to address these problems by automating the coordination aspects of a business process: who has to do what, when, and with which software tools.

Business Workflows

> “The **automation** of a business process where **documents**, **information** to be processed or **tasks** to be carried out are passed from one participant to another following a set of **procedural rules**”

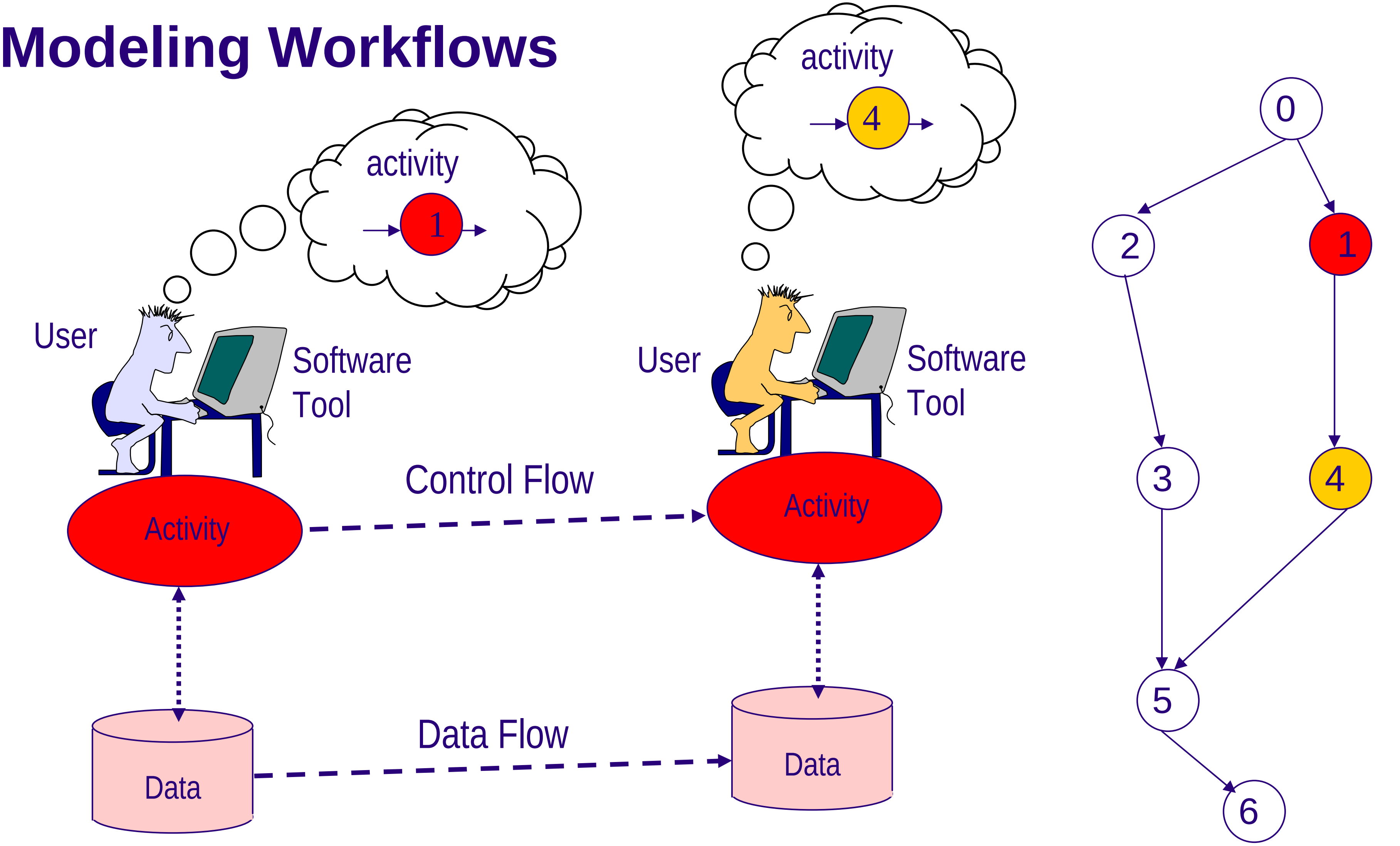
Worfklow Management Coalition (WfMC, 1993)

Scientific Workflows

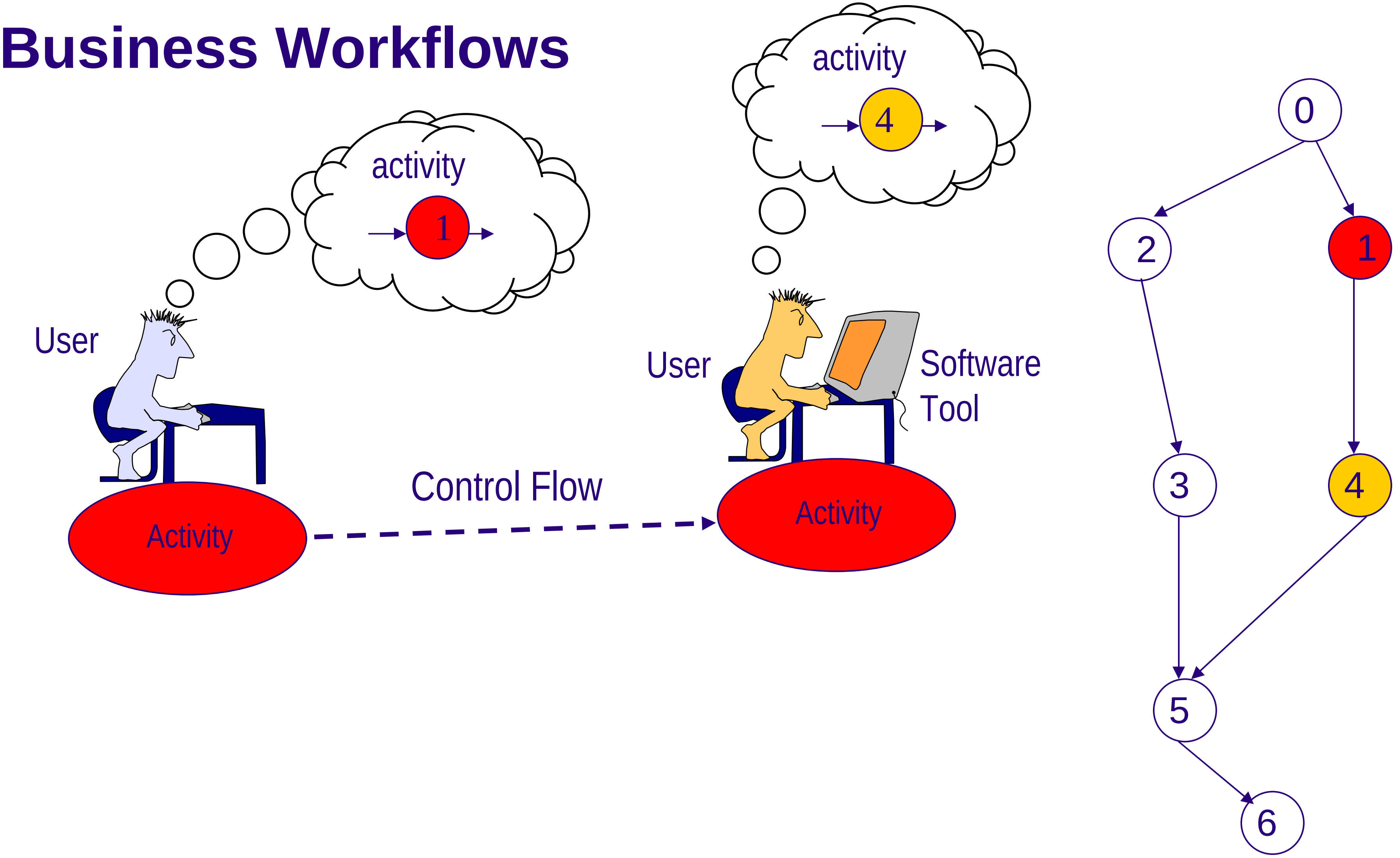
> “ are **networks** of analytical **steps** that may involve, e.g., database access and querying, data analysis and mining, and many other steps including computationally intensive **jobs** submitted to high performance clusters and **Grids** ”

Bertram Ludäscher

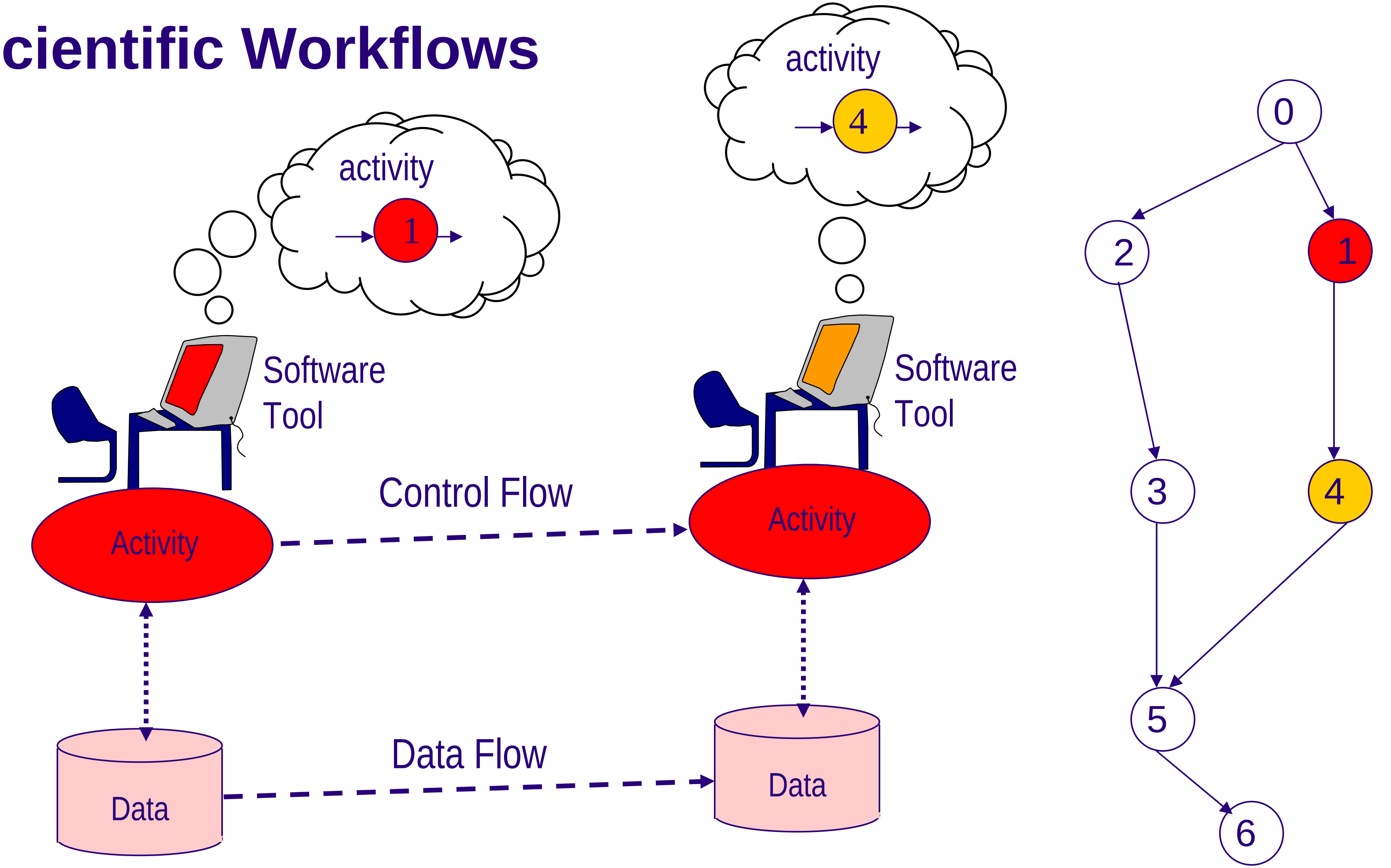
Modeling Workflows



Business Workflows



Scientific Workflows



Similarities:
Are scientists doing e-Business?

Capturing knowledge/best practices

Capture business processes within a company

Capture scientific experiments

Executable Models for Repeated Execution

Run a well defined procedure many times

Ensure that an experiment can be reproduced

Incorporate human decision in the process

Can we always do straight-through processing?

Hard to achieve full automation

Differences:
Do scientists need business transactions?

Rate of change

Changing business procedures requires management approval

Exploratory scientific processes require high flexibility

Which kind of data?

Travel reservations, Loan applications

Large protein sequence databases, Astronomy image catalogs

What is the ultimate goal?

Making profit

Making science

Scientific vs. Grid Workflows

Scientific workflows emphasize the design of virtual experiments:

- Data flow models
- Reusable “scientific computing” component library
- Interactive debugging, monitoring and steering
- Data provenance and lineage tracking for reproducibility
- Model versioning for exploratory customization

Grid workflows focus on the large-scale execution of scientific workflows:

- Mapping and adaptation to a dynamic run-time environment
- Provide access to shared workflows as a Grid service
- Parameterized Execution
- Centralized vs. Distributed Execution Architectures
- Fault Tolerance
- Optimization

Scientific Workflows on the Grid

- How can Scientific WF benefit from the Grid?
  1. Leverage underlying Grid middleware:
     - Resource Management
     - Job Scheduling
     - Large Data Transfers (GridFTP) between Activities
  2. Improved QoS based on the workflow model
     - Grid resource reservation
     - Data replication
     - Data placement
     - Fault Tolerance

Powered by JOpera

http://www.jopera.org/

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Example

PURDUE UNIVERSITY | ITaP Information Technology at Purdue

TeraGrid™

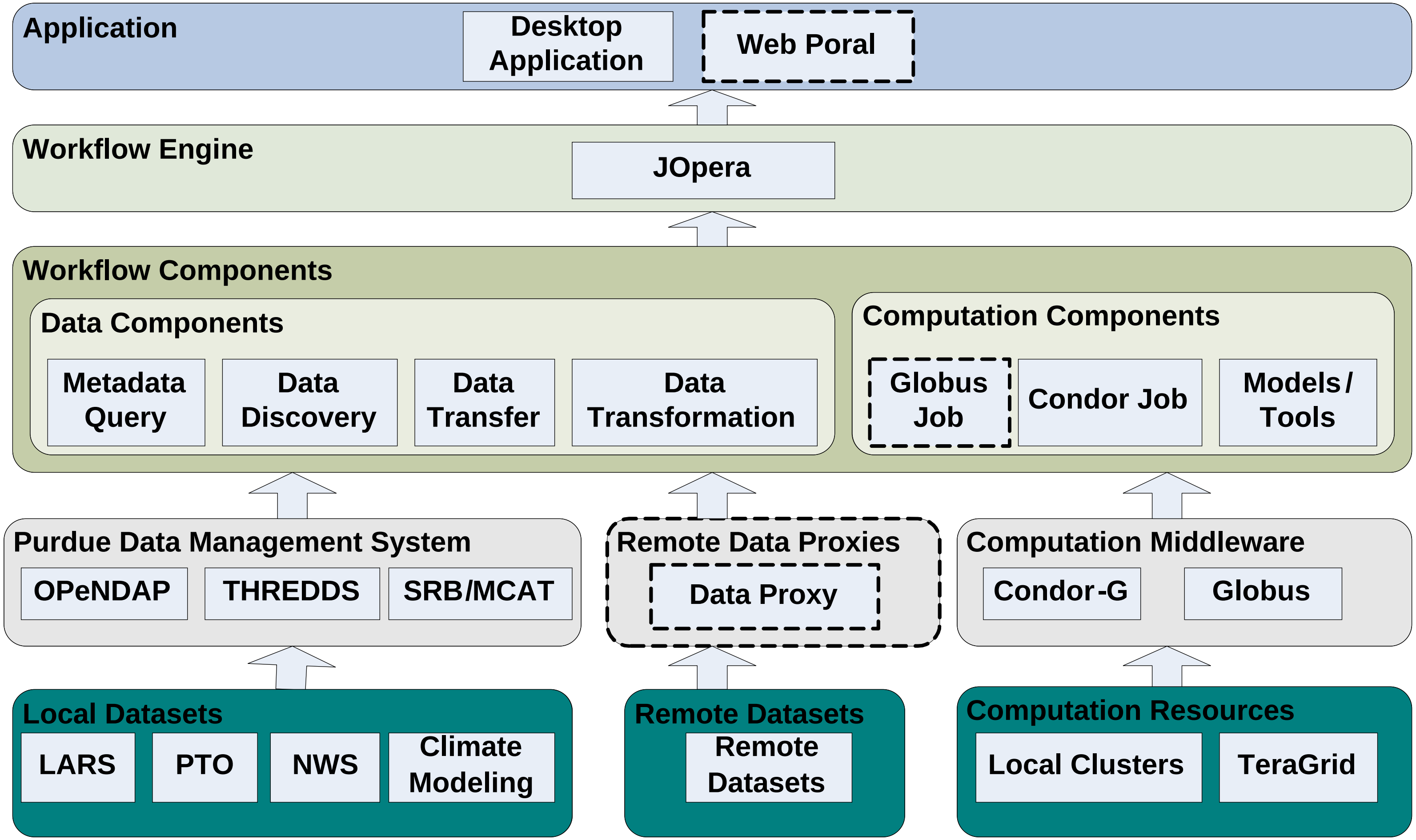
A Web Service-Enabled Workflow System for Climate Modeling Data Processing in TeraGrid

Rajesh Kalyanam

Lan Zhao
Taezoon Park
Sebastien Goasguen

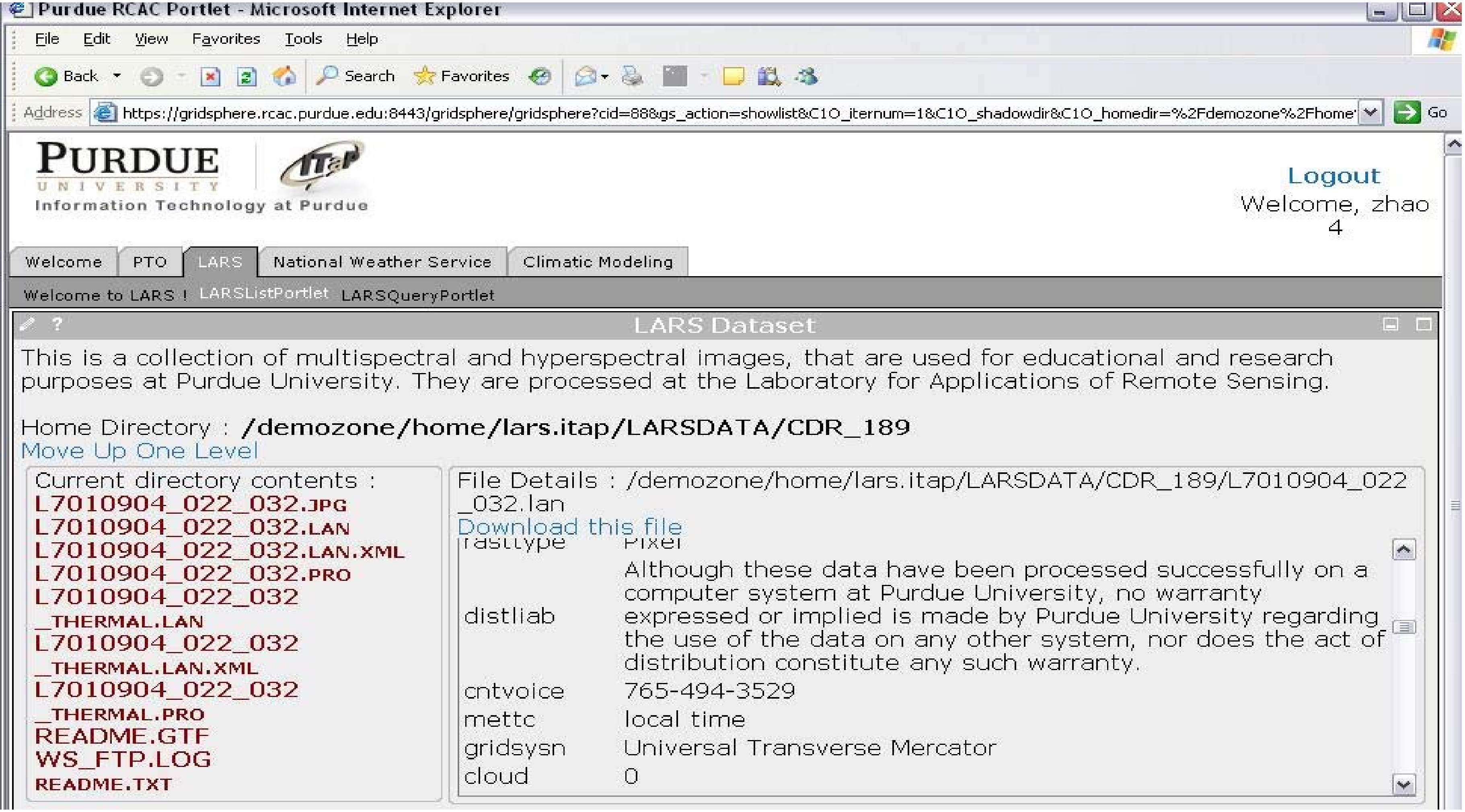
PURDUE UNIVERSITY | ITaP
Information Technology at Purdue

Architecture



From Rajesh Kalyanam

Portal



Purdue RCAC Portlet - Microsoft Internet Explorer
File Edit View Favorites Tools Help
Back Search Favorites
Address https://gridsphere.rcac.purdue.edu:8443/gridsphere/gridsphere?cid=88&gs_action=showlist&C10_iternum=1&C10_shadowdir&C10_homedir=%2Fdemozone%2Fhome
Go
PURDUE UNIVERSITY
Information Technology at Purdue
Logout
Welcome, zhao 4
Welcome PTO LARS National Weather Service Climatic Modeling
Welcome to LARS ! LARSListPortlet LARSQueryPortlet
LARS Dataset

This is a collection of multispectral and hyperspectral images, that are used for educational and research purposes at Purdue University. They are processed at the Laboratory for Applications of Remote Sensing.

Home Directory : **/demozone/home/lars.itap/LARSDATA/CDR_189**

Move Up One Level

Current directory contents :

- L7010904_022_032.JPG
- L7010904_022_032.LAN
- L7010904_022_032.LAN.XML
- L7010904_022_032.PRO
- L7010904_022_032_THERMAL.LAN
- L7010904_022_032_THERMAL.LAN.XML
- L7010904_022_032_THERMAL.PRO
- README.GTF
- WS_FTP.LOG
- README.TXT

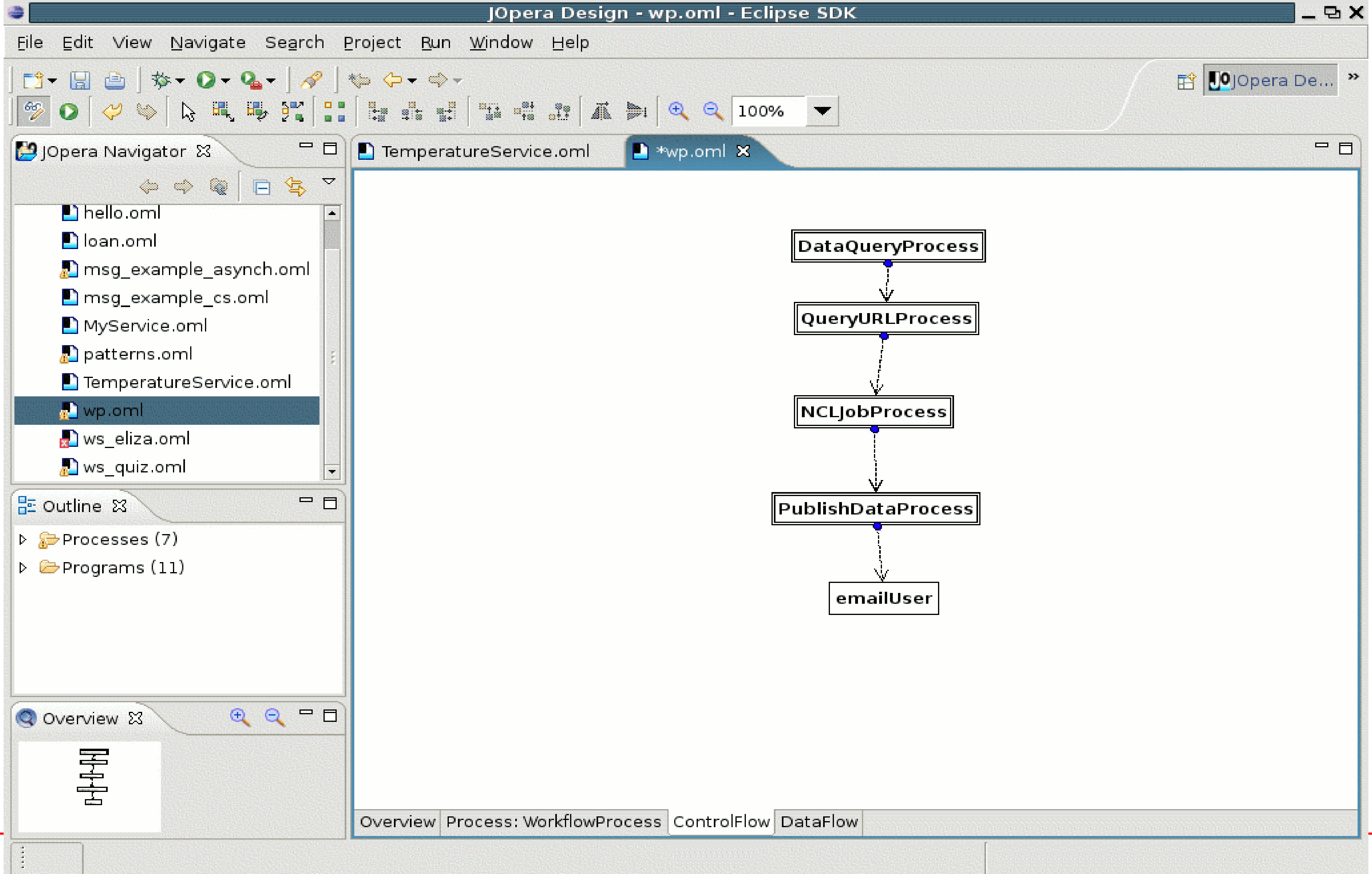
File Details : /demozone/home/lars.itap/LARSDATA/CDR_189/L7010904_022_032.lan

Download this file

rasttype	Pixel
distliab	Although these data have been processed successfully on a computer system at Purdue University, no warranty expressed or implied is made by Purdue University regarding the use of the data on any other system, nor does the act of distribution constitute any such warranty.
cntvoice	765-494-3529
mettc	local time
gridsysn	Universal Transverse Mercator
cloud	0

