

# Scientific workflow management a way to enable e-science on both Grids and Clouds

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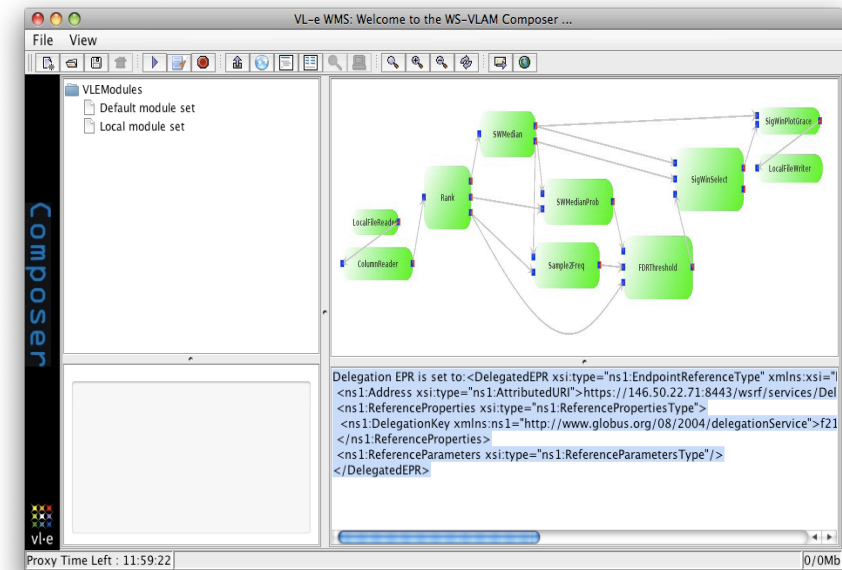
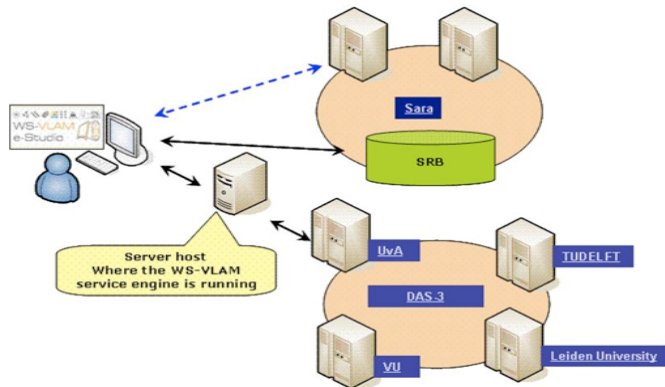
High Performance computing Curriculum, Jan 2015 <http://www.hpc.uva.nl/>

# Outline

- Introduction
- Lifecycle of an e-science workflow
- Workflow management Systems
- Scientific workflows Applications
- Provenance
- Examples of Scientific workflow managements

# Workflow management system

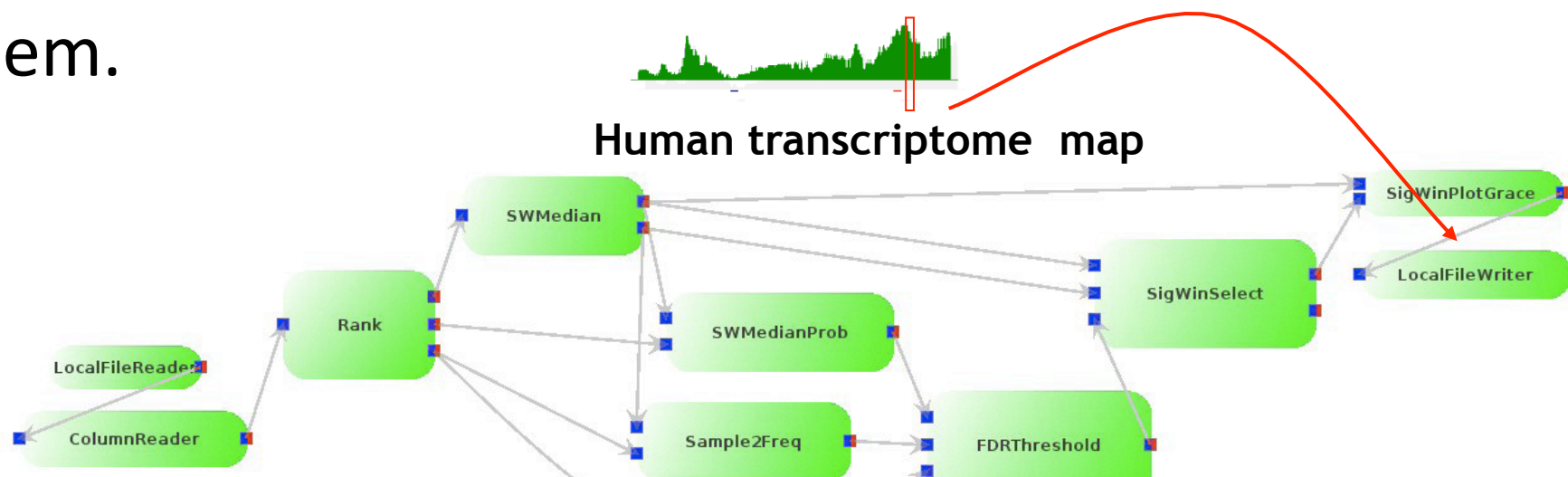
- **Workflow management system** is a computer program that manages the execution of a workflow on a set of computing resources.



*The user interface of the WS-VLAM* a workflow management system developed in the VL-e project to execute application workflow on geographically distributed computing resources

# Application Workflow

A workflow is a model to represent a **reliably repeatable sequence** of operations/tasks by showing explicitly the interdependencies among them.



[http://www.youtube.com/watch?v=R6bTFrzaR\\_w&feature=player\\_embedded](http://www.youtube.com/watch?v=R6bTFrzaR_w&feature=player_embedded)

**SigWin-Detector workflow** has been developed in the VL-e project to detect ridges in for instance a Gene Expression sequence or Human transcriptome map, BMC Research Notes 2008, 1:63 doi: 10.1186/1756-0500-1-63.

# Workflow approach in Science/industry

- **Capturing knowledge/best practices**
  - Capture **business process** based on the company policy
  - Capture **best practices of scientist**, expert from a specific domain
- **Series of structured activities and computations**
  - involves **repeated execution** of certain procedures, and describes tasks within this procedures.
- **Incorporate human decision in the process**
  - There are exceptional cases that can not be automated both in business and scientific workflow

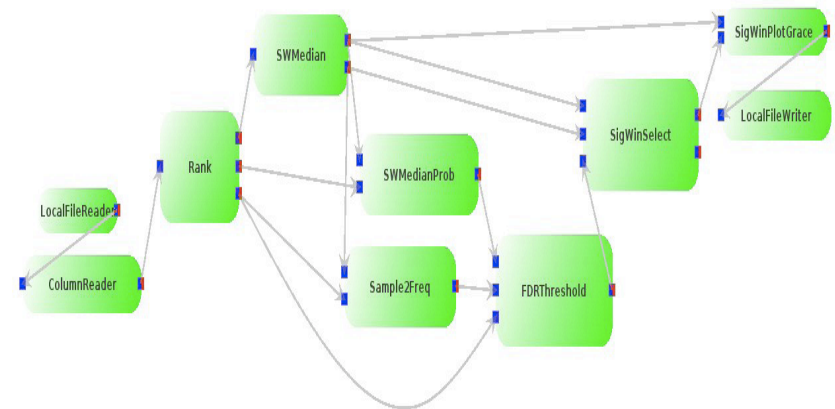
<http://www.csc.ncsu.edu/faculty/mpsingh/papers/databases/workflows/sciworkflows.html>

# Scientific Workflow Specific Needs

- Need for **large data flows** support
- Need to **do parameterized execution** of large number of jobs
- Need to **monitor** and **control workflow execution** including **ad-hoc** changes
- Need to **execute** in **dynamic environment** where resources are not known a priori and may need to adapt to changes
- Hierarchical **execution** with **sub-workflows** created and destroyed when necessary

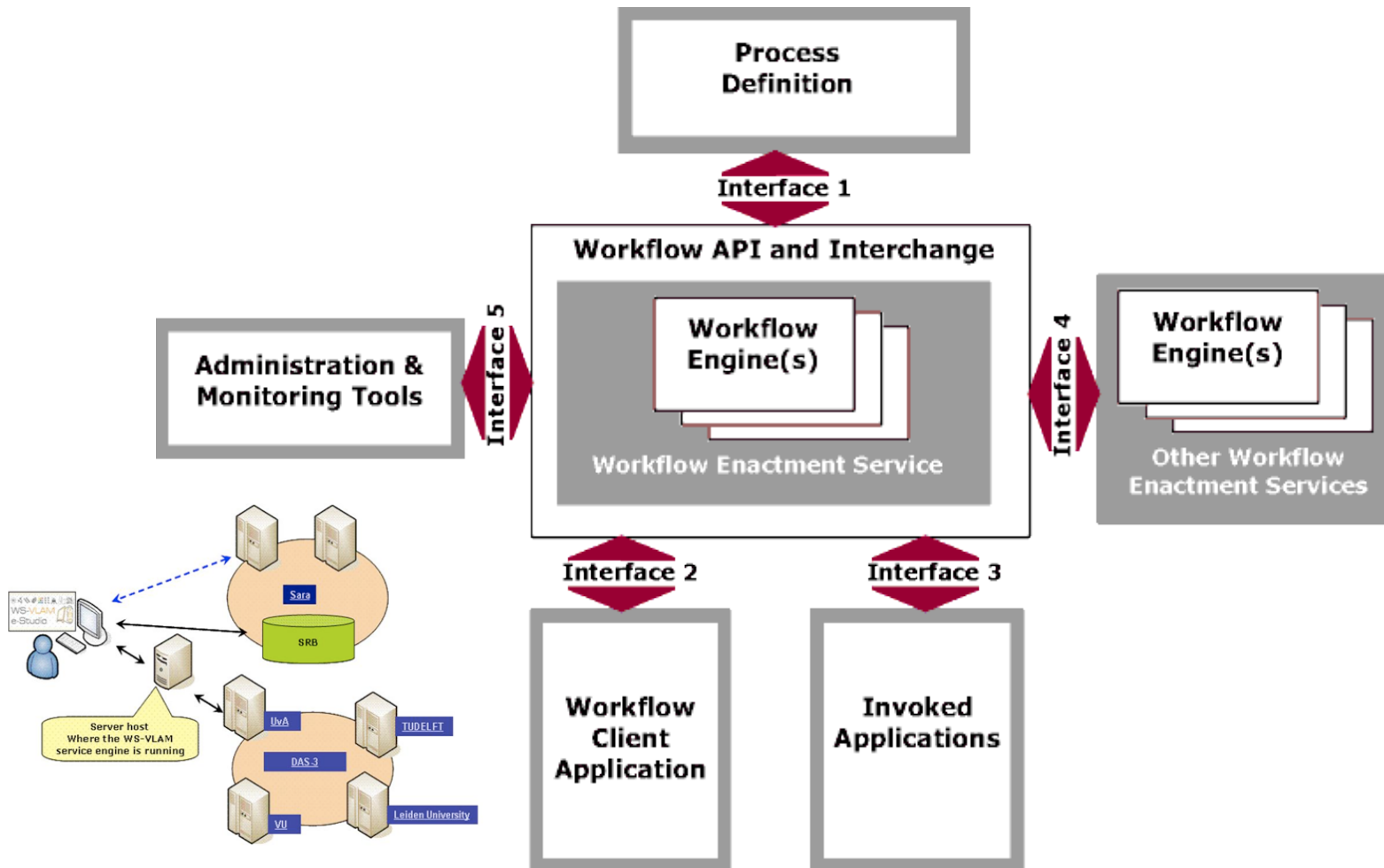
# Challenges of running workflows on e-infrastructure (grids and clouds)

- **co-allocate** resources needed for workflow enactment across multiple domains?
- achieve **QoS** for data centric application workflows that have special requirements on network connections?
- achieve **Robustness** and fault tolerance for workflow running across distributed resources?



- increase **re-usability** of Workflow, workflow components, and refine workflow execution?

# Reference Model From WFMC



The automation of a **business process**, in whole or parts, where **documents, information or tasks** are passed from one participant to another to be processed, according to a set of **procedural rules**. (WFMC definition of a Workflow)



# New Generation of Workflow management systems: Service-Oriented Science

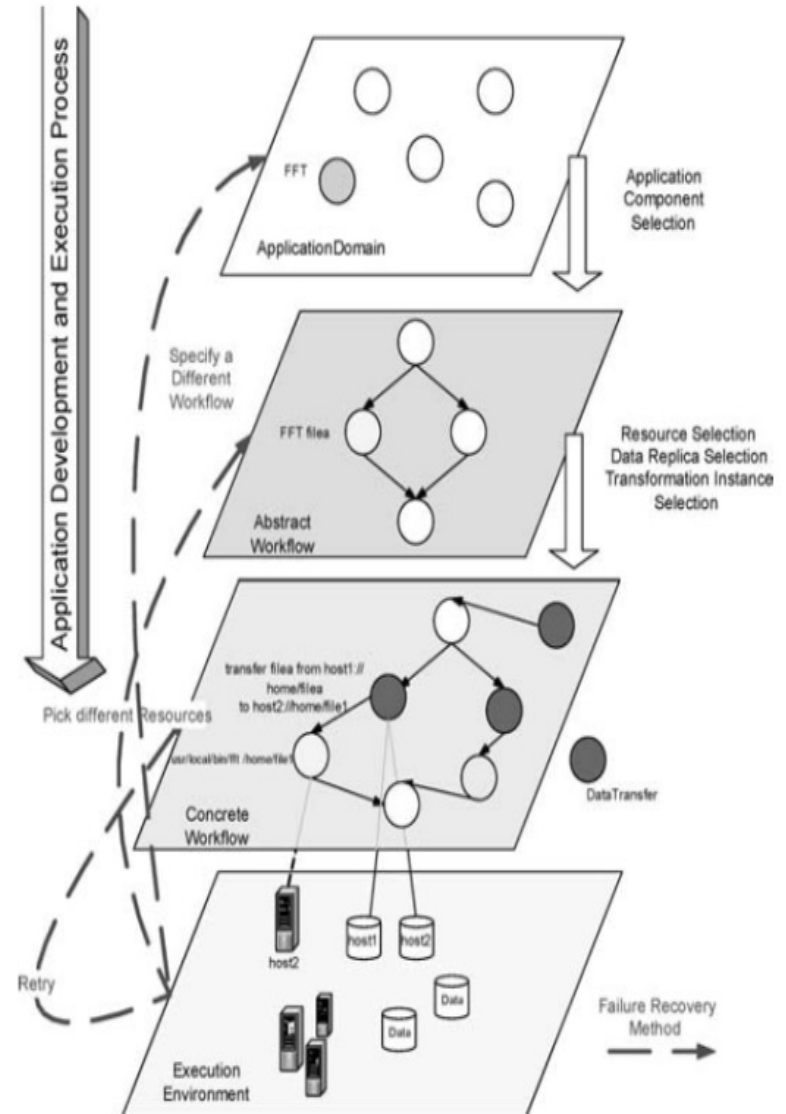
Web Services have been adopted by the new generation of federated and distributed systems

.

