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

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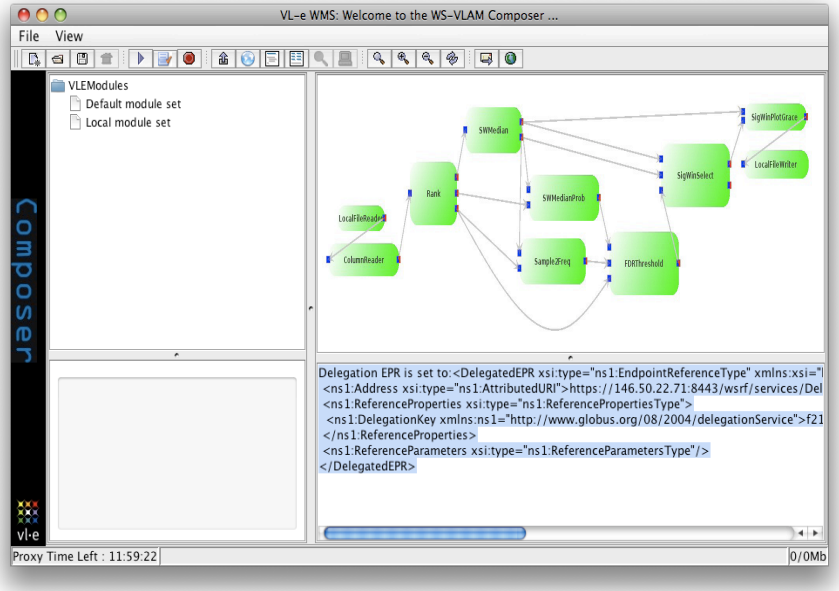
UvA-SURFsara

Outline

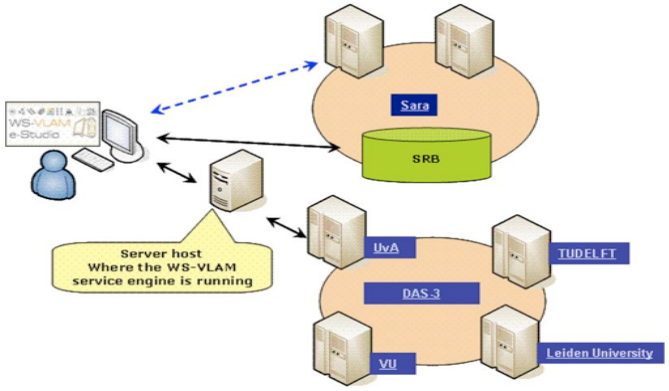
- Introduction
- Lifecycle of an e-science workflow
- Workflow management Systems
- Scientific workflows Applications
- Provenance
- Examples of Scientific workflow managements

Workflow management system

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



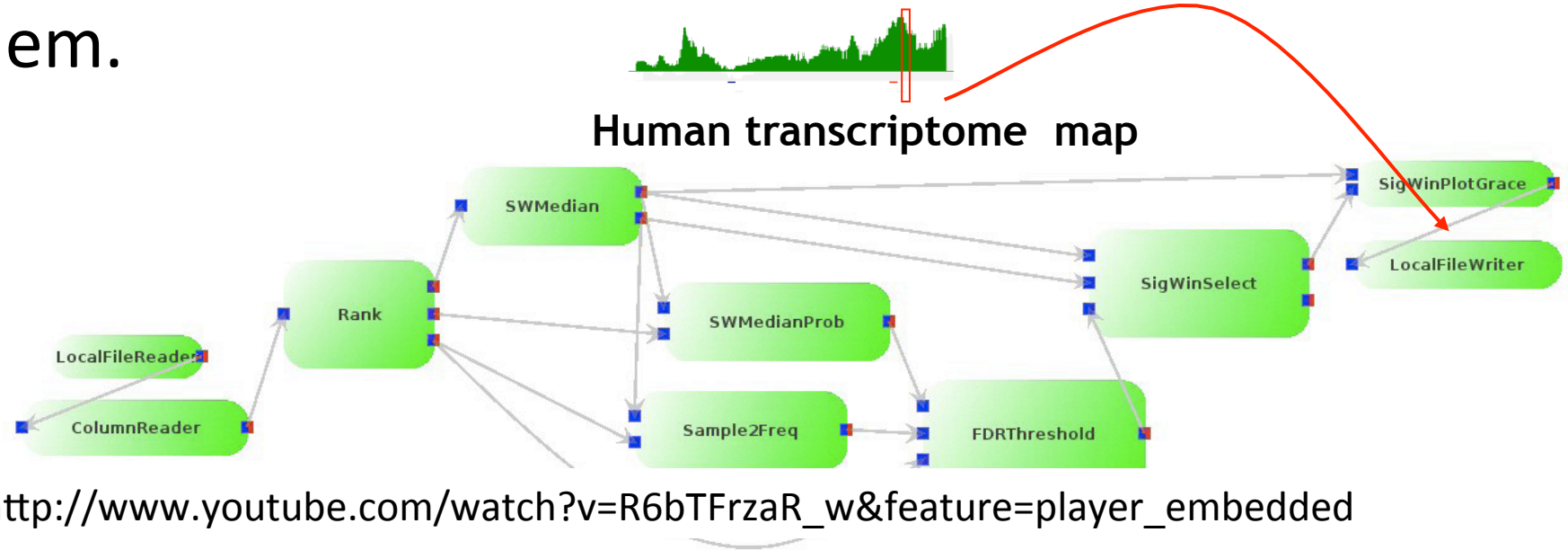
The user interface of the WS-VLAM a workflow management system developed in the VL-e project to execute application workflow on geographically distributed computing resources



Deployed as service on Dutch super Computer (DAS3), and Dutch NGI (BigGrid) Clusters

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

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

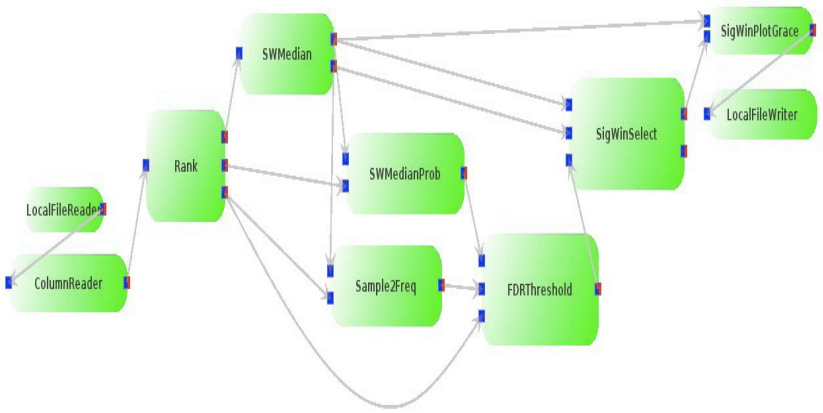
http://www.csc.ncsu.edu/faculty/mpsingh/papers/databases/workflows/sciworkflows.html

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

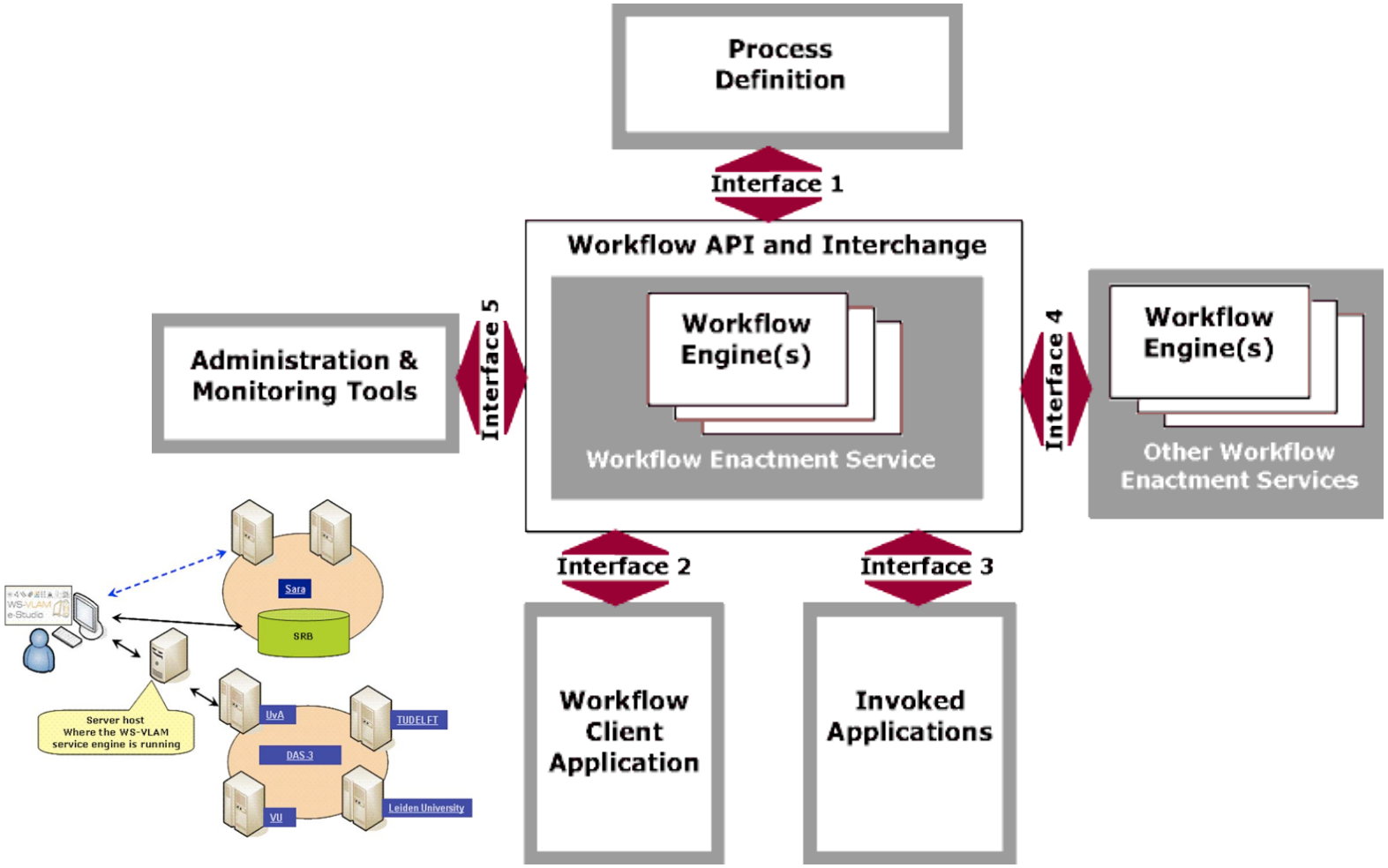
Challenges of running workflows on e-infrastructure (grids and clouds)

- ***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.