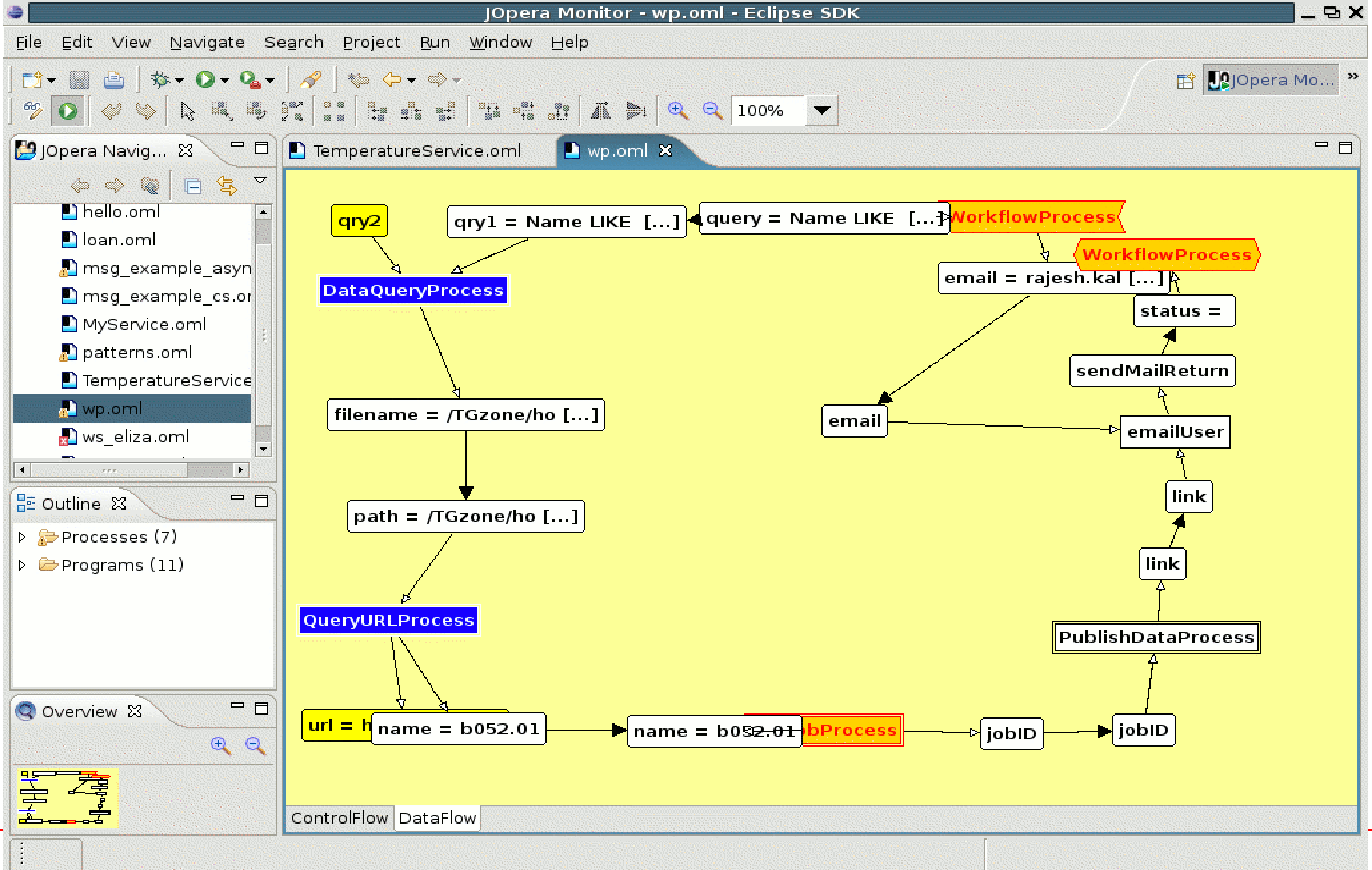
From Rajesh Kalyanam

Workflow Model



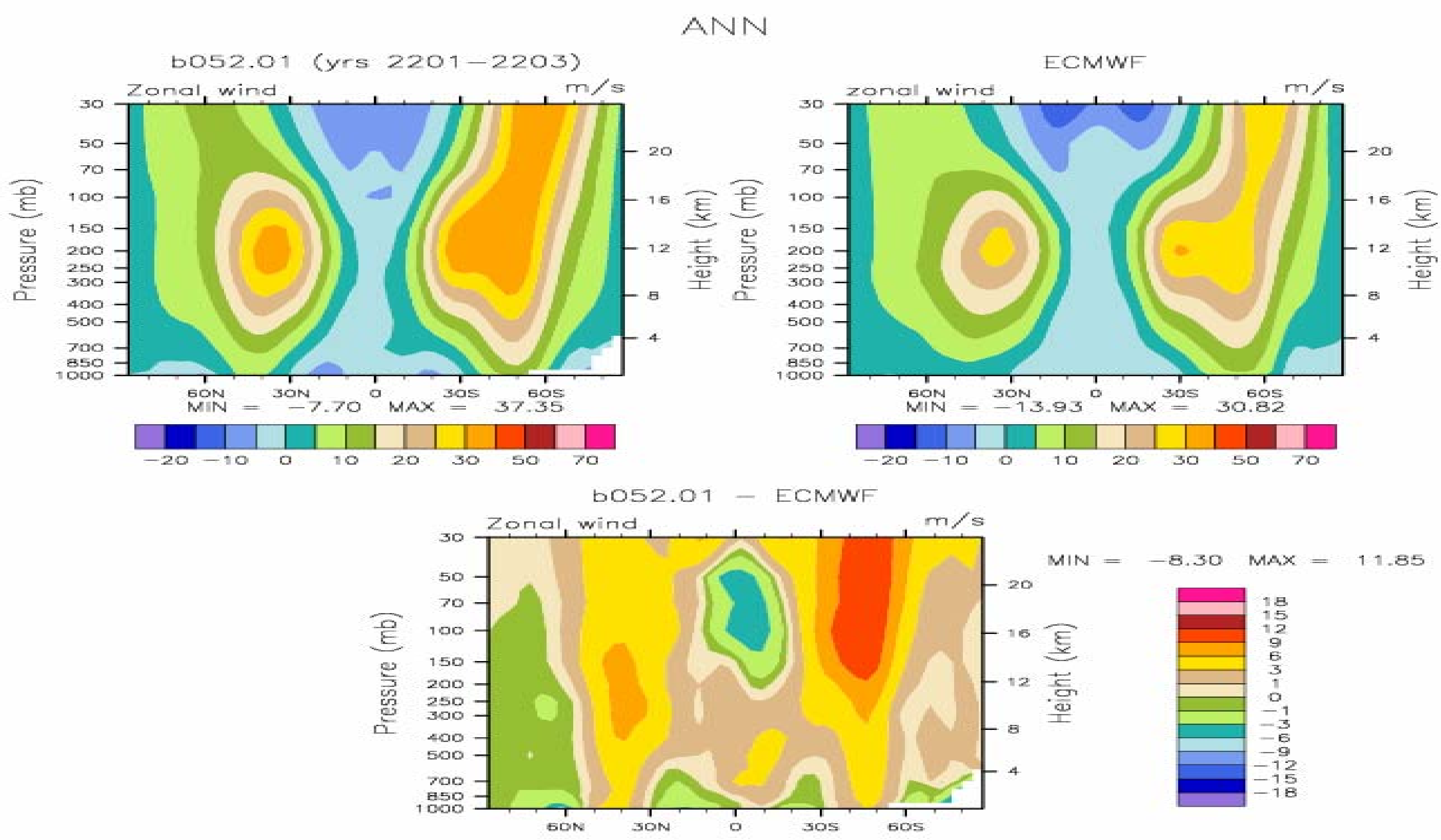
From Rajesh Kalyanam

Workflow Execution



From Rajesh Kalyanam

Workflow Results



From Rajesh Kalyanam

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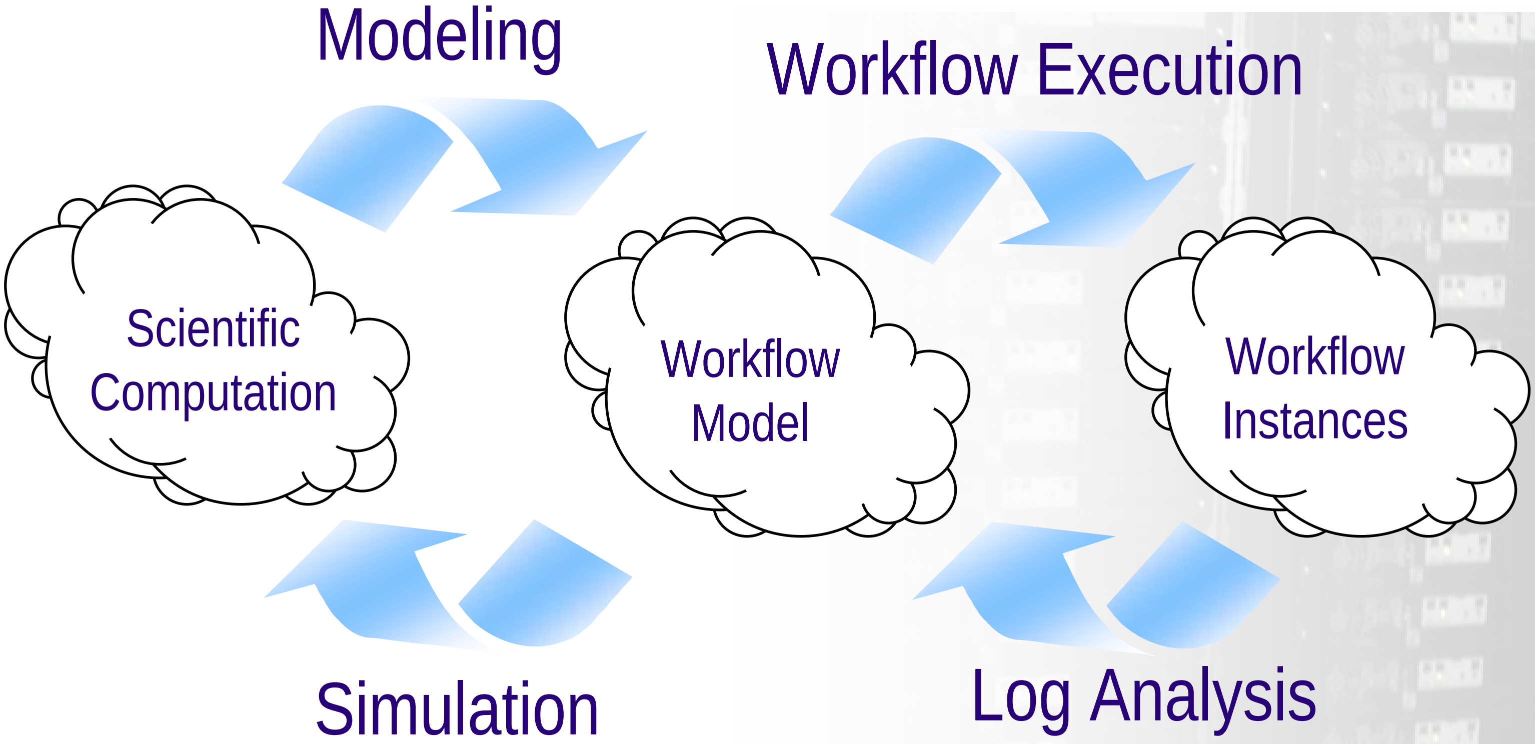
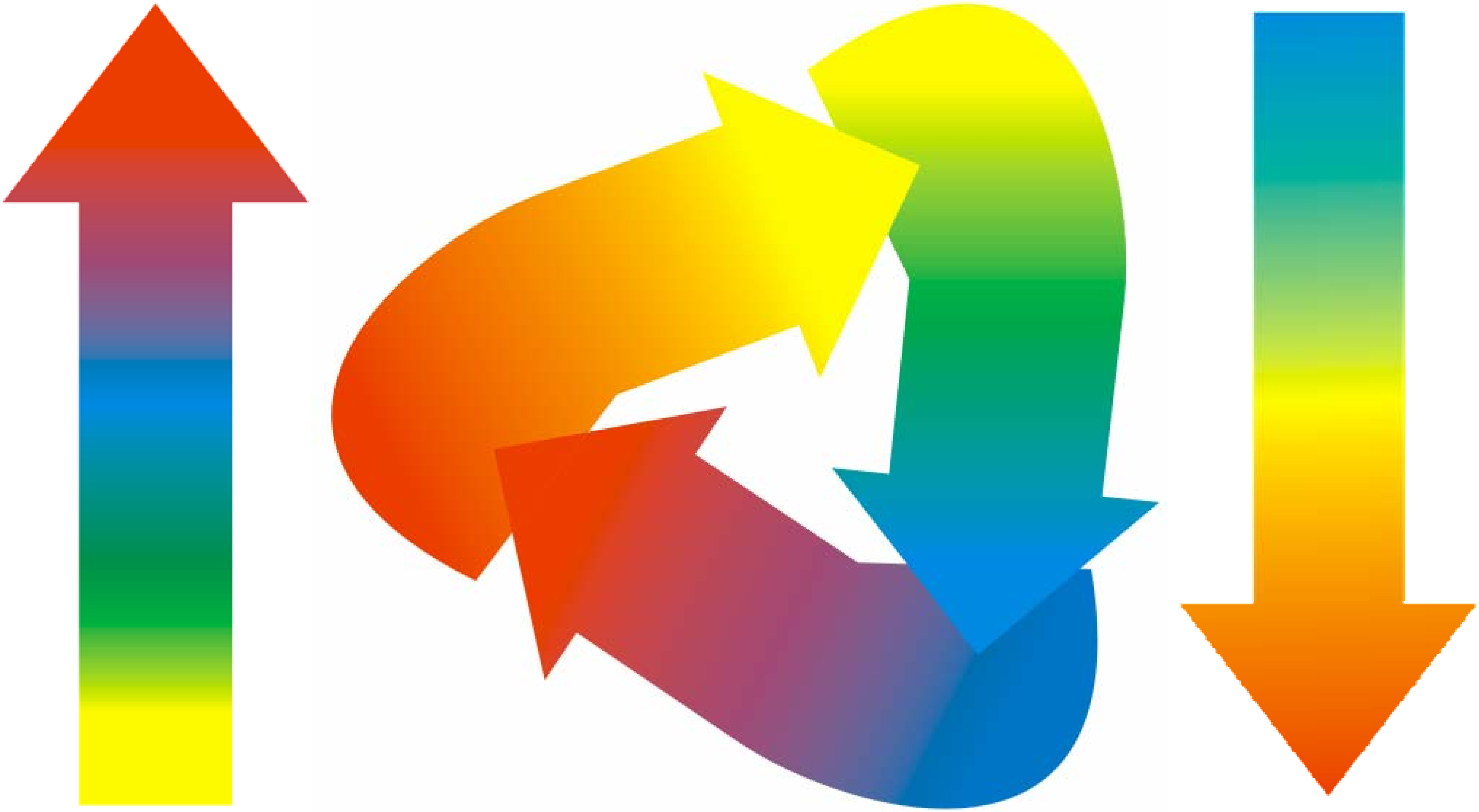
Workflow Lifecycle

Workflow Lifecycle



From Gustavo Alonso

Workflow Modeling Methodologies



Bottom up Composition

4. Share and Publish it as Web Service

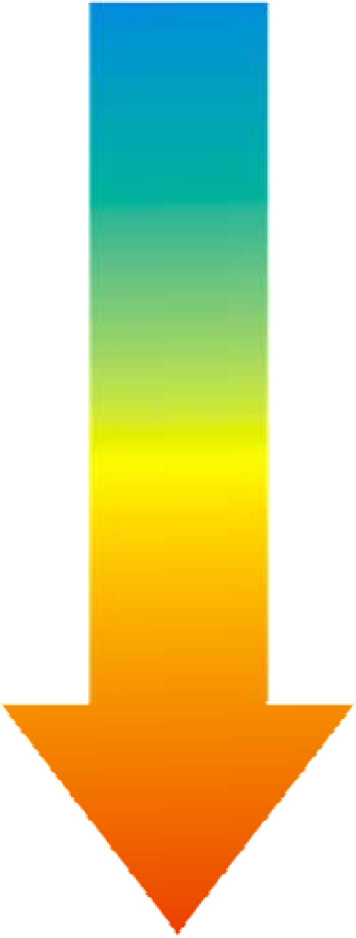
3. Run, Test, and Debug the execution **within the same modeling environment**

2. Build a workflow using a drag, drop and connect **modeling** environment

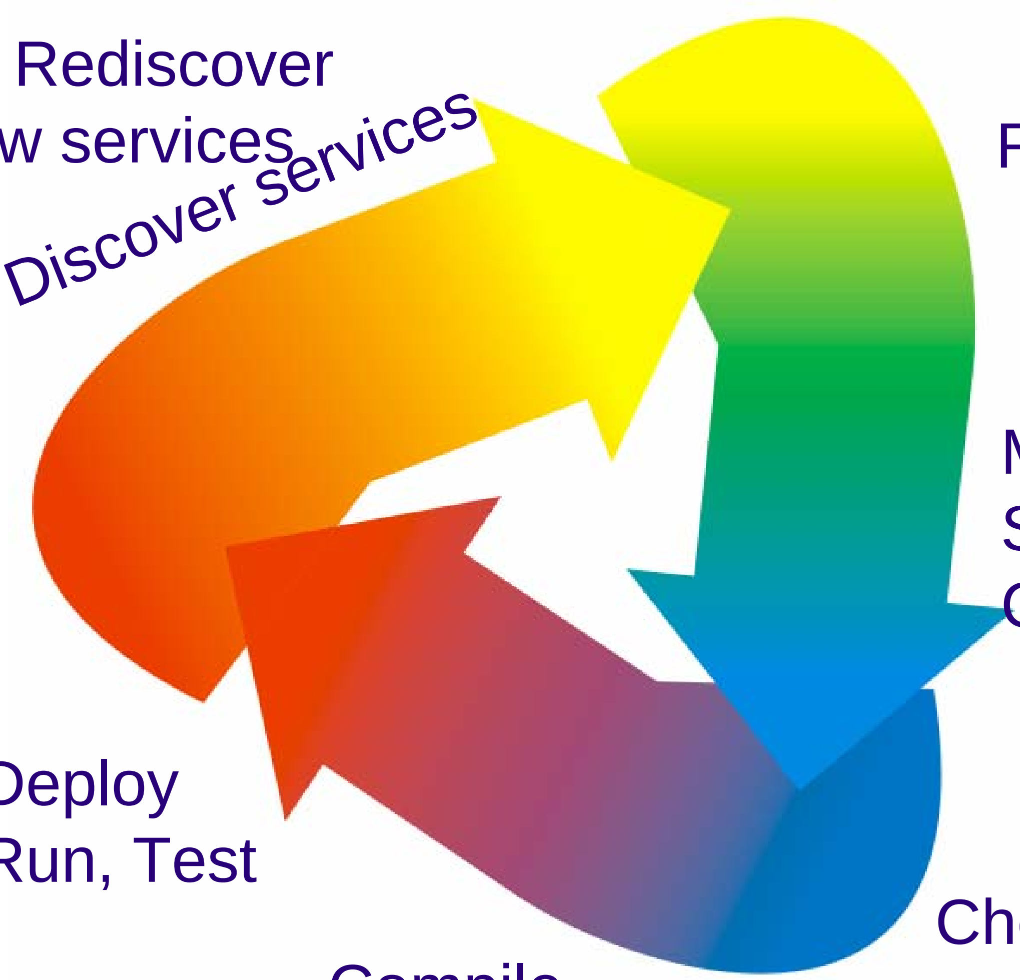
1. Select components from a **library**
   a. Lookup services in a public registry
   b. Import from external Web service (WSDL)
   c. Search the standard library

Top down Decomposition

1. Define a **goal** and Draw a *skeleton of the workflow* that satisfies it
2. Refine it and **Bind** services into it:
   - Search for existing matching services
   - Build missing services (if necessary)
   - Add required data transformations
3. Run, Test, and Debug the execution **within the same modeling environment**
4. Share and Publish it as Web Service



Iterative Composition



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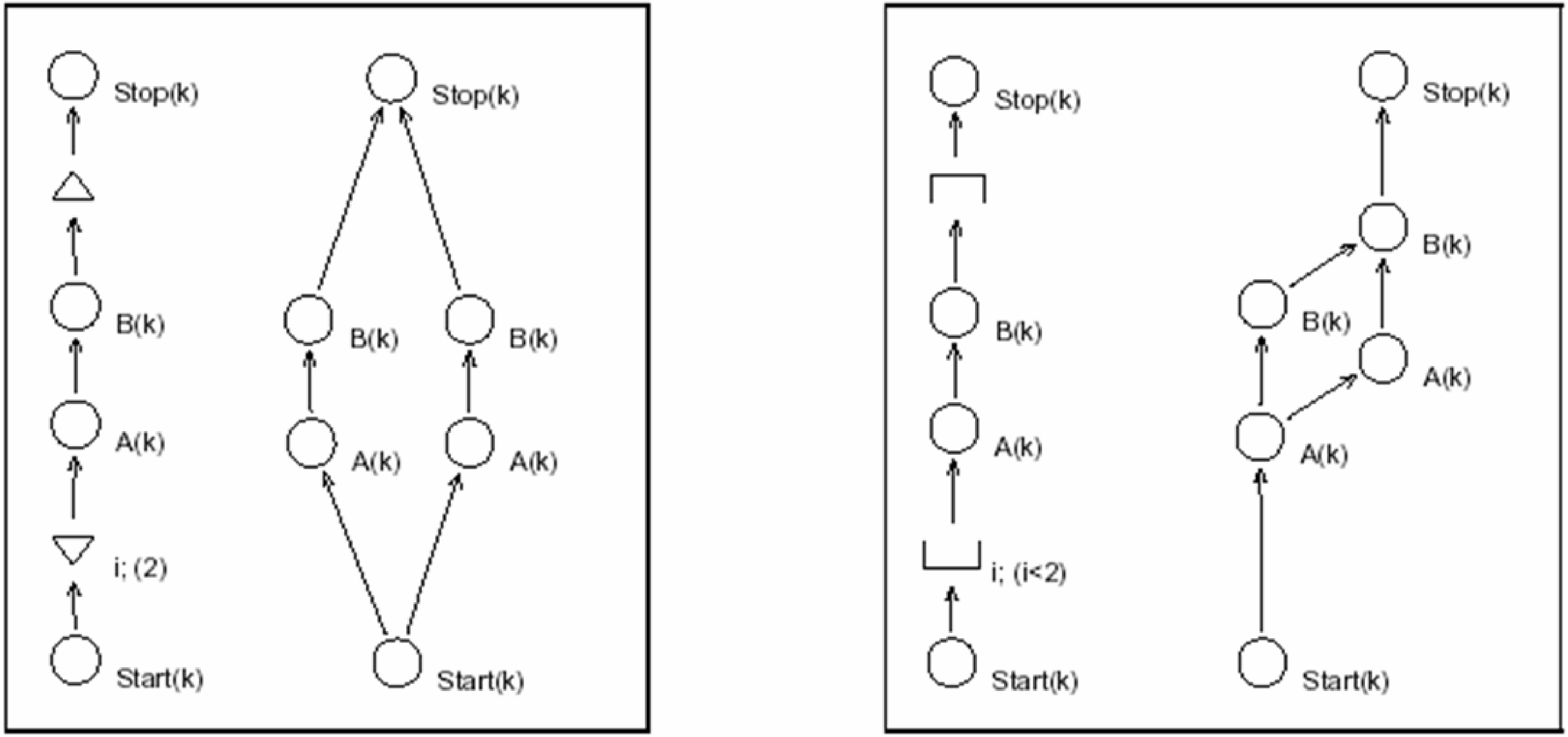
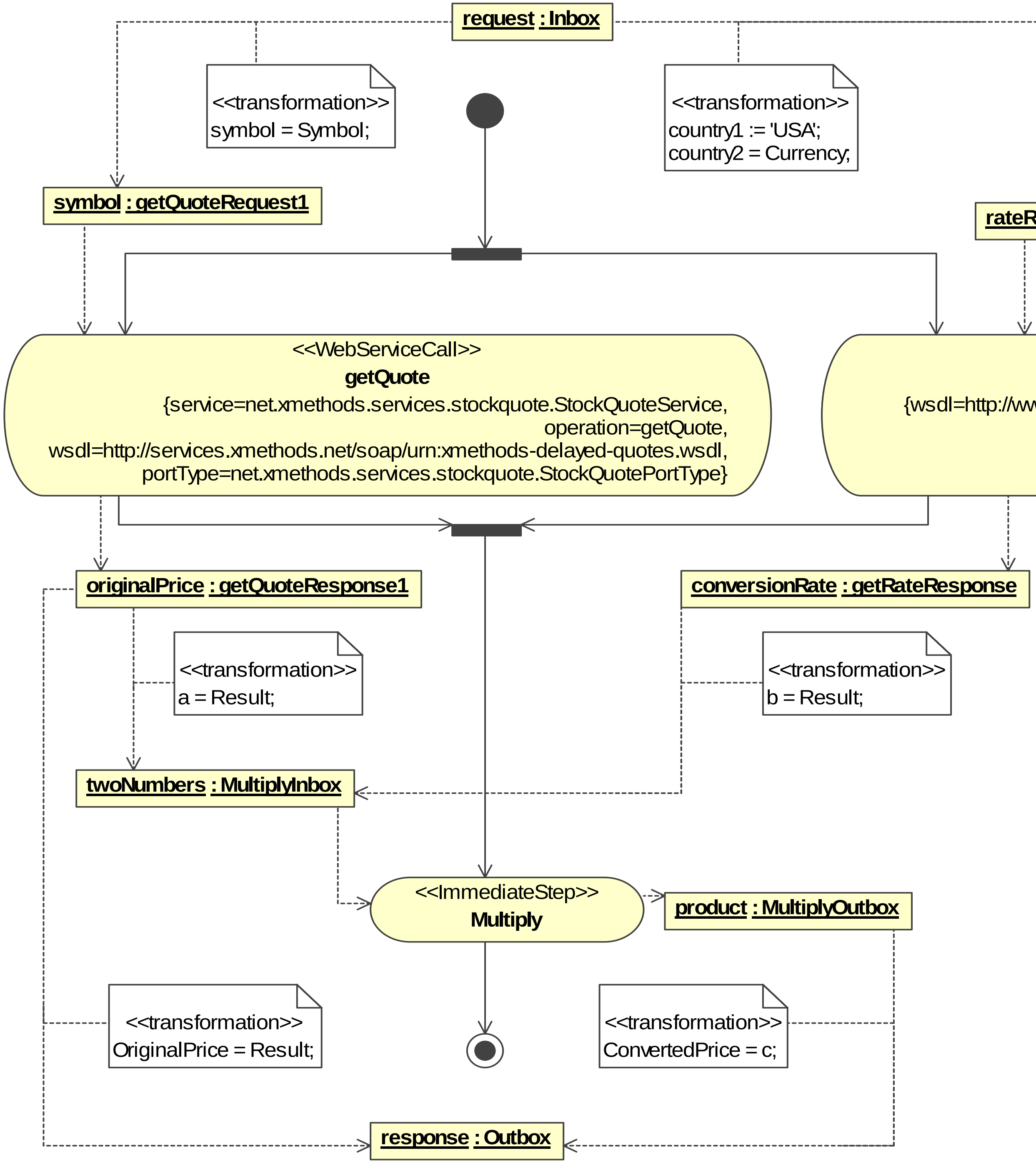
Workflow Modeling Languages and Tools Overview

HeNCE - The Ancestor of Grid Workflows?