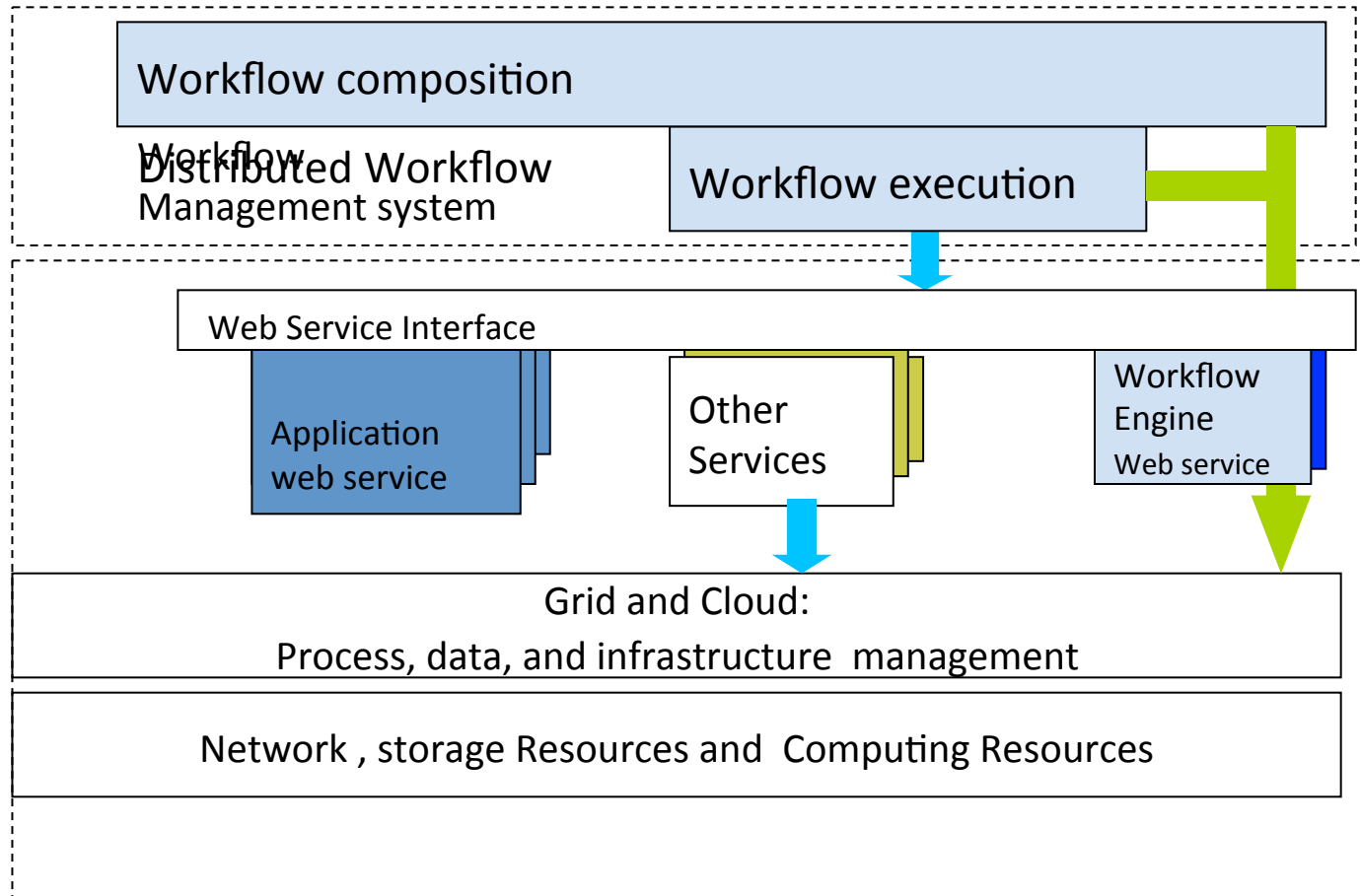
- WS offer **interoperability** and **flexibility** in a large scale distributed environment.
- WS can be **combined** in a **workflow** so that more complex operations may be achieved
  - Application services
  - System services (Grids and Clouds)

# Application development and Execution process

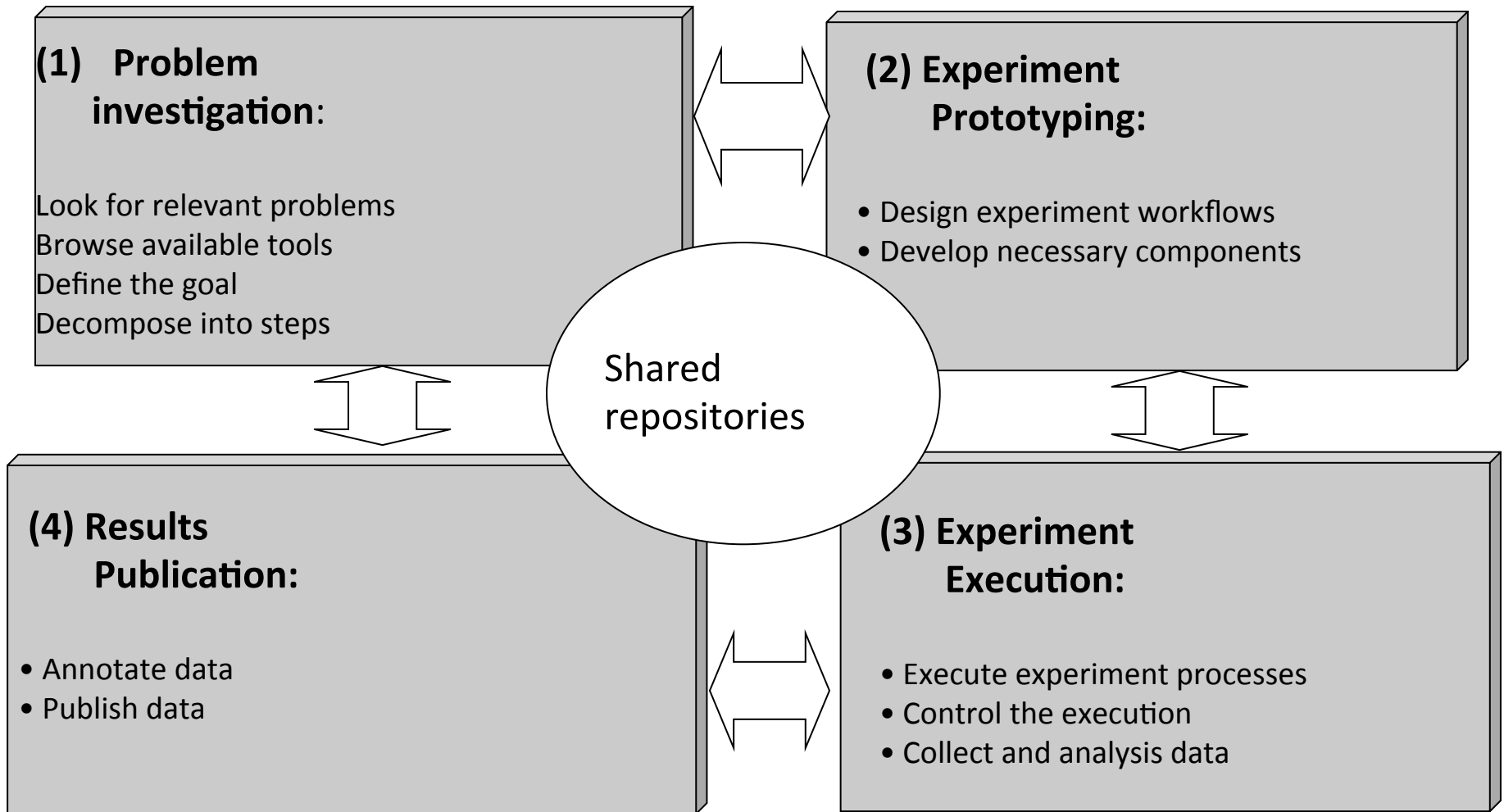
- Select or develop
- Compose the application workflow
- Mapping to actual resource
  - Resource discovery, allocation and management
  - Bind to real computing resource
- Workflow Refinement
  - Modification from the workflow description
  - Reduction of workflow if some data already exist
  - Additional data movement preparation if needed
- Workflow Fault Tolerance & Monitoring of Execution
  - Two level failure recovery techniques
    - Task Level
    - Workflow Level



# Distributed enabled workflow engines

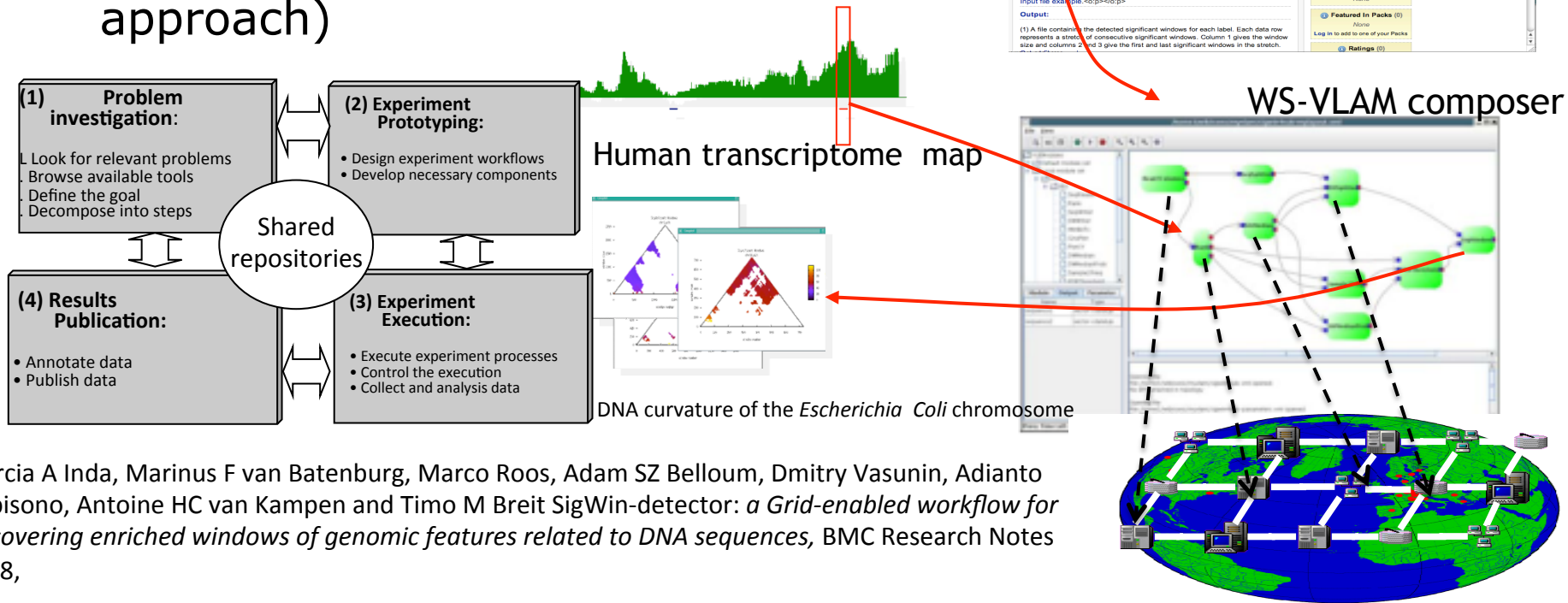


# life cycle of scientific experiments



# life cycle of scientific experiments

- Workflow can be invoked from other systems
- Workflow can be made available to entire community (using Web 2.0 approach)

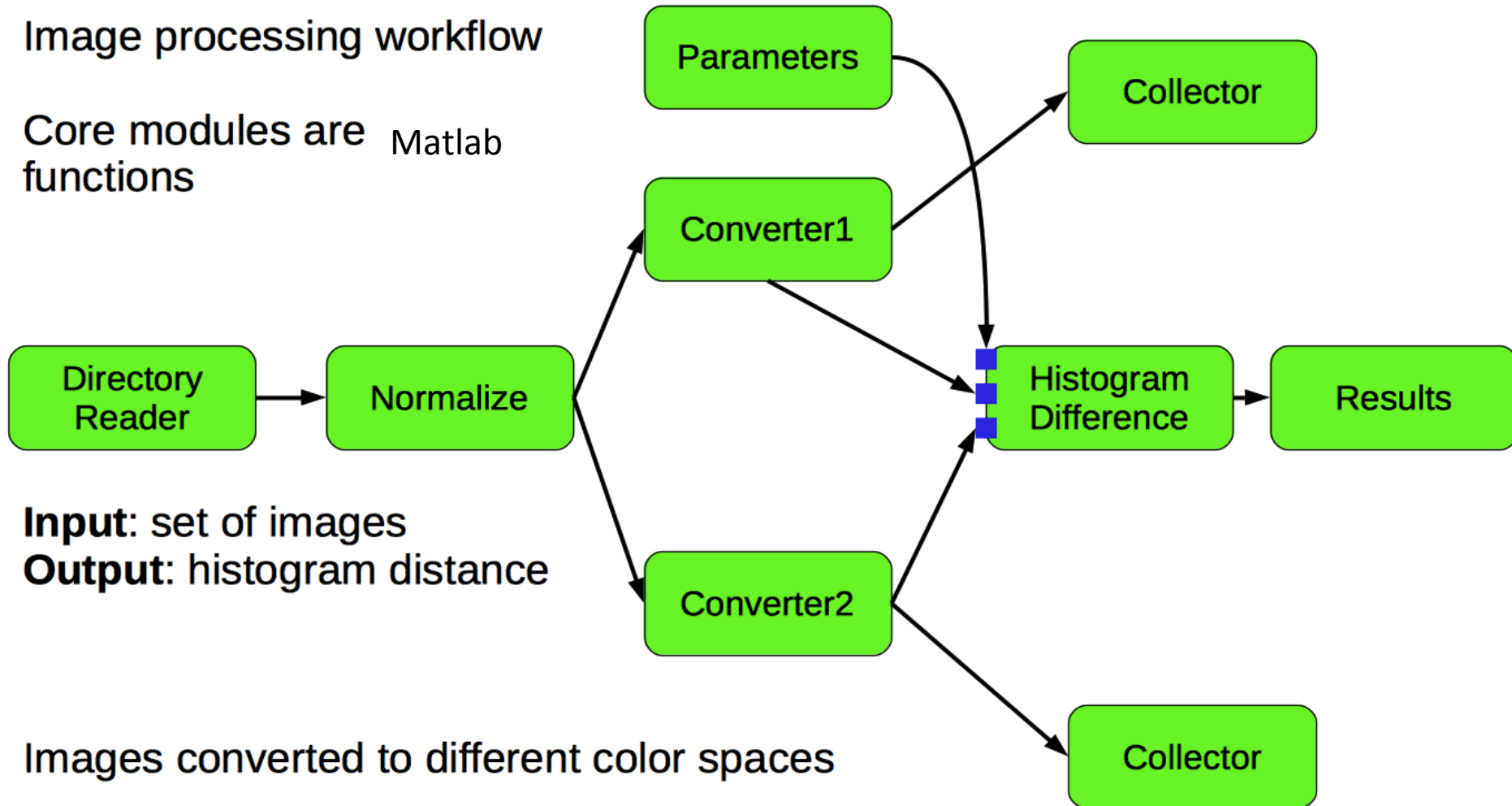


Marcia A Inda, Marinus F van Batenburg, Marco Roos, Adam SZ Belloum, Dmitry Vasunin, Adianto Wibisono, Antoine HC van Kampen and Timo M Breit SigWin-detector: a Grid-enabled workflow for discovering enriched windows of genomic features related to DNA sequences, BMC Research Notes 2008,