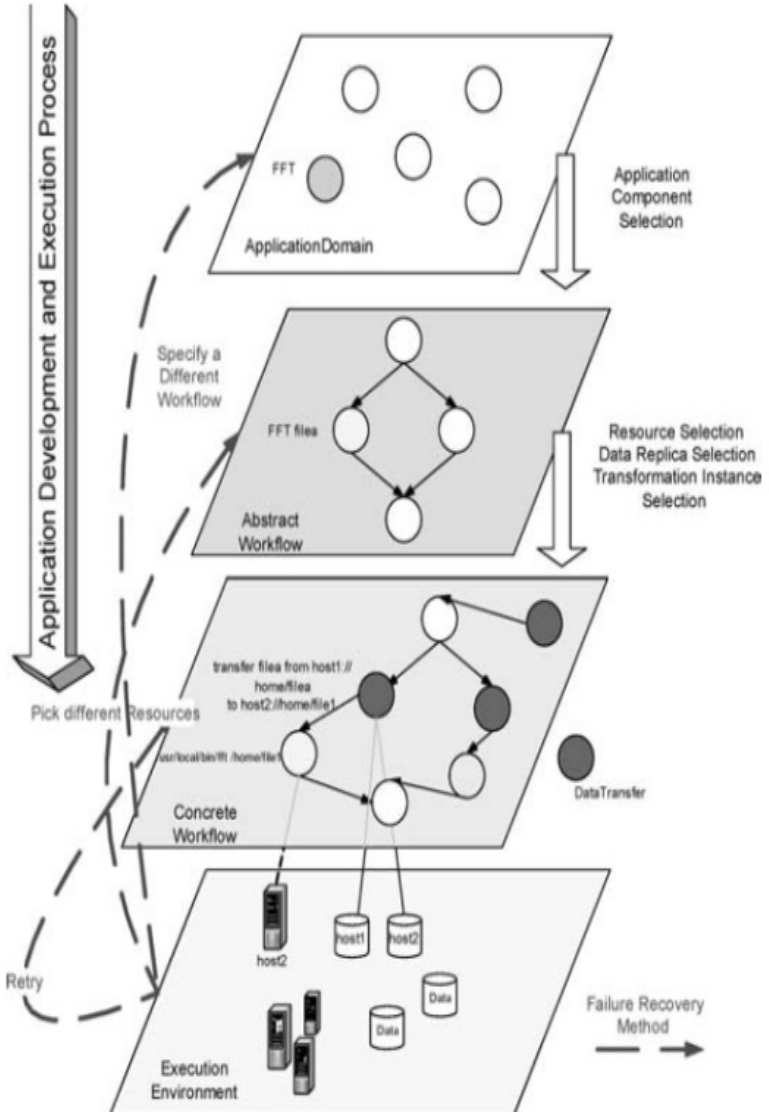
- WS can be **combined** in a **workflow** so that more complex operations may be achieved
  - Application services
  - System services (Grids and Clouds)

Application development and Execution process

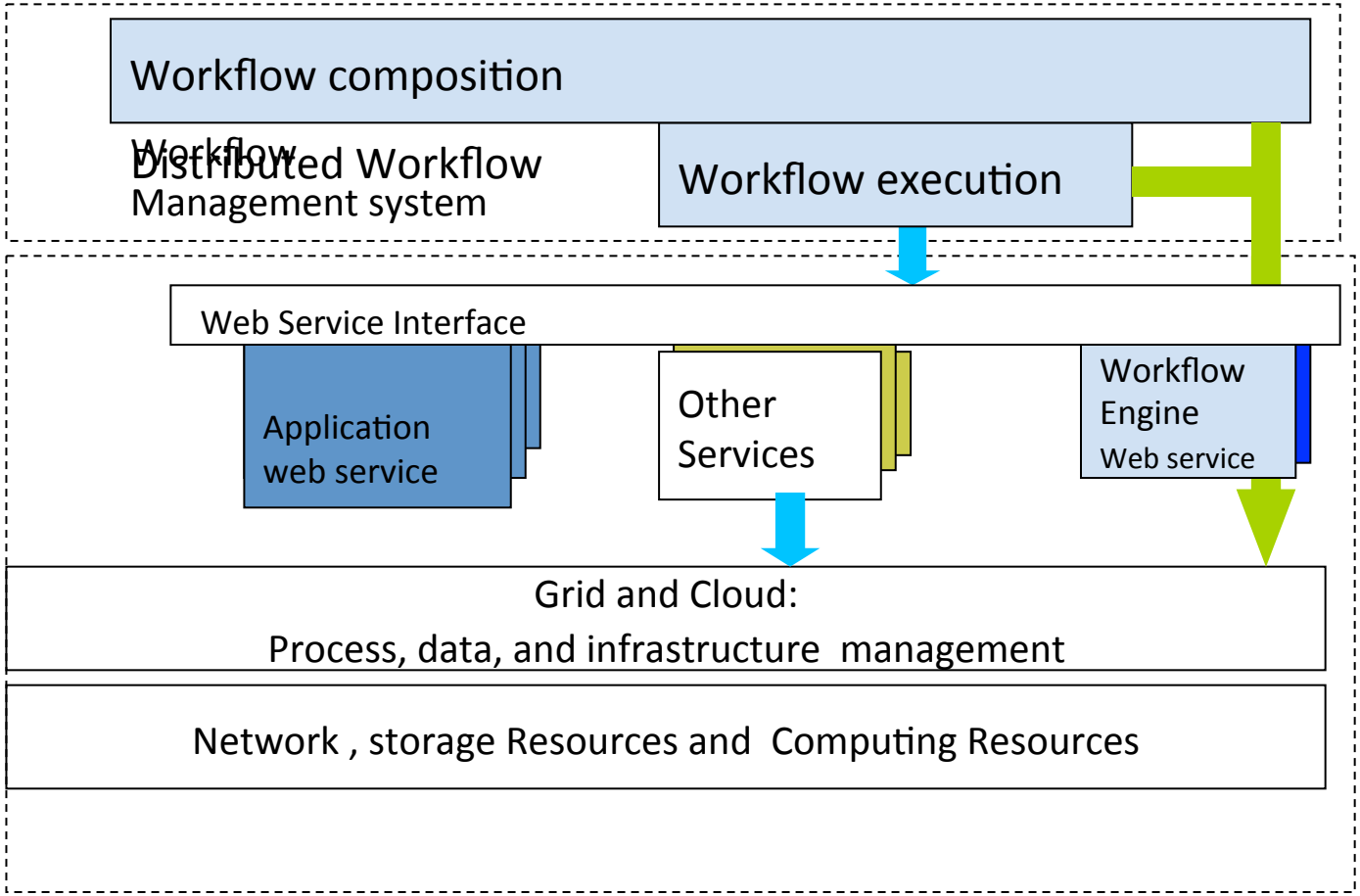
- Select or develop
- Compose the application workflow
- Mapping to actual resource
  - Resource discovery, allocation and management
  - Bind to real computing resource

- 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

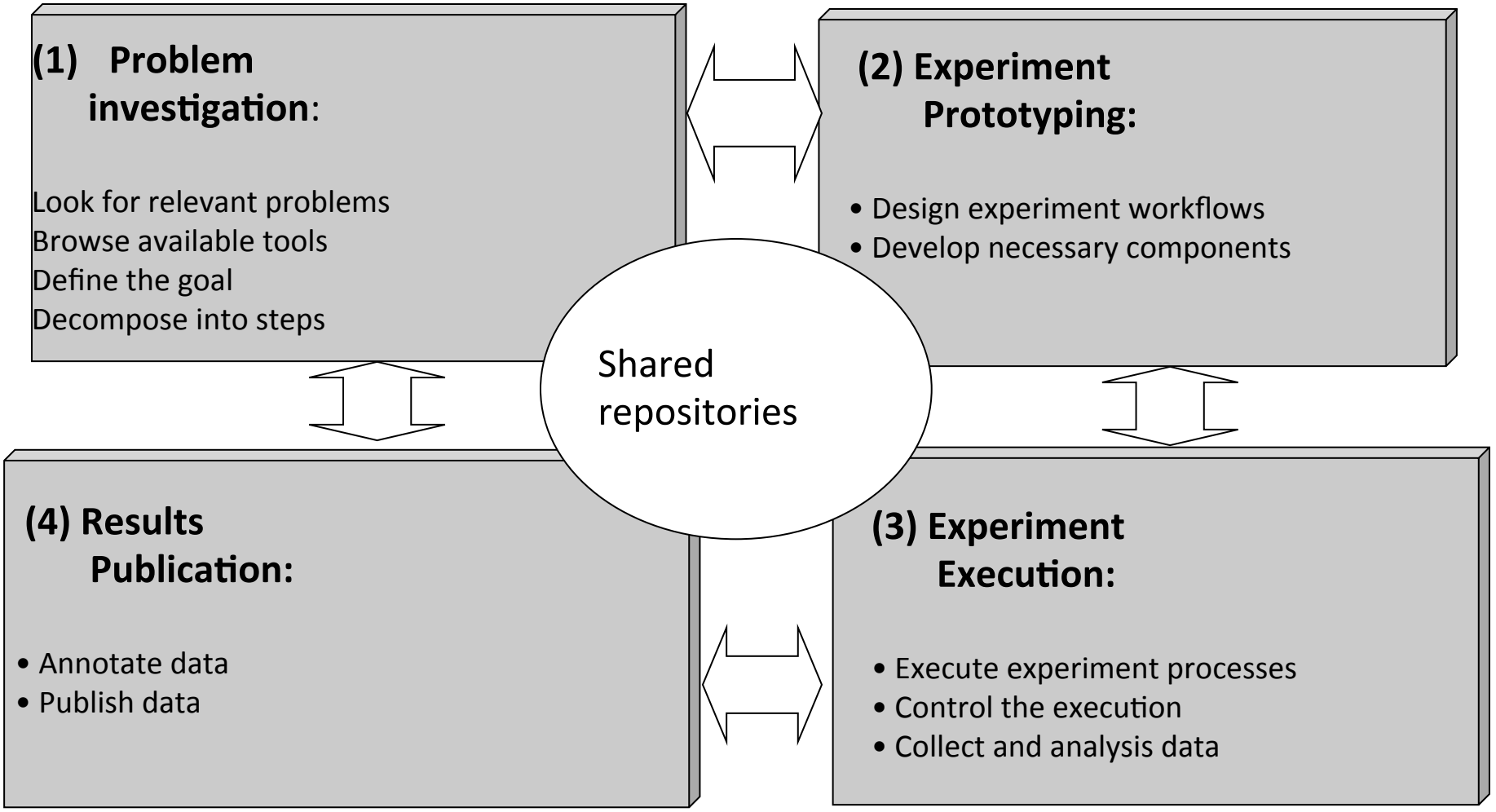


Distributed enabled workflow engines



Bob Hertberger keynote at *2nd IEEE Conf on eScience & grid computing , Amsterdam 2006*

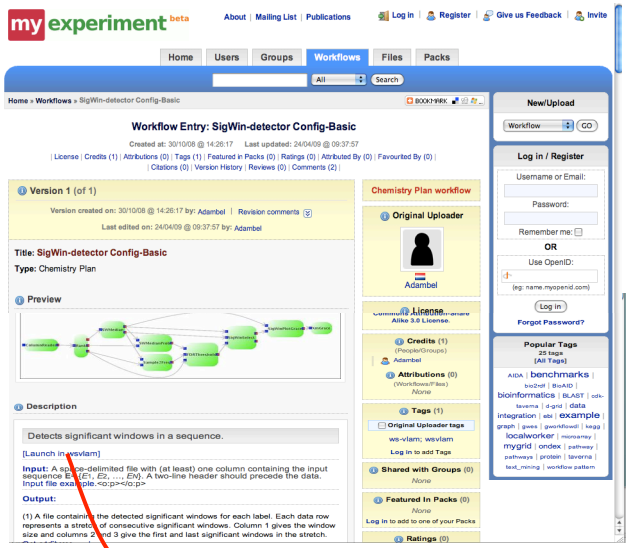
life cycle of scientific experiments

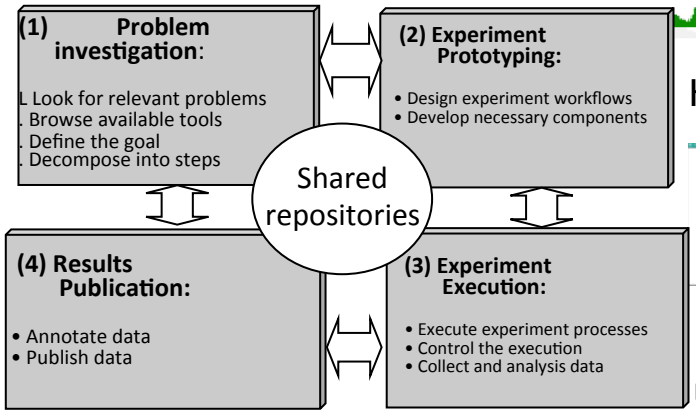


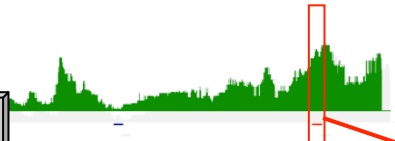
Collaborative e-Science experiments: from scientific workflow to knowledge sharing *A.S.Z. Belloum, Vladimir Korkhov, Spiros Koulouzis, Marcia A Inda, and Marian Bubak JULY/AUGUST, IEEE Internet Computing, 2011*

life cycle of scientific experiments

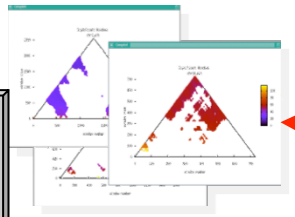
- Workflow can be invoked form other systems
- Workflow can be made available to entire community (using Web 2.0 approach)