A. Beguelin, J. J. Dongarra, G. A. Geist, R. Manchek, V. S. Sunderam, Graphical Development Tools for Network-Based Concurrent Supercomputing, in: Proc. of the 1991 ACM/IEEE conference on Supercomputing, Albuquerque, New Mexico, 1991, pp. 435–444.



request : Inbox

<<transformation>>
symbol = Symbol;

<<transformation>>
country1 := 'USA';
country2 = Currency;

symbol : getQuoteRequest1

rateRequest : getRateRequest

<<WebServiceCall>>
getQuote
{service=net.xmethods.services.stockquote.StockQuoteService,
operation=getQuote,
wsdl=http://services.xmethods.net/soap/urn:xmethods-delayed-quotes.wsdl,
portType=net.xmethods.services.stockquote.StockQuotePortType}

<<WebServiceCall>>
getRate
{wsdl=http://www.xmethods.net/sd/2001/CurrencyExchangeService.wsdl,
service=CurrencyExchangeService,
portType=CurrencyExchangePortType,
operation=getRate}

originalPrice : getQuoteResponse1

conversionRate : getRateResponse

<<transformation>>
a = Result;

<<transformation>>
b = Result;

twoNumbers : MultiplyInbox

<<ImmediateStep>>
Multiply

product : MultiplyOutbox

<<transformation>>
OriginalPrice = Result;

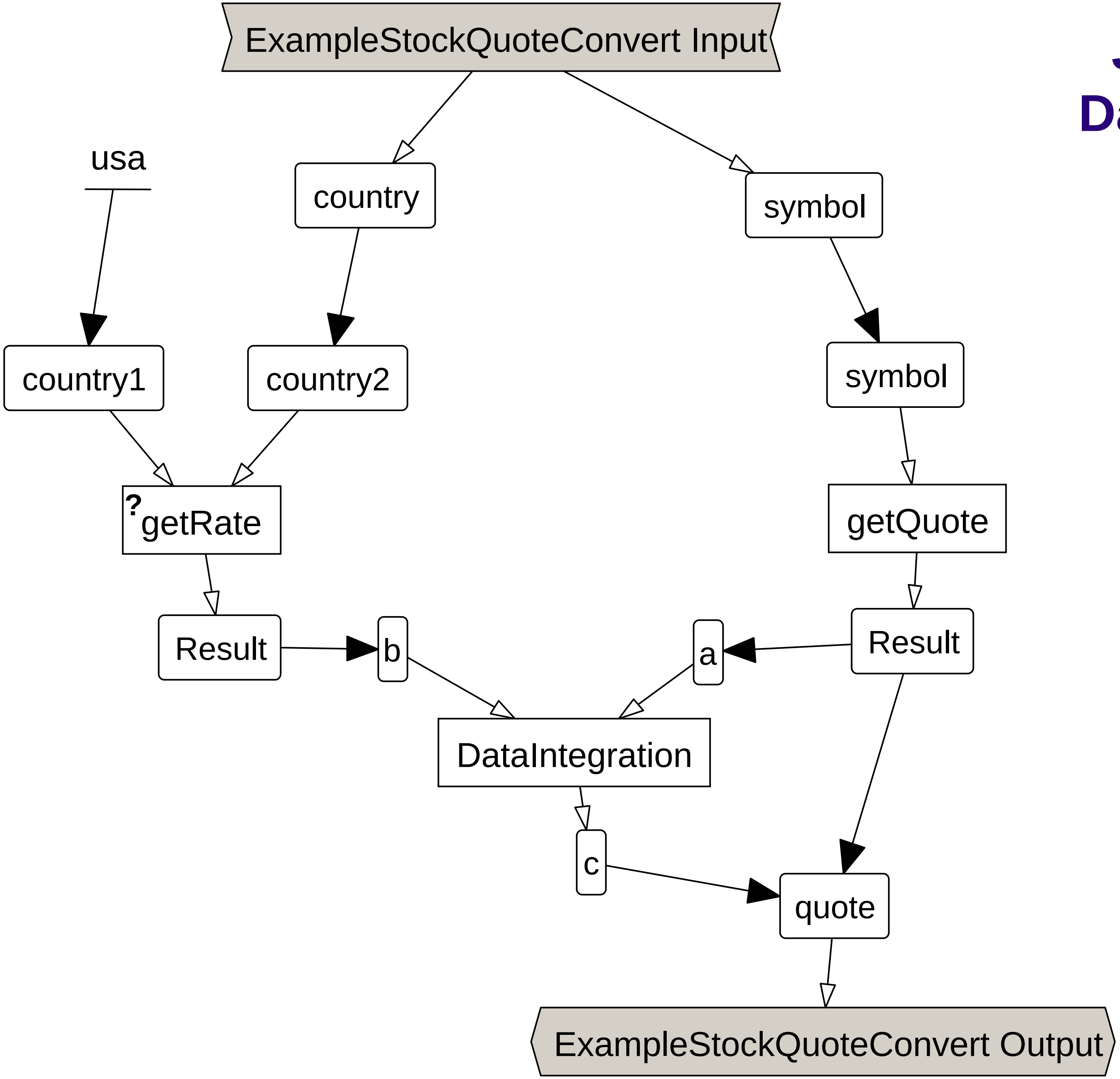
<<transformation>>
ConvertedPrice = c;

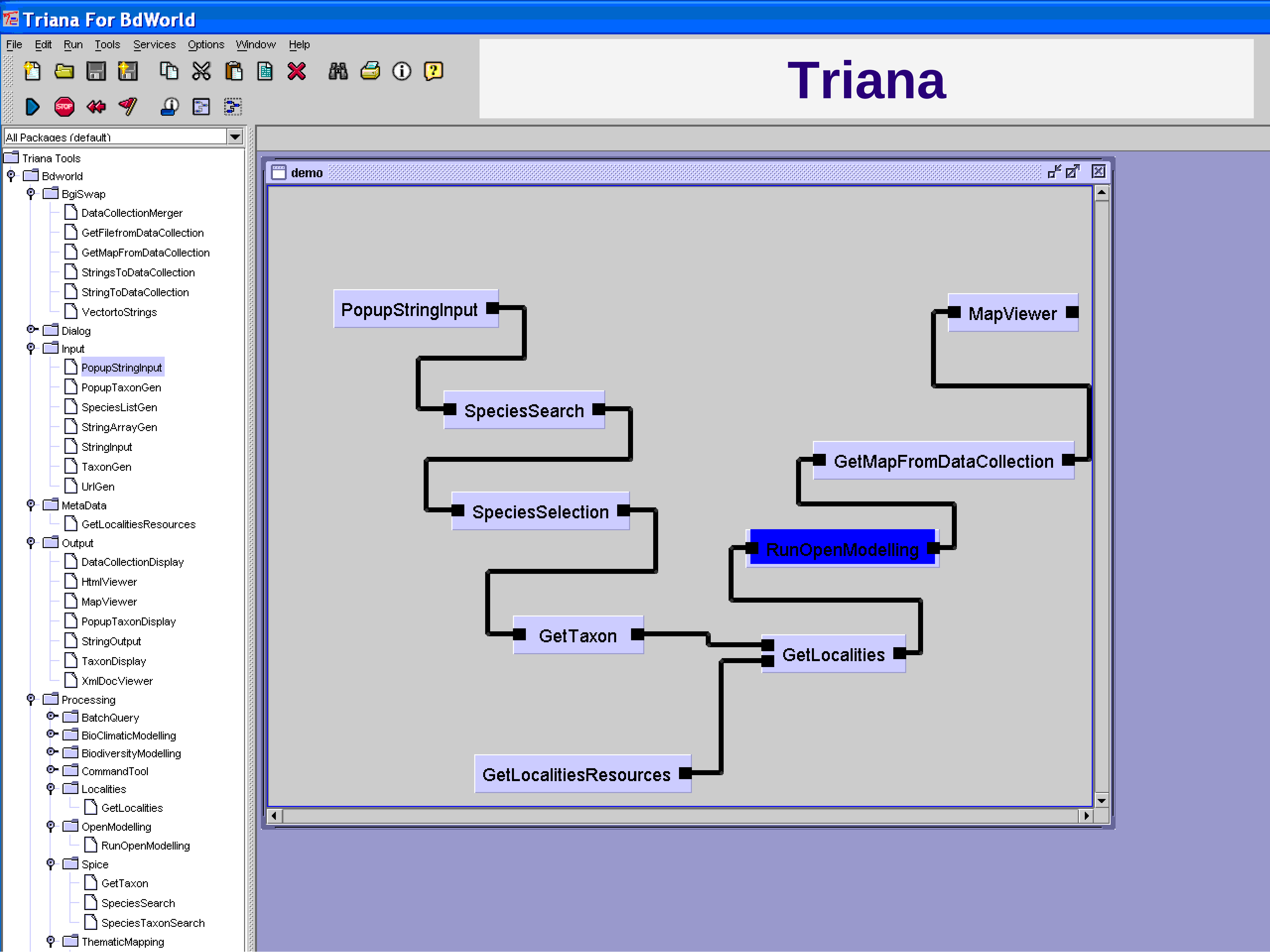
response : Outbox

Extended UML Activity Diagrams

From Roy Gronmo

JOpera Data Flow Graph




Triana For BdWorld
File
Edit
Run
Tools
Services
Options
Window
Help
Triana
All Packages (default)
Triana Tools
Bdworld
BgiSwap
DataCollectionMerger
GetFilefromDataCollection
GetMapFromDataCollection
StringsToDataCollection
StringToDataCollection
VectortoStrings
Dialog
Input
PopupStringInput
PopupTaxonGen
SpeciesListGen
StringArrayGen
StringInput
TaxonGen
UrlGen
MetaData
GetLocalitiesResources
Output
DataCollectionDisplay
HtmlViewer
MapViewer
PopupTaxonDisplay
StringOutput
TaxonDisplay
XmlDocViewer
Processing
BatchQuery
BioClimaticModelling
BiodiversityModelling
CommandTool
Localities
GetLocalities
OpenModelling
RunOpenModelling
Spice
GetTaxon
SpeciesSearch
SpeciesTaxonSearch
ThematicMapping
demo
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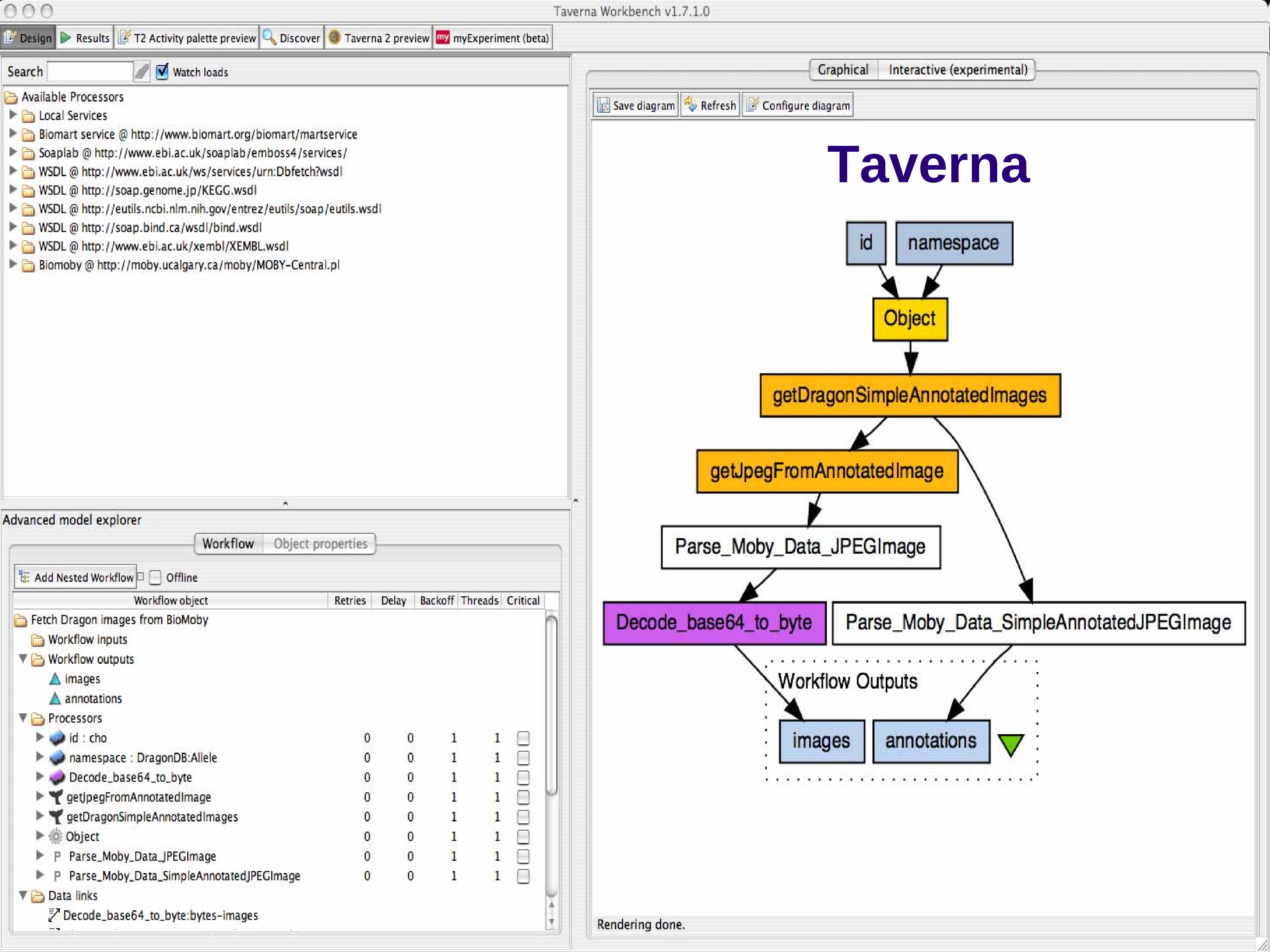
MapViewer
SpeciesSearch
GetMapFromDataCollection
SpeciesSelection
RunOpenModelling
GetTaxon
GetLocalities
GetLocalitiesResources



Taverna

Available Processors
- Local Services
- Biomart service @ http://www.biomart.org/biomart/martservice
- Soaplab @ http://www.ebi.ac.uk/soaplab/emboss4/services/
- WSDL @ http://www.ebi.ac.uk/ws/services/urn:Dbfetch?wsdl
- WSDL @ http://soap.genome.jp/KEGG.wsdl
- WSDL @ http://eutils.ncbi.nlm.nih.gov/entrez/eutils/soap/eutils.wsdl
- WSDL @ http://soap.bind.ca/wsdl/bind.wsdl
- WSDL @ http://www.ebi.ac.uk/xembl/XEMBL.wsdl
- Biomoby @ http://moby.ucalgary.ca/moby/MOBY-Central.pl

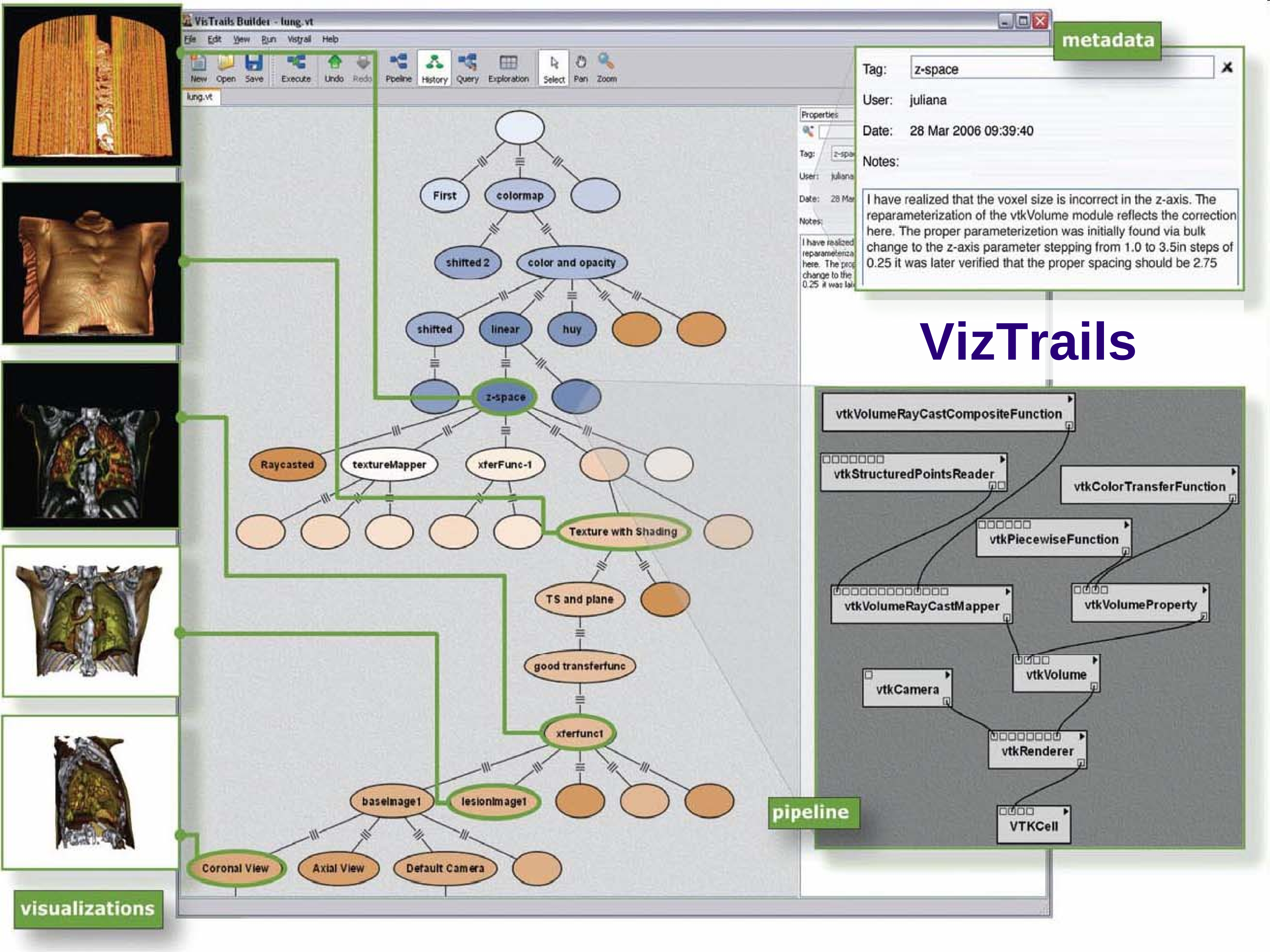
Advanced model explorer

Workflow object	Retries	Delay	Backoff	Threads	Critical
Fetch Dragon images from BioMoby					
Workflow inputs					
Workflow outputs					
images					
annotations					
Processors					
id : cho	0	0	1	1	□
namespace : DragonDB:Allele	0	0	1	1	□
Decode_base64_to_byte	0	0	1	1	□
getJpegFromAnnotatedImage	0	0	1	1	□
getDragonSimpleAnnotatedImages	0	0	1	1	□
Object	0	0	1	1	□
P Parse_Moby_Data_JPEGImage	0	0	1	1	□
P Parse_Moby_Data_SimpleAnnotatedJPEGImage	0	0	1	1	□
Data links					
Decode_base64_to_byte:bytes-images					

id
namespace
Object
getDragonSimpleAnnotatedImages
getJpegFromAnnotatedImage
Parse_Moby_Data_JPEGImage
Decode_base64_to_byte
Parse_Moby_Data_SimpleAnnotatedJPEGImage
Workflow Outputs
images
annotations

Rendering done.

VizTrails



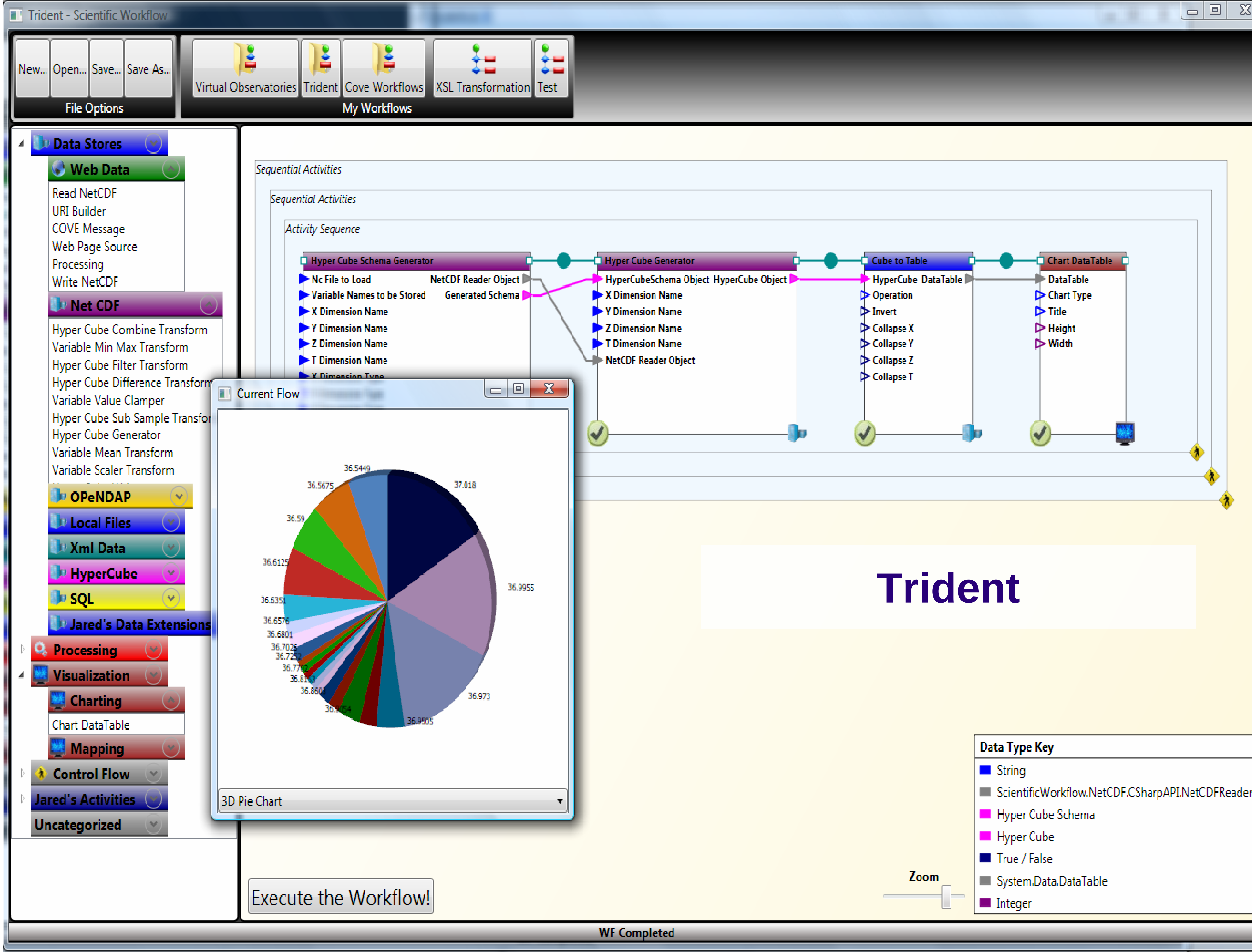
Tag: z-space

User: juliana

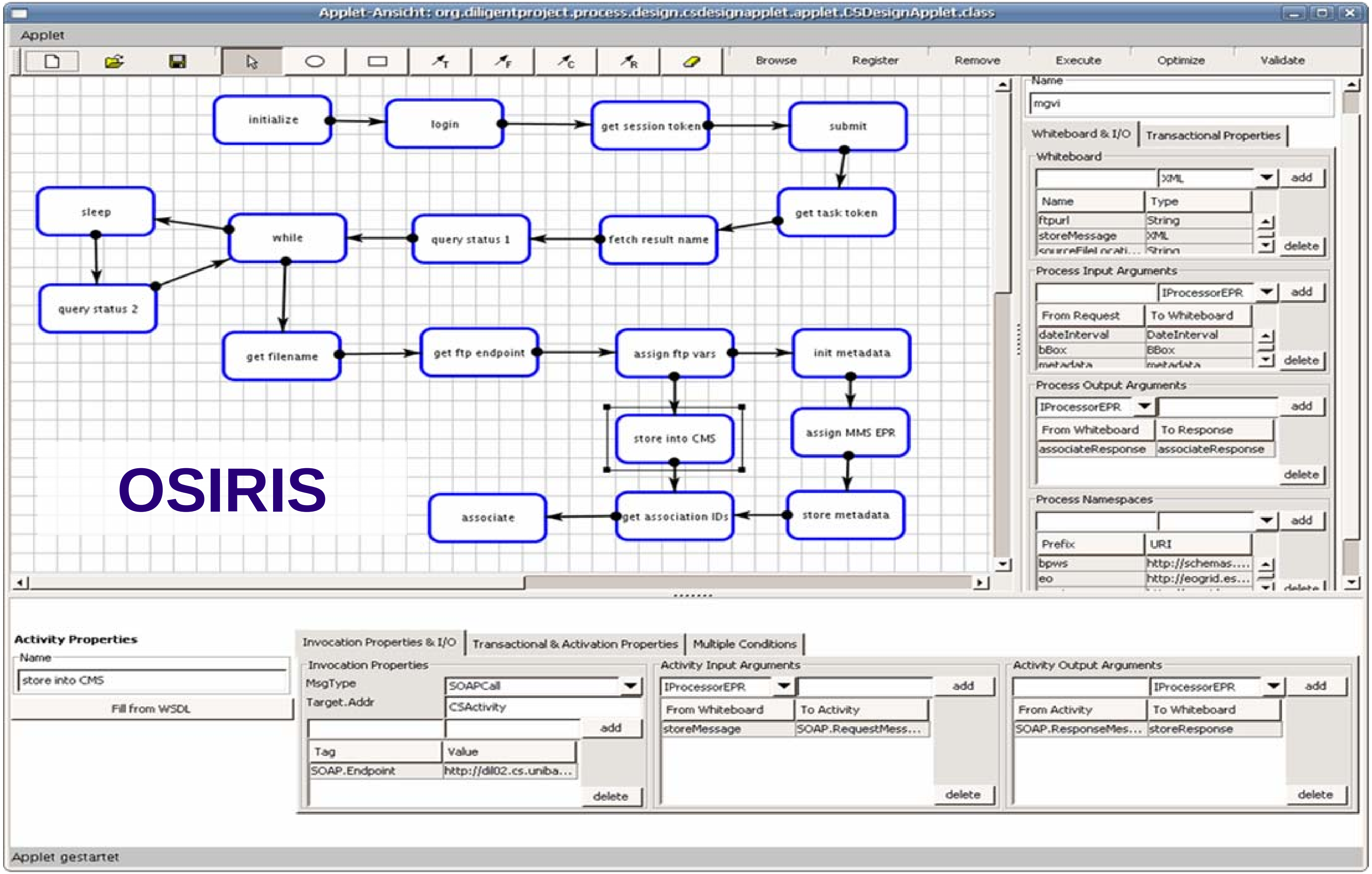
Date: 28 Mar 2006 09:39:40

Notes:

I have realized that the voxel size is incorrect in the z-axis. The reparameterization of the vtkVolume module reflects the correction here. The proper parameterizetion was initially found via bulk change to the z-axis parameter stepping from 1.0 to 3.5in steps of 0.25 it was later verified that the proper spacing should be 2.75


Trident - Scientific Workflow
New...
Open...
Save...
Save As...
File Options
Virtual Observatories
Trident
Cove Workflows
XSL Transformation
Test
My Workflows
Data Stores
Web Data
Read NetCDF
URI Builder
COVE Message
Web Page Source
Processing
Write NetCDF
Net CDF
Hyper Cube Combine Transform
Variable Min Max Transform
Hyper Cube Filter Transform
Hyper Cube Difference Transform
Variable Value Clamper
Hyper Cube Sub Sample Transfor
Hyper Cube Generator
Variable Mean Transform
Variable Scaler Transform
OPeNDAP
Local Files
Xml Data
HyperCube
SQL
Jared's Data Extensions
Processing
Visualization
Charting
Chart DataTable
Mapping
Control Flow
Jared's Activities
Uncategorized
Sequential Activities
Sequential Activities
Activity Sequence
Hyper Cube Schema Generator
Nc File to Load
Variable Names to be Stored
X Dimension Name
Y Dimension Name
Z Dimension Name
T Dimension Name
X Dimension Type
NetCDF Reader Object
Generated Schema
Hyper Cube Generator
HyperCubeSchema Object
HyperCube Object
X Dimension Name
Y Dimension Name
Z Dimension Name
T Dimension Name
NetCDF Reader Object
Cube to Table
HyperCube
DataTable
Operation
Invert
Collapse X
Collapse Y
Collapse Z
Collapse T
Chart DataTable
DataTable
Chart Type
Title
Height
Width
Current Flow
36.5449
37.018
36.5675
36.59
36.6125
36.9955
36.6351
36.6576
36.6801
36.7026
36.7252
36.7702
36.81
36.860
36.9054
36.9505
36.973
3D Pie Chart
Trident
Data Type Key
🟦 String
■ ScientificWorkflow.NetCDF.CSharpAPI.NetCDFReader
🟪 Hyper Cube Schema
🟪 Hyper Cube
■ True / False
■ System.Data.DataTable
■ Integer
Zoom
Execute the Workflow!
WF Completed

OSIRIS



Name: mgvi

Whiteboard: XML

Name	Type
ftpurl	String
storeMessage	XML
sourceFileLocati...	String

Process Input Arguments: IProcessorEPR

From Request	To Whiteboard
dateInterval	DateInterval
bBox	BBox
metadata	metadata

Process Output Arguments: IProcessorEPR

From Whiteboard	To Response
associateResponse	associateResponse

Process Namespaces

Prefix	URI
bpws	http://schemas....
eo	http://eogrid.es...