# Example of Scientific workflow

Image processing workflow

Core modules are Matlab functions



**Input:** set of images

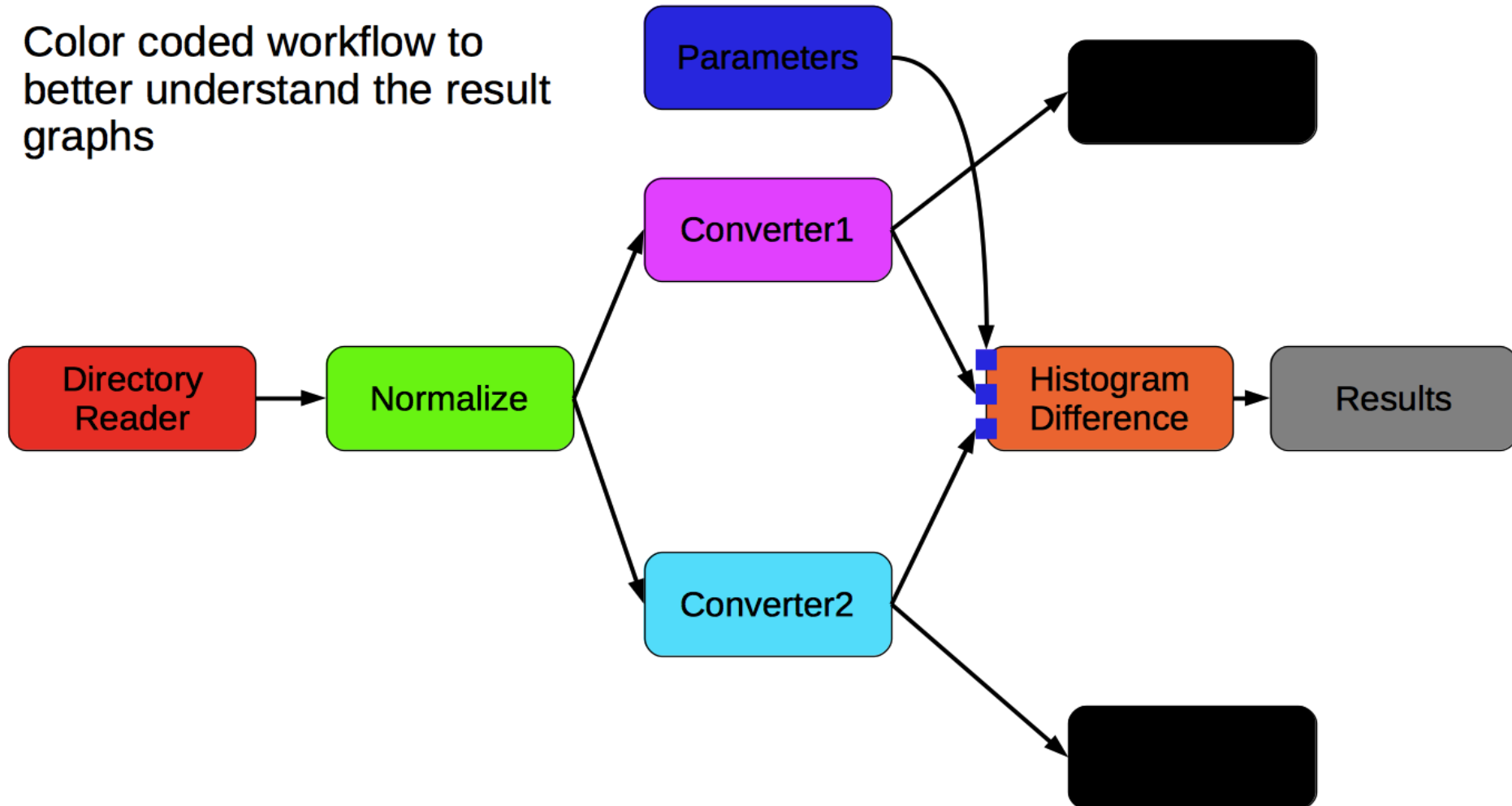
**Output:** histogram distance

Images converted to different color spaces

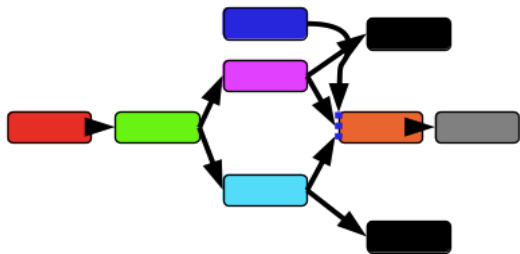
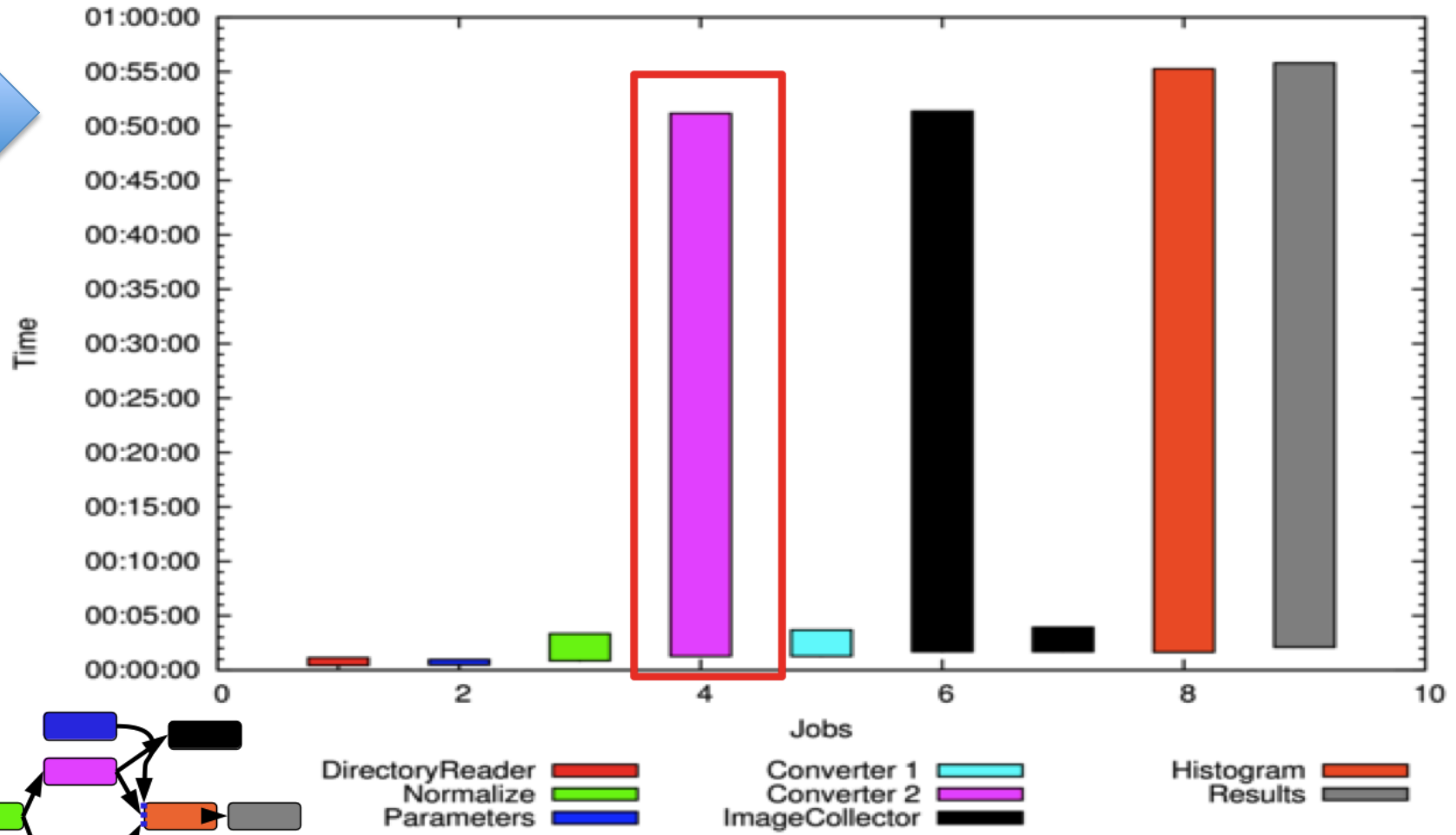
Histogram difference is calculated between color spaces

# Example of Scientific workflow

Color coded workflow to better understand the result graphs



# Workflow Without Scaling

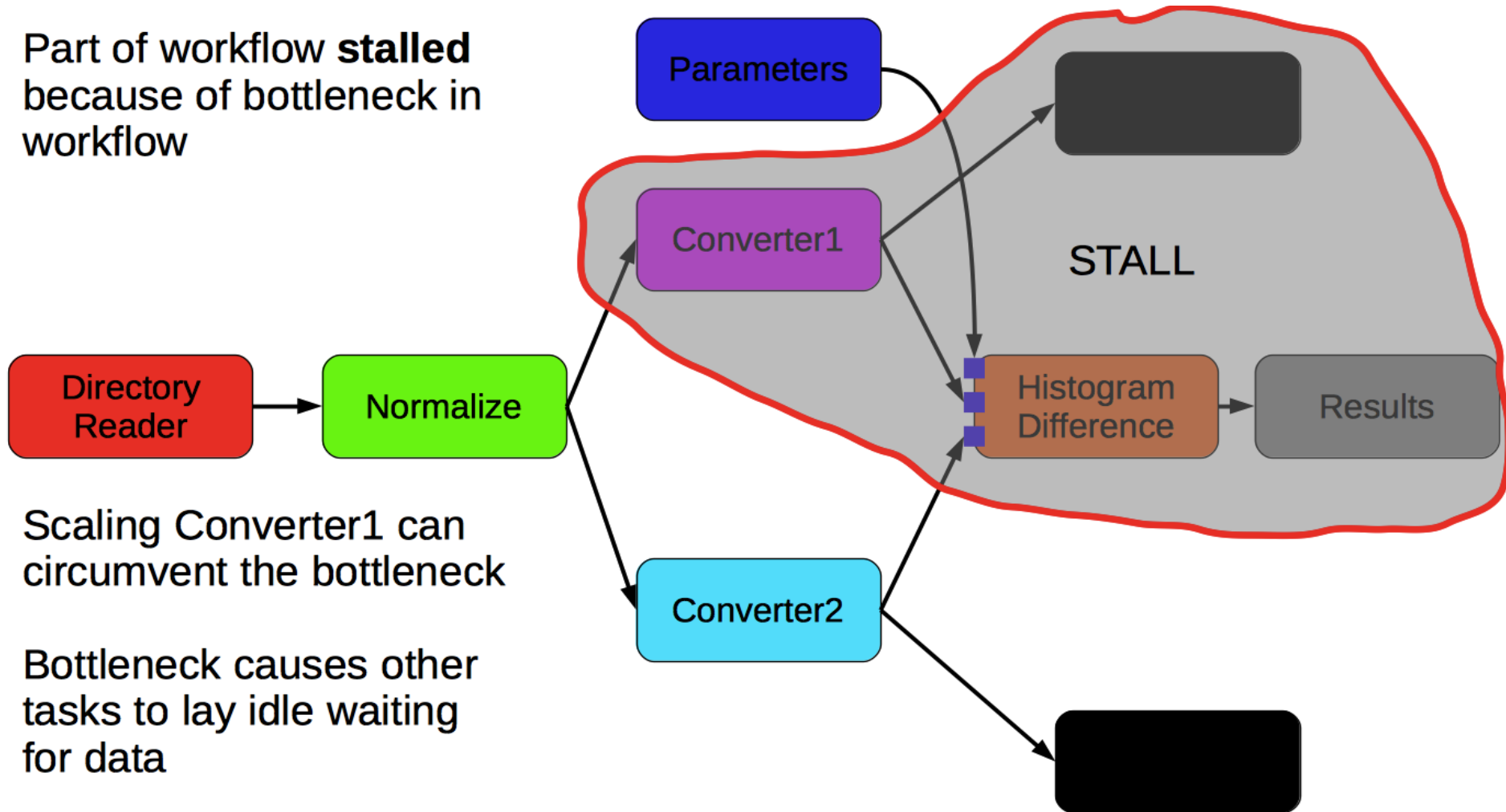


Slow task causing a **bottleneck** in the workflow



# Example of Scientific workflow (1)

Part of workflow **stalled**  
because of bottleneck in  
workflow



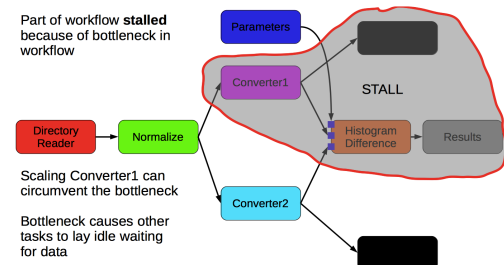
# Zooming into the Task Converter 1



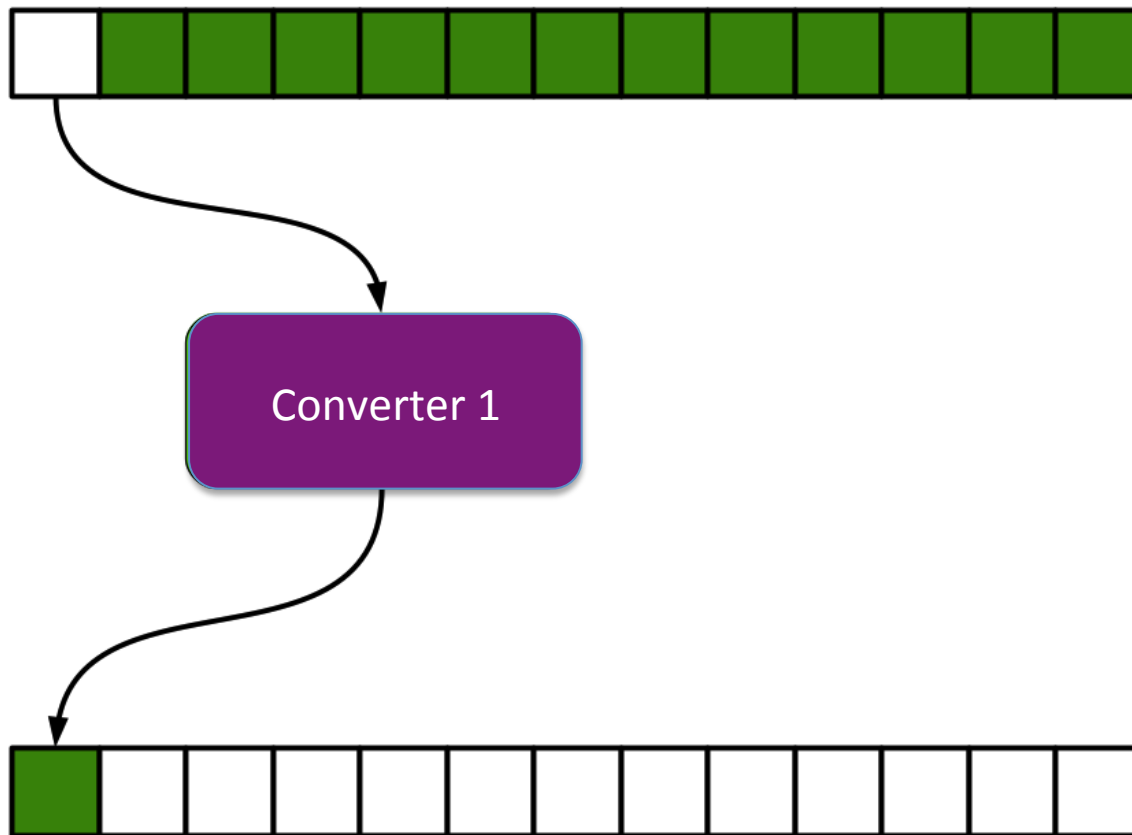
Data organized in  
atomic  
parcels(messages)



Part of workflow **stalled**  
because of bottleneck in  
workflow

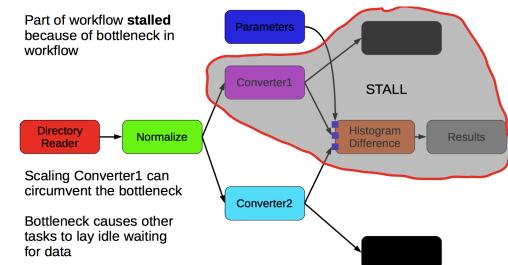


# Zooming into the Task Converter 1

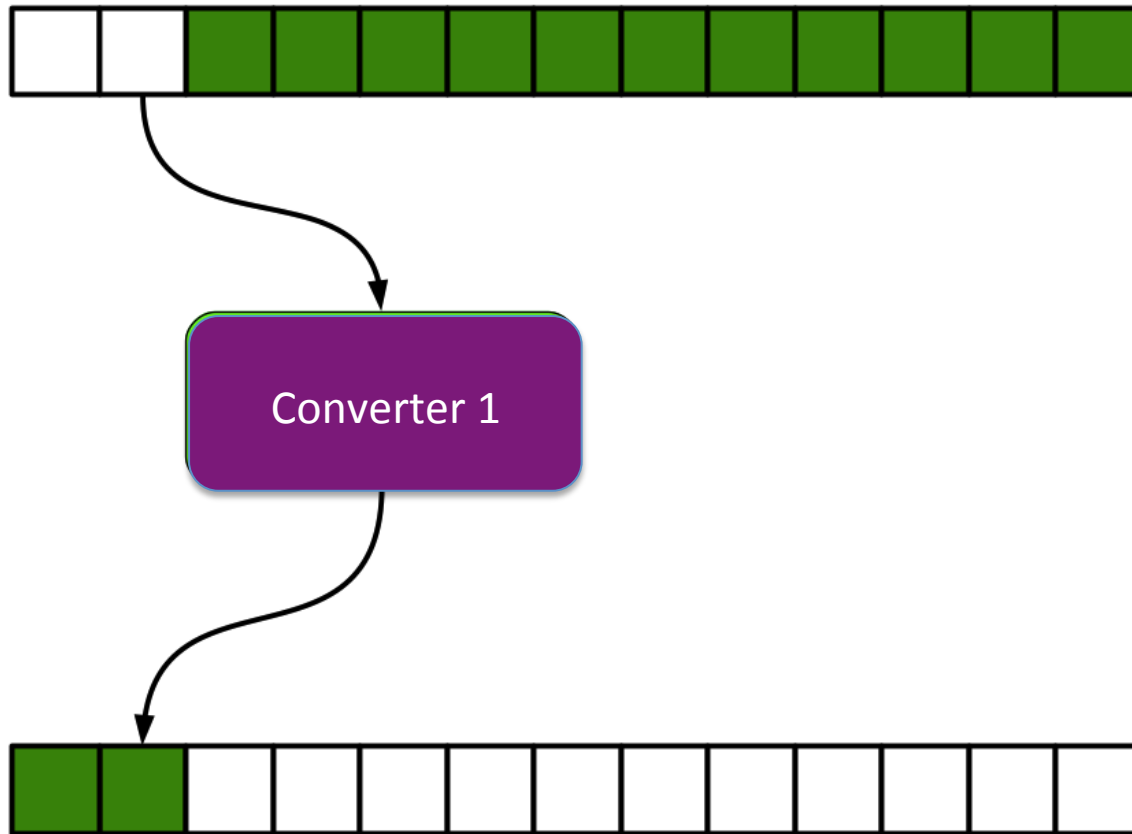


Data organized in atomic parcels(messages)

Task processes data sequentially

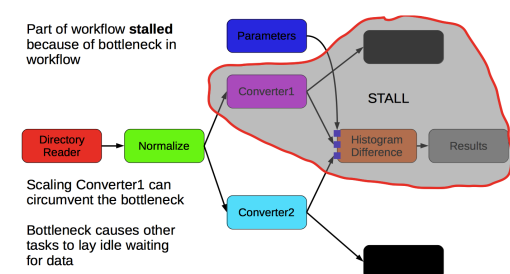


# Scaling Concepts

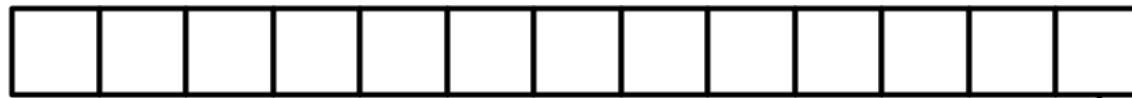


Data organized in atomic parcels(messages)