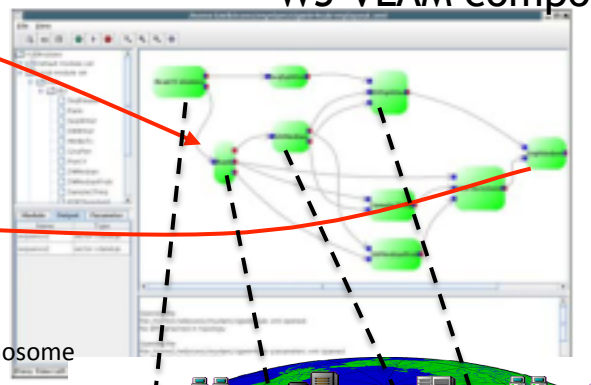


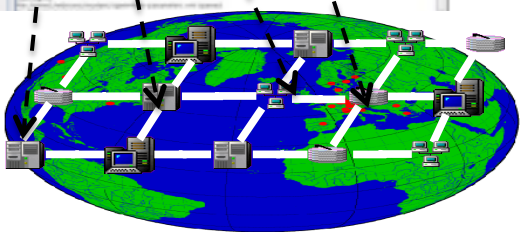
Human transcriptome map



DNA curvature of the *Escherichia Coli* chromosome

WS-VLAM composer



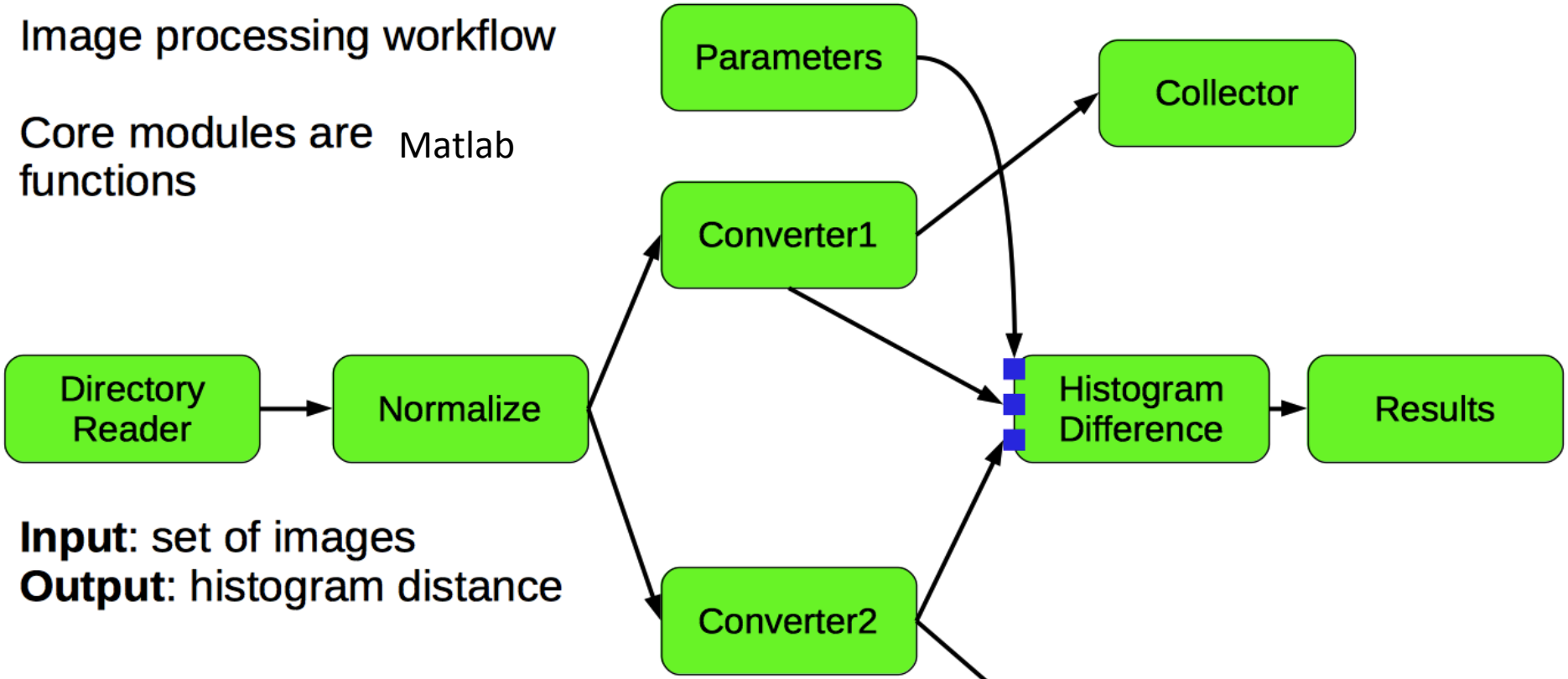


Marcia A Inda, Marinus F van Batenburg, Marco Roos, Adam SZ Belloum, Dmitry Vasunin, Adianto Wibisono, Antoine HC van Kampen and Timo M Breit SigWin-detector: *a Grid-enabled workflow for discovering enriched windows of genomic features related to DNA sequences,* BMC Research Notes 2008,

Example of Scientific workflow

Image processing workflow

Core modules are functions Matlab



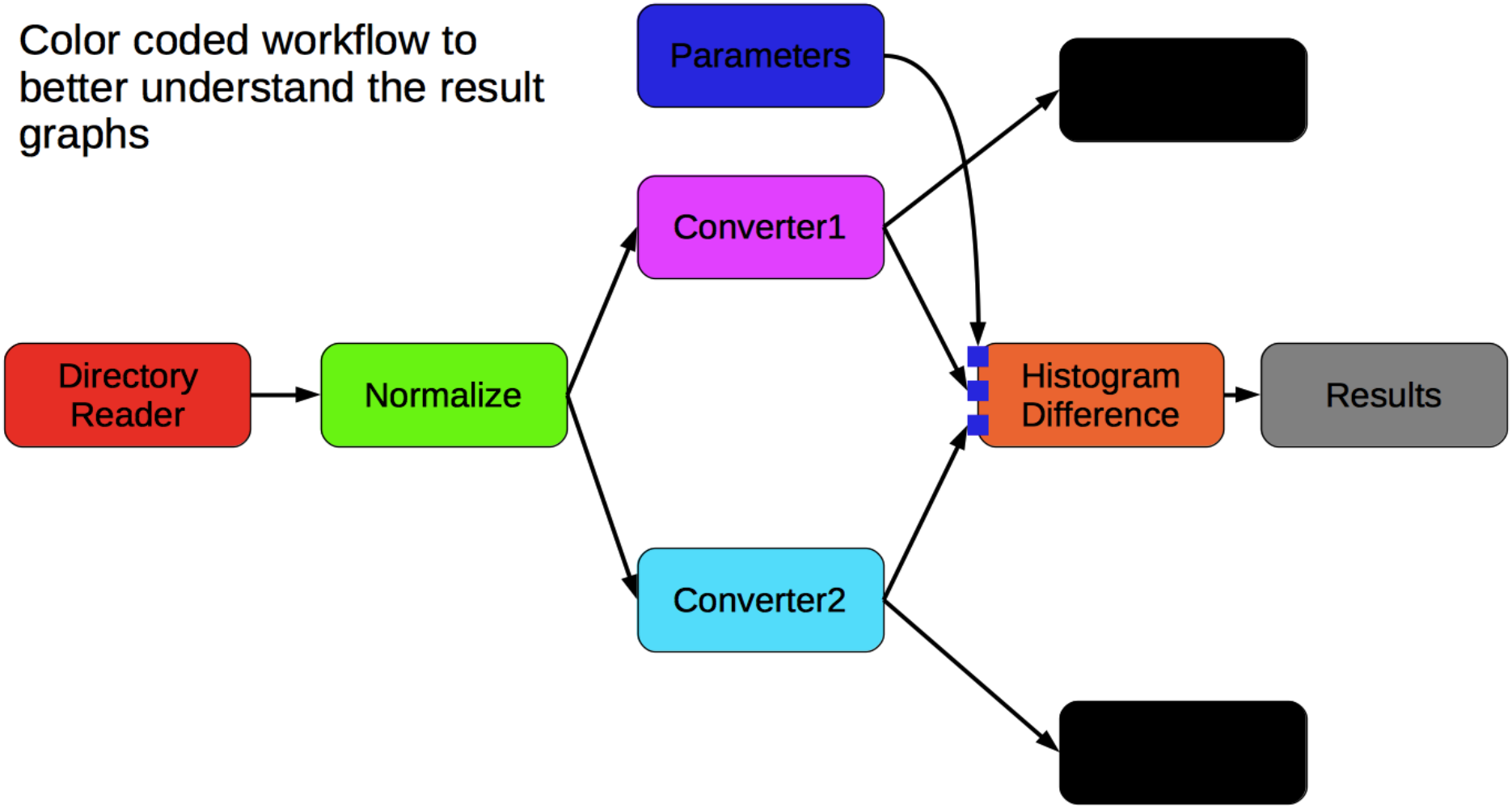
Input: set of images
Output: histogram distance

Images converted to different color spaces

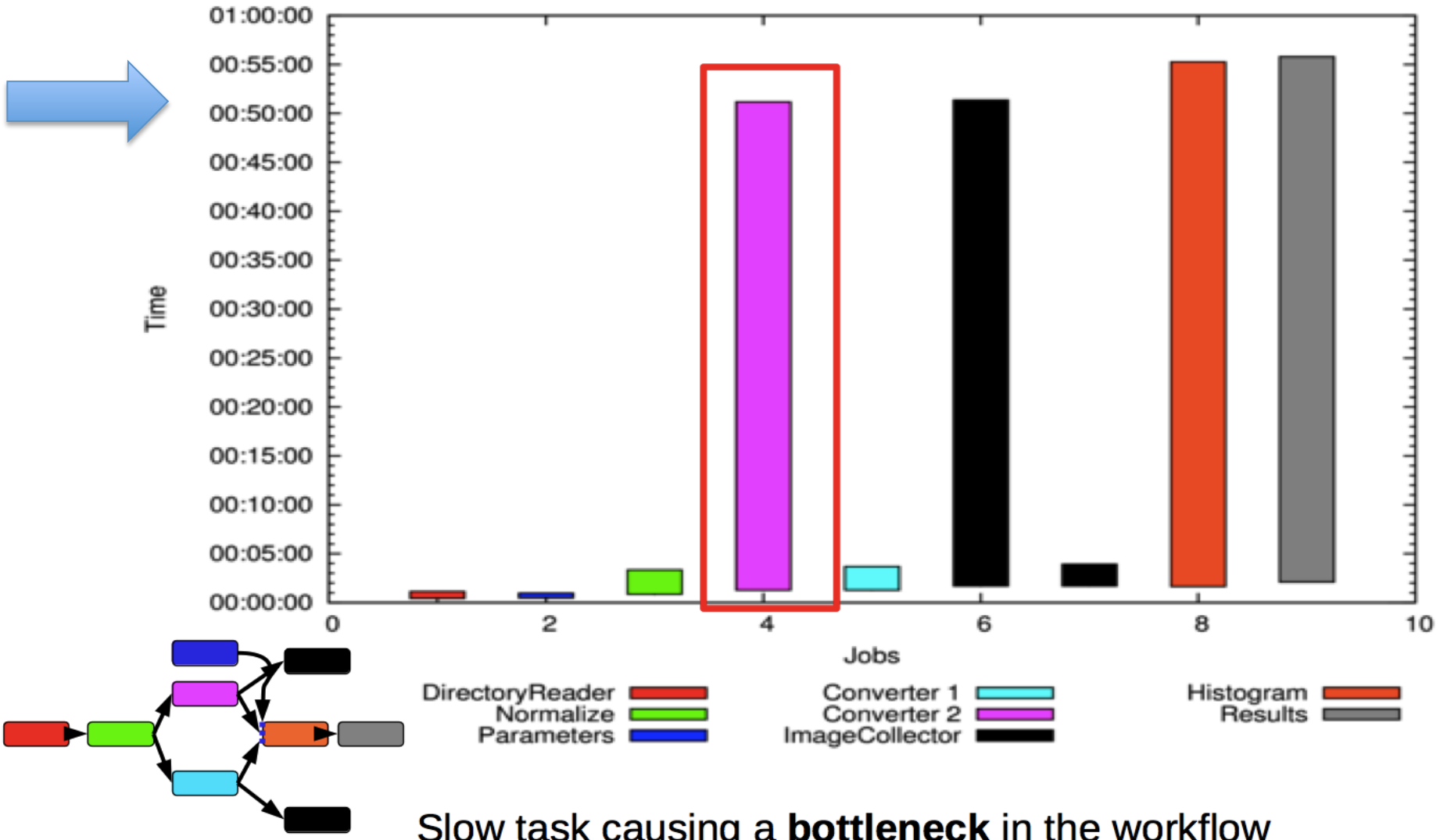
Histogram difference is calculated between color spaces