Activity Properties

Name: store into CMS

Invocation Properties

MsgType: SOAPCall

Target.Addr: CSActivity

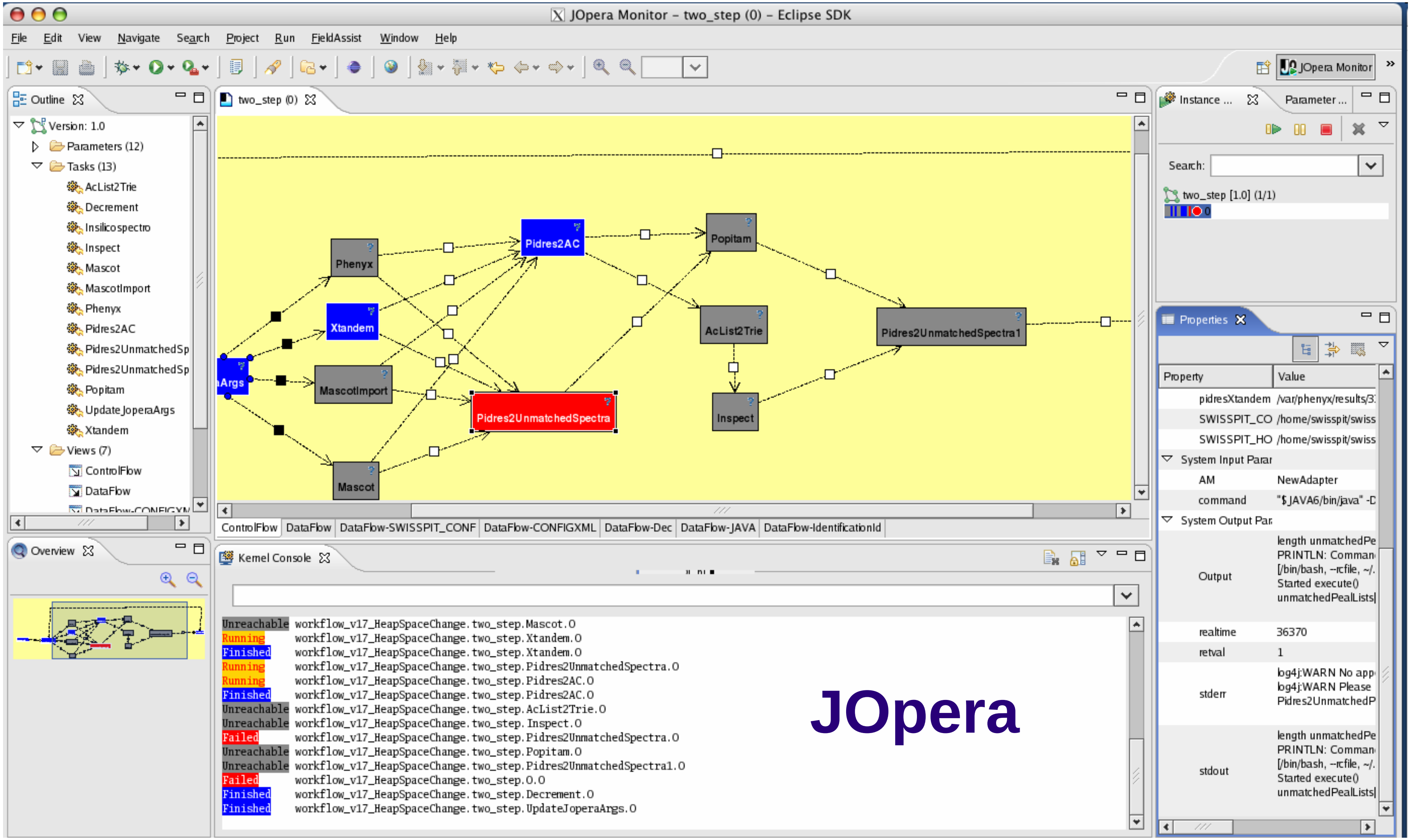
Tag	Value
SOAP.Endpoint	http://dil02.cs.uniba...

Activity Input Arguments: IProcessorEPR

From Whiteboard	To Activity
storeMessage	SOAP.RequestMess...

Activity Output Arguments: IProcessorEPR

From Activity	To Whiteboard
SOAP.ResponseMes...	storeResponse



```
Unreachable workflow_v17_HeapSpaceChange.two_step.Mascot.0
Running     workflow_v17_HeapSpaceChange.two_step.Xtandem.0
Finished    workflow_v17_HeapSpaceChange.two_step.Xtandem.0
Running     workflow_v17_HeapSpaceChange.two_step.Pidres2UnmatchedSpectra.0
Running     workflow_v17_HeapSpaceChange.two_step.Pidres2AC.0
Finished    workflow_v17_HeapSpaceChange.two_step.Pidres2AC.0
Unreachable workflow_v17_HeapSpaceChange.two_step.AcList2Trie.0
Unreachable workflow_v17_HeapSpaceChange.two_step.Inspect.0
Failed      workflow_v17_HeapSpaceChange.two_step.Pidres2UnmatchedSpectra.0
Unreachable workflow_v17_HeapSpaceChange.two_step.Popitam.0
Unreachable workflow_v17_HeapSpaceChange.two_step.Pidres2UnmatchedSpectra1.0
Failed      workflow_v17_HeapSpaceChange.two_step.0.0
Finished    workflow_v17_HeapSpaceChange.two_step.Decrement.0
Finished    workflow_v17_HeapSpaceChange.two_step.UpdateJoperaArgs.0
```

Property	Value
pidresXtandem	/var/phenyx/results/3:
SWISSPIT_CO	/home/swisspit/swiss
SWISSPIT_HO	/home/swisspit/swiss
System Input Parar	
AM	NewAdapter
command	"$JAVA6/bin/java" -D
System Output Par	
Output	length unmatchedPe PRINTLN: Comman [/bin/bash, --rcfile, ~/. Started execute() unmatchedPealLists|
realtime	36370
retval	1
stderr	log4j:WARN No app log4j:WARN Please Pidres2UnmatchedP
stdout	length unmatchedPe PRINTLN: Comman [/bin/bash, --rcfile, ~/. Started execute() unmatchedPealLists|

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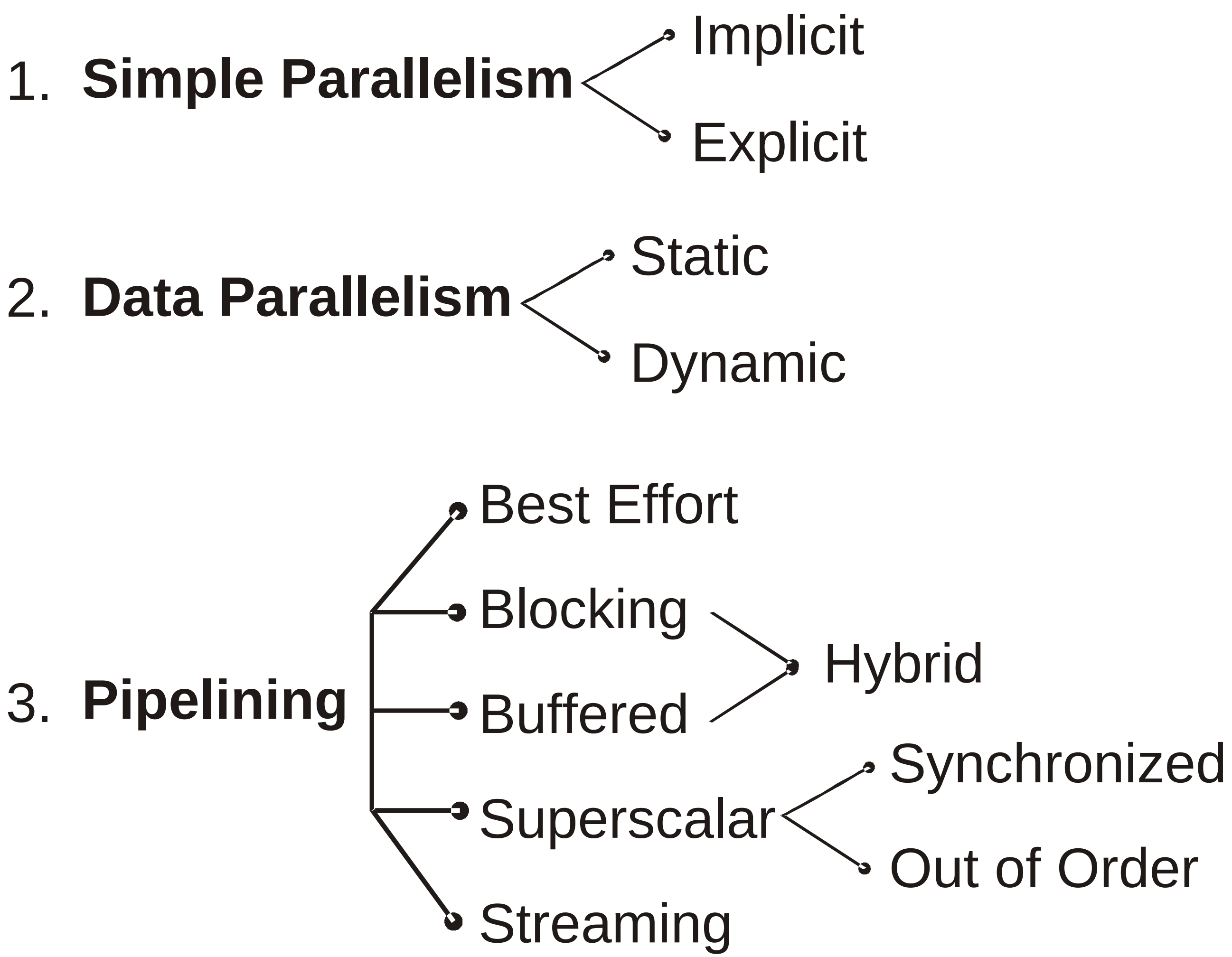
Grid Workflow Language Patterns

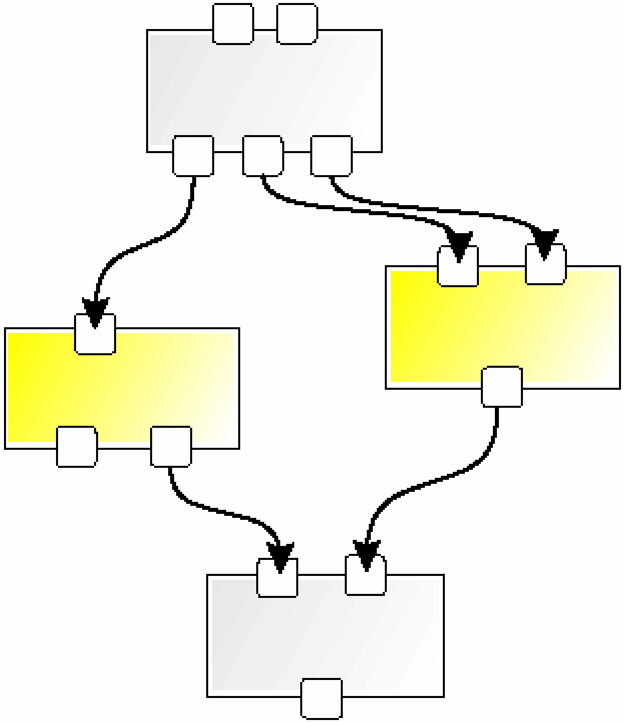
Workflow Pattern **Variants**



1. **Simple Parallelism**
   - Implicit
   - Explicit
2. **Data Parallelism**
   - Static
   - Dynamic
3. **Pipelining**
   - Best Effort
   - Blocking
   - Buffered
   - Hybrid
   - Superscalar
     - Synchronized
     - Out of Order
   - Streaming