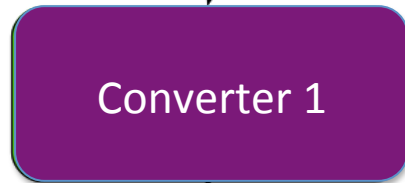
Task processes data sequentially



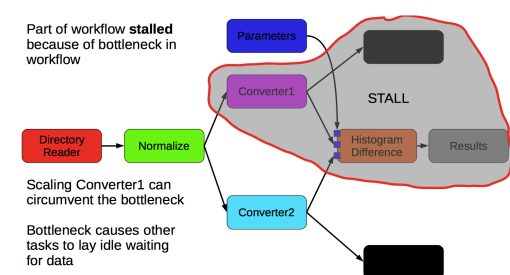
# Zooming into the Task Converter 1



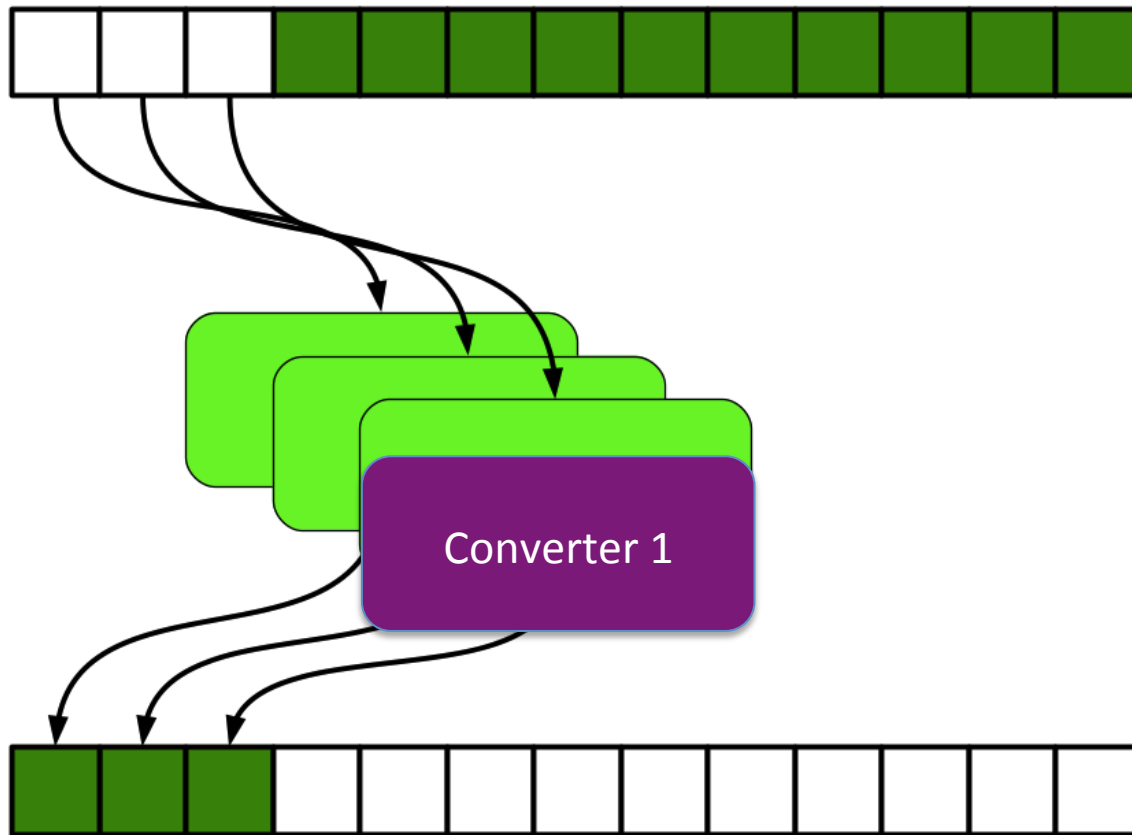
Data organized in atomic parcels(messages)



Task processes data sequentially



# Zooming into the Task Converter 1

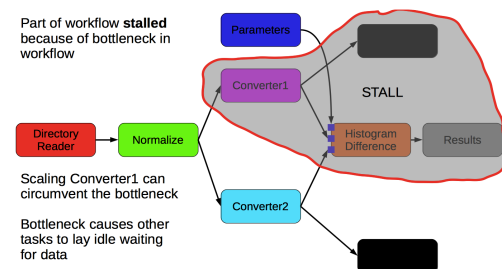


Data organized in  
atomic  
parcels(messages)

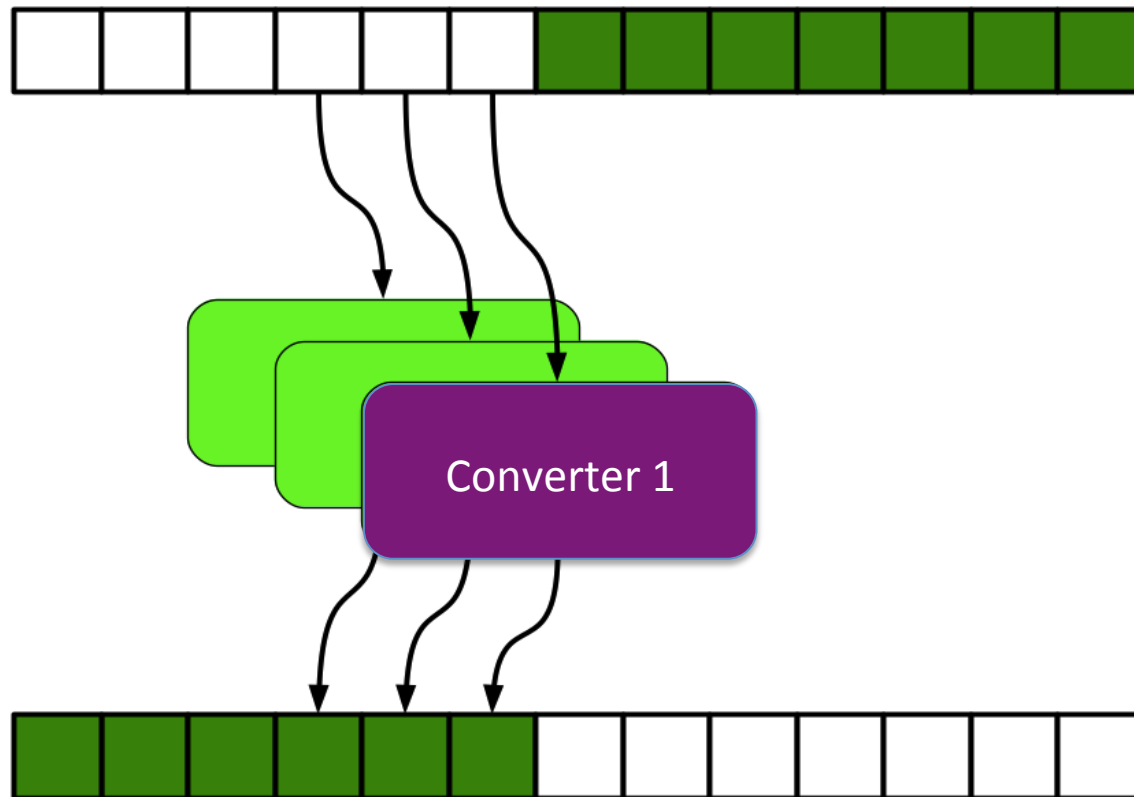
Tasks processes  
data **concurrently**

Adding more tasks  
increases **message  
consumption** rate

Part of workflow **stalled**  
because of bottleneck in  
workflow



# Zooming into the Task Converter 1



Data organized in atomic parcels(messages)

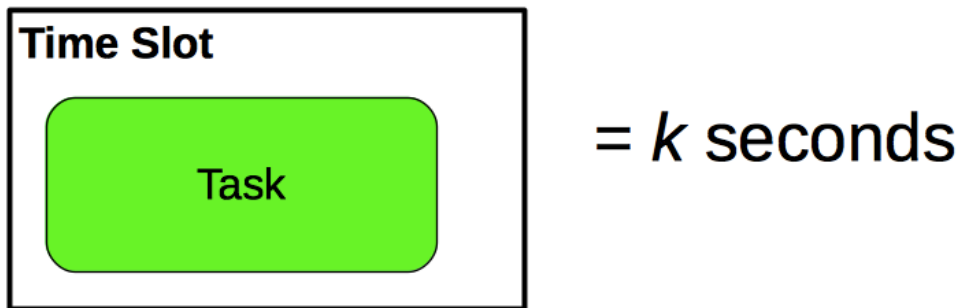
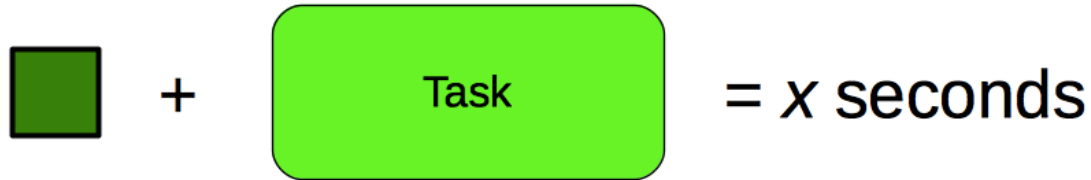
Task processes data sequentially

Adding more tasks increases **message consumption** rate

**Challenge:** How many tasks to create?

Too **many** and tasks get stuck on queues. Too **few** and optimal performance not achieved

# Load Prediction

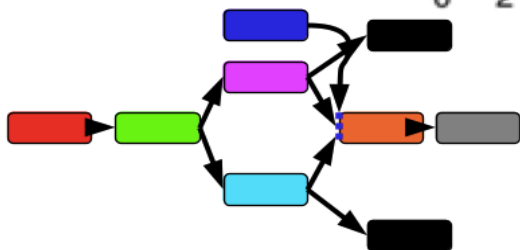
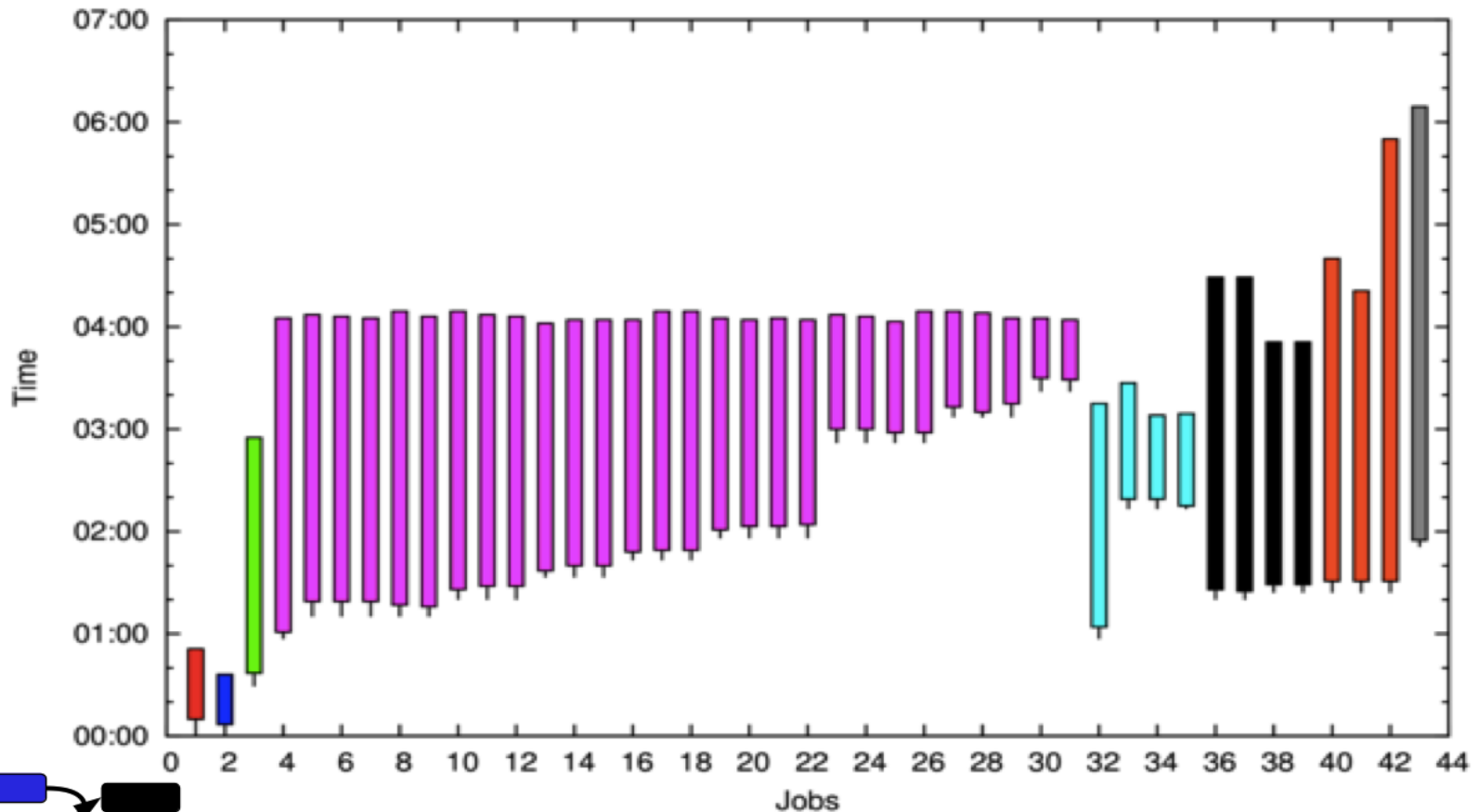


**Simplified Load** =  $6x/k$  time slots

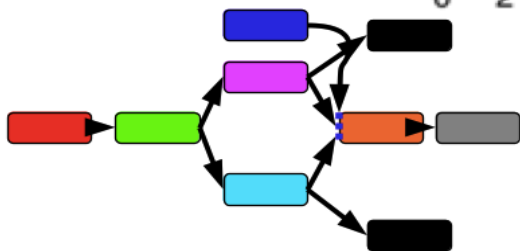
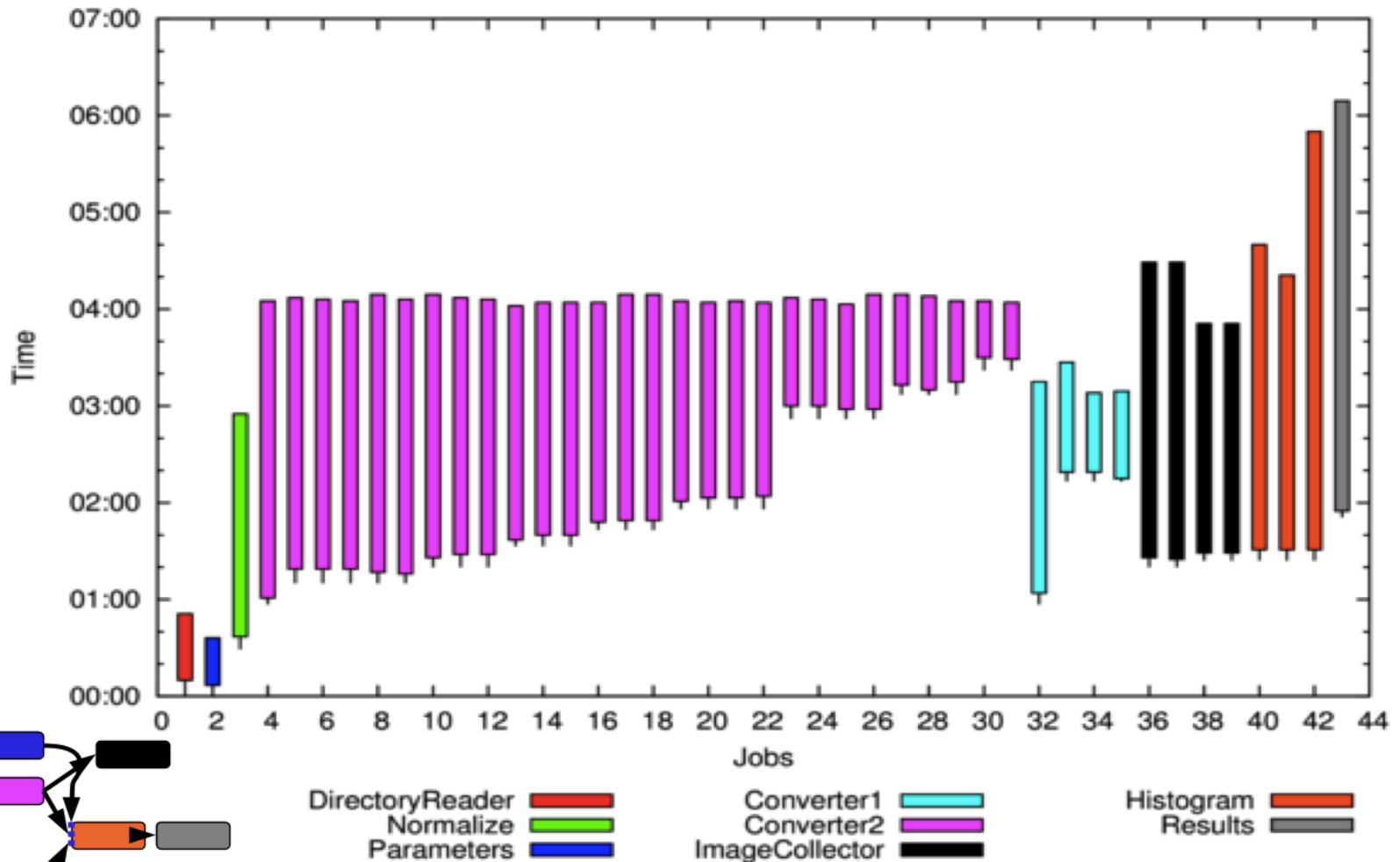
**Assumption:** Size of data directly proportional to computation time. May not always be the case