Example of Scientific workflow

Color coded workflow to better understand the result graphs



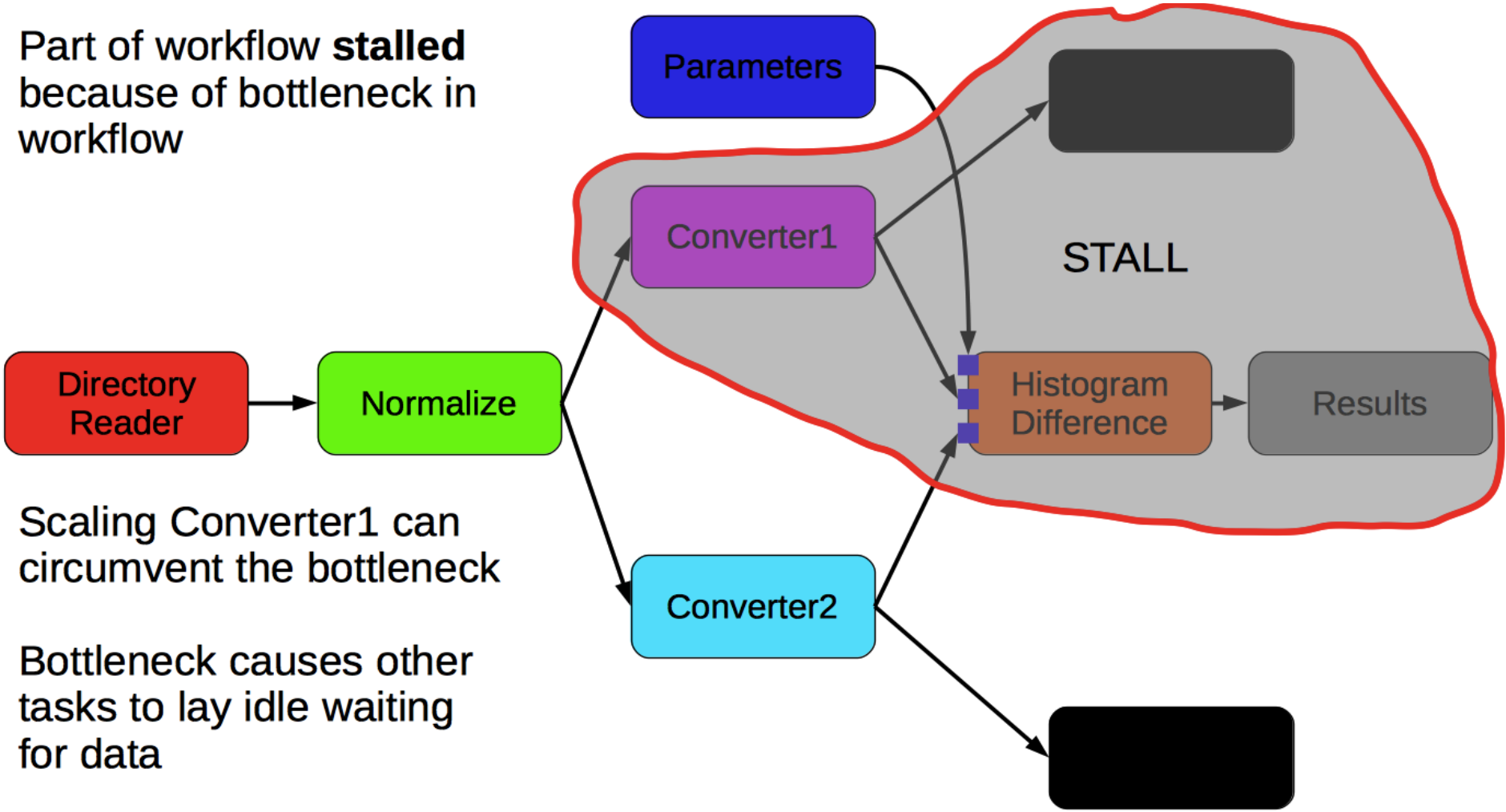
Workflow Without Scaling



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

Example of Scientific workflow (1)

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



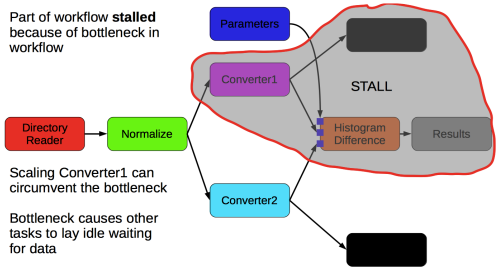
Scaling Converter1 can circumvent the bottleneck

Bottleneck causes other tasks to lay idle waiting for data

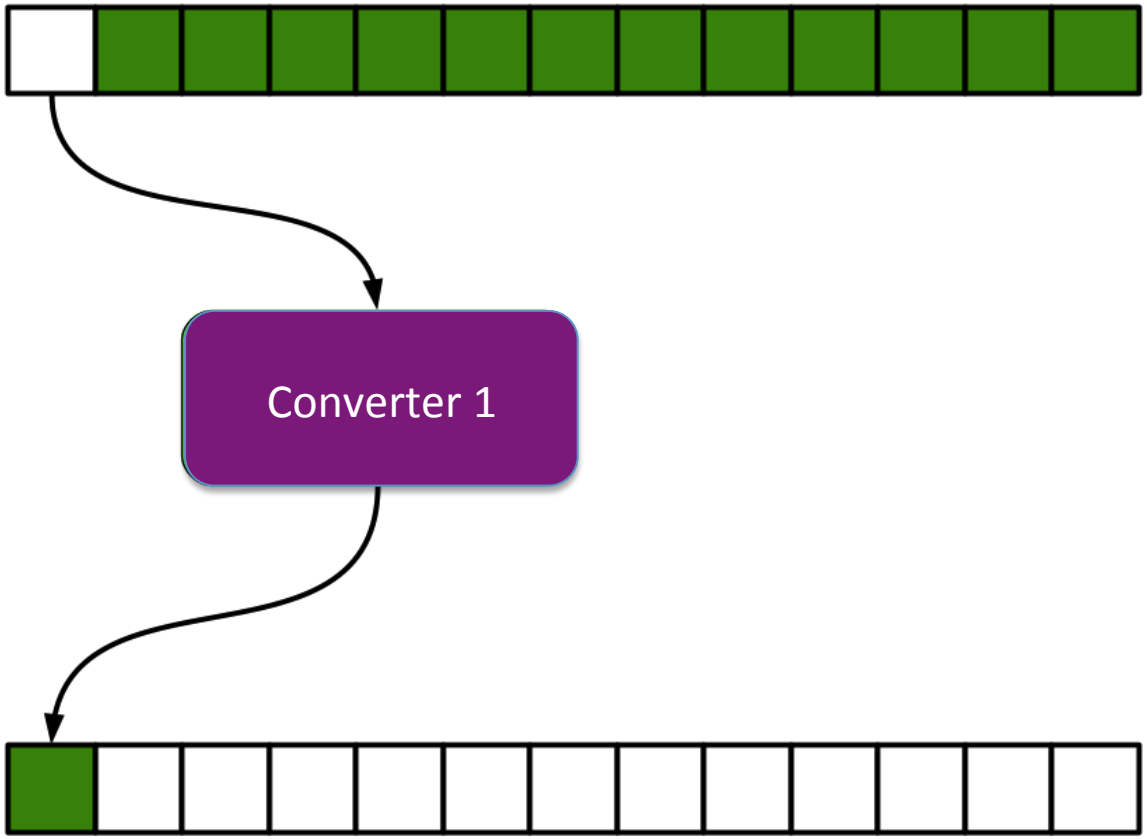
Zooming into the Task Converter 1

Data organized in atomic parcels(messages)

Converter 1

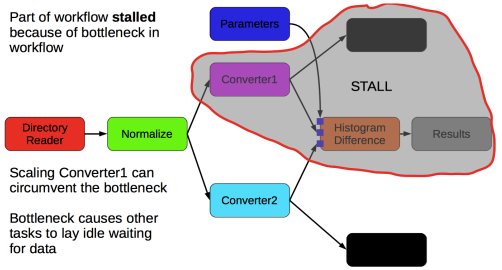


Zooming into the Task Converter 1

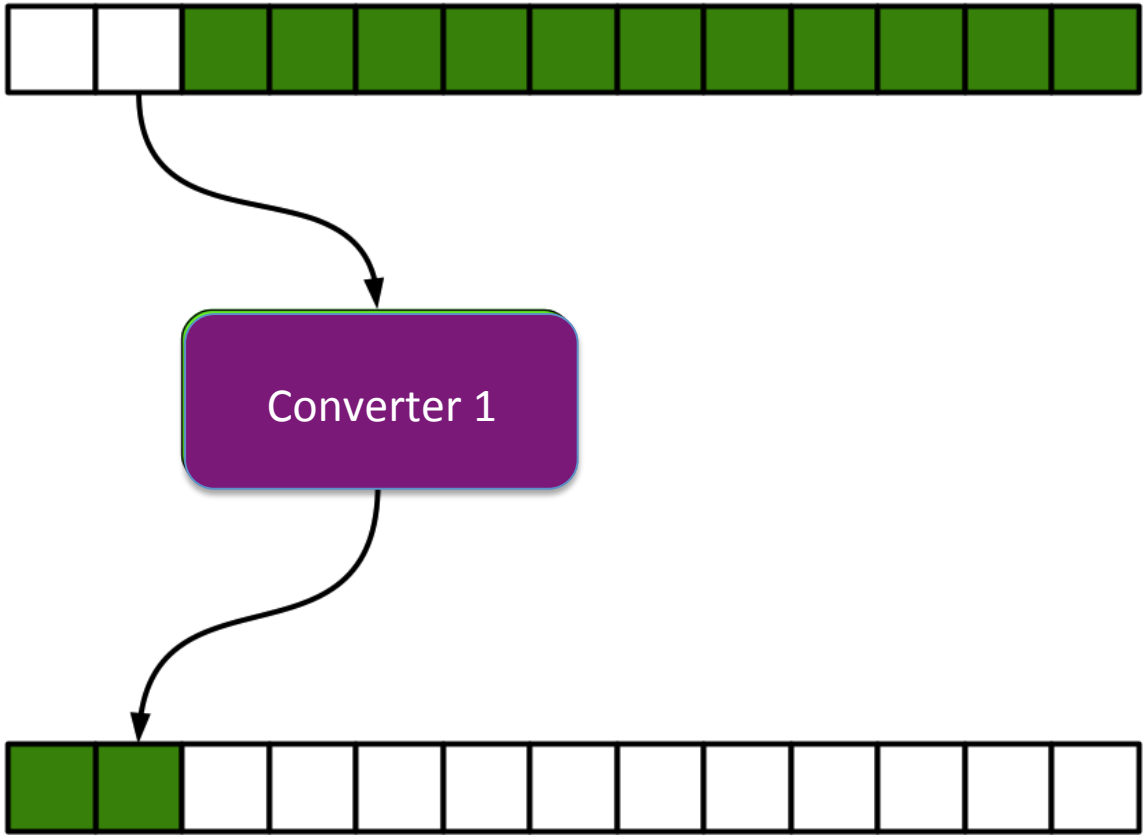


Data organized in atomic parcels(messages)