Modeling Simple Parallelism

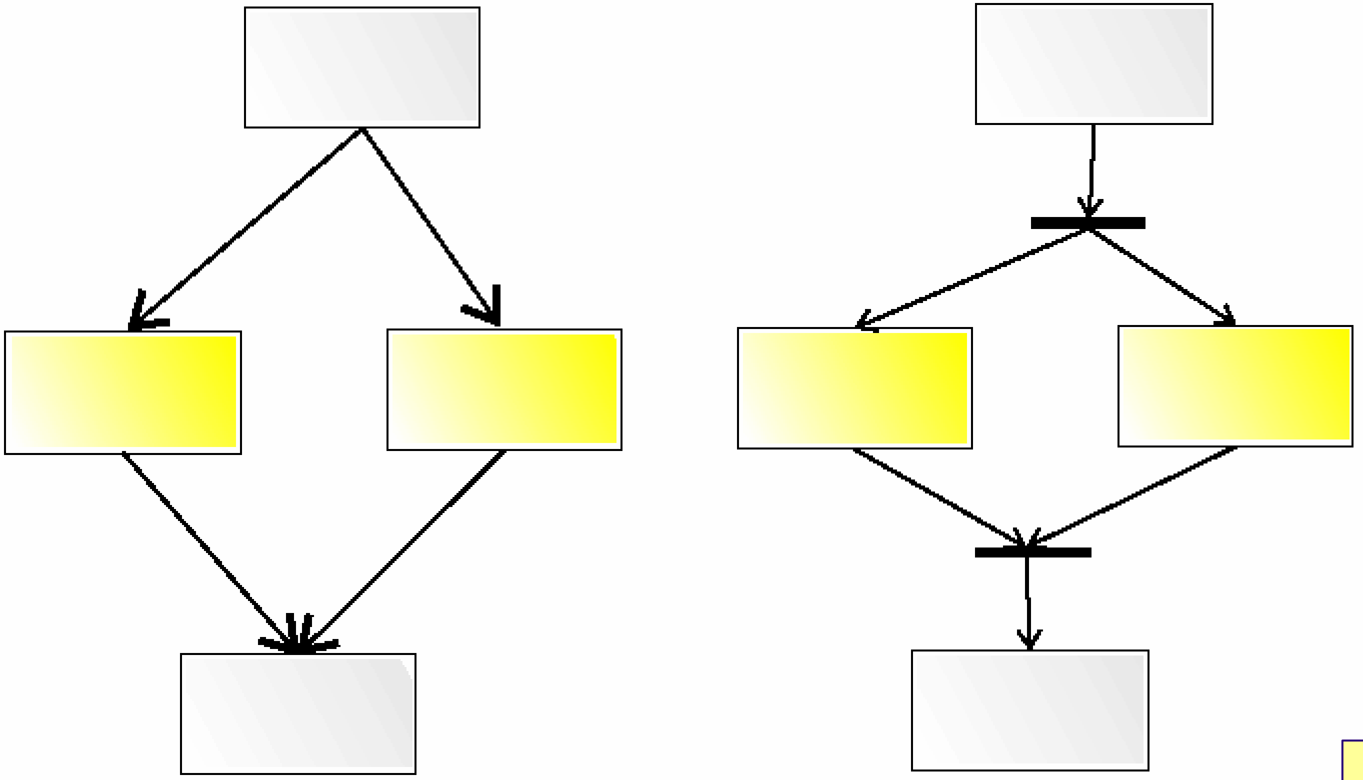
Data Flow, Graph Based



SCIRun
Kepler
Triana

Modeling Simple Parallelism

Control Flow, Graph Based

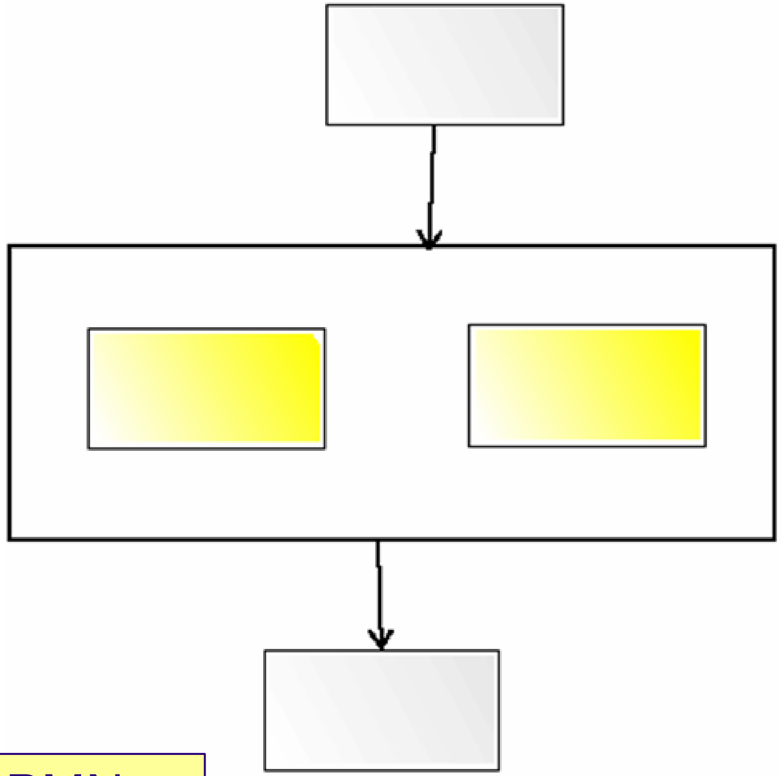


JOpera
GEL

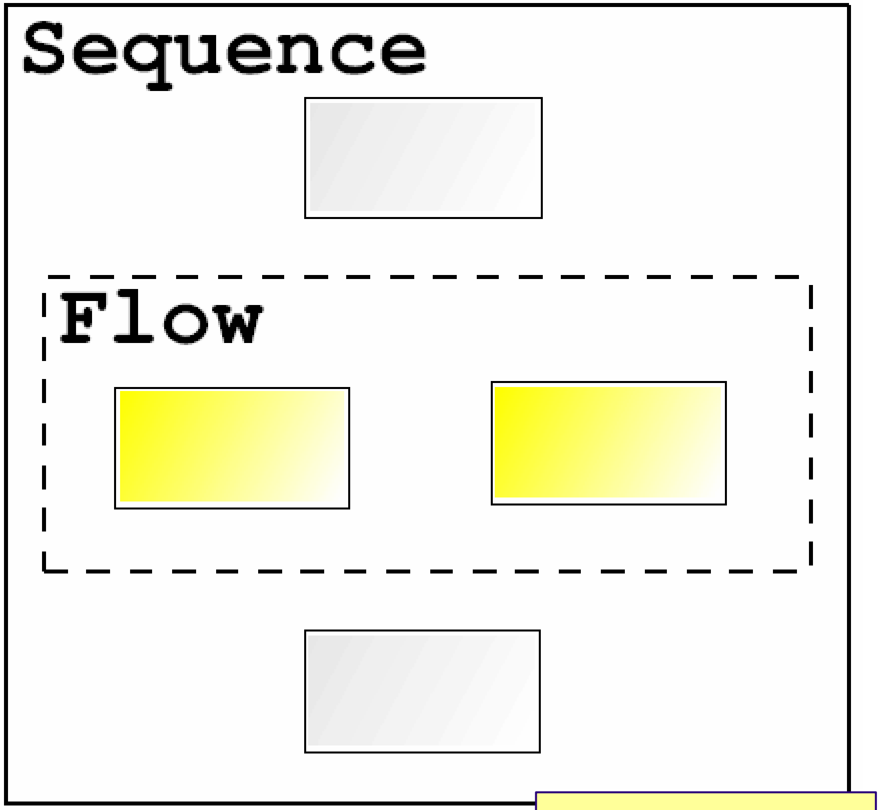
UML

Modeling Simple Parallelism

Control Flow, Block Based



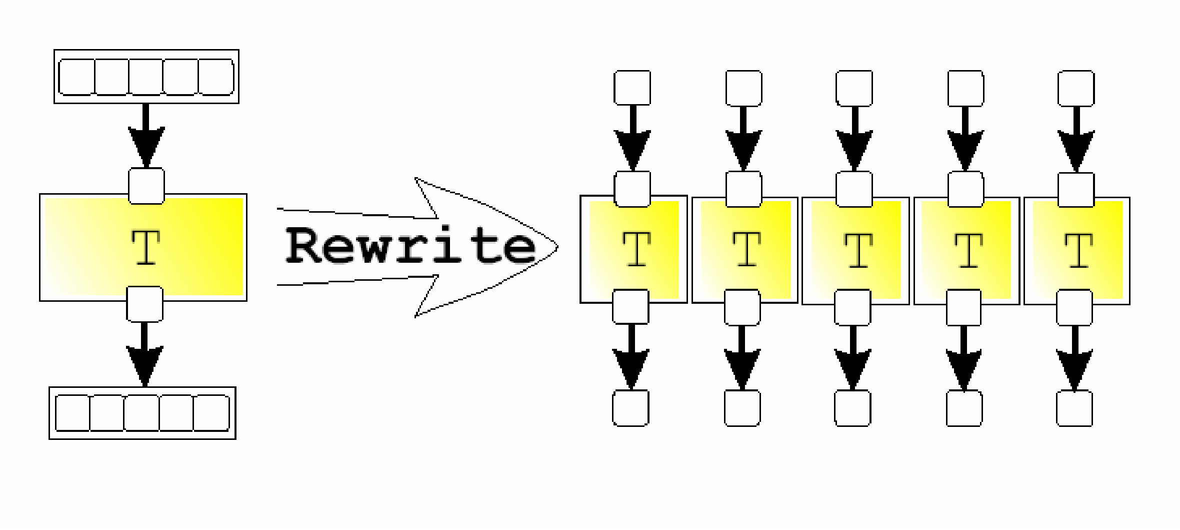
BPMN

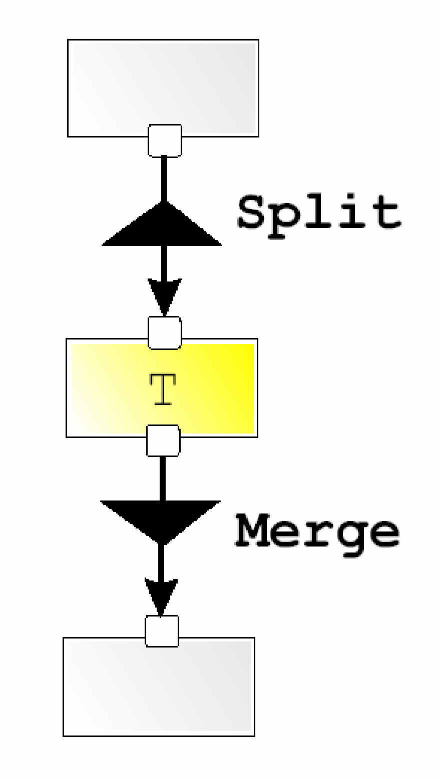


WS-BPEL

Modeling Data Parallelism

Data Flow, Graph Rewriting





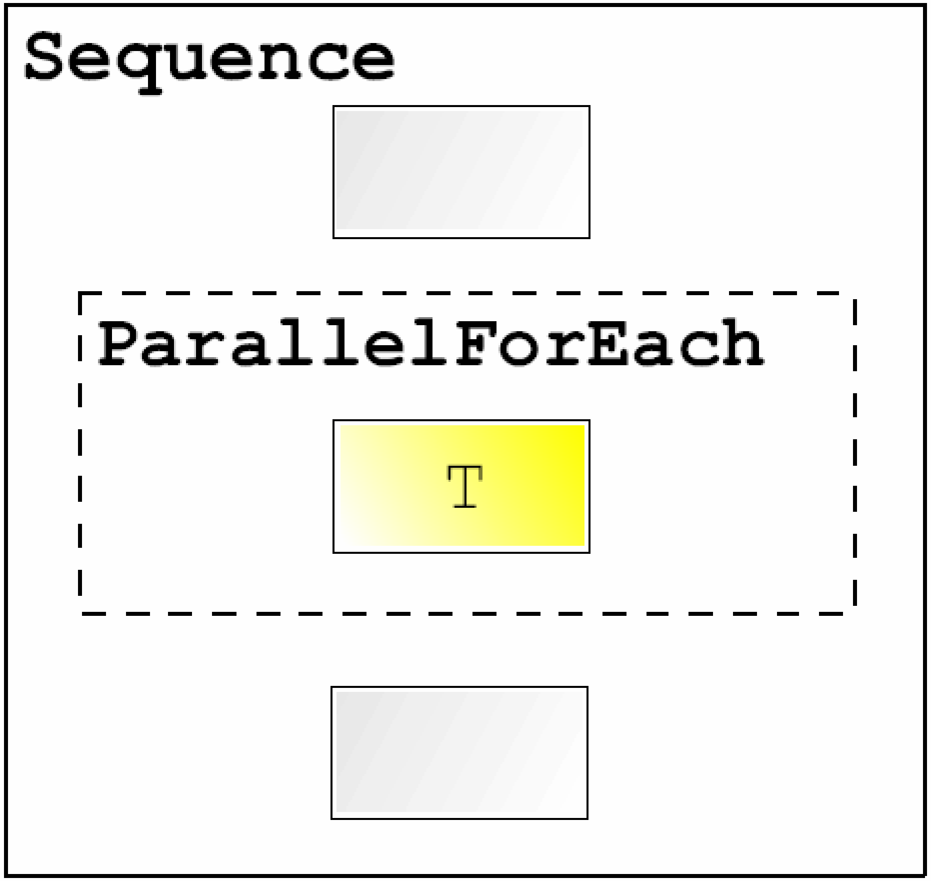
Static or Dynamic

Triana

Taverna
JOpera

Modeling Data Parallelism

Control Flow, Block Based, Dynamic



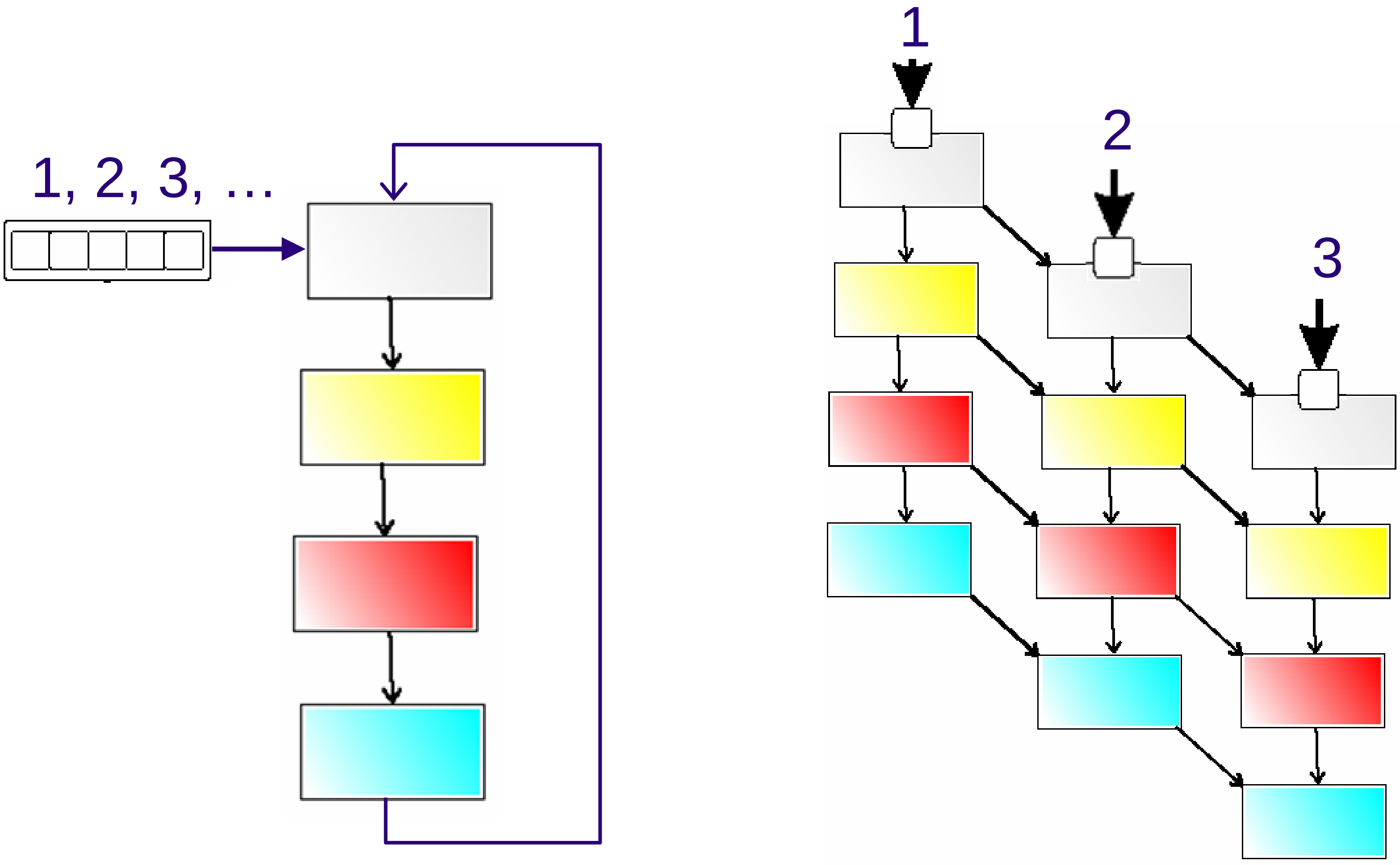
WS-BPEL

AGWL

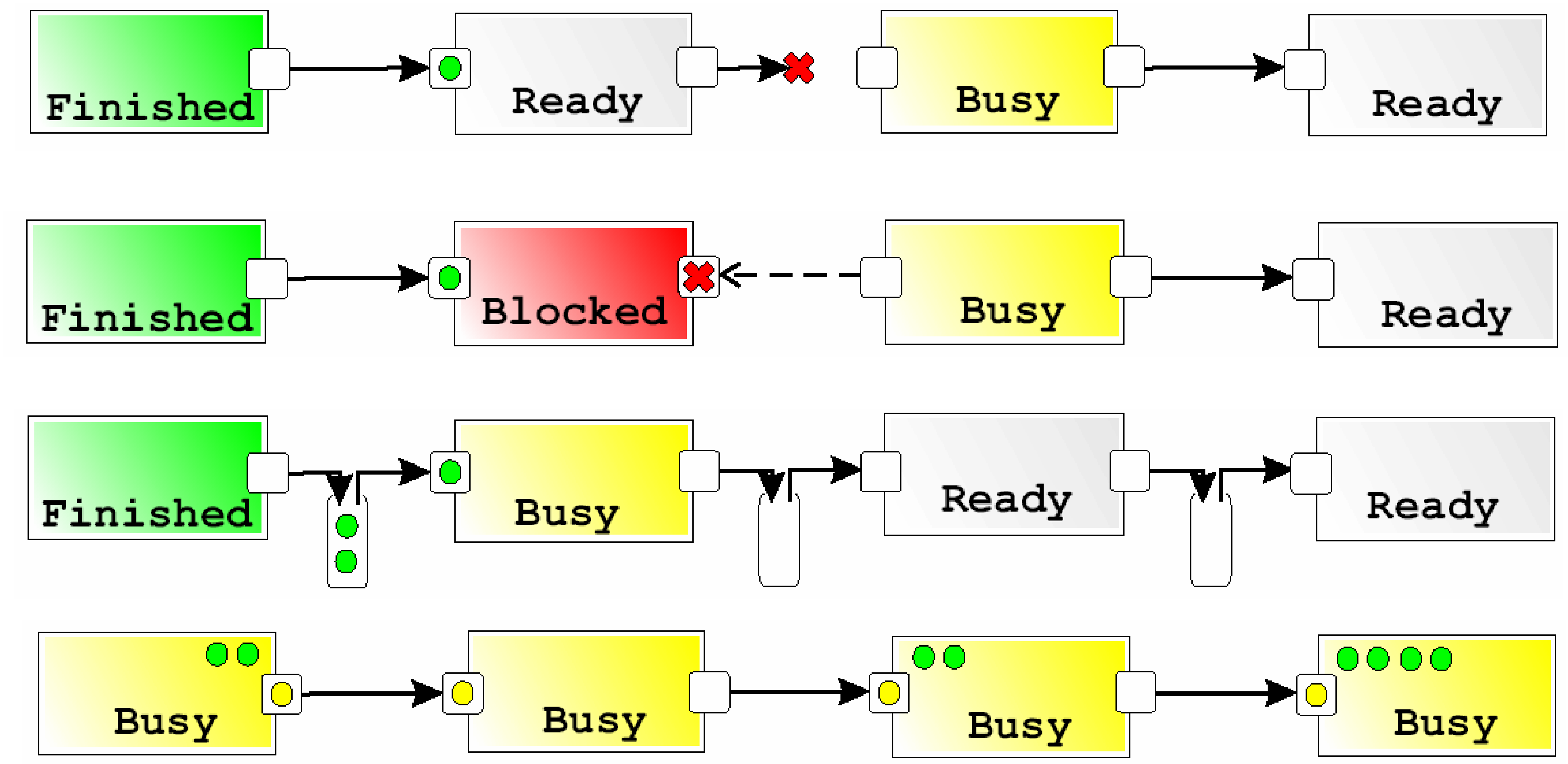
Karajan

GEL

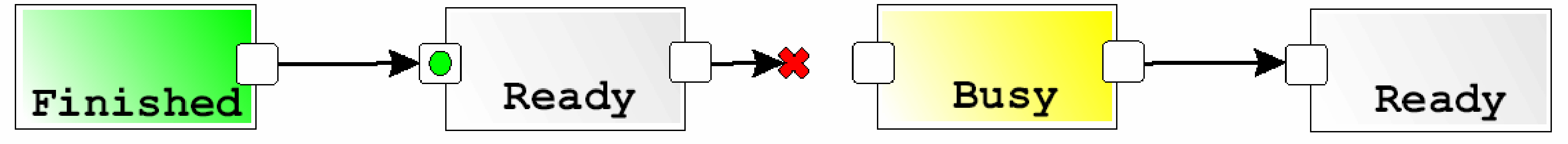
Modeling Pipelined Execution



Pipelining Semantics



Best Effort Pipelined Execution



Drop data elements on pipeline collisions

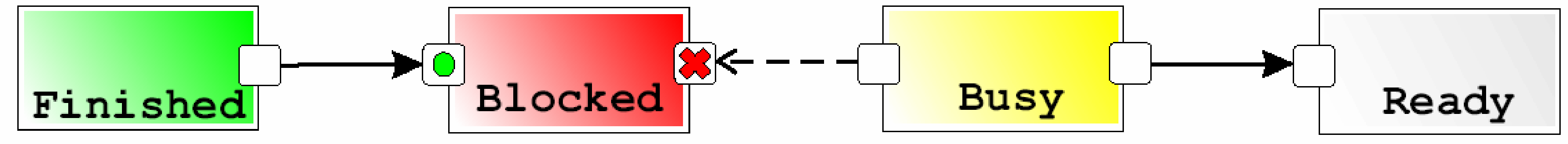
Advantages:

- Simplified implementation
- Some applications may tolerate data loss

Problem:

- Downsampling is non deterministic

Blocking Pipelined Execution



Tasks are blocked if successors are busy

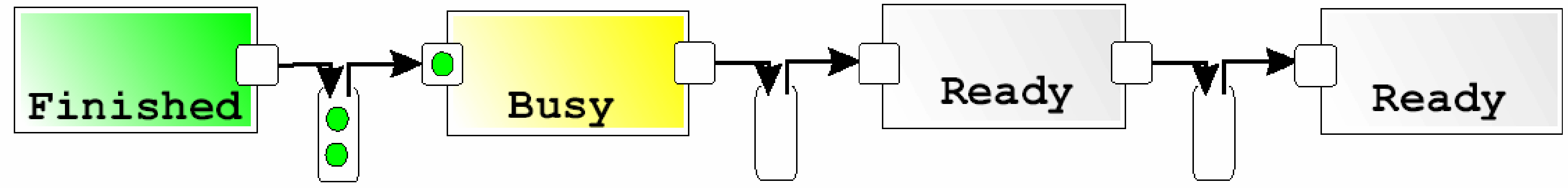
Advantages:

- Avoid data loss in the pipeline

Problem:

- Pipeline speed limited by slowest task
- Data may be lost before it enters the pipeline

Buffered Pipelined Execution



Tasks are decoupled by buffers

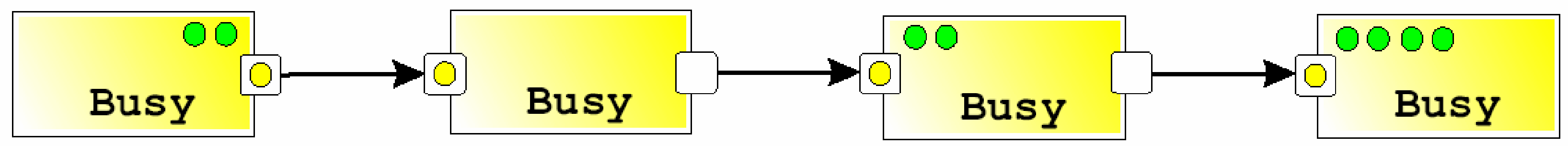
Advantages:

- Collisions are prevented
- Best applied to tasks having variable speed

Problem:

- Buffer capacity is limited
(Blocking still needed – Hybrid semantics)

Streaming Pipelined Execution



Tasks exchange data while running

Advantages:

- Suitable for a distributed (P2P) engine

Problems:

- Shifts complexity from the workflow engine to the tasks
- Tasks exchange data while running
- Workflow/Task interface more complex

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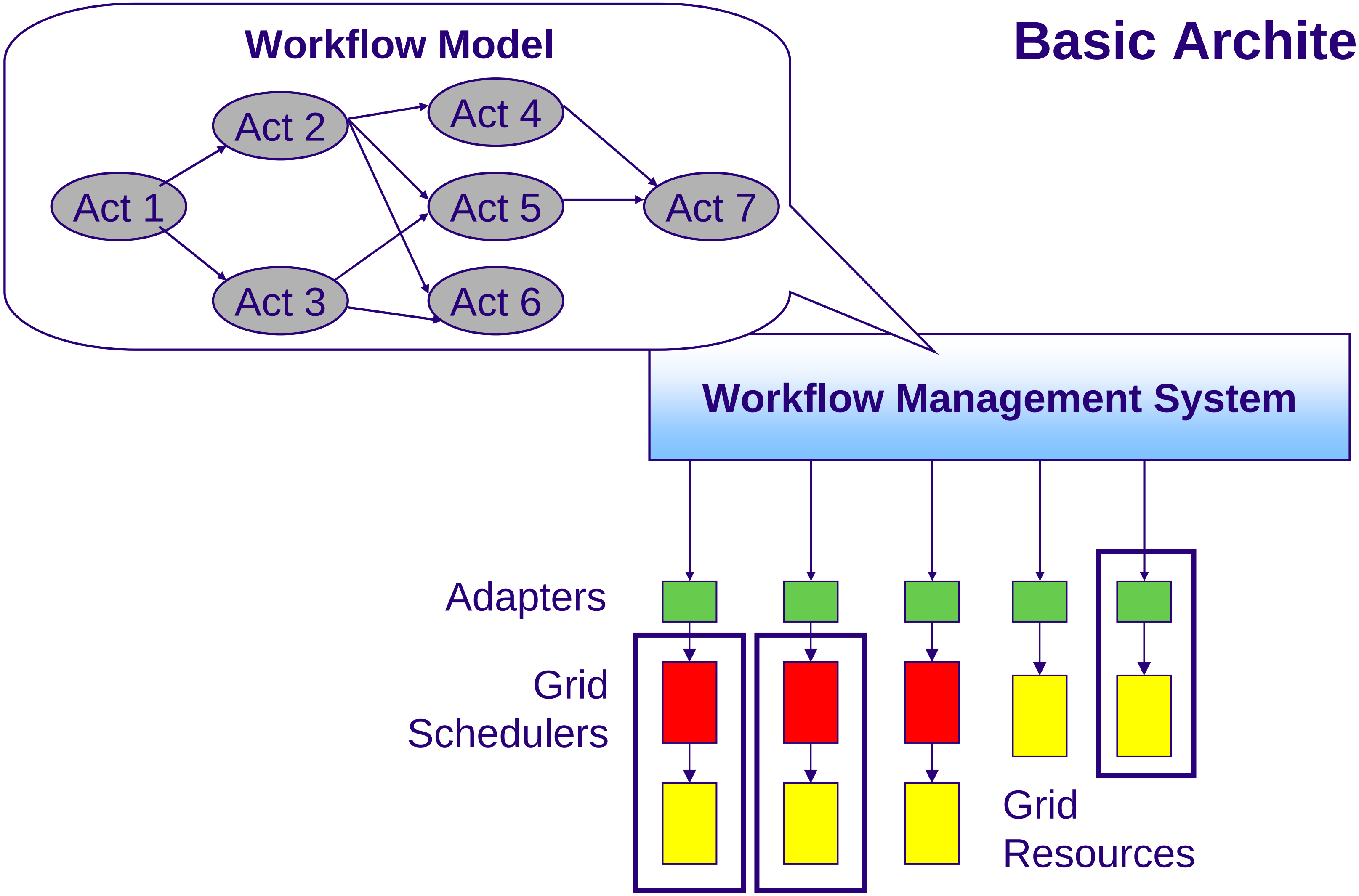
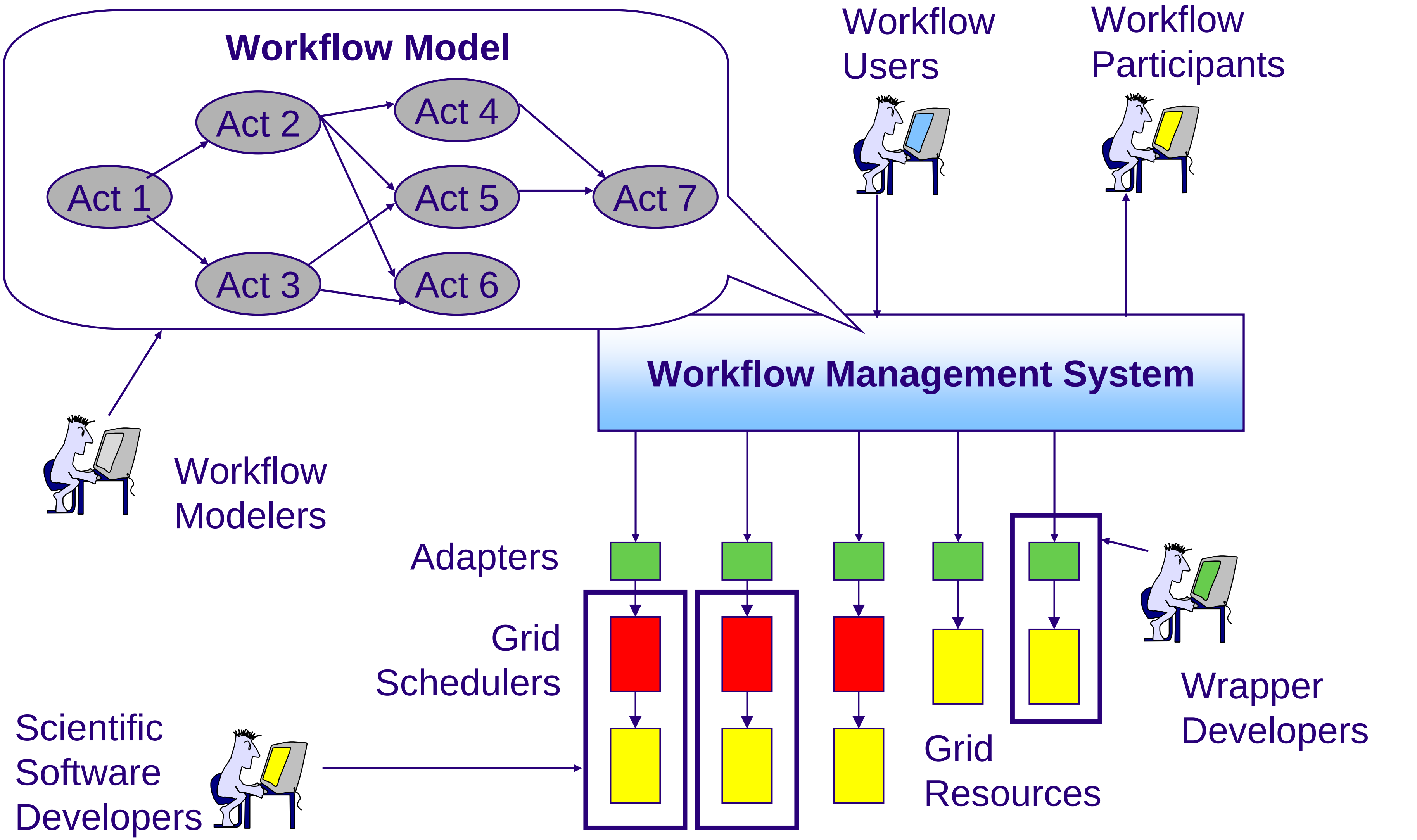
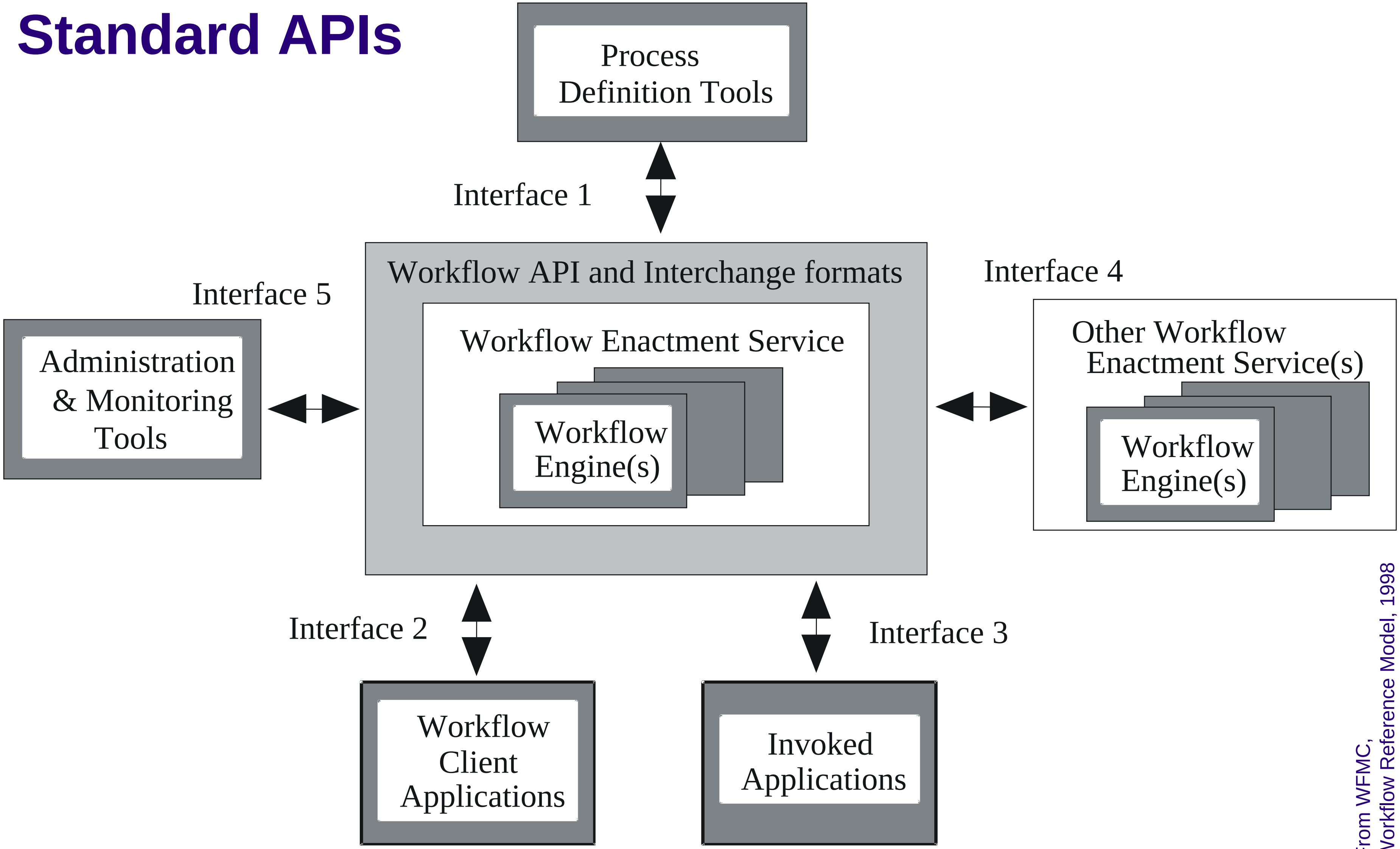
Running Workflows on the Grid

Basic Architecture



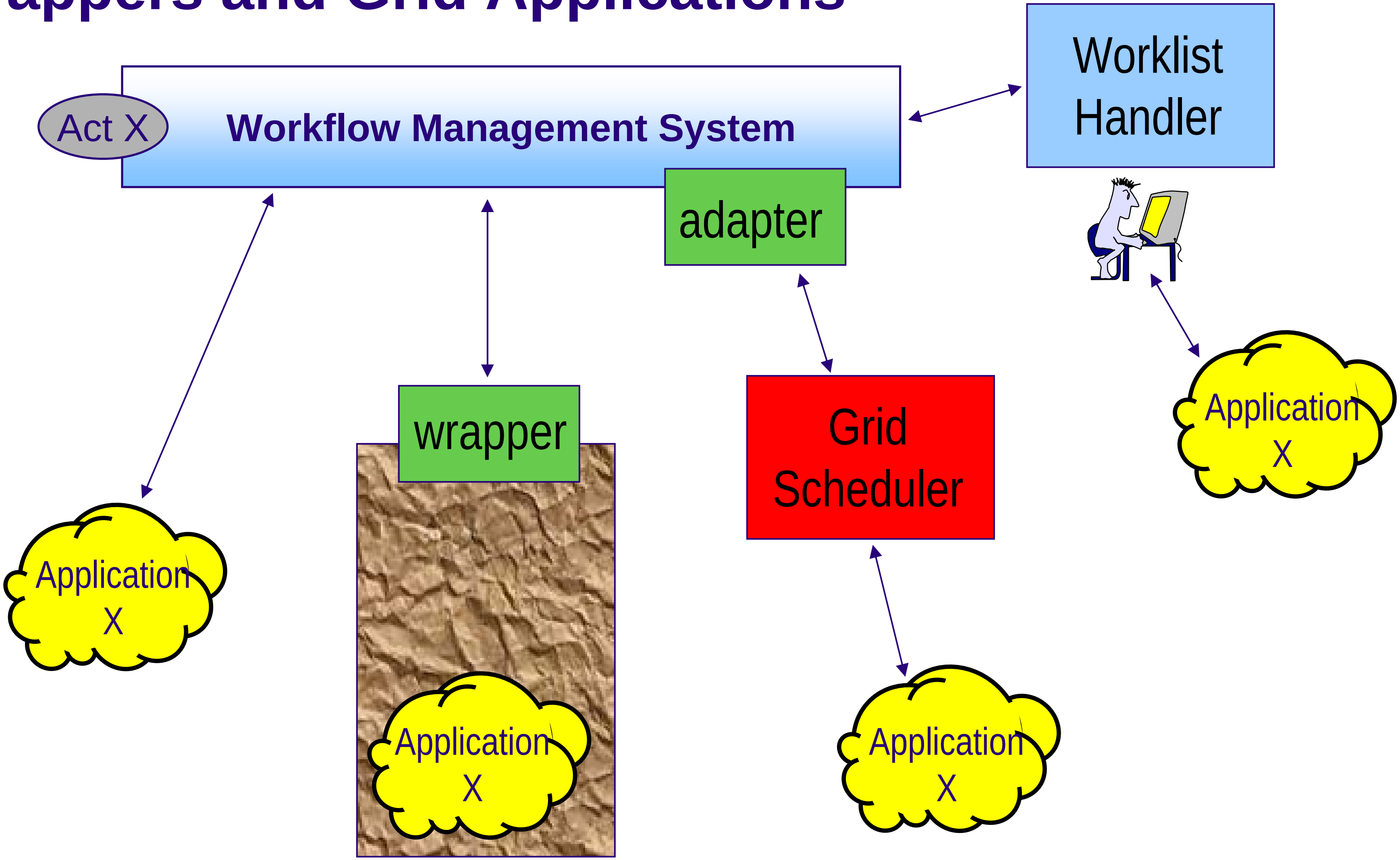

Workflow Model
Act 1
Act 2
Act 3
Act 4
Act 5
Act 6
Act 7
Workflow Users
Workflow Participants
Workflow Management System
Workflow Modelers
Adapters
Grid Schedulers
Grid Resources
Wrapper Developers
Scientific Software Developers

Standard APIs


Process Definition Tools
Interface 1
Workflow API and Interchange formats
Workflow Enactment Service
Workflow Engine(s)
Interface 5
Administration & Monitoring Tools
Interface 4
Other Workflow Enactment Service(s)
Workflow Engine(s)
Interface 2
Interface 3
Workflow Client Applications
Invoked Applications

From WFMC,
Workflow Reference Model, 1998

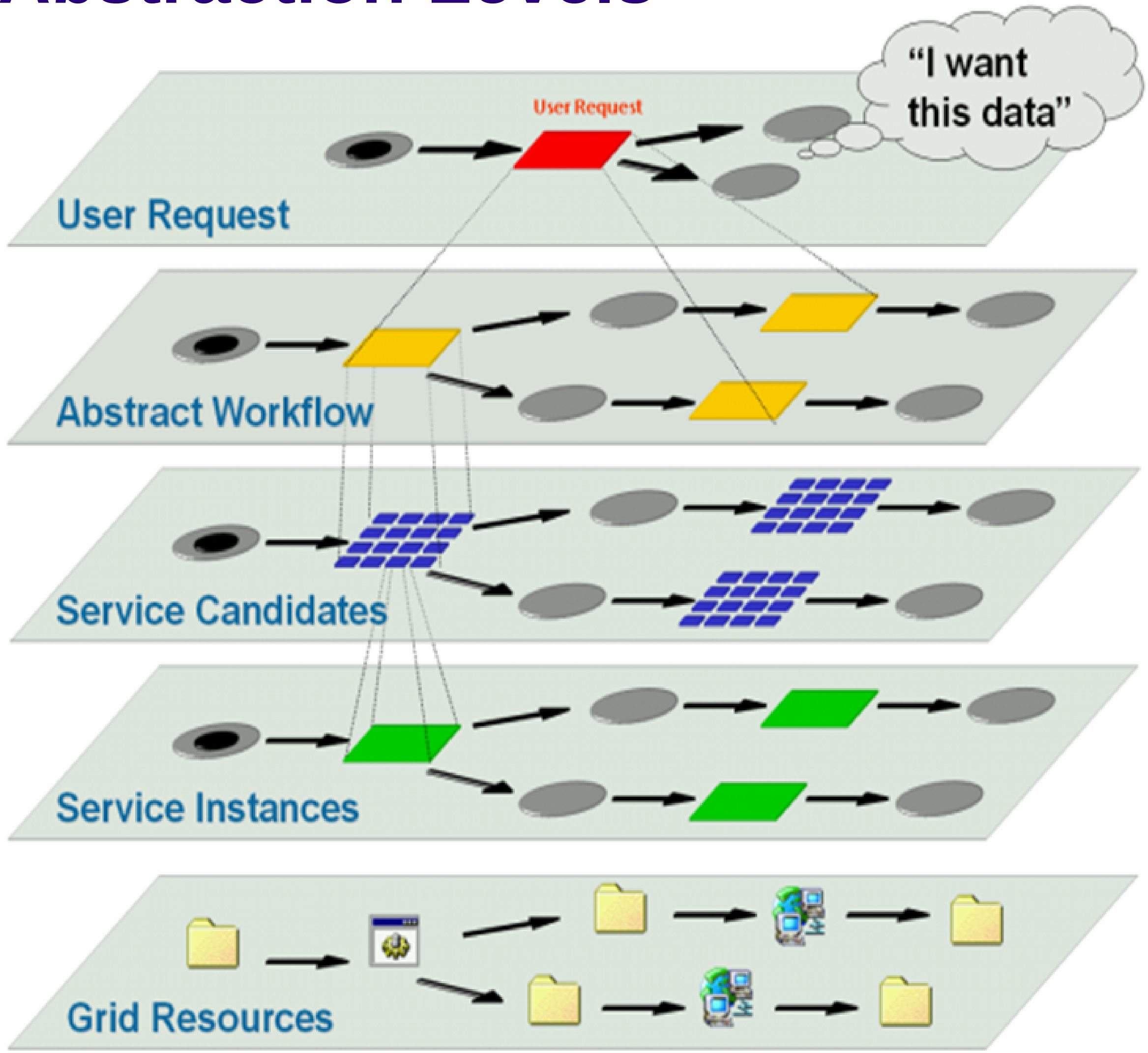
Wrappers and Grid Applications



Wrappers and Legacy Applications

- The workflow engine is also in charge of connecting the different scientific applications.
- These applications do not have to talk directly to each other, they do it through the workflow engine.
- Most engines target a service oriented applications for which they provide very good connectivity through standardized protocols. Otherwise, the interface adapters must be developed on a case by case basis (as a last resort manual integration may be required!)
- For legacy application, a wrapper must be built so that the workflow engine can communicate with the application. The wrapper can be a simple relay of commands and data, or a complete translation program implementing functionality not present in the legacy application.
- For most Grid applications, the interaction takes place through a Grid scheduler, which is responsible for managing the distributed execution of the applications.