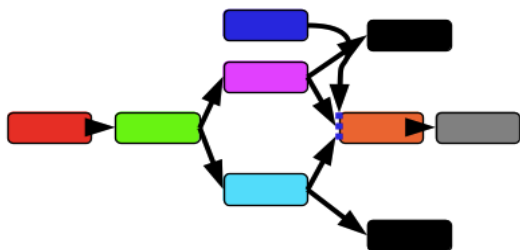
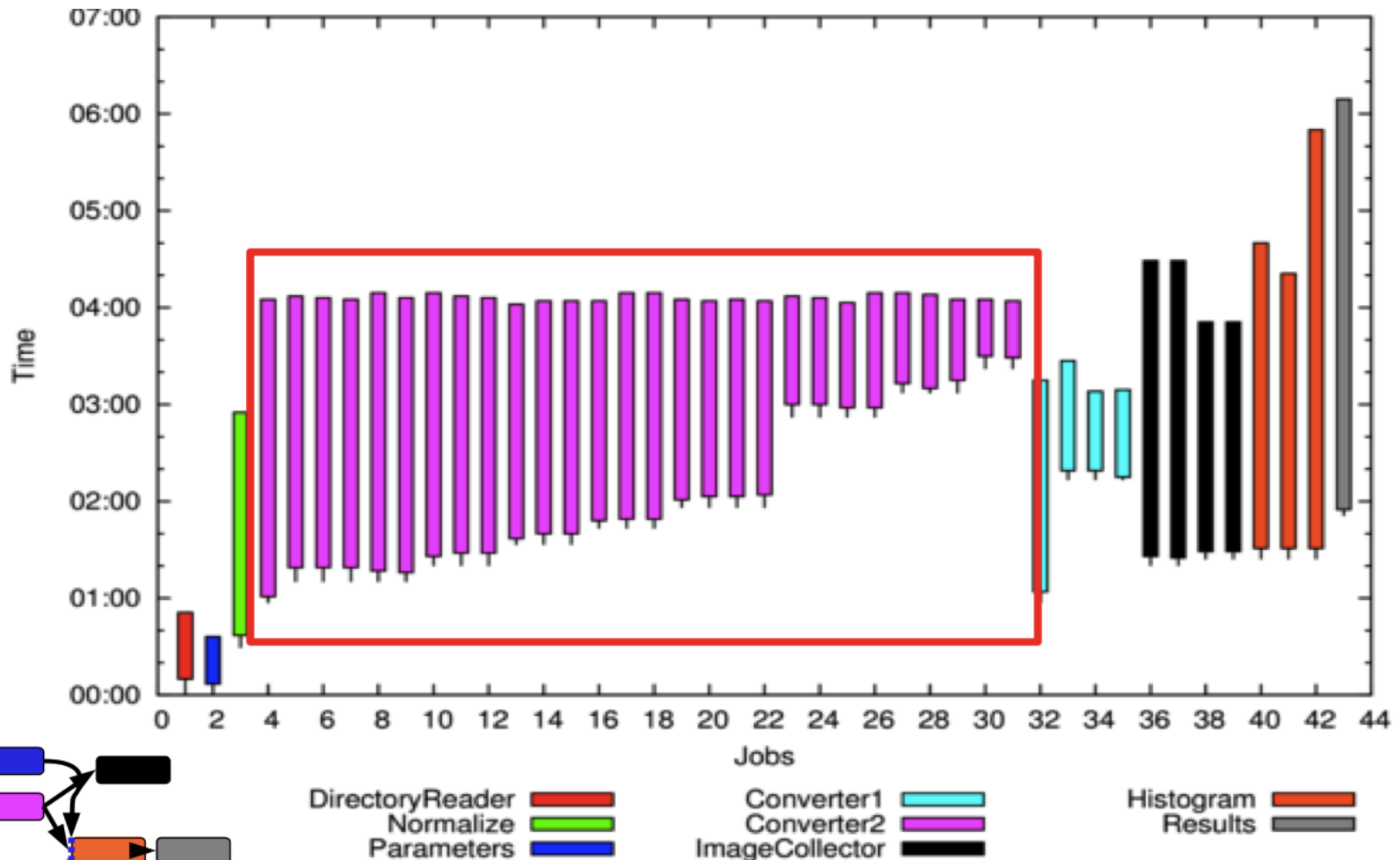
# Workflow execution with Scaling



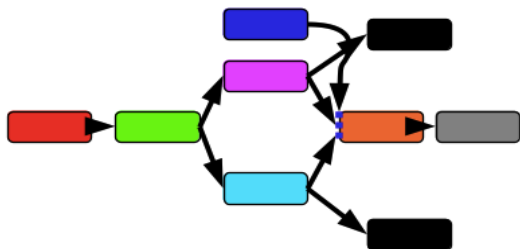
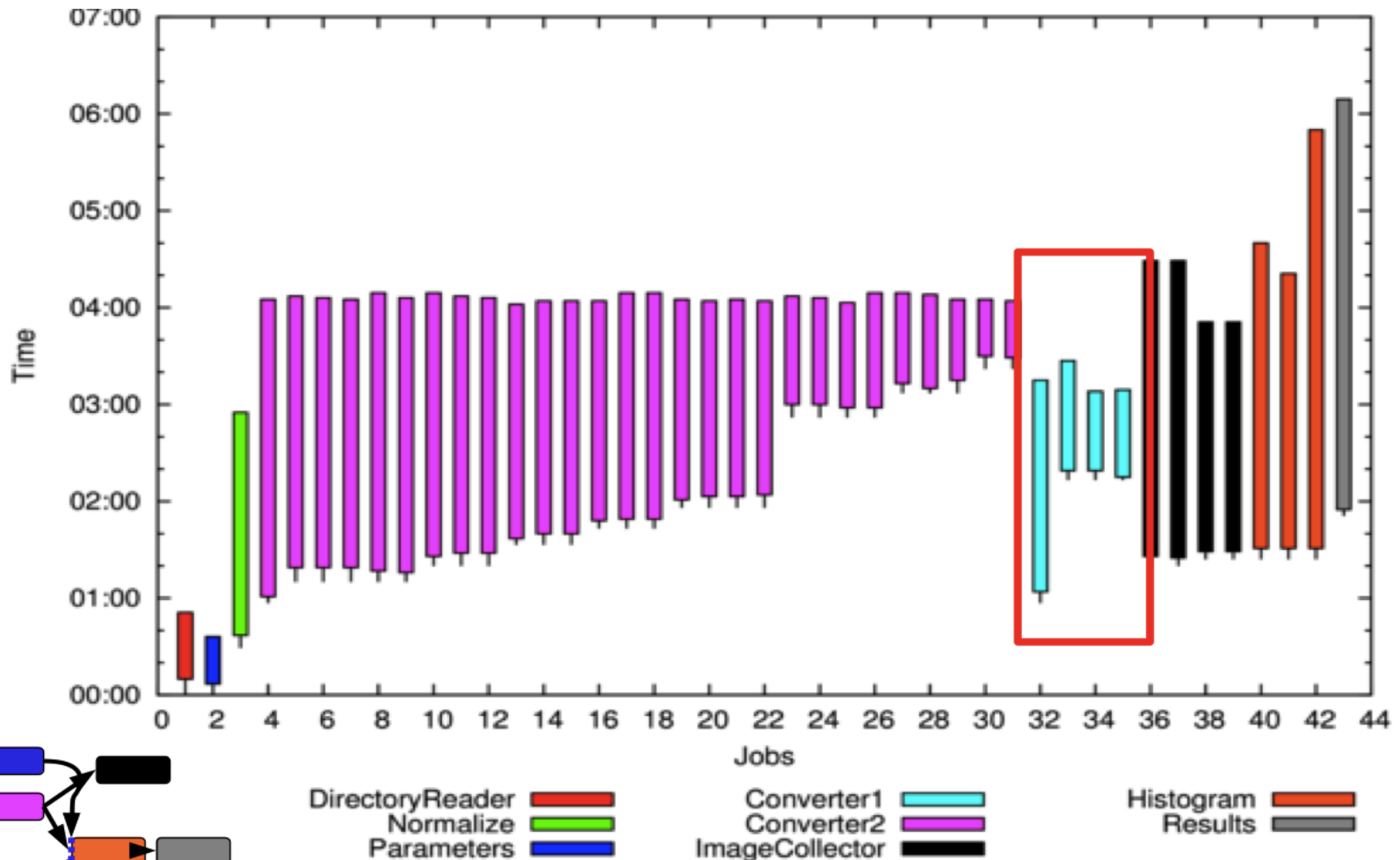
# Workflow execution with Scaling



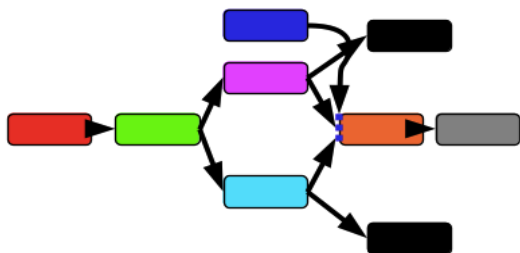
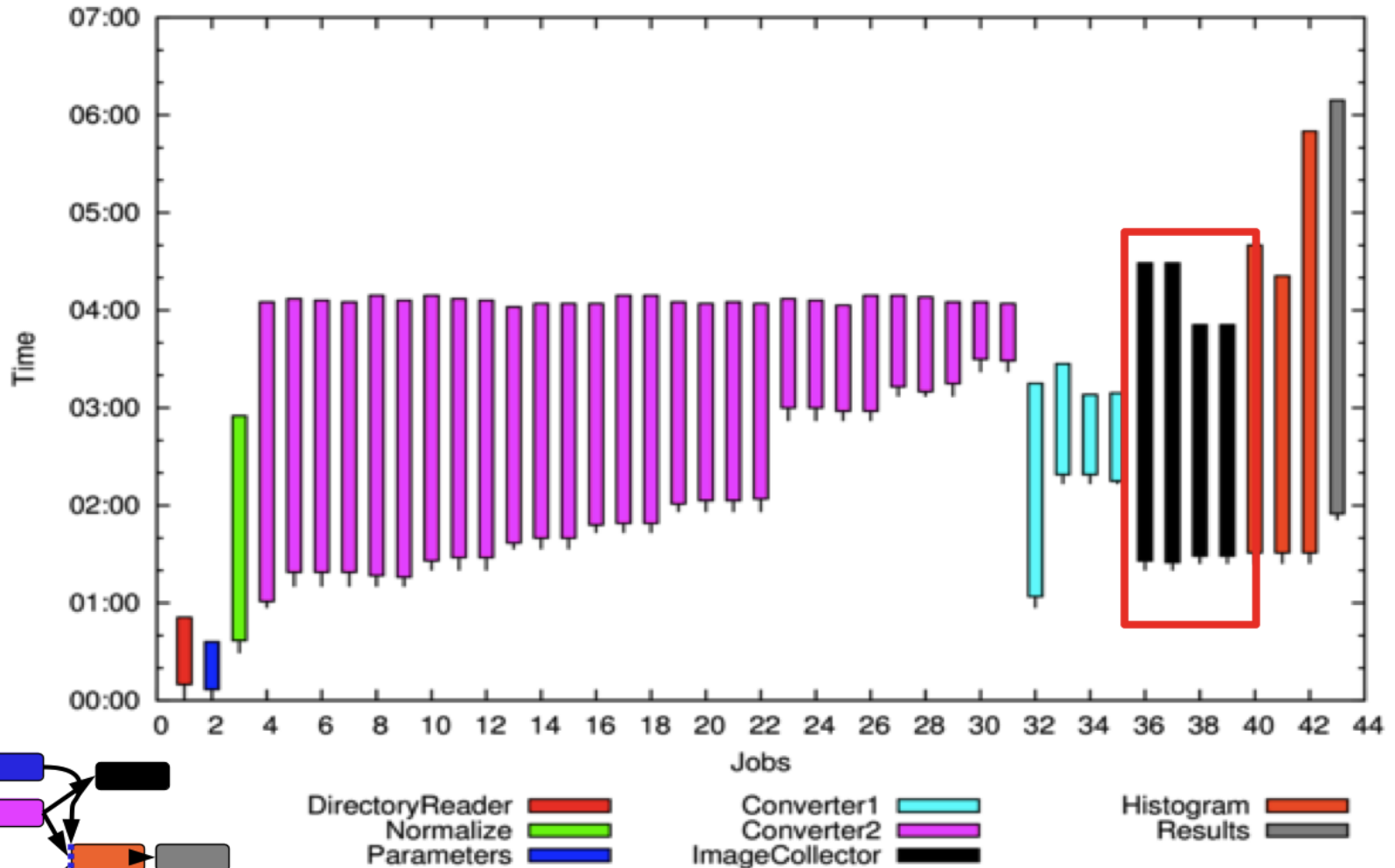
# Workflow execution with Scaling Task -1



# Workflow execution with Scaling Task -2

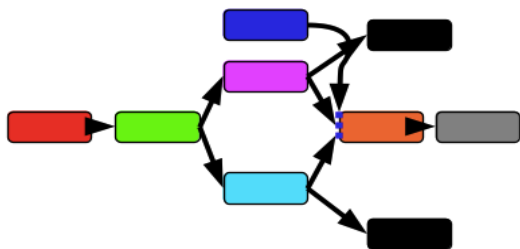
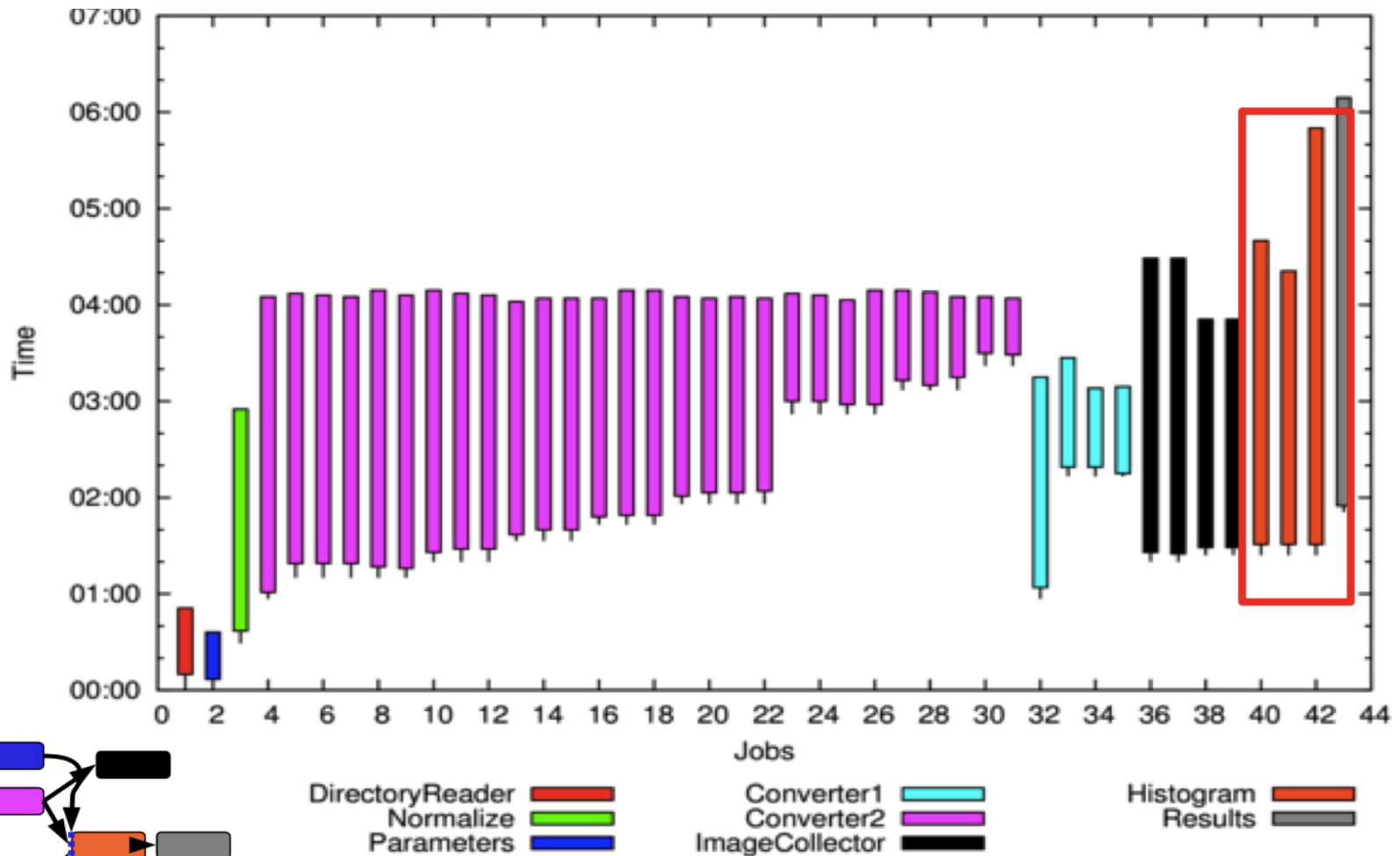