Task processes data sequentially

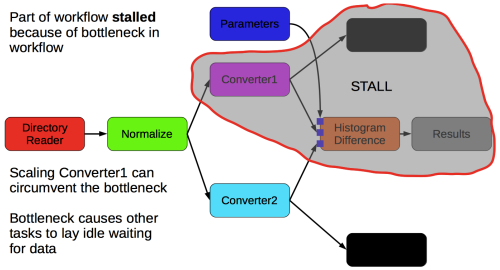


Scaling Concepts

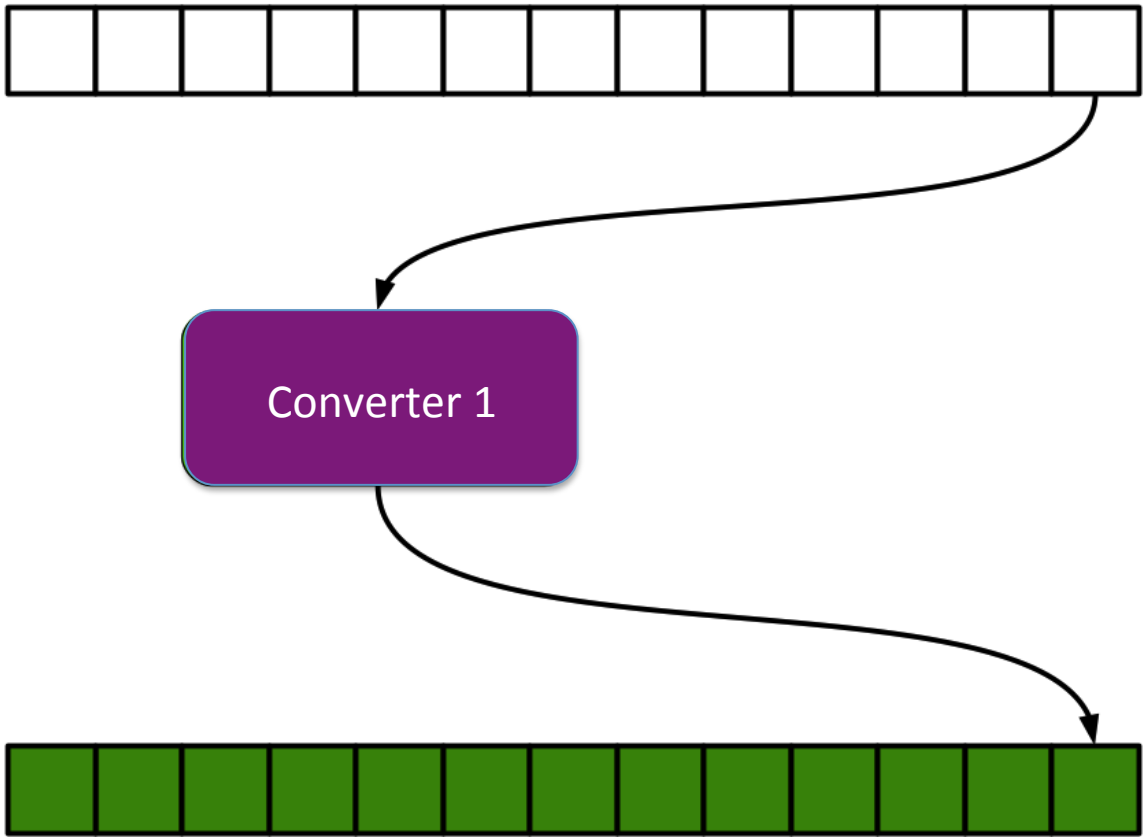


Data organized in atomic parcels(messages)

Task processes data sequentially

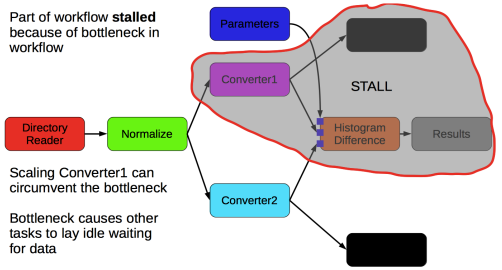


Zooming into the Task Converter 1

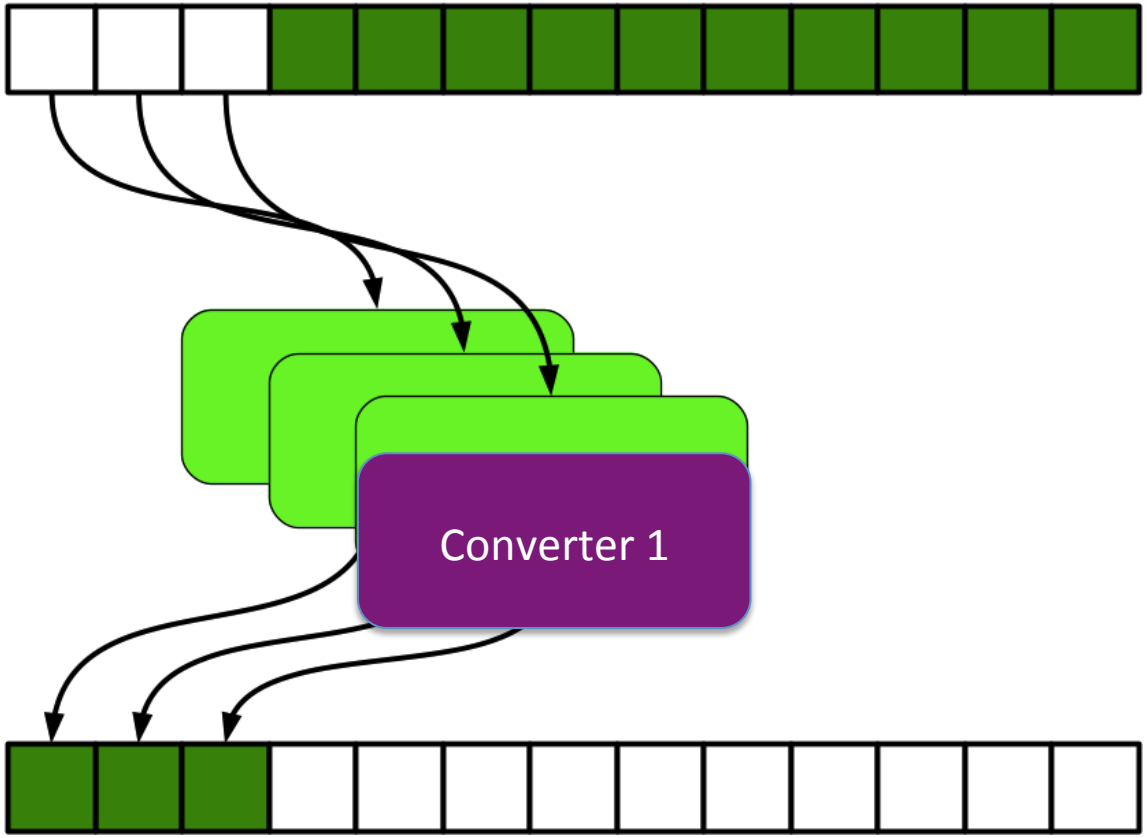


Data organized in atomic parcels(messages)

Task processes data sequentially



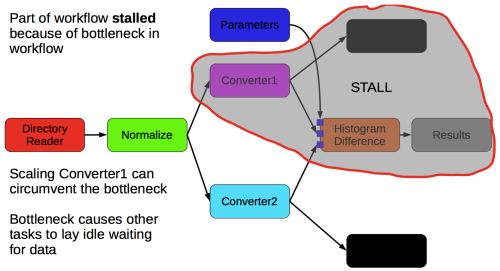
Zooming into the Task Converter 1



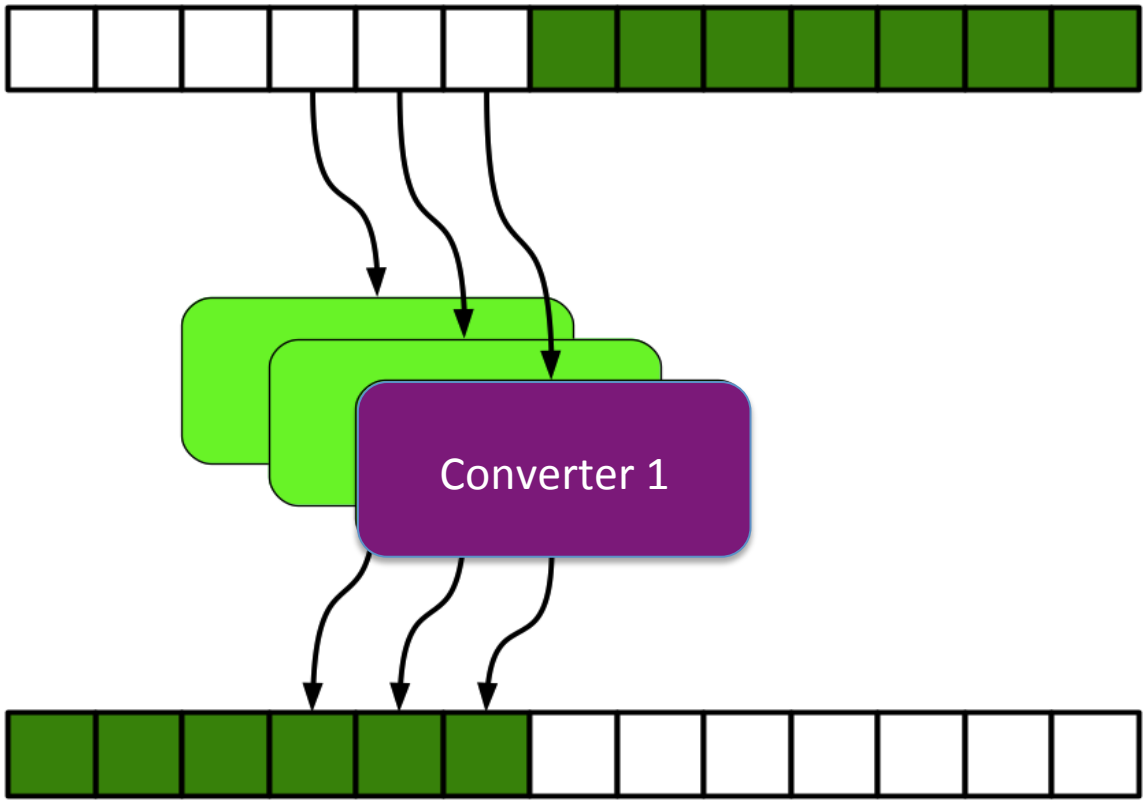
Data organized in atomic parcels(messages)

Tasks processes data **concurrently**

Adding more tasks increases **message consumption** rate



Zooming into the Task Converter 1



Data organized in atomic parcels(messages)