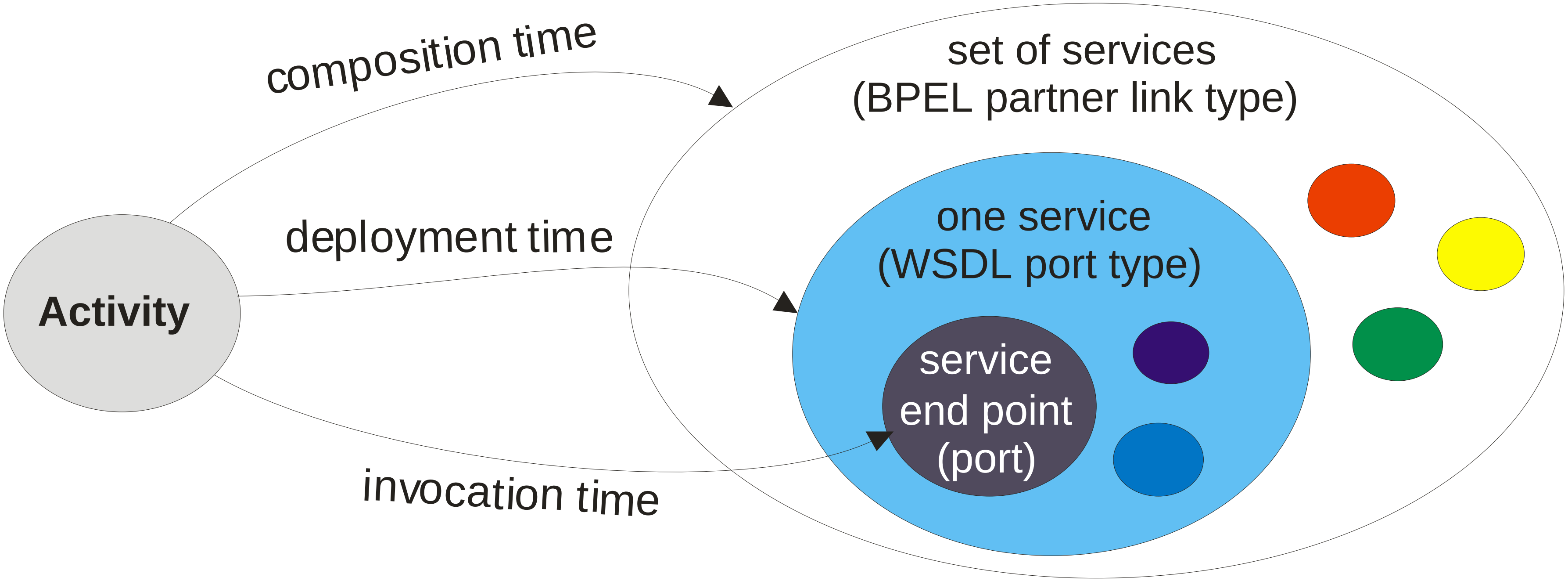
Run-time Abstraction Levels



Run-time Abstraction Levels

- A design-time workflow model needs to be mapped across different abstraction levels in order to be executed at run time.
- User request the execution of a new workflow instance.
- The abstract workflow is mapped to an executable instance by:
  - Finding suitable service implementations and binding them to the tasks
  - Rewriting the workflow graph based on a set of refinement rules
  - Planning required data staging, registration, placement, replication and transfer operations
- Each task of the resulting executable workflow is then submitted to a Grid resource manager so that it can be scheduled on suitable resources
- The mapping can be done:
  - when the workflow is started at instantiation time (statically)
  - incrementally as the workflow runs (adaptive execution with dynamic late binding)

Example: Binding with WS-BPEL



Workflow Binding Lifecycle

- Library Registration time *(classification)*
- Modeling time *(**static early binding**)*
- Compilation time *(blacklisting)*
- Deployment time *(customization)*
- Startup time *(testing)*
- Task Execution time *(**dynamic late binding**)*
- Failed invocation time *(rebind on retry)*

Powered by JOpera

http://www.jopera.org/

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JOpera
Scientific Workflow for Eclipse

- **High Level Workflow Language**
  - Data and Control Aspects (Visual Representation)
  - Recursion, Iteration, Parallelism and Pipelining

- **Open and Extensible Component Model**
  - Run existing code without changes
  - Synchronous, Asynchronous, and Streaming interaction
  - Web services support (Axis, WSIF)
  - Secure access to remote file systems and hosts (SSH)
  - Easy to integrate with existing schedulers (e.g. Condor)

- **High Level Workflow Language**
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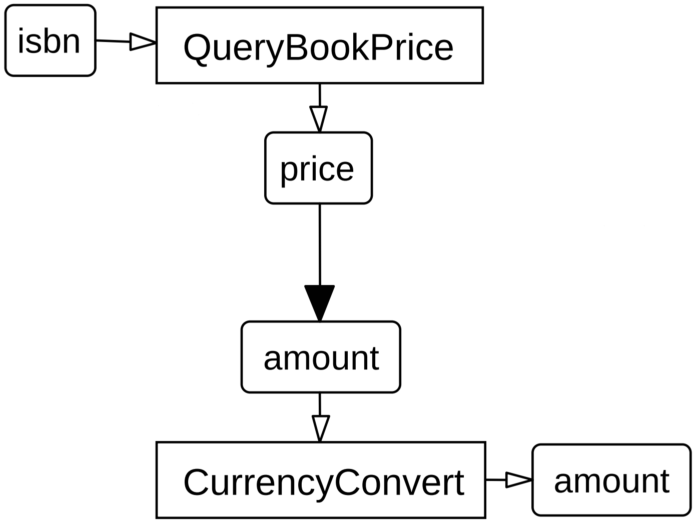
  - Web services support (Axis, WSIF)
  - Secure access to remote file systems and hosts (SSH)
  - Easy to integrate with existing schedulers (e.g. Condor)
- **Strong Eclipse Foundation**
  - Platform Independent (Eclipse/Java)
  - Flexible, Extensible, Modular and Embeddable

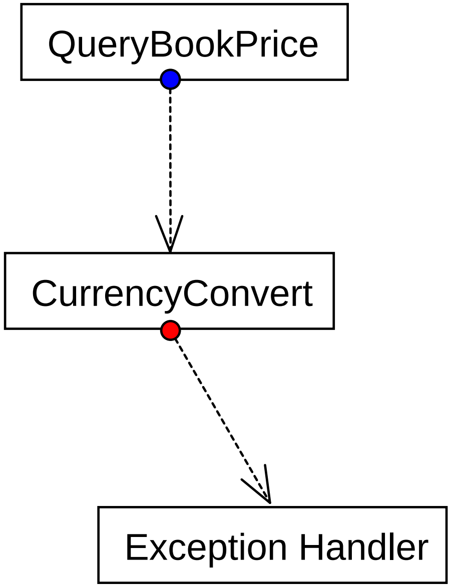
JOpera Visual Composition Language

Workflows are modeled using multiple viewpoints:

1. Data Flow Graph



2. Control Flow Graph



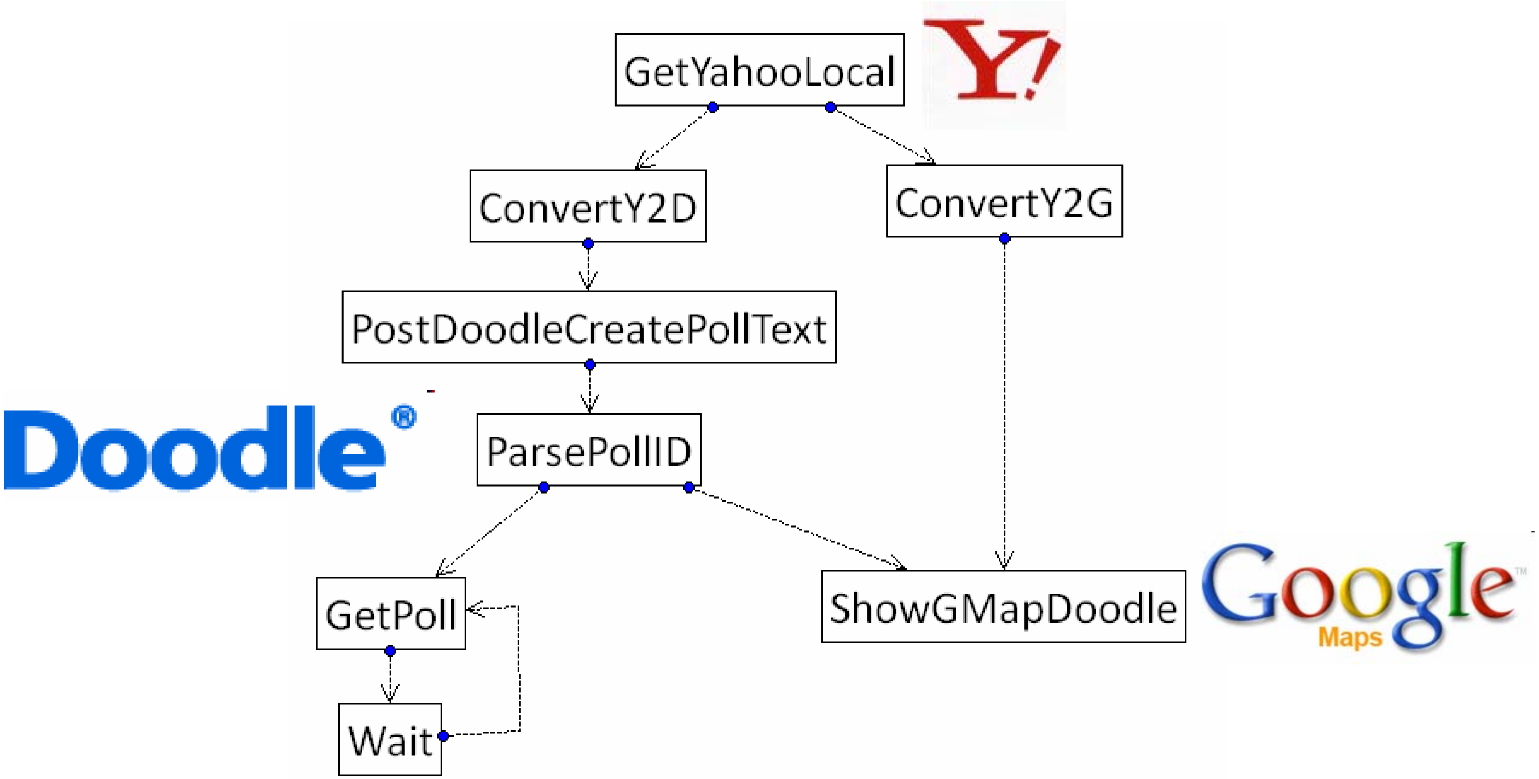
3. Service Bindings

QueryBookPrice
Amazon.com

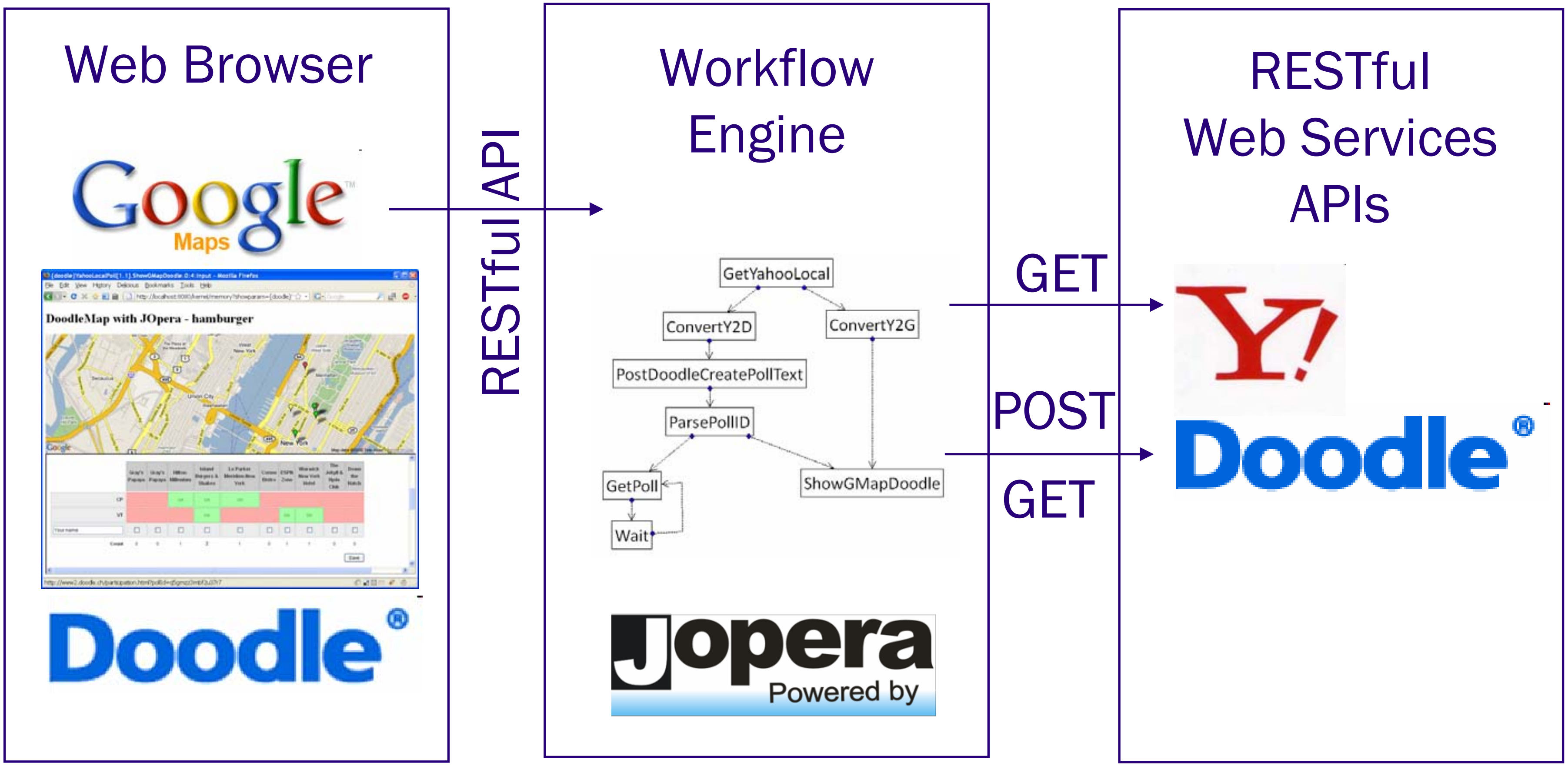
CurrencyConvert
XE.com

JOpera Example: Doodle Map Mashup

Setup a Doodle with Yahoo! Local search and visualize the results of the poll on Google Maps

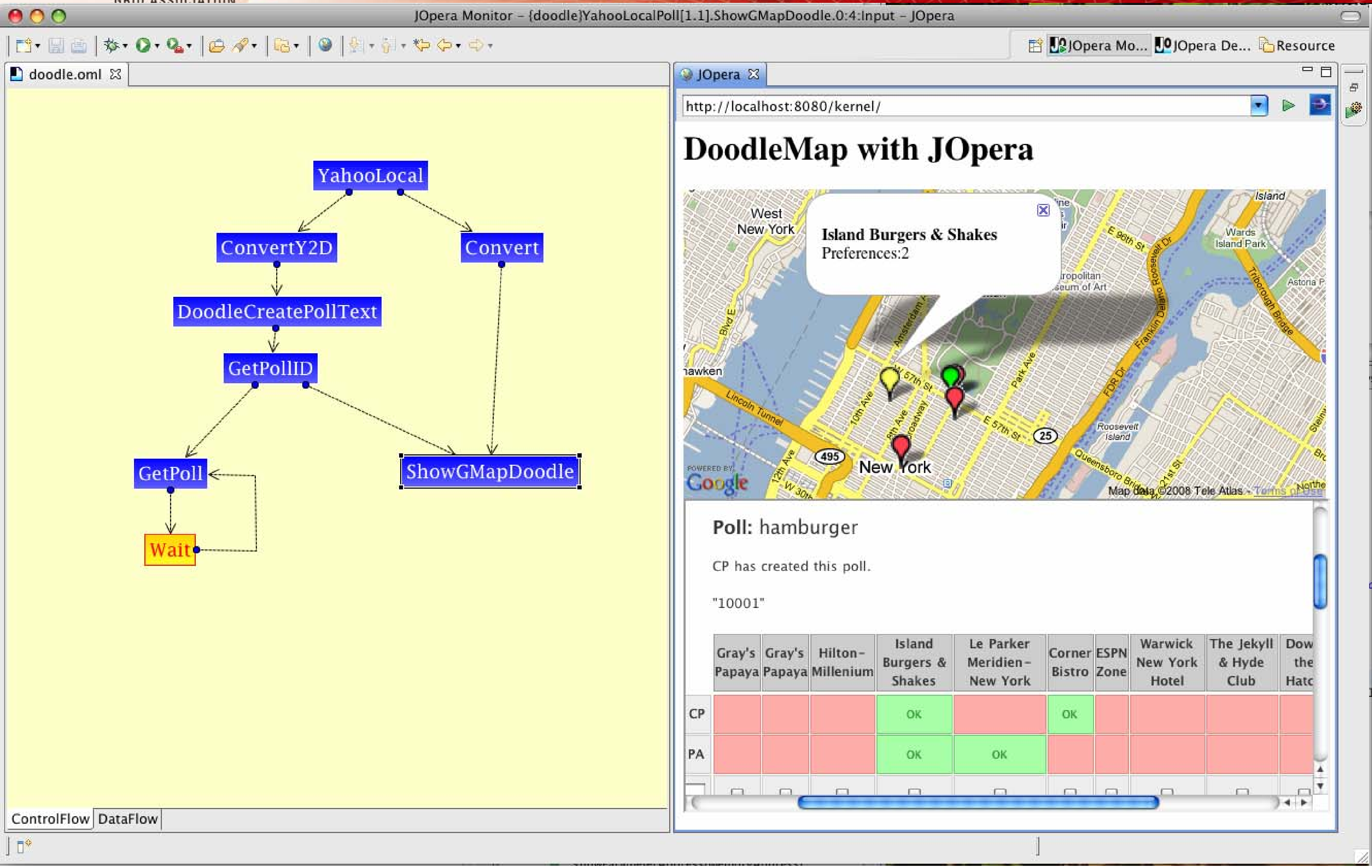


Doodle Map Mashup Architecture



[doodle] YahooLocalPoll[1.1].ShowGMapDoodle.0:4 Input - Mozilla Firefox

DoodleMap with JOpera - hamburger



DoodleMap with JOpera

Island Burgers & Shakes
Preferences:2

Poll: hamburger

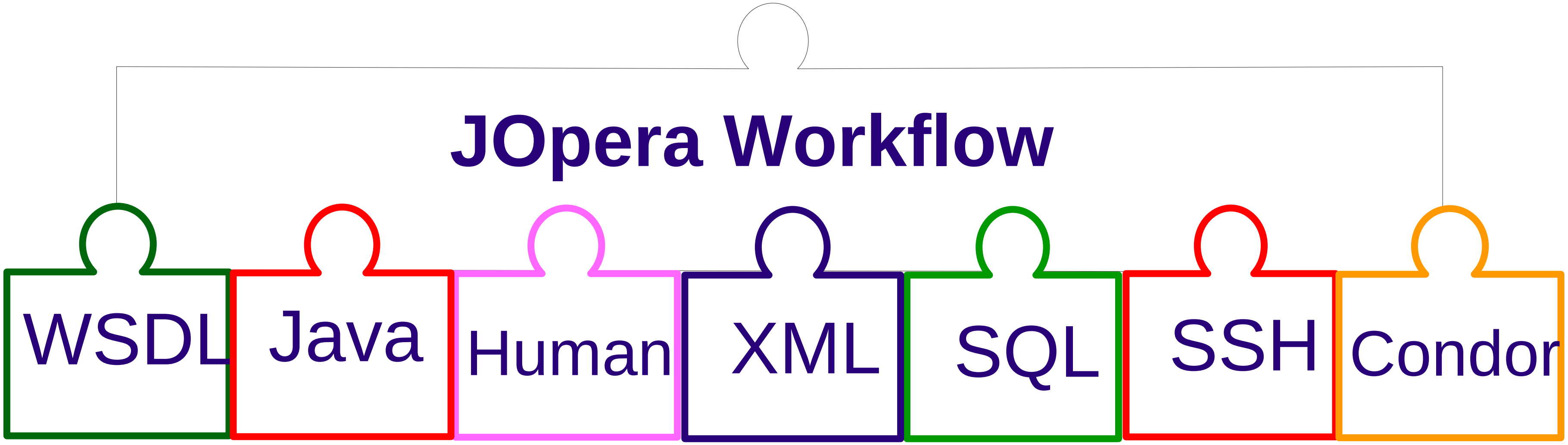
CP has created this poll.

"10001"

	Gray's Papaya	Gray's Papaya	Hilton-Millenium	Island Burgers & Shakes	Le Parker Meridien-New York	Corner Bistro	ESPN Zone	Warwick New York Hotel	The Jekyll & Hyde Club	Dow the Hatc
CP				OK		OK				
PA				OK	OK					
☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Extensible JOpera Component Model

Combine in the same workflow jobs implemented using an open and extensible set of technologies

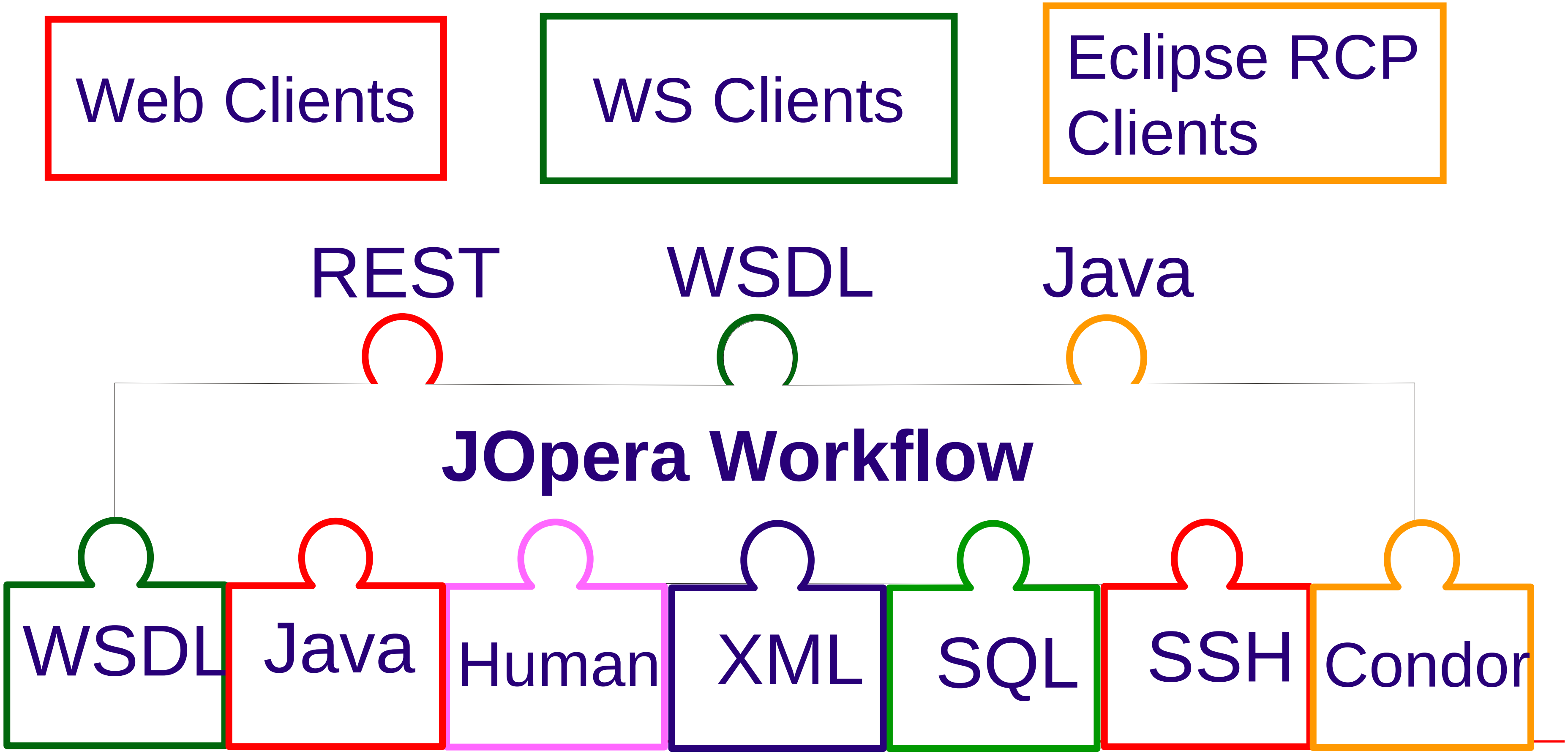


- Snippets
- Methods

- XSLT
- XPath

Sharing Workflows as a Service

JOpera processes are automatically published to clients using a variety of access protocols



Web Clients

WS Clients

Eclipse RCP Clients

REST

WSDL

Java

JOpera Workflow

WSDL

Java

Human

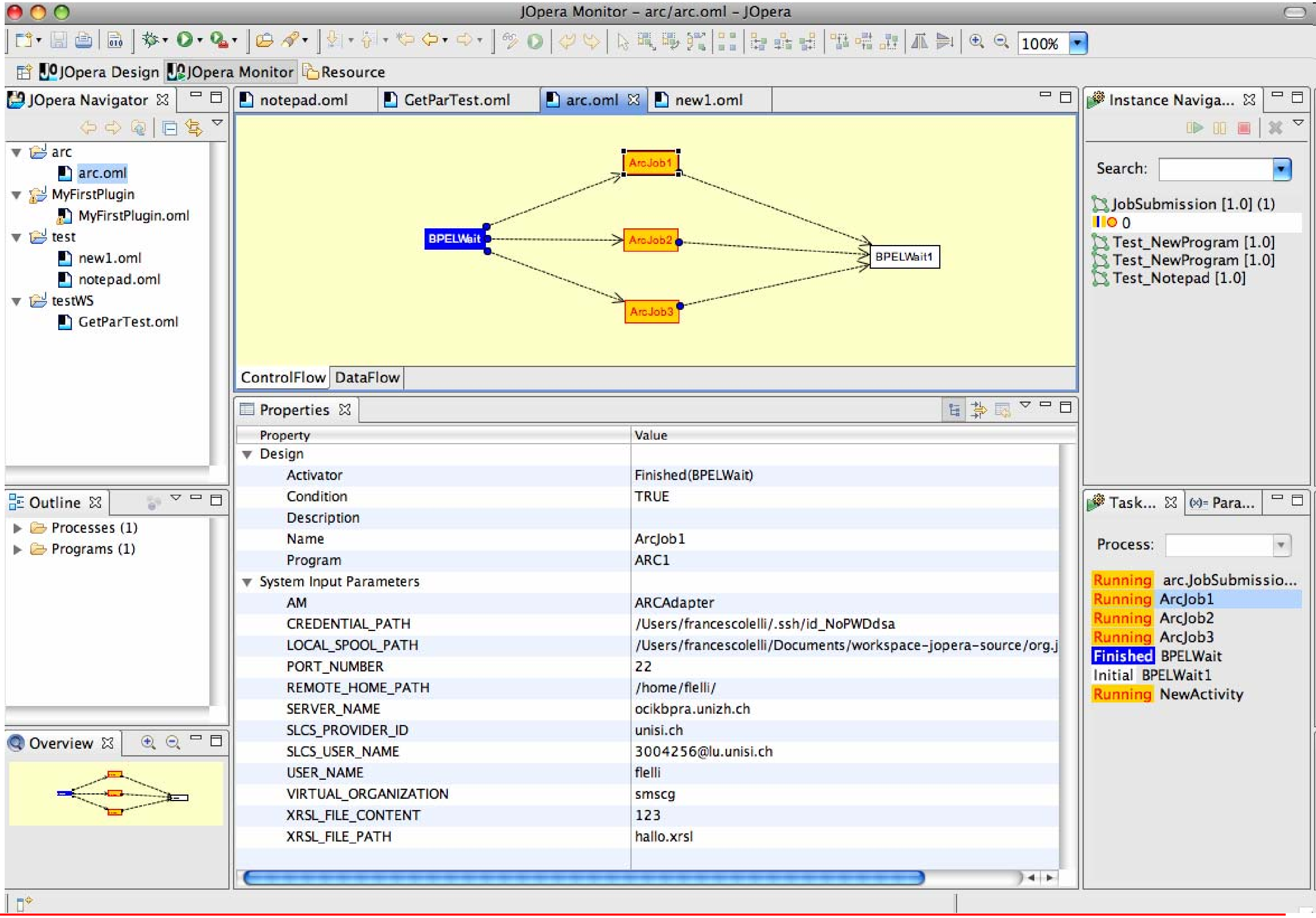
XML

SQL

SSH

Condor

JOpera ARC Integration Demo



Property	Value
Design	
Activator	Finished(BPELWait)
Condition	TRUE
Description	
Name	ArcJob1
Program	ARC1
System Input Parameters	
AM	ARCAdapter
CREDENTIAL_PATH	/Users/francescolelli/.ssh/id_NoPWDdsa
LOCAL_SPOOL_PATH	/Users/francescolelli/Documents/workspace-jopera-source/org.j
PORT_NUMBER	22
REMOTE_HOME_PATH	/home/flelli/
SERVER_NAME	ocikbpra.unizh.ch
SLCS_PROVIDER_ID	unisi.ch
SLCS_USER_NAME	3004256@lu.unisi.ch
USER_NAME	flelli
VIRTUAL_ORGANIZATION	smscg
XRSL_FILE_CONTENT	123
XRSL_FILE_PATH	hallo.xrsl

Running	arc.JobSubmissio...
Running	ArcJob1
Running	ArcJob2
Running	ArcJob3
Finished	BPELWait
Initial	BPELWait1
Running	NewActivity

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Workflows and Provenance

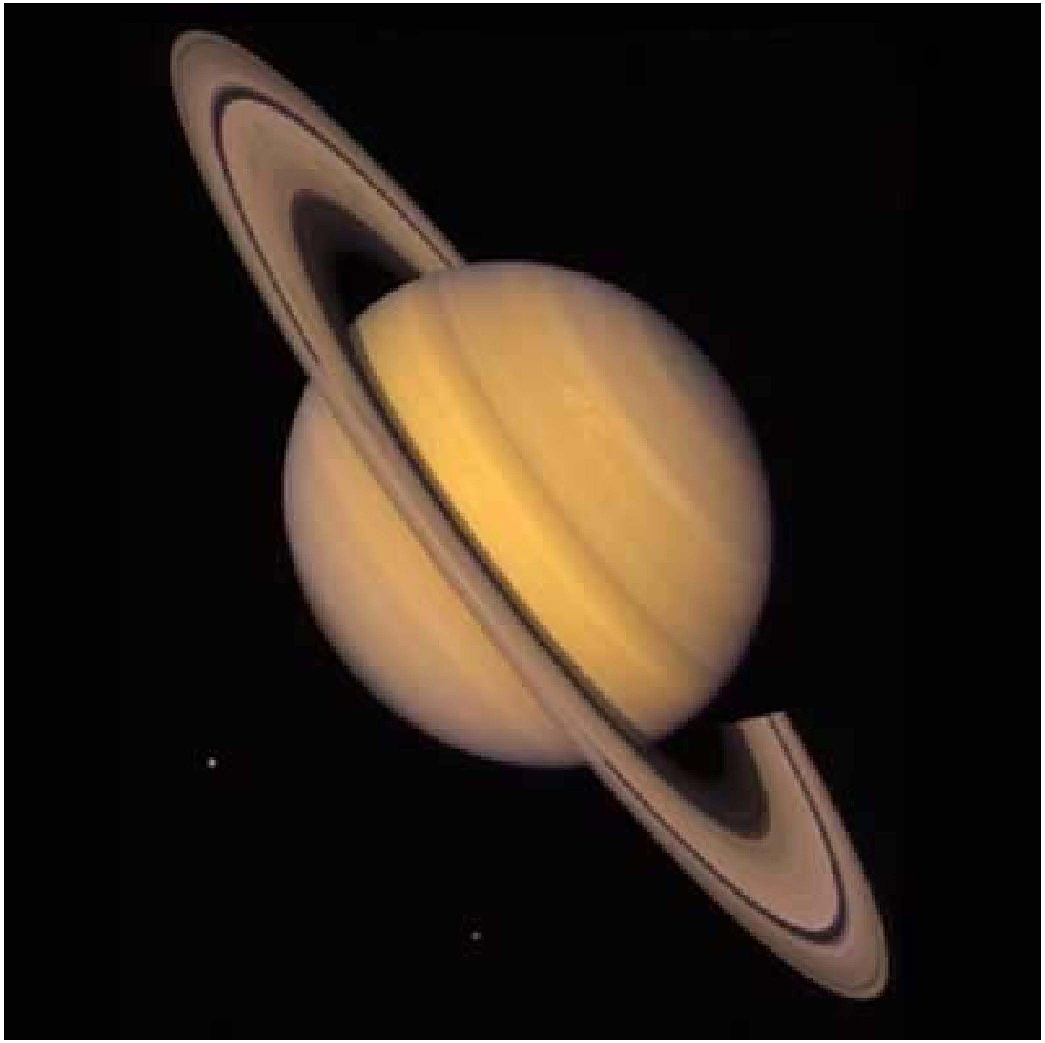
Lineage in Scientific Workflows

Scientists consider the “capture and generation of provenance information as a critical part of the workflow-generated data”

“Sharing workflows is an essential element of education, and acceleration of knowledge dissemination.”