# Other Scaled Task -1



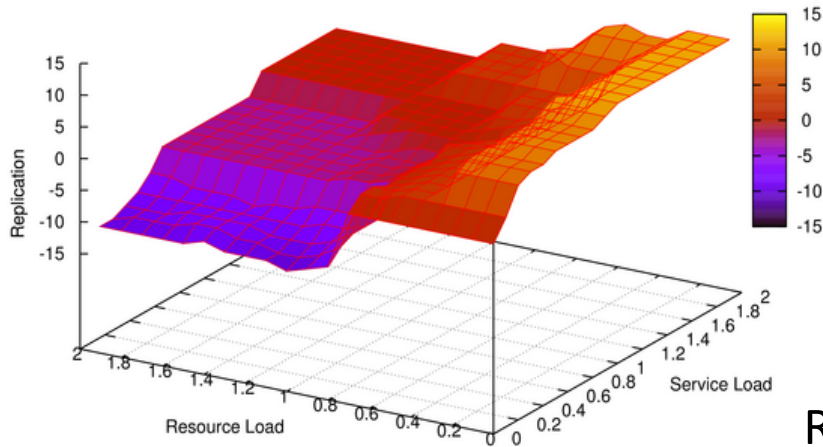
ImageCollector was set to a **fixed** amount (4)

# Auto Scaling Task -2



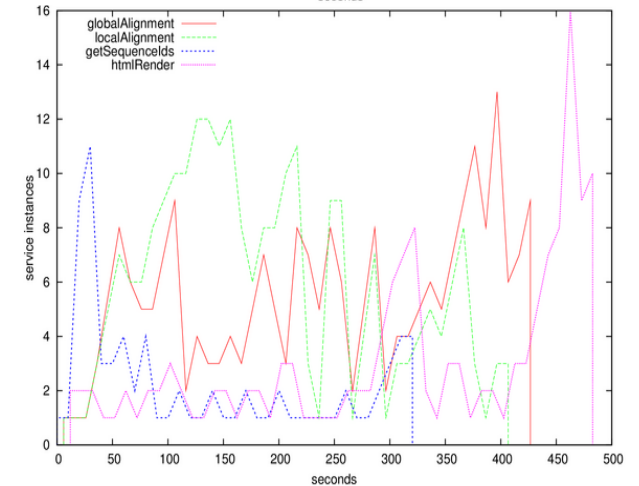
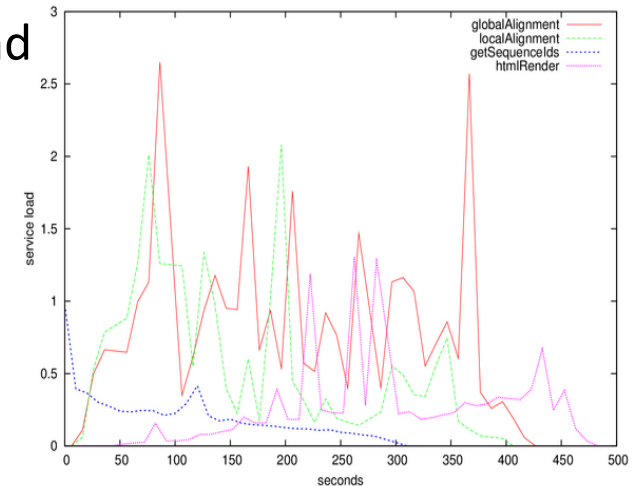
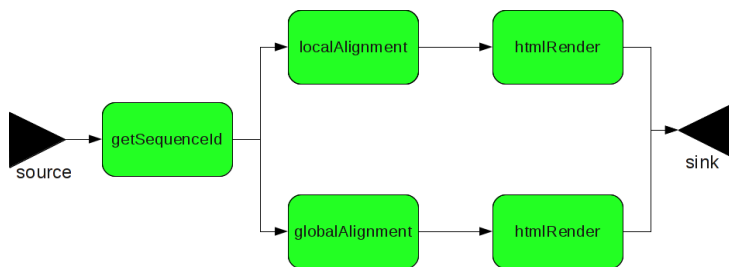
HistogramDifference was set to **one-to-one** scaling.  
Each parameter generates a new task

# Example of Scientific workflow (2)



Service Load

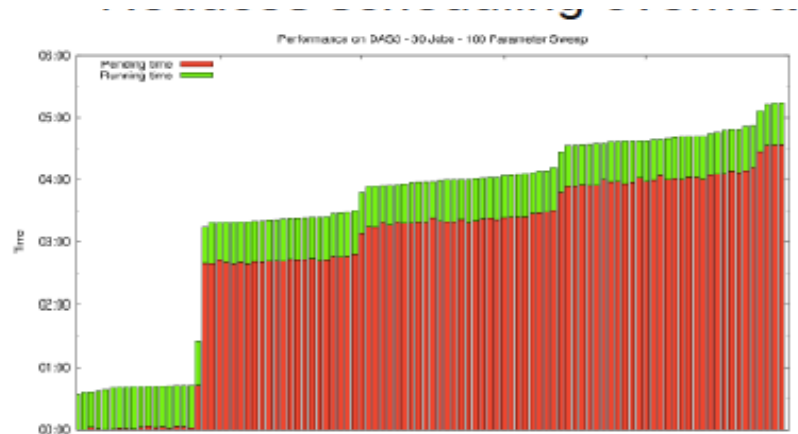
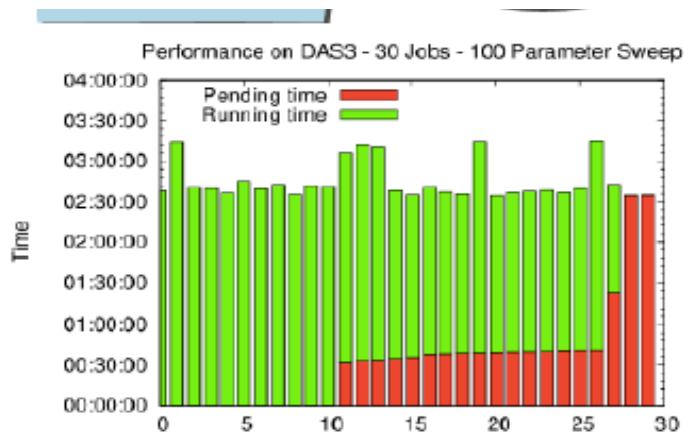
Running Service instances



Reginald Cushing, Spiros Koulouzis, Adam S. Z. Belloum, Marian Bubak, **Dynamic Handling for Cooperating Scientific Web Services**, 7th IEEE International Conference on e-Science, December 2011, Stockholm, Sweden

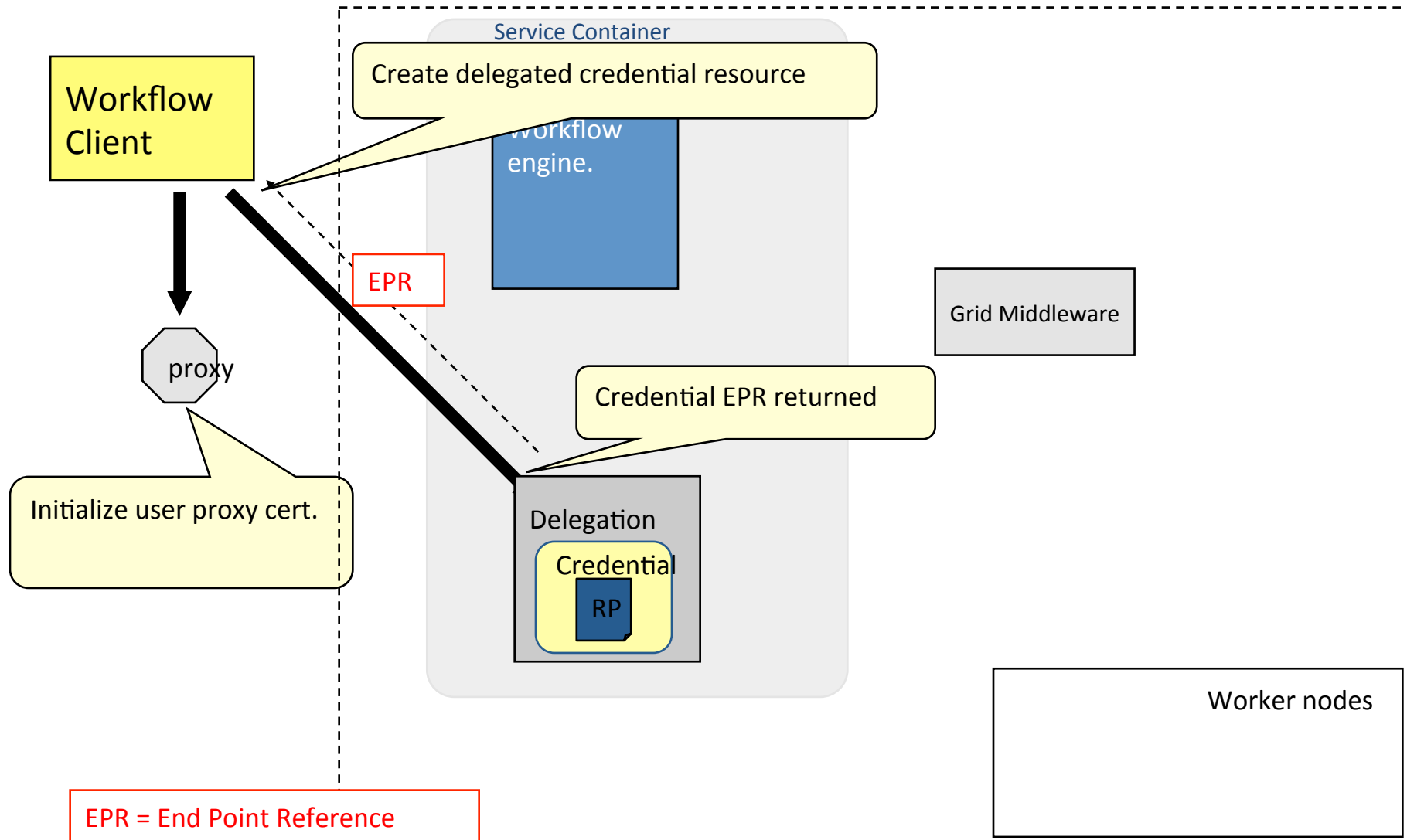
# Workflow as a Service (WFaaS)

- Once a workflow is initiated on the resources it stays alive and process data/jobs continuously
- Reduce the scheduling overhead