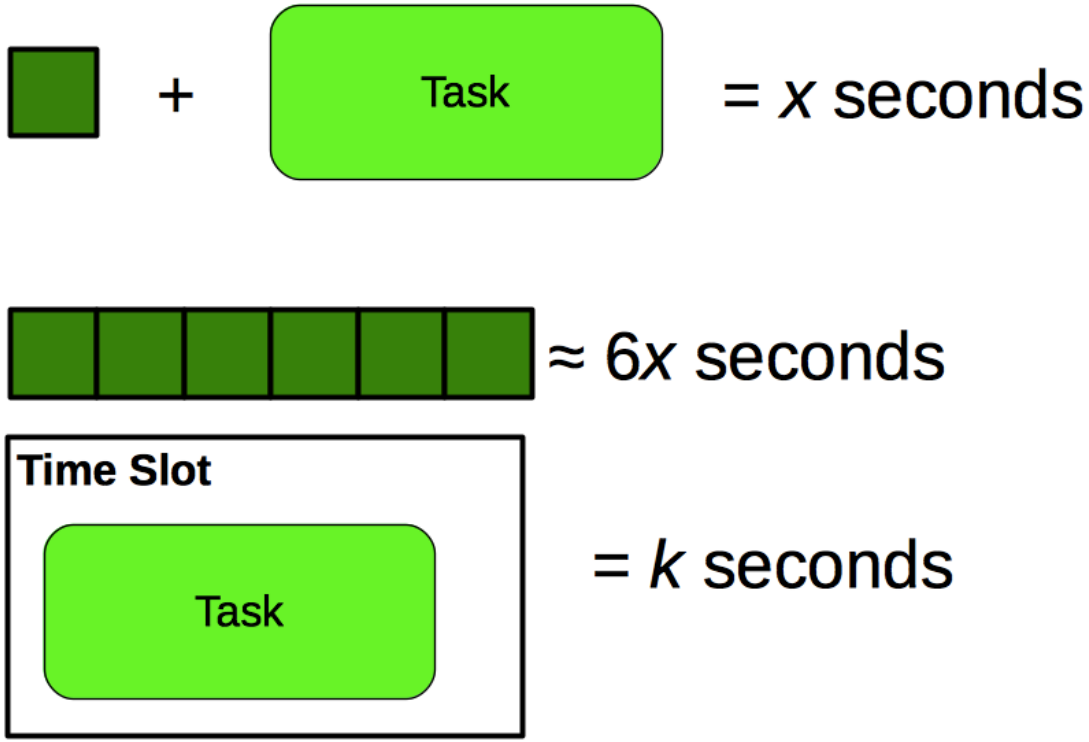
Task processes data sequentially

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

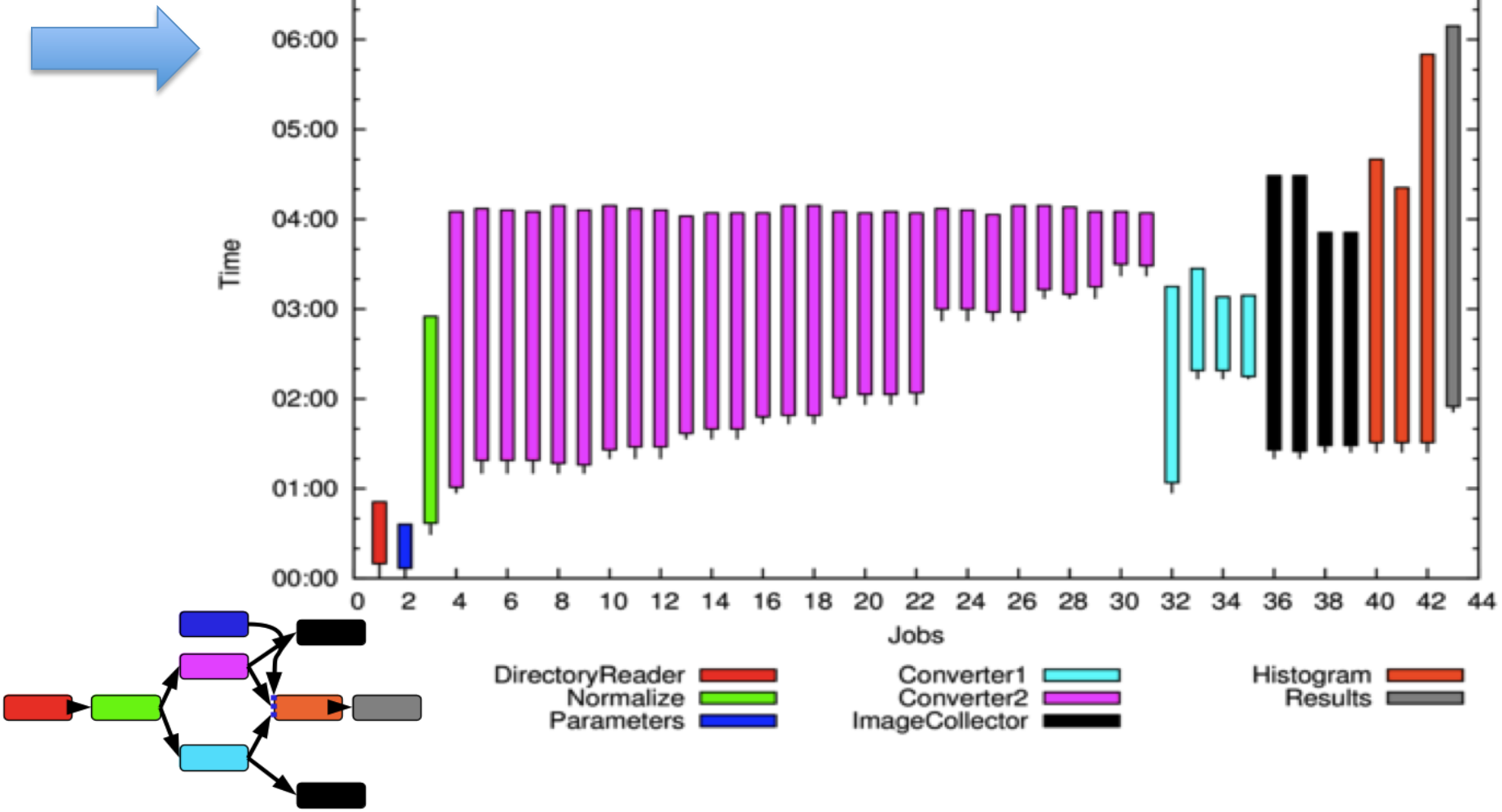
Load Prediction



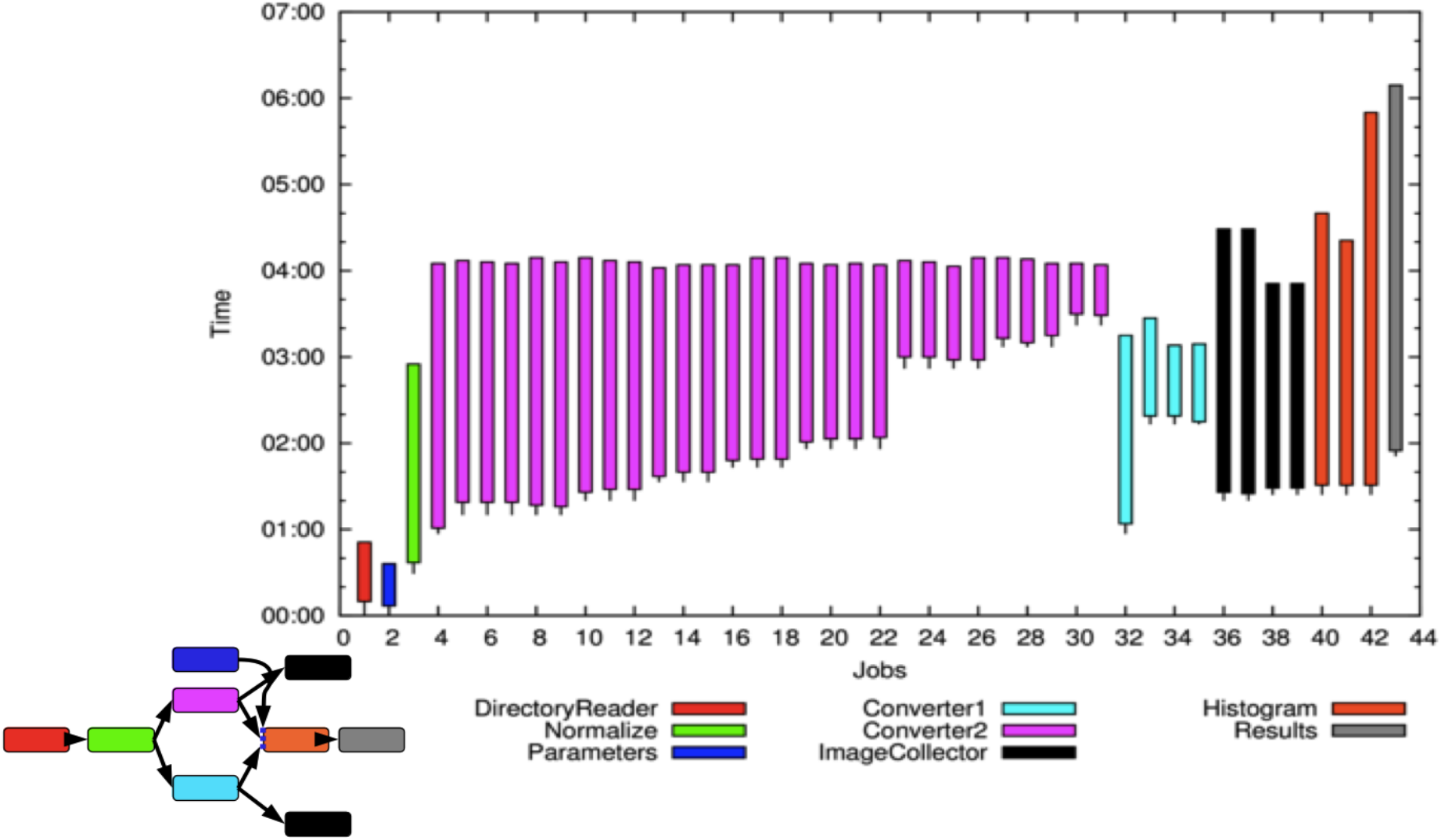
Simplified Load = 6*x*/*k* time slots

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

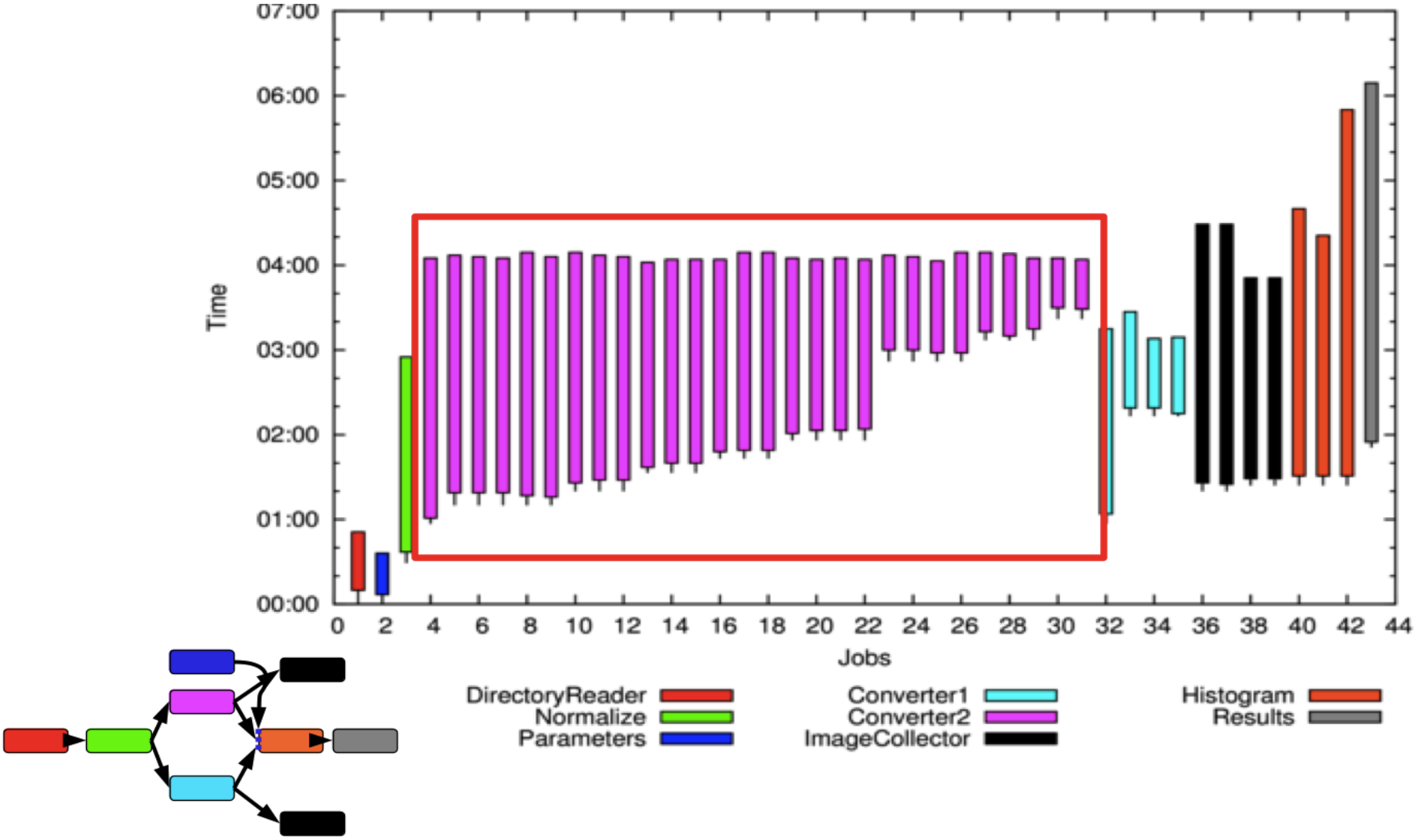
Workflow execution with Scaling



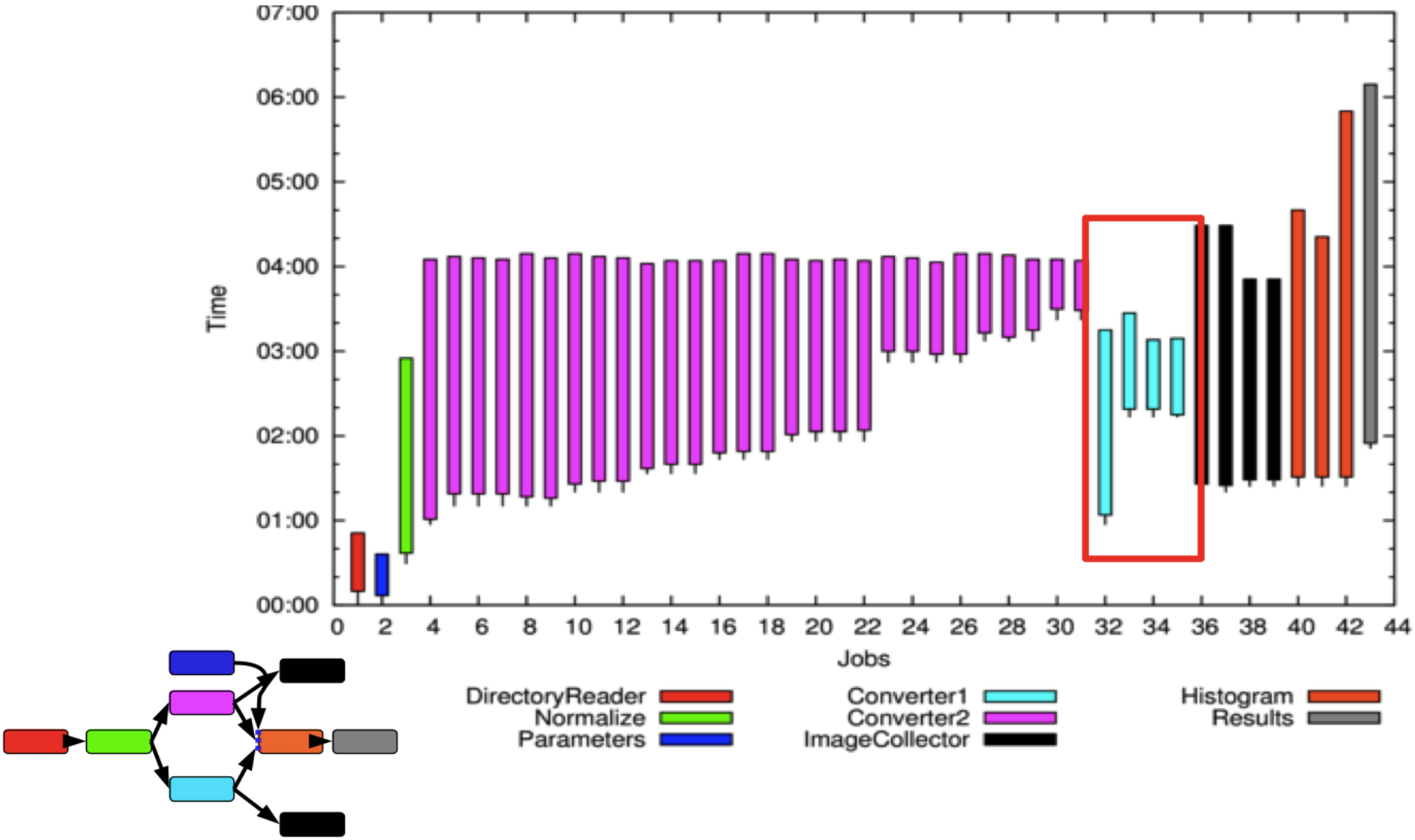
Workflow execution with Scaling



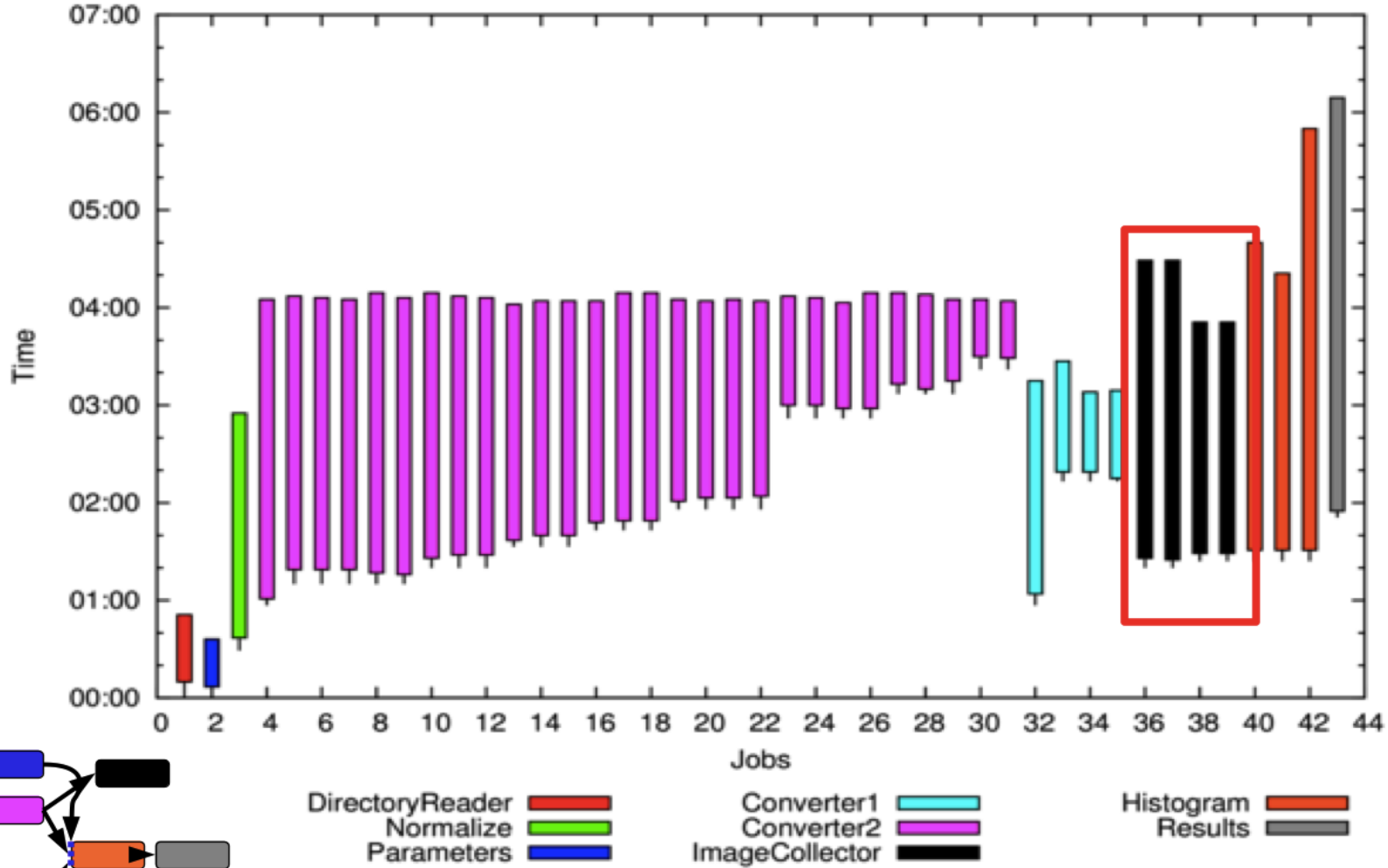