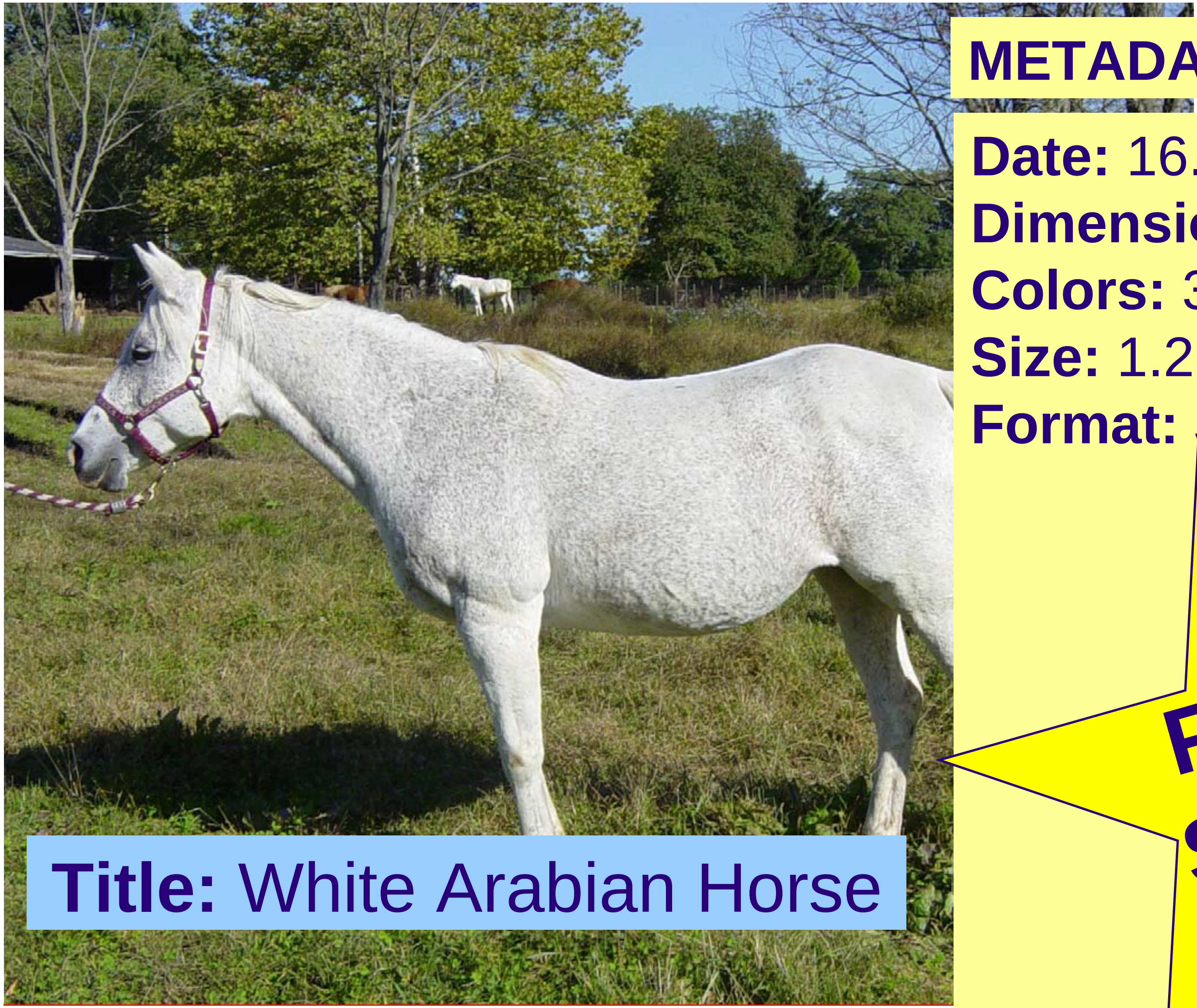
Ewa Deelman *et al.*

Where does this picture come from?



METADATA

This photo was taken
July 21, 1981,
when the Voyager 2
spacecraft
was 33.9 million km
from the Saturn planet



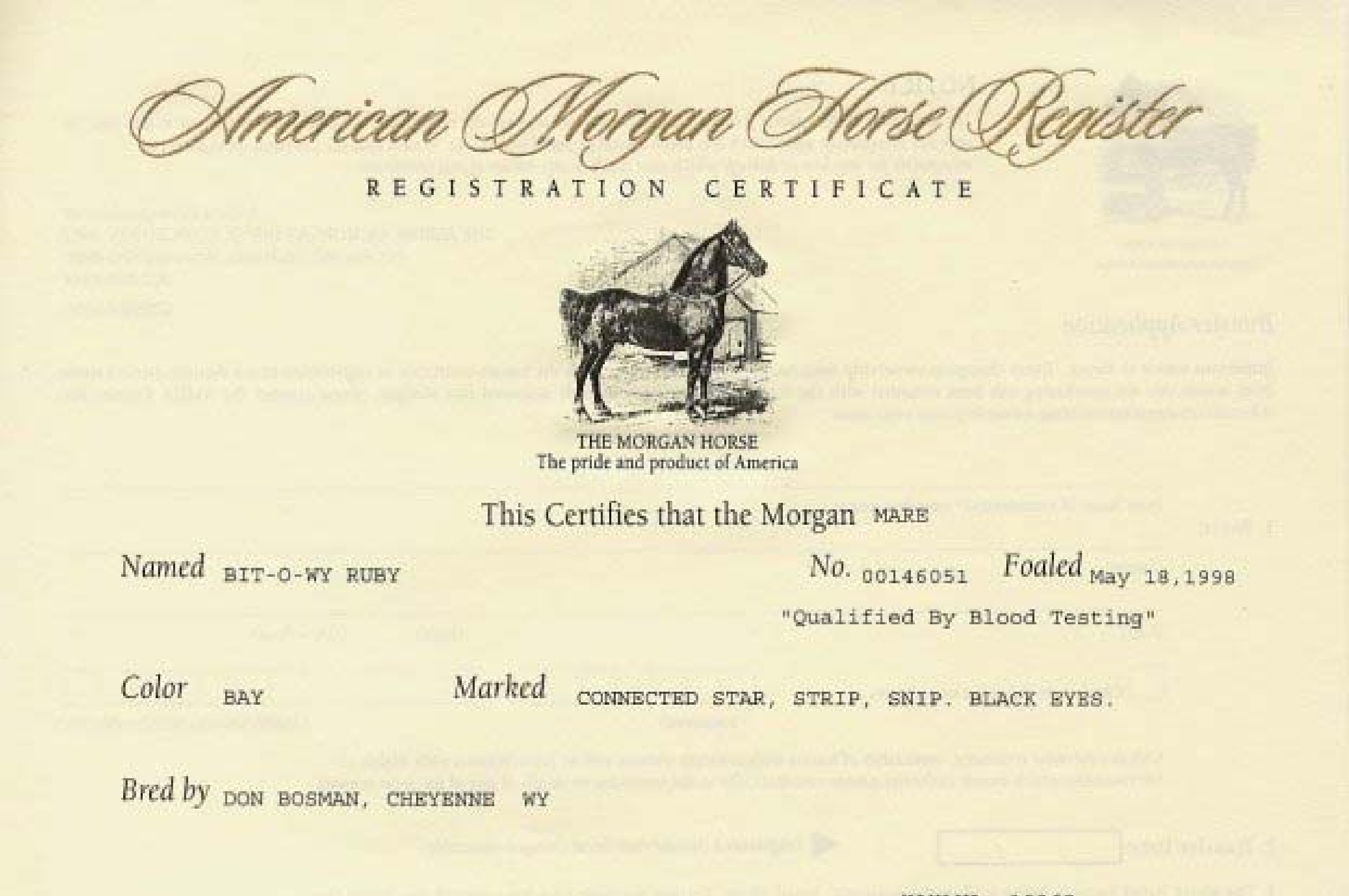
METADATA

Date: 16.4.2005
Dimension: 640x480
Colors: 32bits
Size: 1.2MB
Format: JPEG

FOR SALE

Title: White Arabian Horse

Would you buy a horse without this?



American Morgan Horse Register

REGISTRATION CERTIFICATE

THE MORGAN HORSE
The pride and product of America

This Certifies that the Morgan MARE

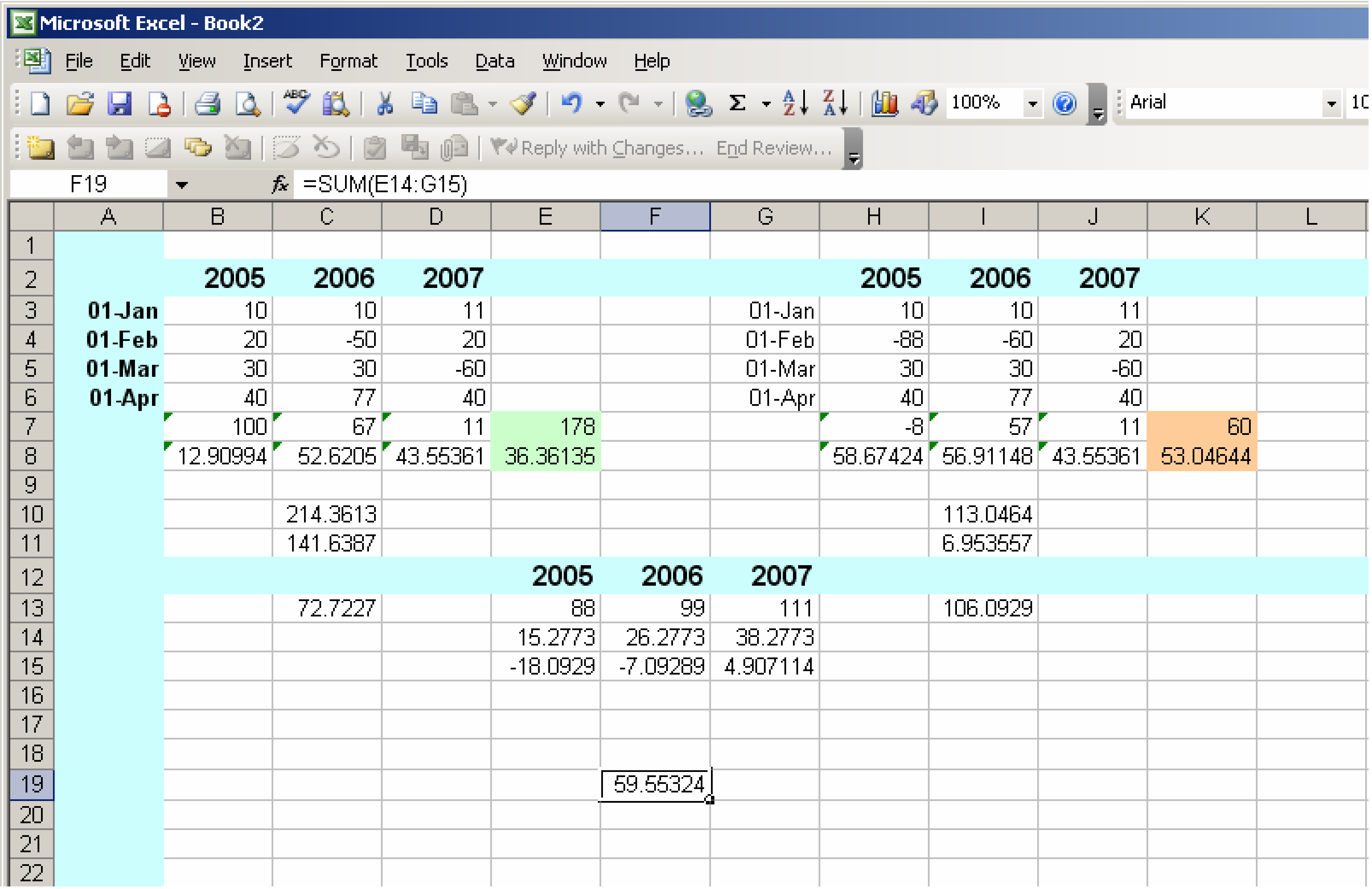
Named BIT-O-WY RUBY No. 00146051 Foaled May 18,1998

"Qualified By Blood Testing"

Color BAY Marked CONNECTED STAR, STRIP, SNIP. BLACK EYES.

Bred by DON BOSMAN, CHEYENNE WY

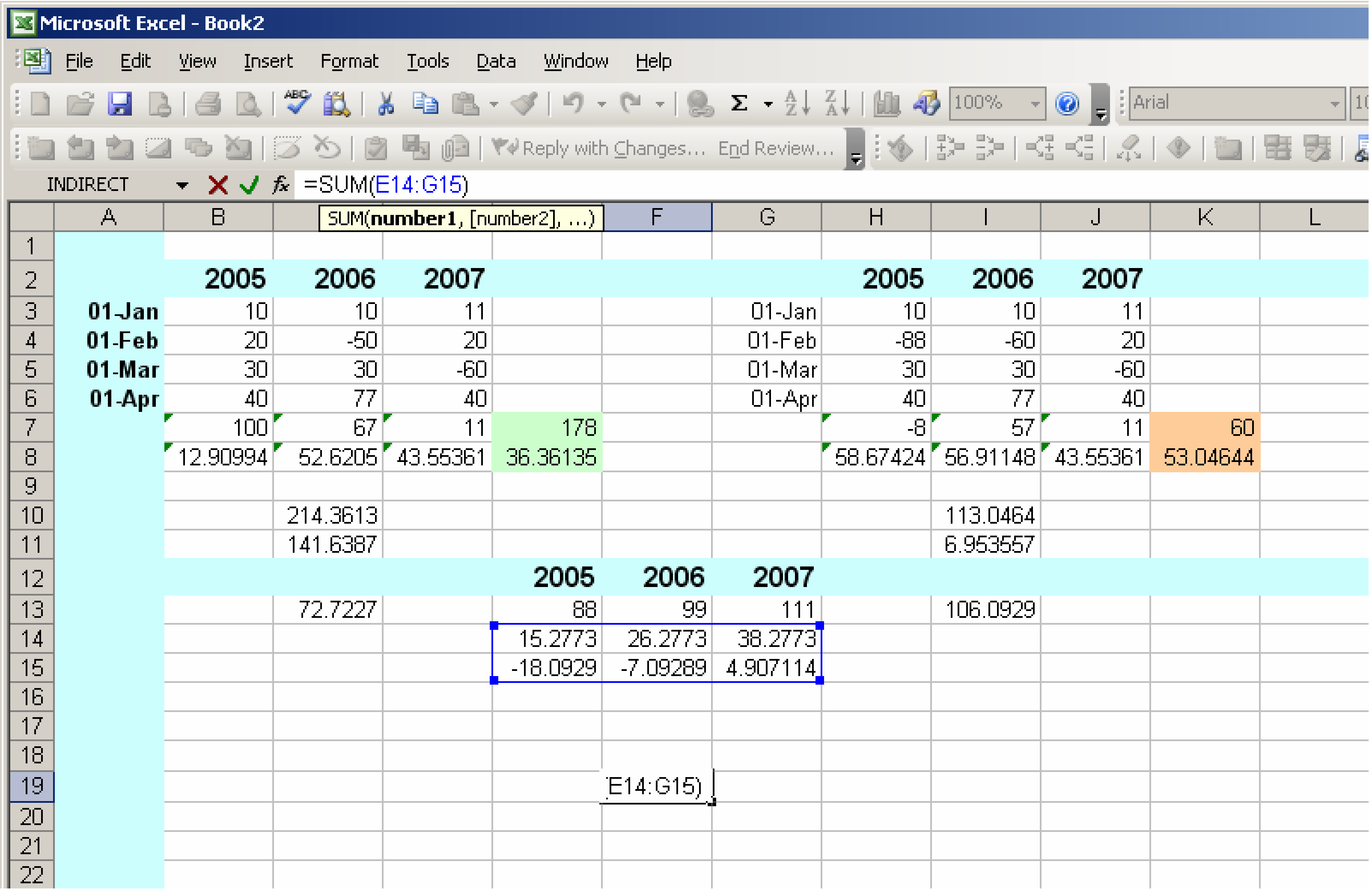
Lineage in Spreadsheets



F19 fx =SUM(E14:G15)

	A	B	C	D	E	F	G	H	I	J	K	L
1												
2		2005	2006	2007				2005	2006	2007		
3	01-Jan	10	10	11			01-Jan	10	10	11		
4	01-Feb	20	-50	20			01-Feb	-88	-60	20		
5	01-Mar	30	30	-60			01-Mar	30	30	-60		
6	01-Apr	40	77	40			01-Apr	40	77	40		
7		100	67	11	178			-8	57	11	60	
8		12.90994	52.6205	43.55361	36.36135			58.67424	56.91148	43.55361	53.04644	
9												
10			214.3613						113.0464			
11			141.6387						6.953557			
12					2005	2006	2007					
13			72.7227		88	99	111		106.0929			
14					15.2773	26.2773	38.2773					
15					-18.0929	-7.09289	4.907114					
16												
17												
18												
19						59.55324						
20												
21												
22												

Lineage in Spreadsheets

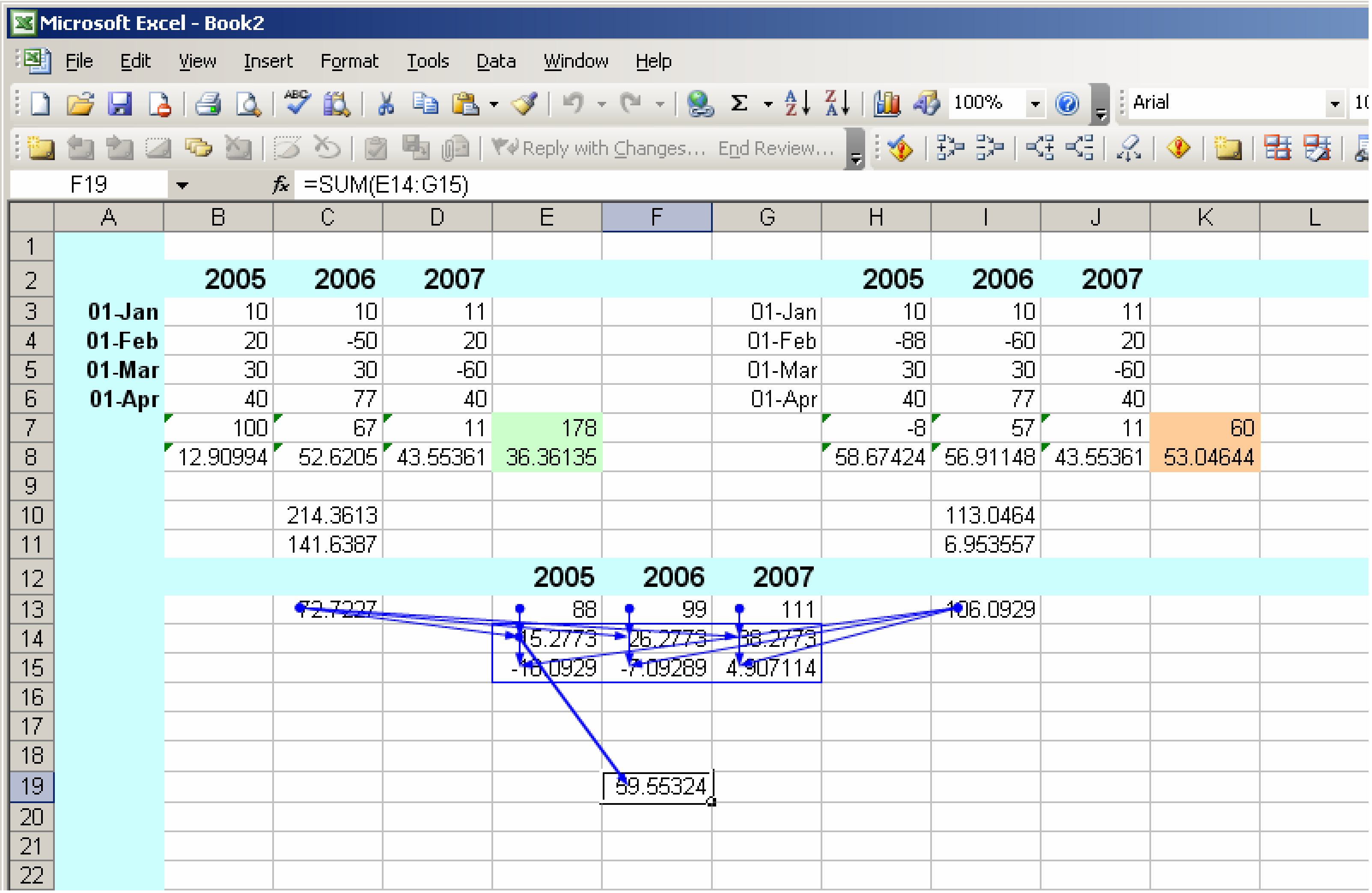


INDIRECT =SUM(E14:G15)

SUM(**number1**, [number2], ...)