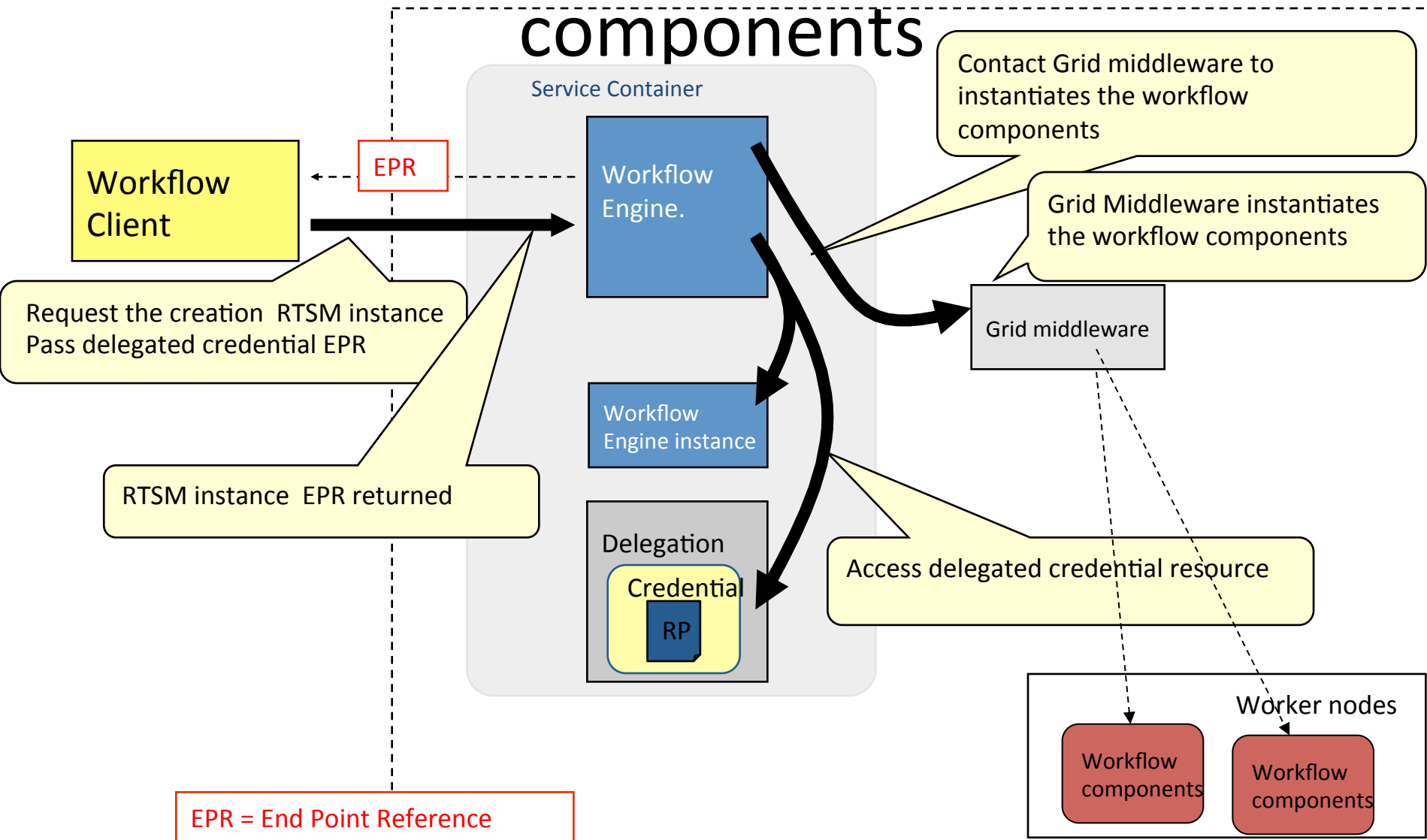




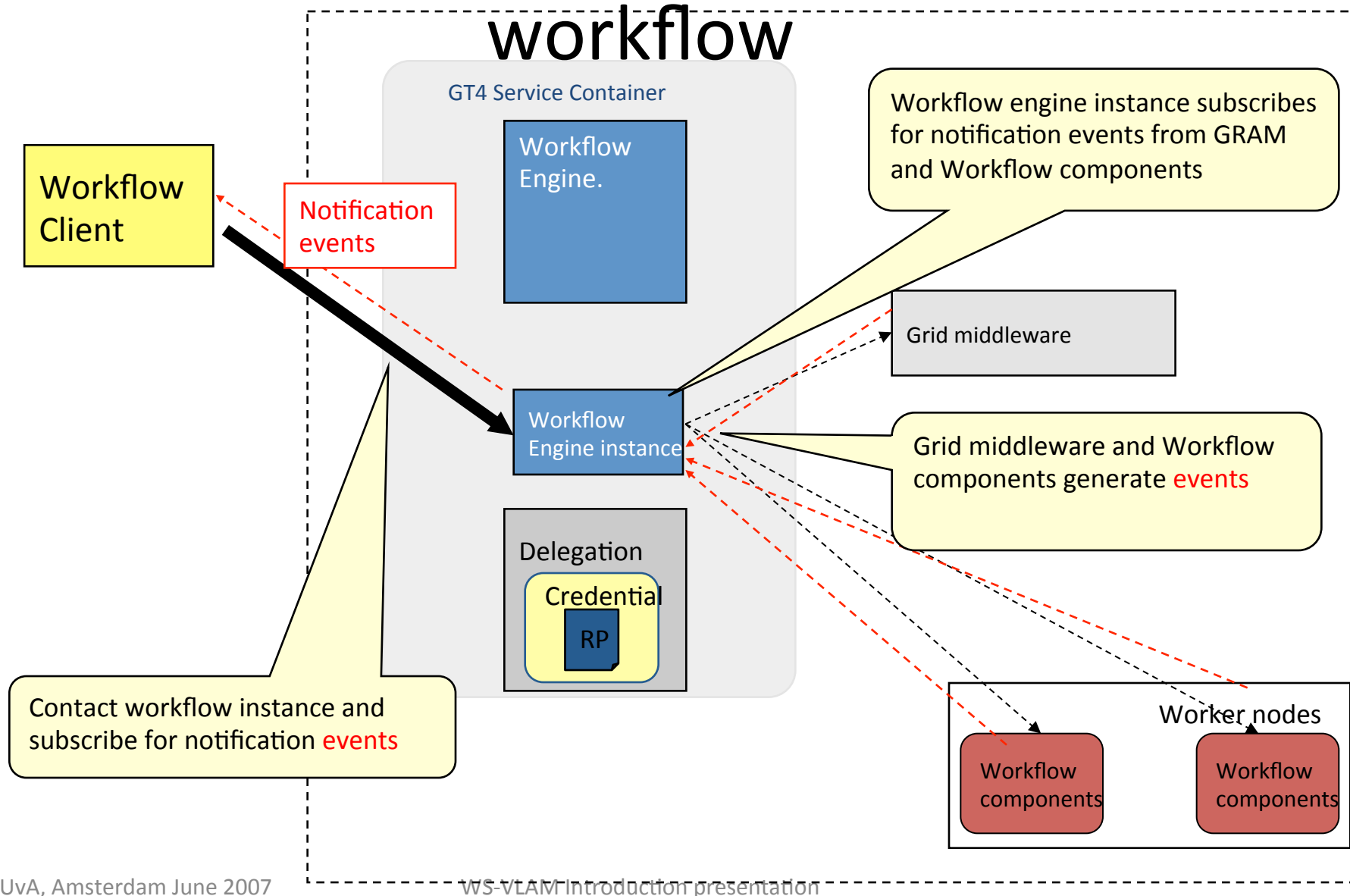
# Step1: Create Delegated Credential



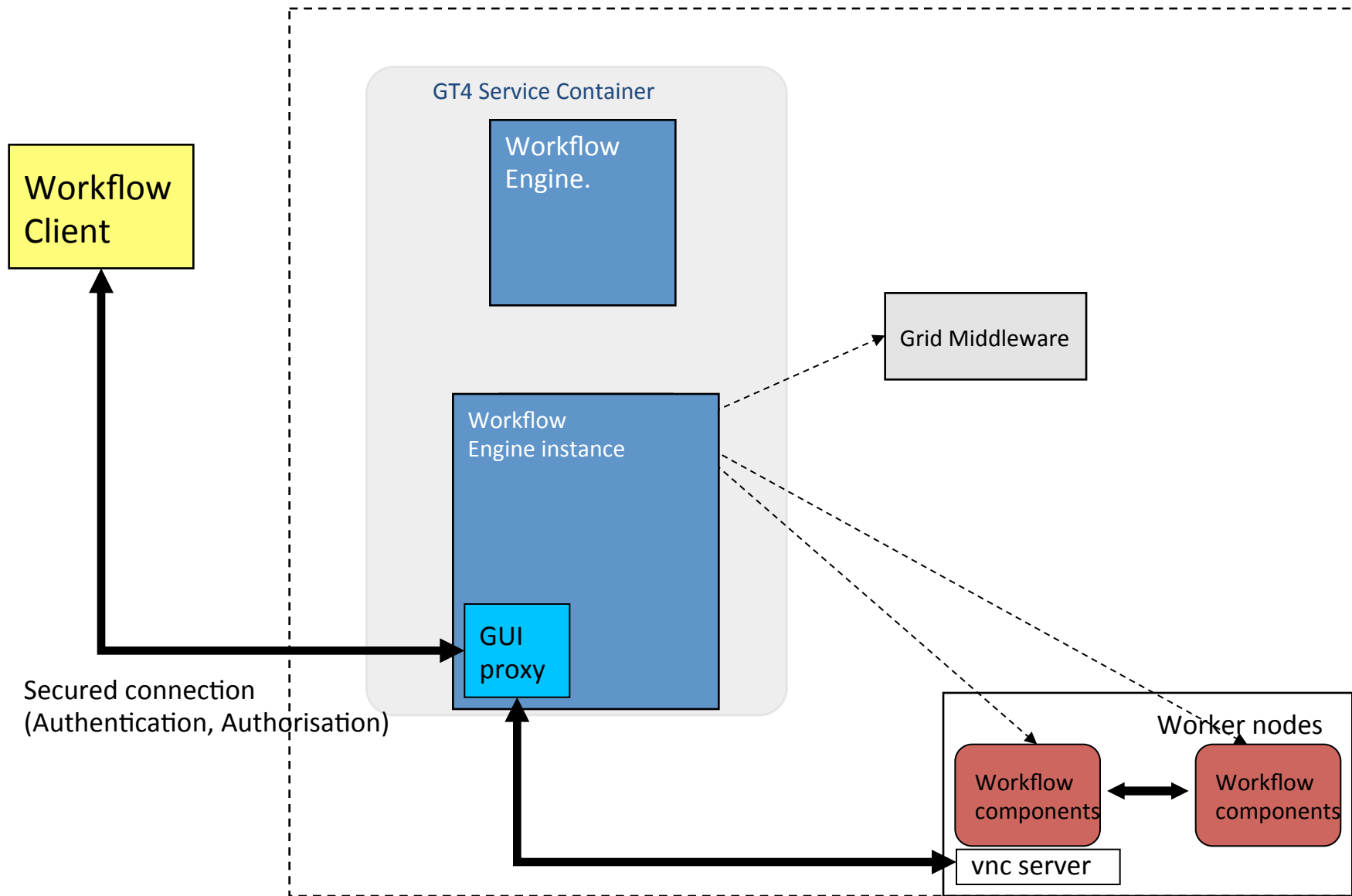
# Step 2: instantiates the workflow



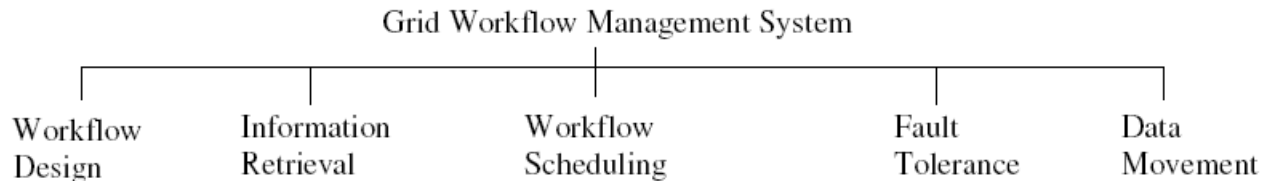
# Step3: monitors the application



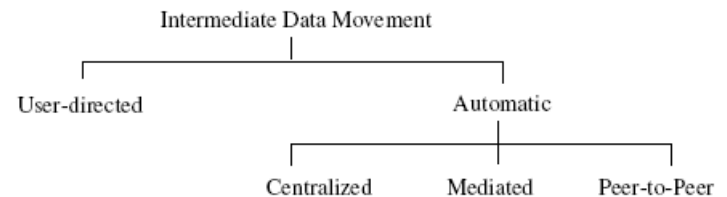
# Workflow components with graphical output



# Workflow Taxonomy



- For Grid workflow applications,
  - the **input files** of tasks need to be staged to a remote site before processing the task.
  - Similarly, **output files** may be required by their children tasks which are processed on other resources.
- The **intermediate** data has to be staged out to the corresponding Grid sites.



A Taxonomy of Workflow Management Systems for Grid Computing

Jia Yu and Rajkumar Buyya, <http://www.cloudbus.org/reports/GridWorkflowTaxonomy.pdf>

# Component Based Workflow Description: Triana

PROBLEM SOLVING THE OPEN SOURCE ENVIRONMENT

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## Feature Highlights

⚙️ Modular Java Workflow Environment

📊 Triana Cloud Job Queuing

🔧 10 Plus Years of Proven Technology

🖱️ Sophisticated Drag & Drop Composition

🌐 Web Services

📦 Comprehensive Toolbox Libraries

## What is it?

An open source problem solving environment developed at Cardiff University that combines an intuitive visual interface with powerful data analysis tools. Already used by scientists for a range of tasks, such as signal, text and image processing, Triana includes a large library of pre-written analysis tools and the ability for users to easily integrate their own tools.

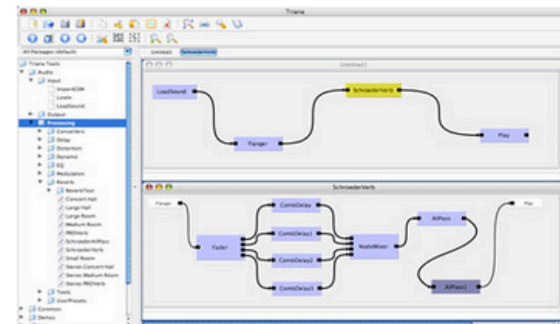
[Learn more](#)

## How do I get it?

Go to our [DOWNLOADS](#) page to get our latest build release.



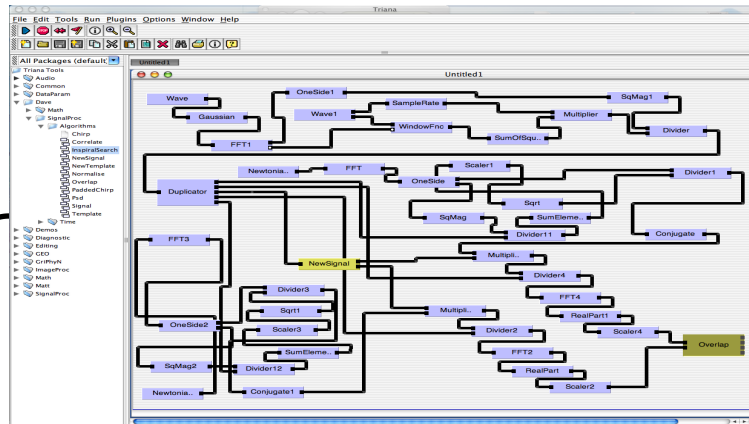
## What does it look like?



# Triana, the GAT and the GAP

## Grid Computing:

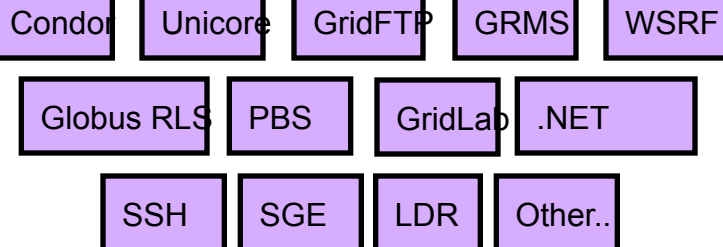
Job Submission,  
data services  
On top of a  
number of Grid  
Middleware



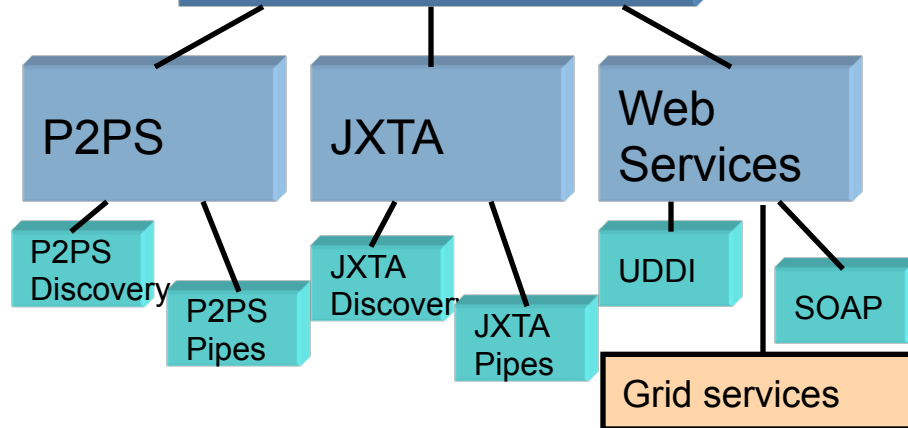
## Service Based Computing:

Deployment,  
discovery and  
communication  
with distributed  
services e.g. P2P  
and (GSI) Web  
services


GAT Interface



GAP Interface



# Component Based Workflow Description: Kepler



The banner features the Kepler logo with the tagline "Your Science. Enabled." on the left. In the center is a diagram of a workflow with green rectangular components connected by blue arrows. On the right is a search bar with the text "Search Site" and a "search" button, with a checkbox option "only in current section" below it.

user developer

you are here: home

navigation

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- Add-on Modules
- Kepler Features
- Sample Workflows
- Example Projects Using Kepler
- Documentation
- What's New
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## The Kepler Project

The Kepler Project is dedicated to furthering and supporting the capabilities, use, and awareness of the free and open source, scientific workflow application, Kepler. Scientists, analysts, and computer programmers create, execute, and share models and analyses across a broad range of scientific and engineering disciplines. Kepler supports a variety of formats, locally and over the internet, and is an effective environment for integrating disparate software components, such as merging "R" scripts with compiled code. Kepler also supports the distributed execution of models. Using Kepler's graphical user interface, users simply select and then connect pertinent analytical components and data sources to create an executable representation of the steps required to generate results. The Kepler software helps users share and reuse data, workflows, and components developed by others to address common needs.

The Kepler software is developed and maintained by the cross-project Kepler collaboration, which is led by a team consisting of several of the key institutions that have contributed to the development of Kepler, including the University of California, Santa Barbara, and UC San Diego. Primary responsibility for achieving the goals of the Kepler Project reside with the Leadership Team, which works to assure the long-term viability of Kepler by making strategic decisions on behalf of the Kepler user community, as well as providing an official and durable point-of-contact to articulate the vision and goals of the Kepler Project and the Kepler software application. Details about how to get more involved with the Kepler Project can be found in the [developer](#) section of this website.


Kepler is a java-based application that is maintained for the Windows, OSX, and Linux operating systems. The Kepler Project supports the official code-base for Kepler and provides materials and mechanisms for learning how to use Kepler, sharing experiences with other workflow developers, reporting bugs, suggesting enhancements, etc.

Download Kepler





# Program/Application: workflow Based: Taverna



## Taverna

myGrid

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### Taverna Workflow Management System

Powerful, scalable, open source & domain independent tools for designing and executing workflows. Access to 3500+ resources.

#### RECENT NEWS

- Data Refinement paper published
- AstroTaverna—Building workflows with Virtual Observatory services
- Modelling the sun with Taverna
- Starting now — the Taverna Open Development Workshop

[Workbench](#) [Server](#) [Player](#) [Command Line](#) [Taverna Online](#)

#### COMMUNITY

- Taverna for astronomy, bioinformatics, biodiversity, digital preservation
- Workflow components
- Taverna 3 OSGi
- Taverna Online
- Next generation sequencing on Amazon cloud
- Taverna-Galaxy

**Taverna** is an open source and domain-independent [Workflow Management System](#) – a suite of tools used to design and execute scientific workflows and aid *in silico* experimentation.

Taverna has been created by the [myGrid team](#) and is currently funded through FP7 projects [BioVeL](#), [SCAPE](#) and [Wf4Ever](#).

The Taverna tools include the [Workbench](#) (desktop client application), the [Command Line Tool](#) (for a quick execution of workflows from a terminal), the [Server](#) (for remote execution of workflows) and the [Player](#) (Web interface plugin for submitting workflows for remote execution). [Taverna Online](#) lets you create Taverna workflows from a Web browser.

#### Taverna is moving to the Apache Incubator


Taverna has been [accepted as an Apache Incubator project](#). In short, this means:

- Taverna 2.5.1 will be last non-Apache release
- Open Development process
- Development infrastructure hosted by [apache.org](#)

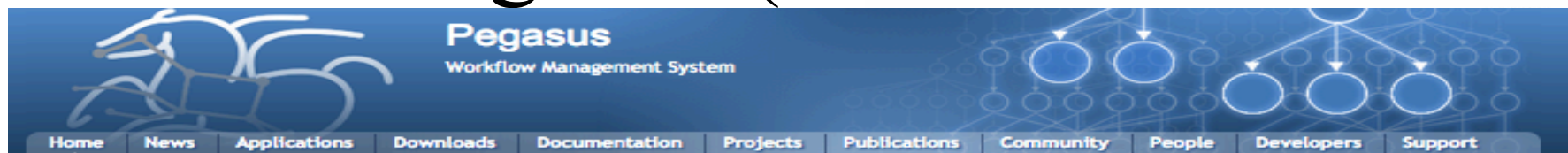
#### See Taverna in action



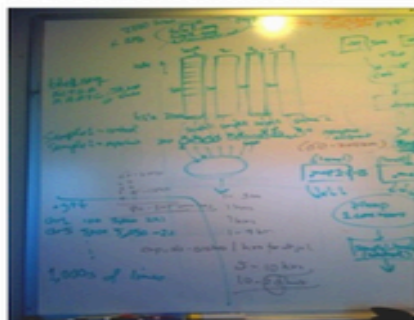
#### Integrated with other myGrid tools

- [my experiment](#) – workflow sharing environment for scientists
- [BioCatalogue](#)  – curated catalogue of Web services

# Pegasus (GriPhyN)



If You can draw....

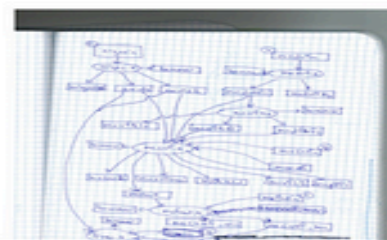


We can make it run....



Epigenomics,  
Ben Berman,  
USC

PSOCI  
( Solar  
Fuels )  
Jeff  
Tilson,  
RENCI



Helio-Seismology : Laurent Gizon, Max Planck

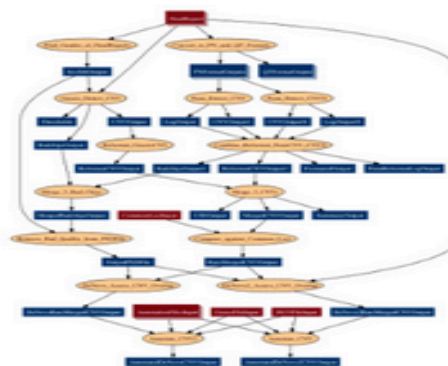
Pegasus receives a new round of NSF funding

## What are scientific workflows?

Scientific workflows allow users to easily express multi-step computational tasks, for example retrieve data from an instrument or a database, reformat the data, and run an analysis. A scientific workflow describes the dependencies between the tasks and in most cases the workflow is described as a directed acyclic graph (DAG), where the nodes are tasks and the edges denote the task dependencies. A defining property for a scientific workflow is that it manages data flow. The tasks in a scientific workflow can be everything from short serial tasks to very large parallel tasks (MPI for example) surrounded by a large number of small, serial tasks used for pre- and post-processing.