Workflow execution with Scaling Task -1

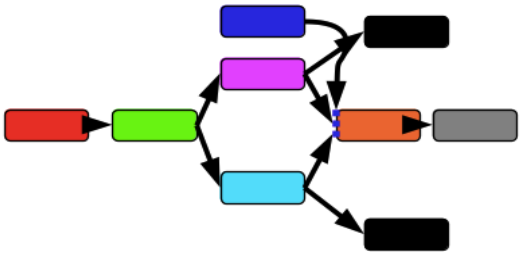


Workflow execution with Scaling Task -2



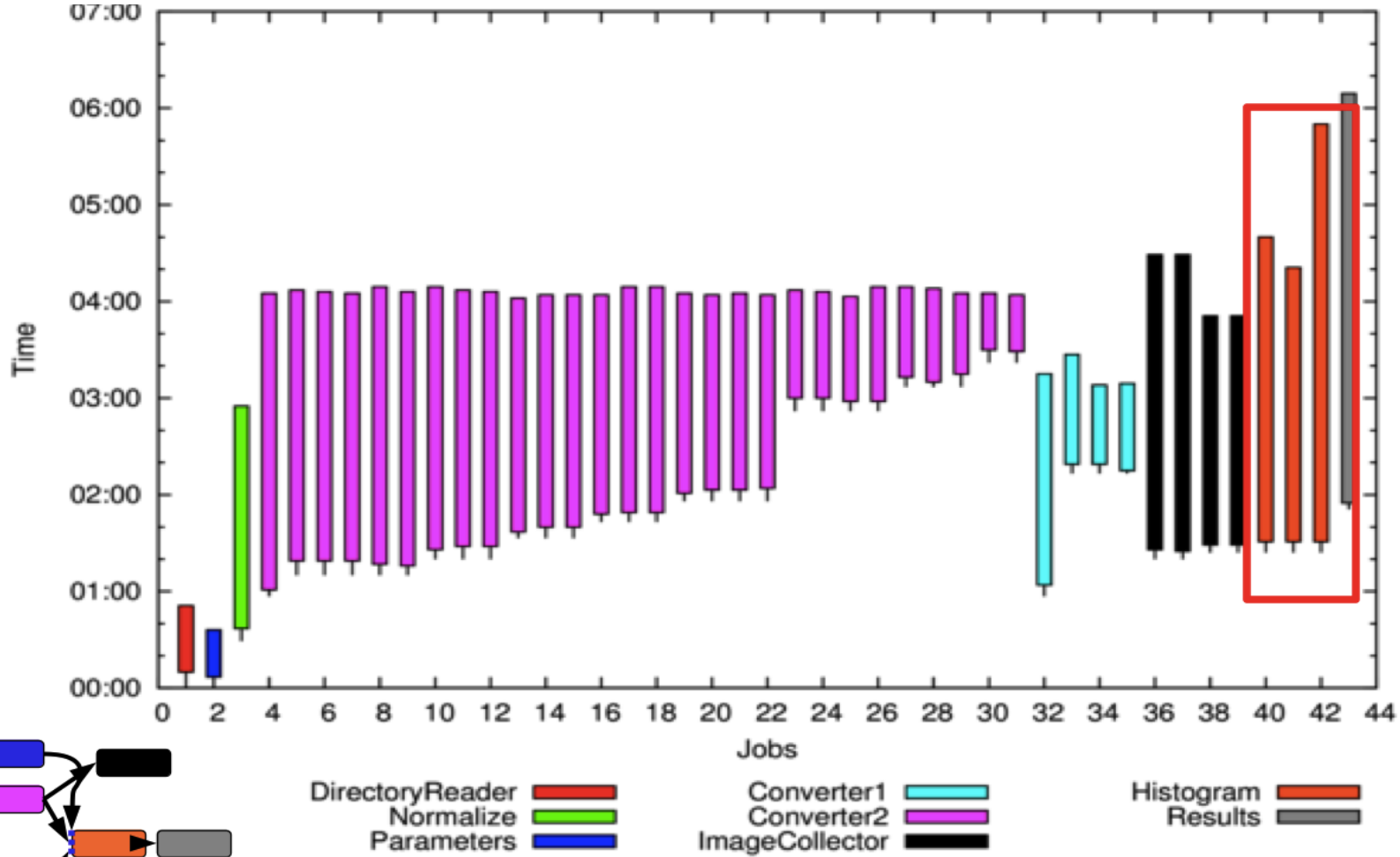
Other Scaled Task -1

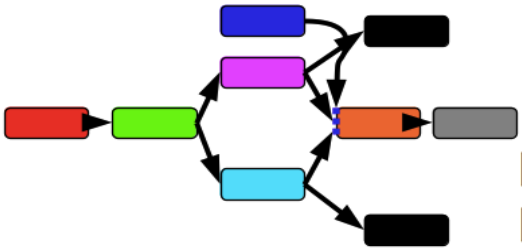




ImageCollector was set to a **fixed** amount (4)

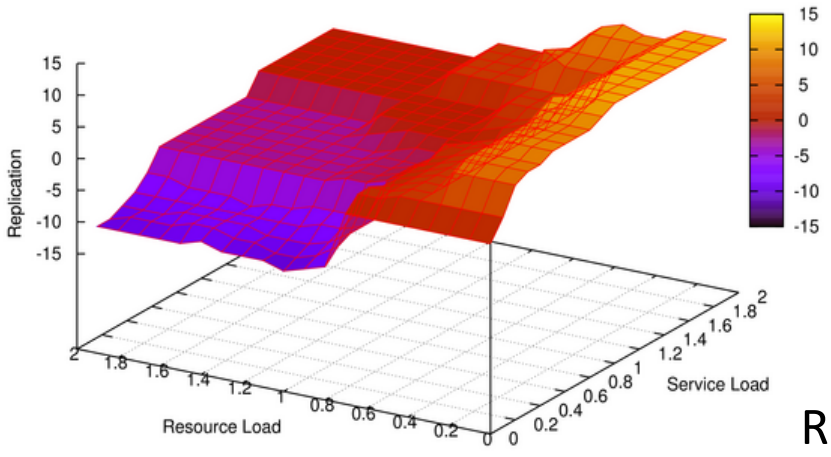
Auto Scaling Task -2



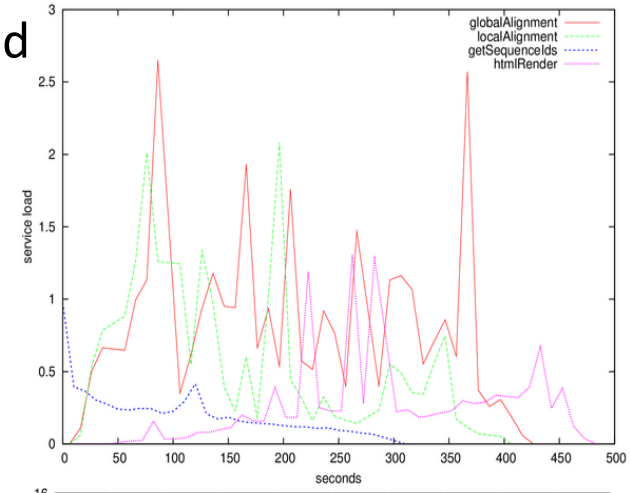


HistogramDifference was set to **one-to-one** scaling.
Each parameter generates a new task