	A	B				F	G	H	I	J	K	L
1												
2		2005	2006	2007				2005	2006	2007		
3	01-Jan	10	10	11			01-Jan	10	10	11		
4	01-Feb	20	-50	20			01-Feb	-88	-60	20		
5	01-Mar	30	30	-60			01-Mar	30	30	-60		
6	01-Apr	40	77	40			01-Apr	40	77	40		
7		100	67	11	178			-8	57	11	60	
8		12.90994	52.6205	43.55361	36.36135			58.67424	56.91148	43.55361	53.04644	
9												
10			214.3613						113.0464			
11			141.6387						6.953557			
12					2005	2006	2007					
13			72.7227		88	99	111		106.0929			
14					15.2773	26.2773	38.2773					
15					-18.0929	-7.09289	4.907114					
16												
17												
18												
19						E14:G15)						
20												
21												
22												

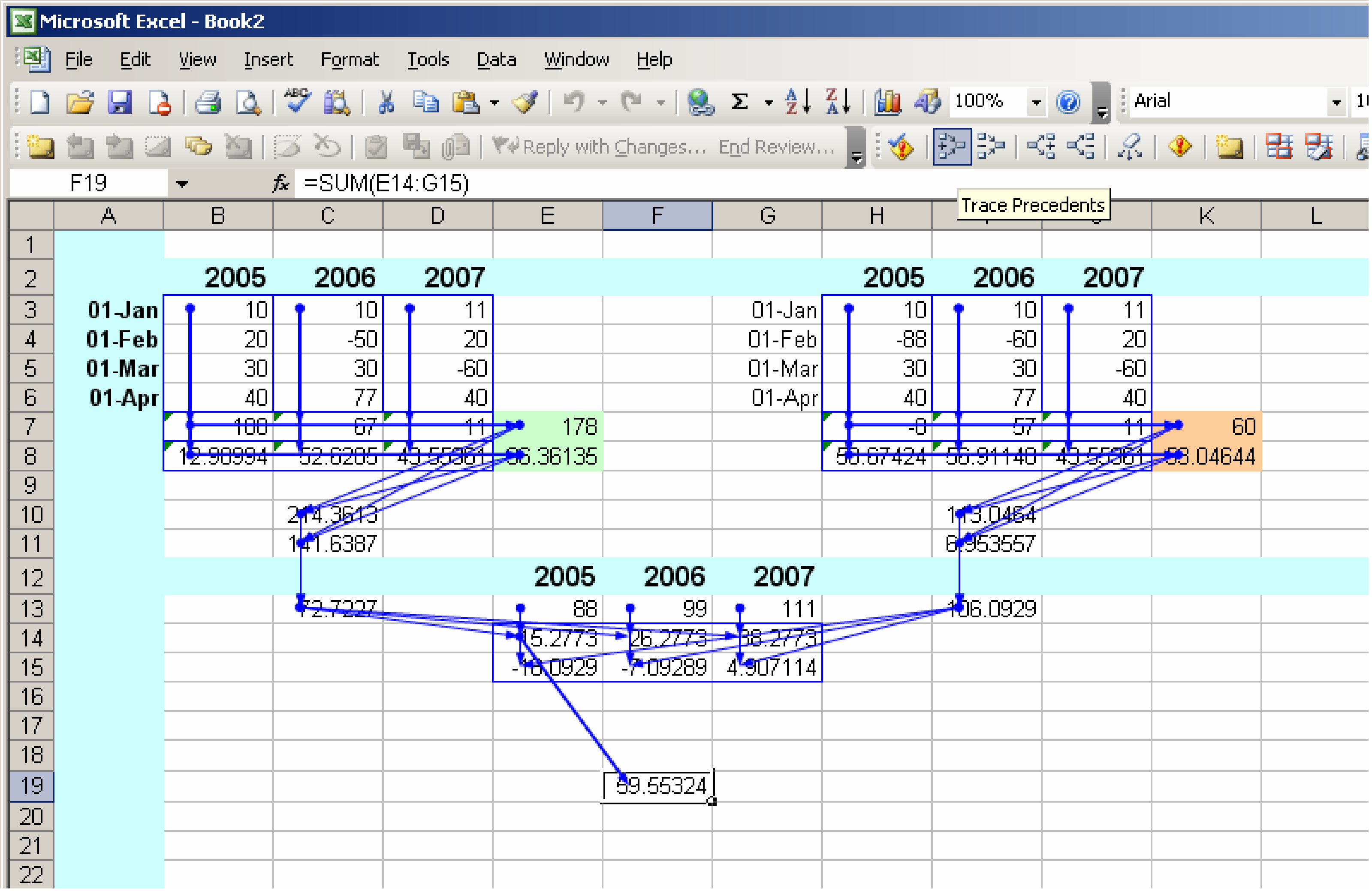
Lineage in Spreadsheets



F19 =SUM(E14:G15)

	A	B	C	D	E	F	G	H	I	J	K	L
1												
2		**2005**	**2006**	**2007**				**2005**	**2006**	**2007**		
3	**01-Jan**	10	10	11			01-Jan	10	10	11		
4	**01-Feb**	20	-50	20			01-Feb	-88	-60	20		
5	**01-Mar**	30	30	-60			01-Mar	30	30	-60		
6	**01-Apr**	40	77	40			01-Apr	40	77	40		
7		100	67	11	178			-8	57	11	60	
8		12.90994	52.6205	43.55361	36.36135			58.67424	56.91148	43.55361	53.04644	
9												
10			214.3613						113.0464			
11			141.6387						6.953557			
12					**2005**	**2006**	**2007**					
13			72.7227		88	99	111		106.0929			
14					15.2773	26.2773	38.2773					
15					-16.0929	-7.09289	4.907114					
16												
17												
18												
19						59.55324						
20												
21												
22												

Lineage in Spreadsheets

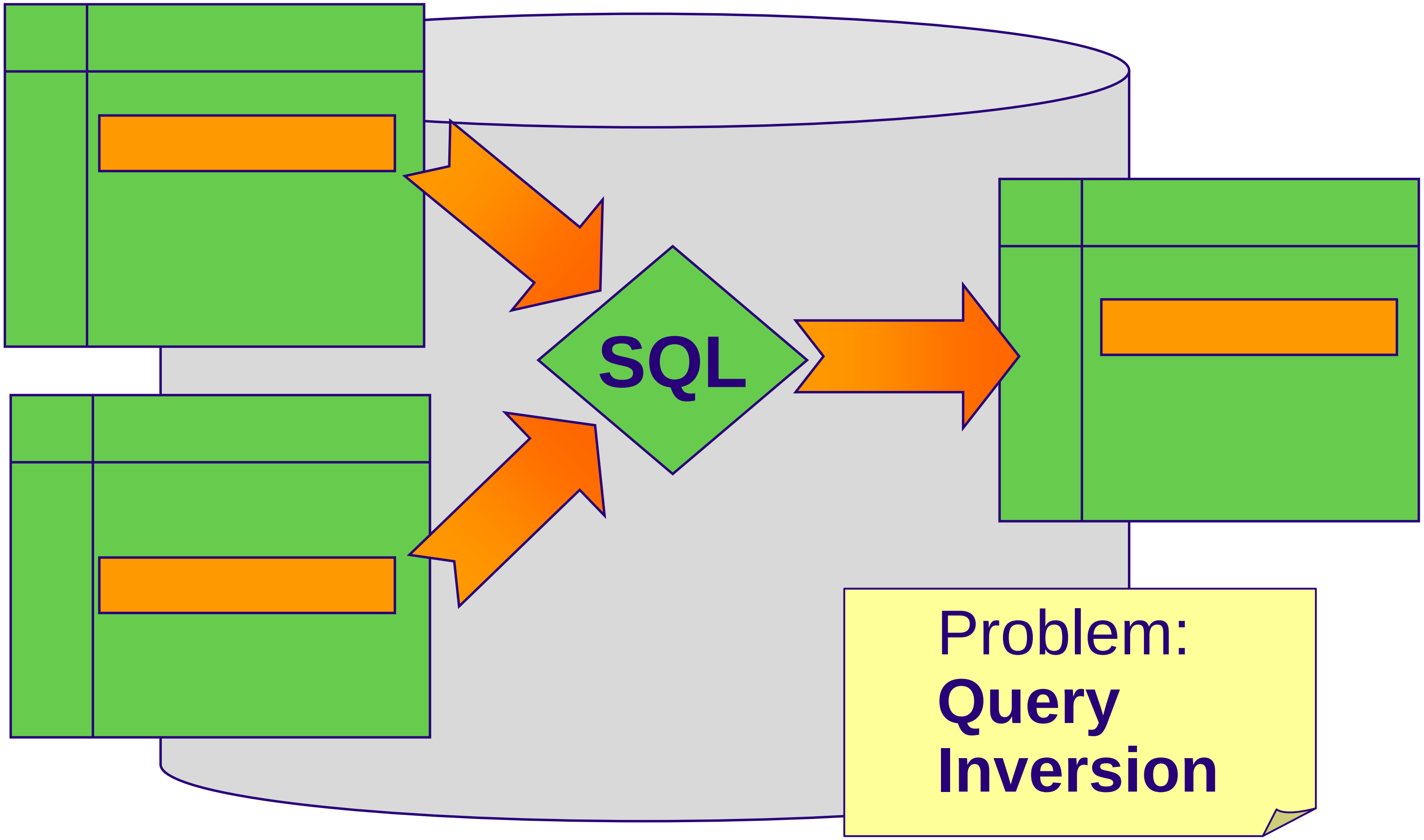


F19 =SUM(E14:G15)

	A	B	C	D	E	F	G	H	I	J	K	L
1												
2		2005	2006	2007				2005	2006	2007		
3	01-Jan	10	10	11			01-Jan	10	10	11		
4	01-Feb	20	-50	20			01-Feb	-88	-60	20		
5	01-Mar	30	30	-60			01-Mar	30	30	-60		
6	01-Apr	40	77	40			01-Apr	40	77	40		
7		100	67	11	178			-8	57	11	60	
8		12.90994	52.6205	43.55961	66.36135			50.67424	56.91140	43.55961	53.04644	
9												
10			214.3613						113.0464			
11			141.6387						6.953557			
12					2005	2006	2007					
13			72.7227		88	99	111		106.0929			
14					15.2773	26.2773	38.2773					
15					-16.0929	-7.09289	4.907114					
16												
17												
18												
19						59.55324						
20												
21												
22												

Lineage in Databases

What is the relationship between these tuples?



Problem: **Query Inversion**

Lineage in Software Development

What’s in a Makefile?

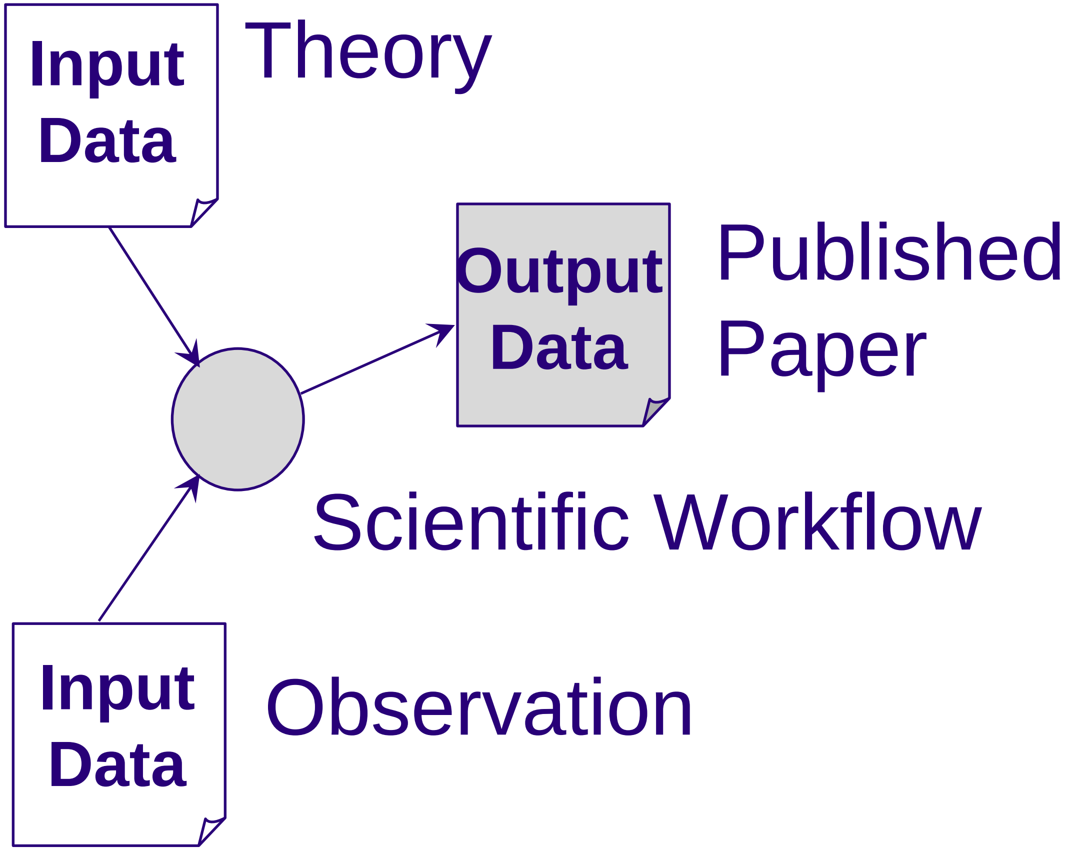
```
CC = gcc
CFLAGS = -Wall -g

program: main.o input.o output.o logic.o
       $(CC) $(CFLAGS) main.o input.o output.o logic.o -o program

main.o: main.c input.h output.h logic.h
       $(CC) $(CFLAGS) -c main.c
input.o: input.c input.h
       $(CC) $(CFLAGS) -c input.c
output.o: output.c output.h
       $(CC) $(CFLAGS) -c output.c
logic.o: logic.c logic.h
       $(CC) $(CFLAGS) -c logic.c
```

Lineage in Software Development

Where does my program come from?

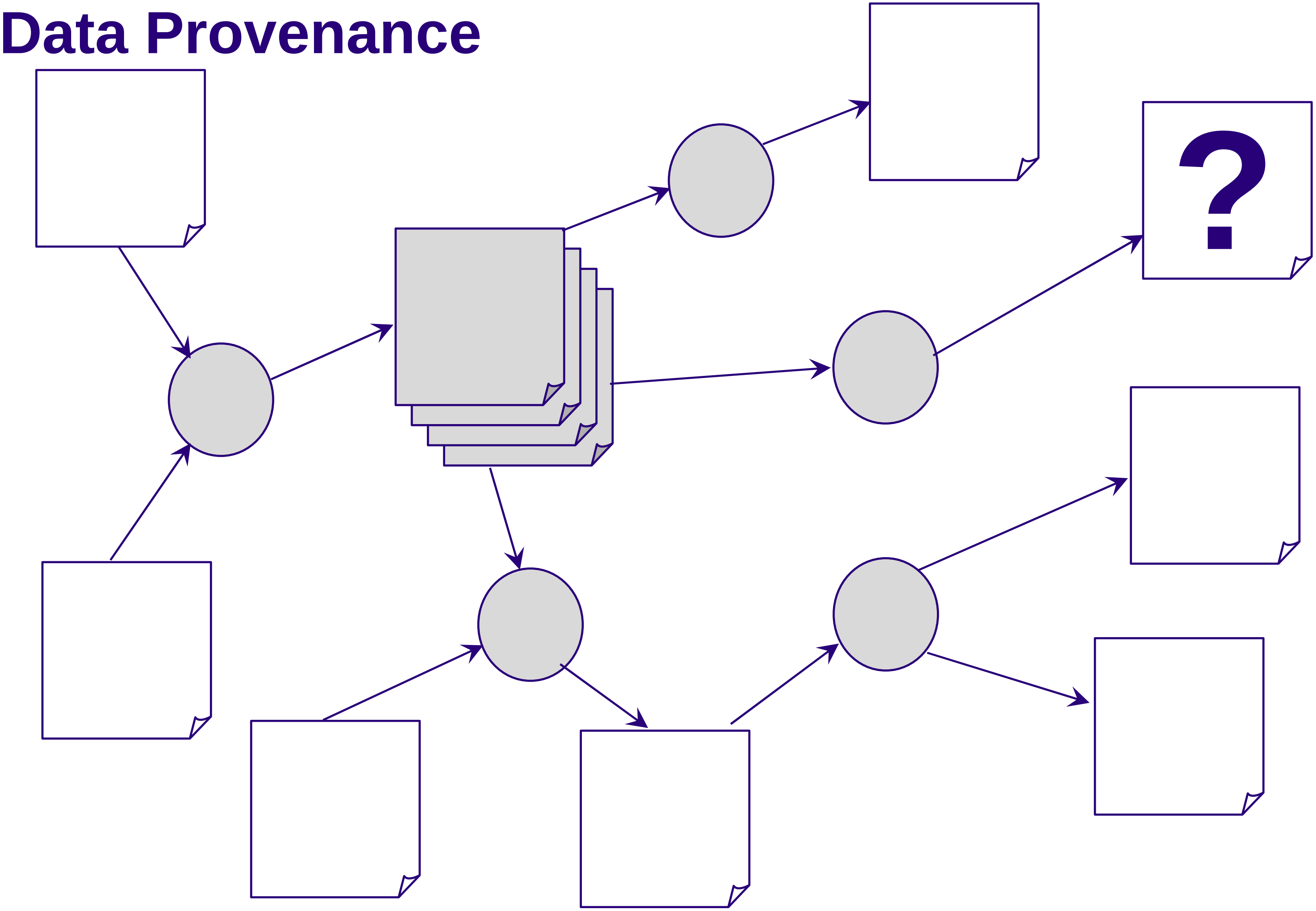
```
CC = gcc
CFLAGS = -Wall -g

program: main.o input.o output.o logic.o
	$(CC) $(CFLAGS) main.o input.o output.o logic.o -o program

main.o: main.c input.h output.h logic.h
	$(CC) $(CFLAGS) -c main.c
input.o: input.c input.h
	$(CC) $(CFLAGS) -c input.c
output.o: output.c output.h
	$(CC) $(CFLAGS) -c output.c
logic.o: logic.c logic.h
	$(CC) $(CFLAGS) -c logic.c
```

Lineage in Scientific Workflows



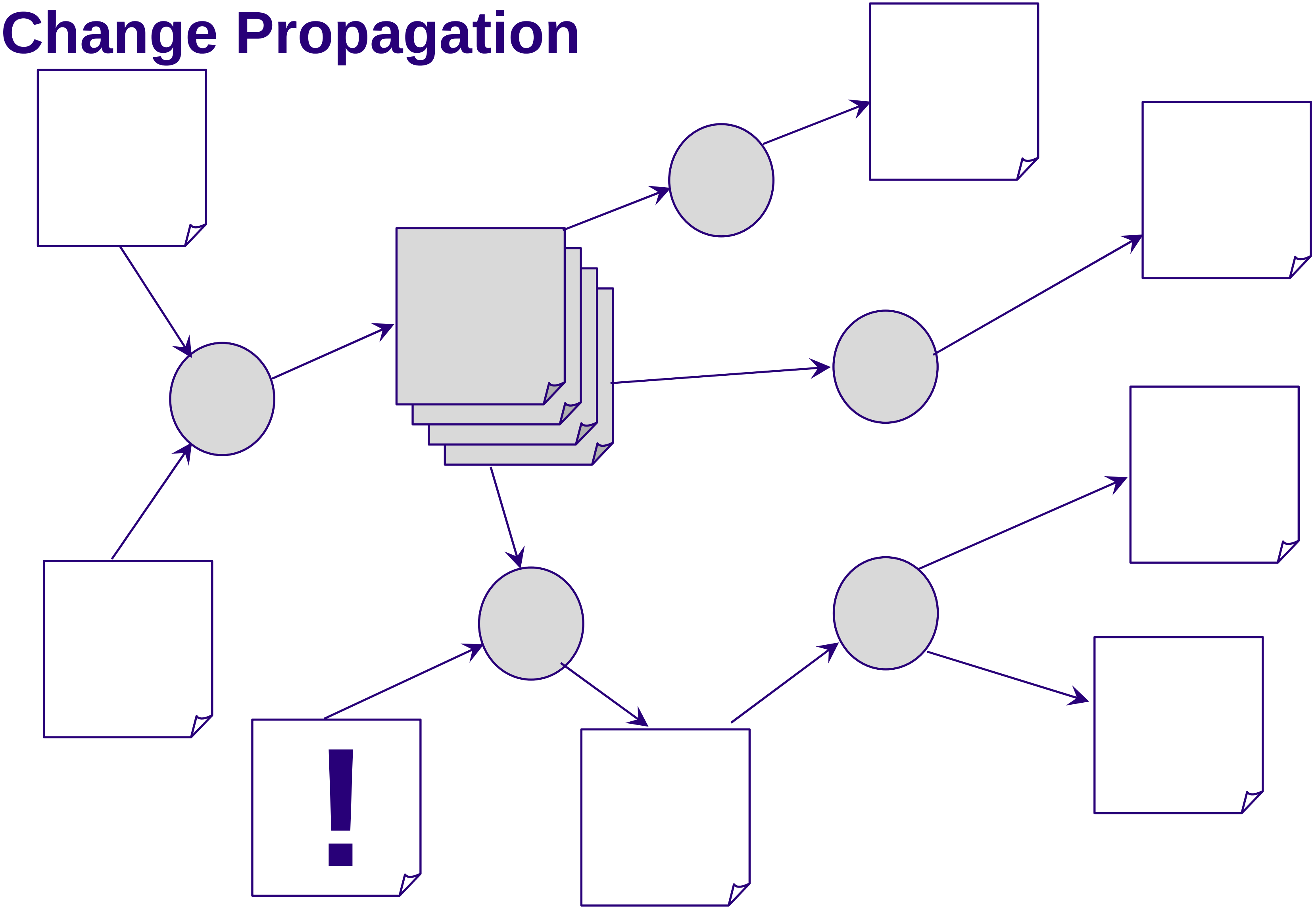
An ideal scientific workflow should document all of the steps linking the original observations with the final published results so that the process can be reproduced

Data Provenance



Where does this output document come from?

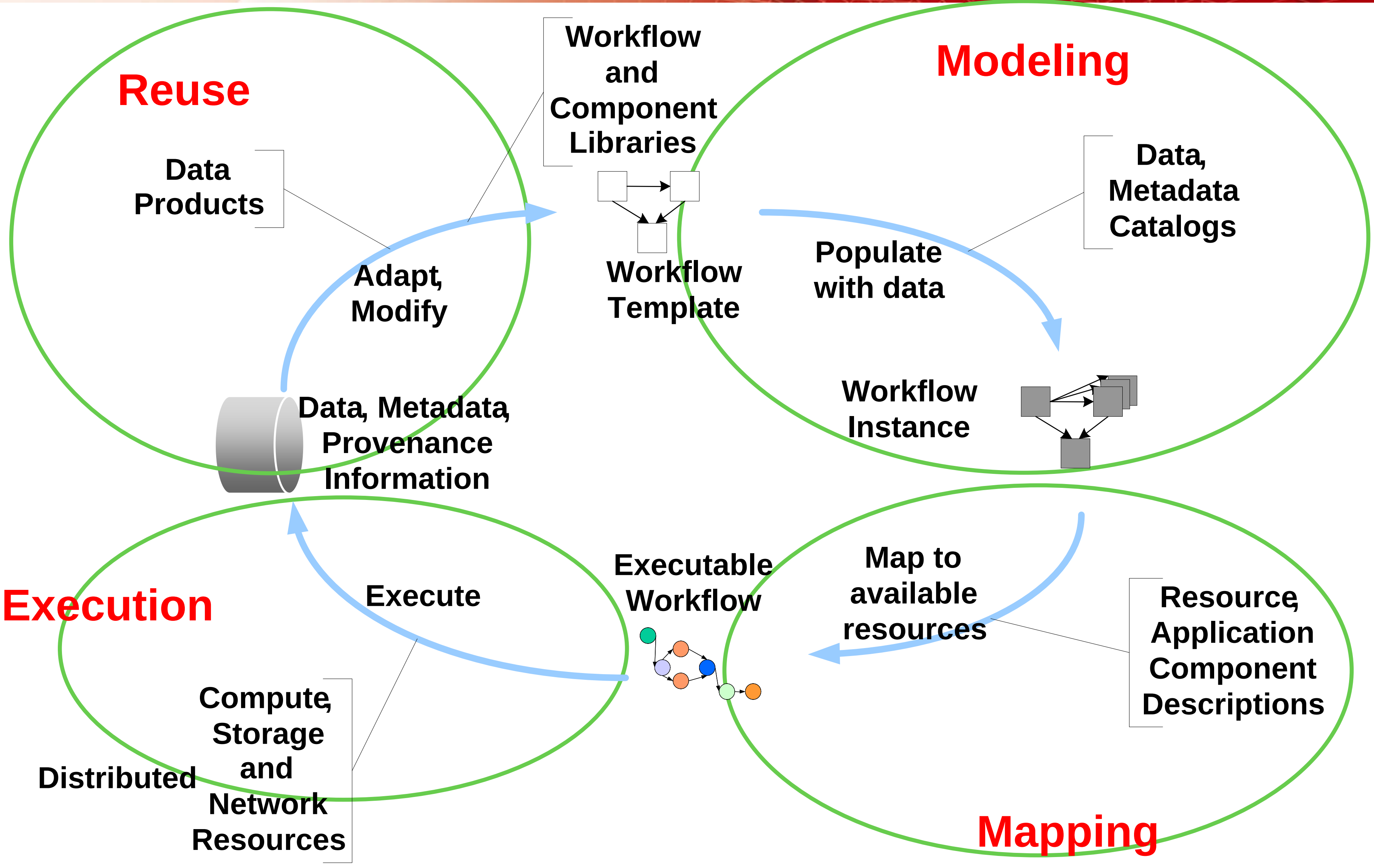
Change Propagation



What to recompute if this input changes?

SwiNG
SWISS NATIONAL
GRID ASSOCIATION

Conclusion


Reuse
Data Products
Workflow and Component Libraries
Modeling
Data, Metadata Catalogs
Adapt, Modify
Workflow Template
Populate with data
Workflow Instance
Data, Metadata, Provenance Information
Executable Workflow
Map to available resources
Execute
Execution
Resource, Application Component Descriptions
Distributed
Compute, Storage and Network Resources
Mapping

From Ewa Deelman

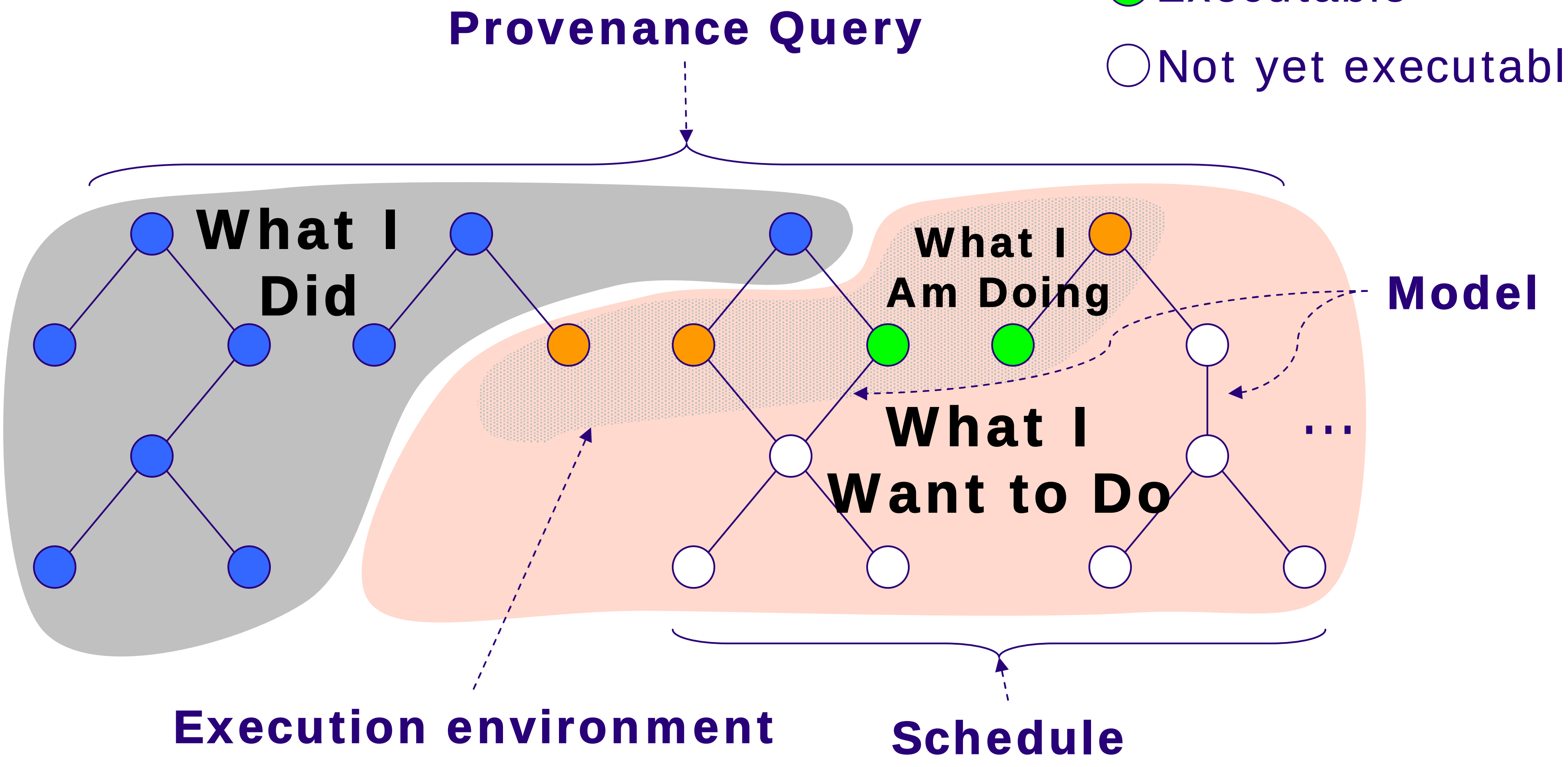
e-Science as Workflow?

🔵 Executed

🟠 Executing

🟢 Executable

○ Not yet executable



Provenance Query

What I Did

What I Am Doing

What I Want to Do

Model

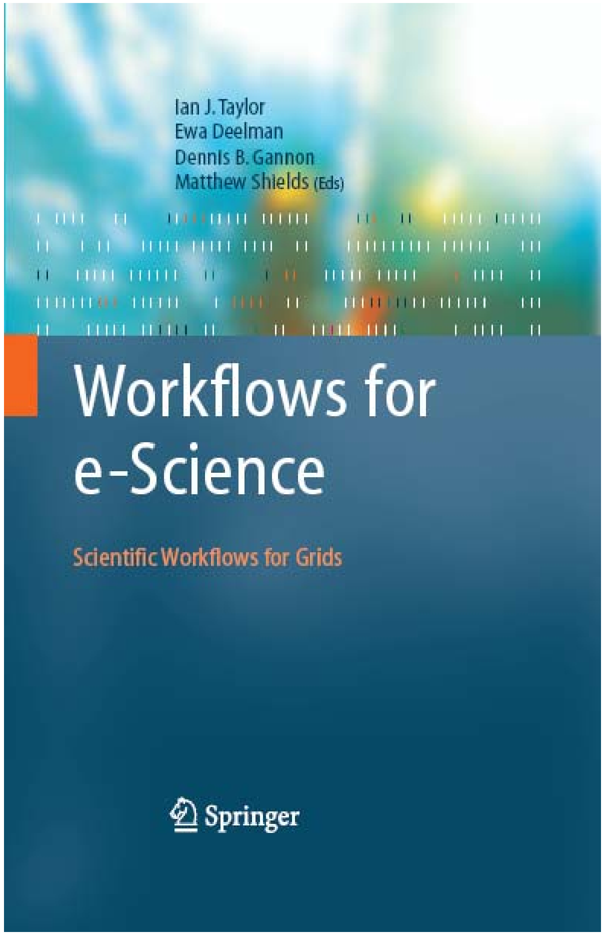
...

Execution environment

Schedule

From Ian Foster

Some References



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OGF Workflow Research Group
http://www.isi.edu/~deelman/wf–rg/

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