## Pegasus overview

The Pegasus project encompasses a set of technologies that help workflow-based applications execute in a number of different environments including desktops, campus clusters, grids, and clouds. Pegasus bridges the scientific domain and the execution environment by automatically mapping high-level workflow descriptions onto distributed resources. It automatically



## News

Pegasus 4.4.1 Released - Dec 2014

Seminar by Dan Katz:  
Building and Linking Local,  
Regional, and National  
Cyberinfrastructure to  
Advance Science - Dec  
2014

Seminar by Rizos  
Sakellariou: Scheduling  
workflows on platforms  
where energy matters -  
Nov 2014

Pegasus at SC'14 - Nov  
2014

The Pegasus team along  
with researchers at ORNL:  
Jeff Vetter, LBNL: Brian  
Tierney, RENC: Anirban  
Mandal, and RPI: Chis  
Carothers receive funding  
from DOE for the  
Panorama project:  
Predictive Modeling and  
Diagnostic Monitoring of  
Extreme Science  
Workflows - Nov 2014

Pegasus GT-FAR Cloud  
Solution at ASHG 2014 -  
Oct 2014

Seminar by Michael  
McLennan: HUBzero:  
Gateways to Pegasus and  
More - Oct 2014

Workflow and Data  
Management Research  
Project Funded by NSF -  
Sep 2014

# Workflow Refinement

- Example of a simple **abstract workflow** in which
  - the logical component *Extract* is applied to an input file with a logical filename *F.a*.
  - The resulting files *F.b1* and *F.b2*, are used as inputs to the components identified by logical filenames *Resample* and *Decimate*.
  - Finally, the results are *Concatenated*

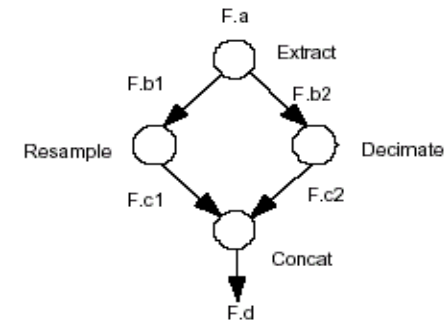


Figure 1.2. An example abstract workflow.

- If we **assume that F.c2** is already available
  1. Reduces the workflow to 3 components, namely *Extract*, *Resample*, and *Concat*.
  2. Adds the transfer nodes for transferring F.c2 and F.a from their current locations.
  3. Adds transfer nodes between jobs that will run on different locations.
  4. Adds output transfer nodes to stage data out and registration nodes if the user requested that the resulting data be published and made available at a particular location.

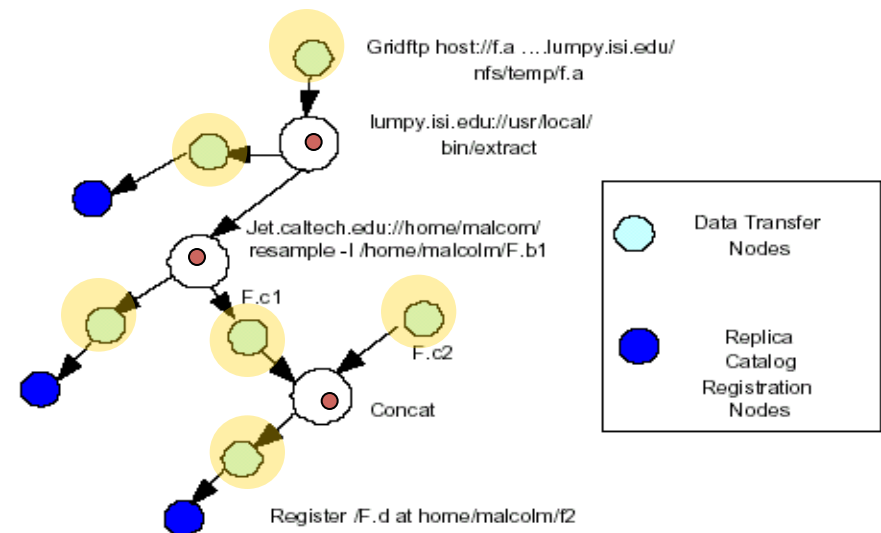


Figure 1.3. An example reduced, concrete workflow.

# WS-VLAM



University of Amsterdam - UvA  
Faculty of Science

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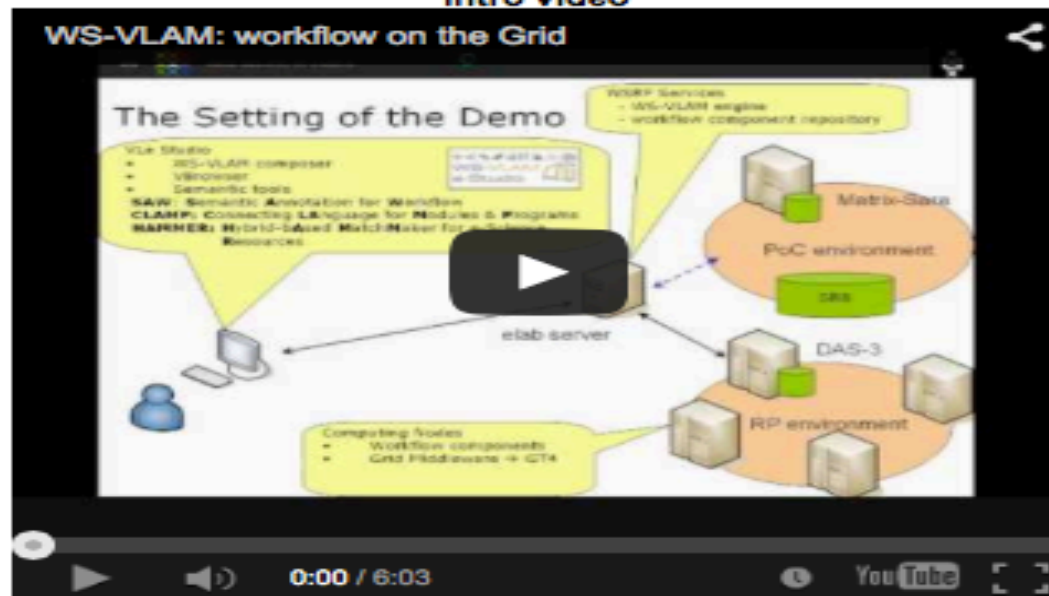


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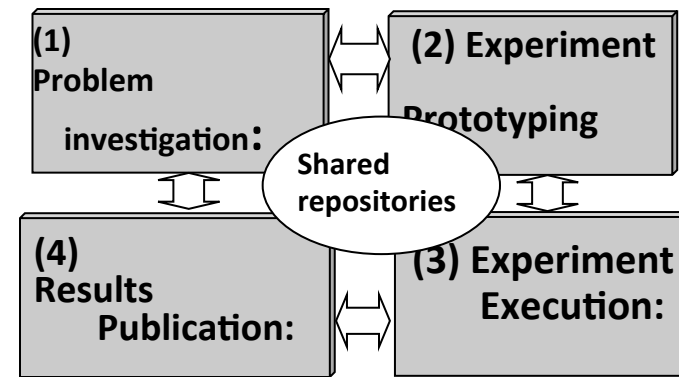
# WS-VLAM

[Intro video](#)



# Outline

- Introduction
- Lifecycle of an e-science workflow
- Different approach to workflow scheduling
  - Workflow Process Modeling & Management In Grid/Cloud
  - Workflow and Web services (intrusive/non-intrusive)
- provenance





# Provenance/ reproducibility

- “A complete provenance record for a data object allows the possibility to **reproduce the result** and reproducibility is a critical component of the scientific method”
- Provenance: The recording of metadata and provenance information during the various stages of the workflow lifecycle

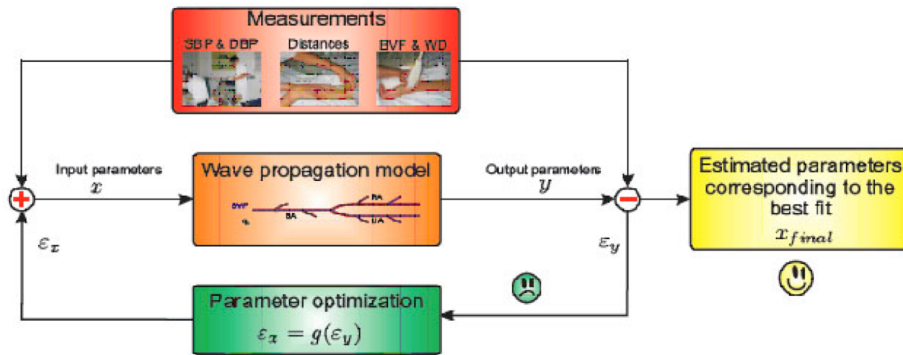
Workflows and e-Science: An overview of workflow system features and capabilities Ewa Deelman<sup>a</sup>, Dennis Gannon<sup>b</sup>, Matthew Shields<sup>c</sup>, Ian Taylor, Future Generation Computer Systems 25 (2009)

# History-tracing XML (FH Aachen)

- provides data/process provenance following an approach that
  - maps the workflow graph to a layered structure of an XML document.
  - This allows an intuitive and easy processable representation of the workflow execution path,
  - which can be, eventually, electronically signed.

```
<patternMatch>
  <events>
    <PortResolved> provenance
data</PortResolved>
    <ConDone>provenance data
      </ConDone>
    ...
  </events>
  <fileReader2>
    <events> ... </events>
    <sign-fileReader2> ...
      </signfileReader2>
  </fileReader2>
  <sffToFasta>
    Reference
  </sffToFasta>
  <sign-patternMatch> ...
    </sign-patternMatch>
</patternMatch>
```

# wave propagation model applications

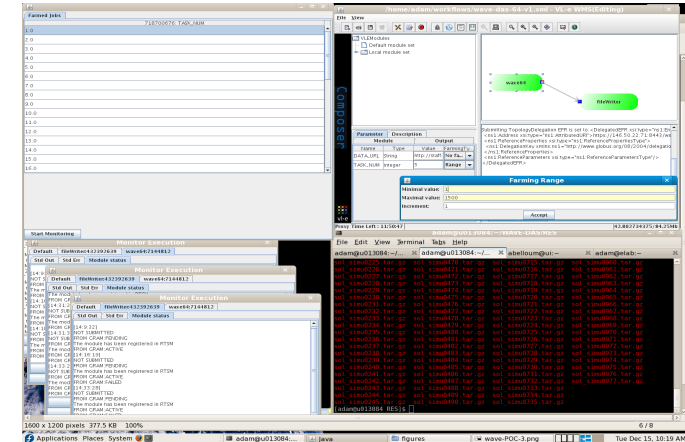


[Biomedical engineering Cardiovascular biomechanics group TUE]

wave propagation model of blood flow in large vessels using an approximate velocity profile function:

a biomedical study for which **3000 runs** were required to perform a global sensitivity analysis of a blood pressure wave propagation in arteries

User Interface to compose workflow (top right), monitor the execution of the farmed workflows (top left), and monitor each run separately (bottom left) data



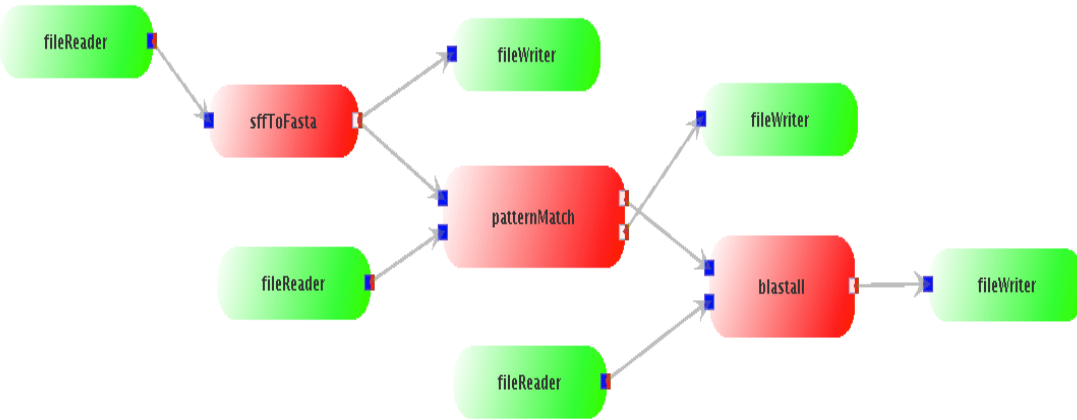
The screenshot shows the 'Cardiovascular Provenance Query Interface'. It includes a search bar for 'Experiment' and 'Timestamp'. Below the search bar, there is a table of simulation results. The table has columns for Name, Start, Time, and various parameters (P0, P1, P2, P3, P4, P5, P6, P7, P8, P9). The table lists 3000 runs, with the first few rows showing results for 'Wave\_CardioV...'.

Name	Start	Time	P0	P1	P2	P3	P4	P5	P6	P7	P8	P9
Wave_CardioV...	01:58:43	01:58:43	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:57:51	01:57:51	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:56:35	01:56:35	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:56:53	01:56:53	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:56:52	01:56:52	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:56:49	01:56:49	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:56:28	01:56:28	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:57:05	01:57:05	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:57:04	01:57:04	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:56:51	01:56:51	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:56:18	01:56:18	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:55:12	01:55:12	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:56:00	01:56:00	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:54:37	01:54:37	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:55:05	01:55:05	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:55:23	01:55:23	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:54:50	01:54:50	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:55:27	01:55:27	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:54:54	01:54:54	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:52:08	01:52:08	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:52:35	01:52:35	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...
Wave_CardioV...	01:52:53	01:52:53	1.000	2.000	2.37...	2.37...	0.00	0.00	3.56...	3.56...	4.18...	4.18...

Query interface for the provenance data collected from 3000 simulations of the “wave propagation model of blood flow in large vessels using an approximate velocity profile function”

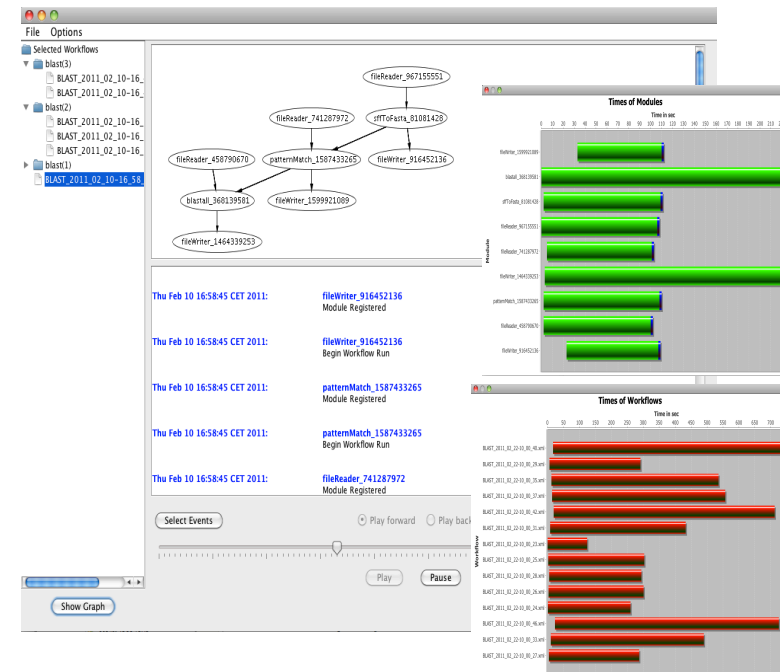


# Blast Application



*[Department of Clinical  
Epidemiology, Biostatistics and  
Bioinformatics (KEBB), AMC ]*

The aim of the application is the **alignment of DNA sequence** data with a given reference database. A workflow approach is currently followed to run this application on distributed computing resources.



on-going work UvA-AMC-fh-aachen

For Each workflow run  
The provenance data is collected and stored following the XML-tracing system  
User interface allows to reproduce events that occurred at runtime (replay mode)  
User Interface can be customized (User can select the events to track)  
User Interface show resource usage

# More References

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2. Ilkay Altintas, Manish Kumar Anand, Daniel Crawl, Shawn Bowers, Adam Belloum, Paolo Missier, Bertram Ludascher, Carole A. Goble, Peter M.A. Sloot, Understanding Collaborative Studies Through Interoperable Workflow Provenance, IPAW2010, Troy, NY, USA
3. A. Belloum, Z. Zhao, and M. Bubak Workflow systems and applications , Future Generation Comp. Syst. 25 (5): 525-527 (2009)
4. Z. Zhao, A.S.Z. Belloum, et al., Distributed execution of aggregated multi domain workflows using an agent framework The 1st IEEE International Workshop on Scientific Workflows, Salt Lake City, U.SA, 2007
5. Zhiming Zhao, Adam Belloum, Cees De Laat, Pieter Adriaans, Bob Hertzberger Using Jade agent framework to prototype an e-Science workflow bus, International Conference on Cluster Computing and the Grid, 2007. CCGRID 2007