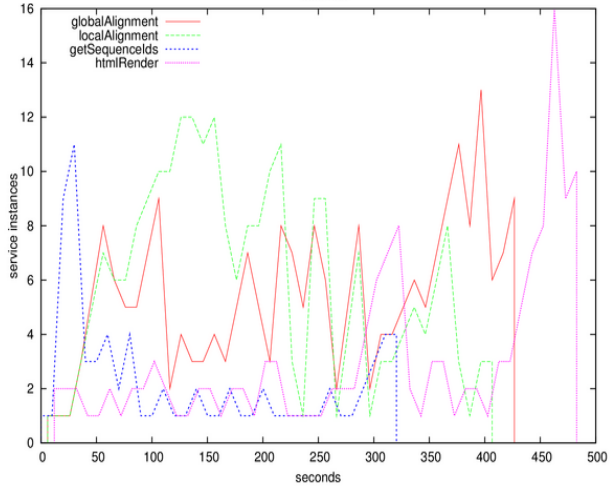
Example of Scientific workflow (2)

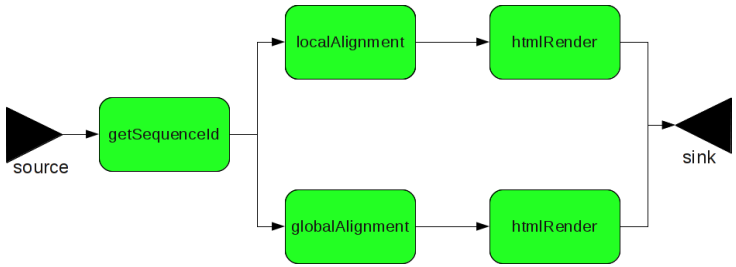


Service Load



Running Service instances

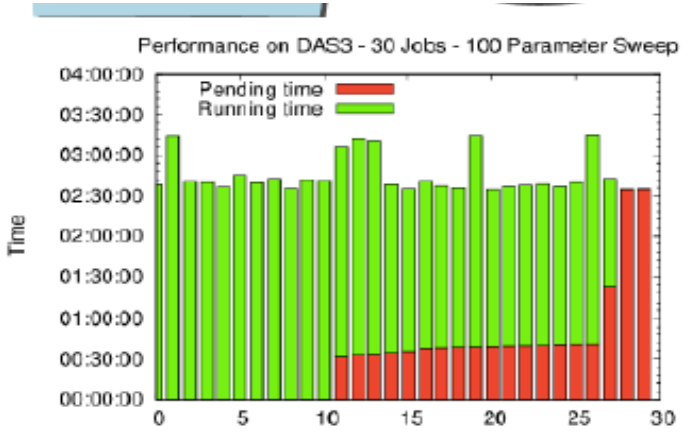


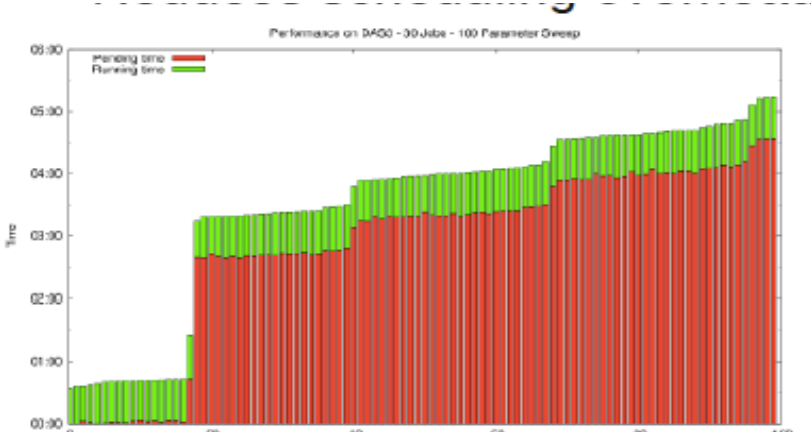


Reginald Cushing, Spiros Koulouzis, Adam S. Z. Belloum, Marian Bubak, **Dynamic Handling for Cooperating Scientific Web Services**, 7th IEEE International Conference on e-Science, December 2011, Stockholm, Sweden

Workflow as a Service (WFaaS)

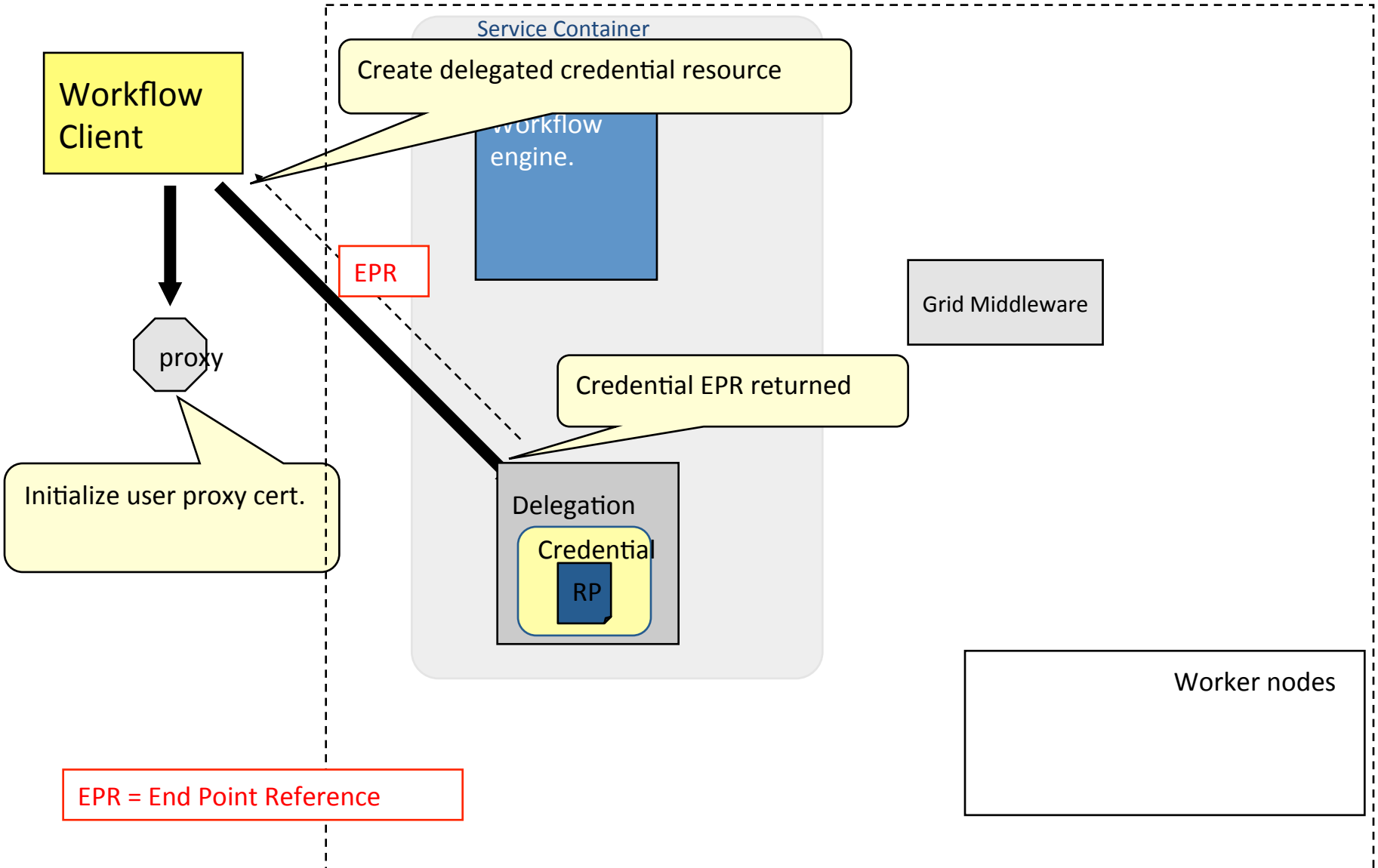
- Once a workflow is initiated on the resources it stays alive and process data/jobs continuously
- Reduce the scheduling overhead



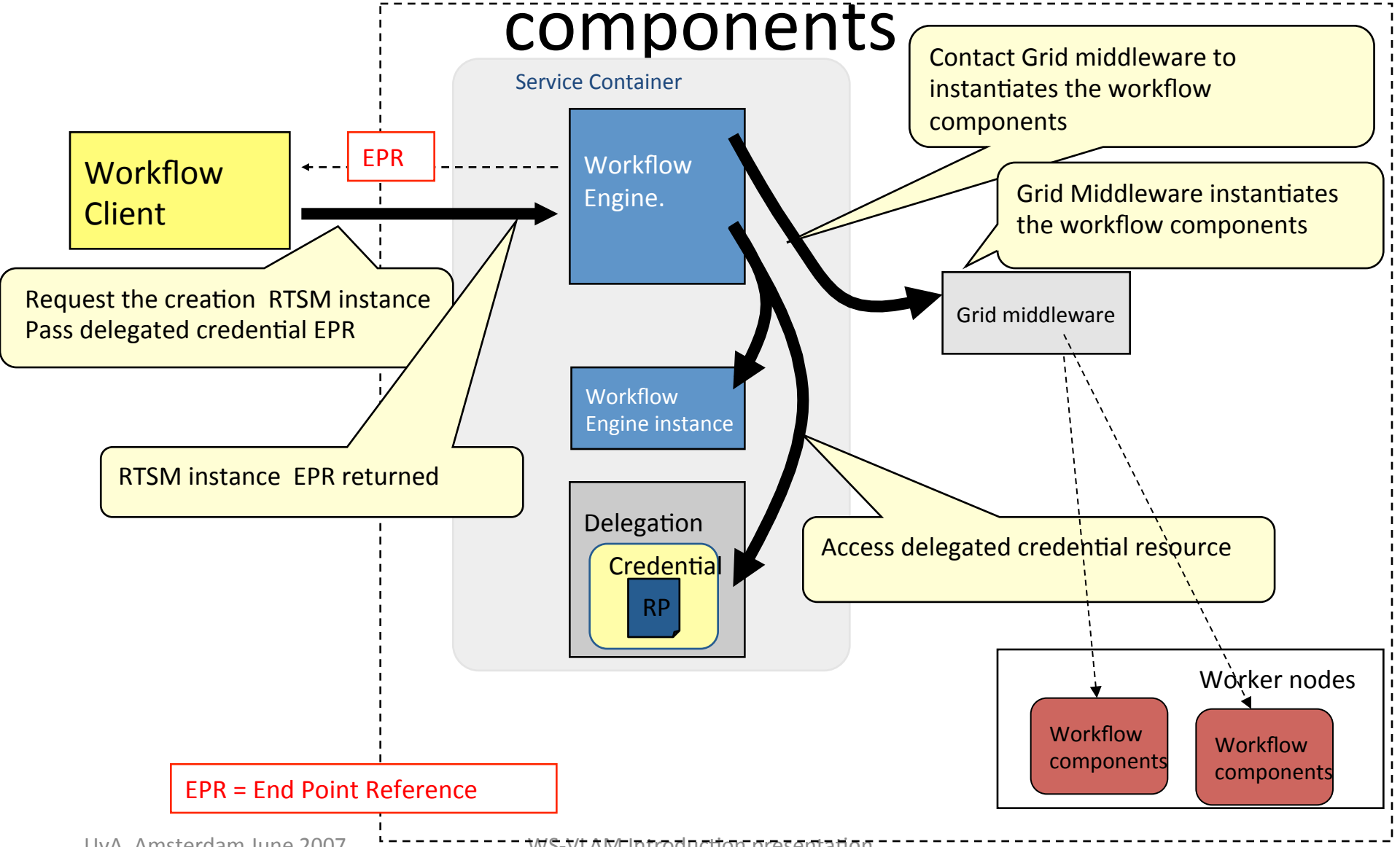


Reginald Cushing, Adam S. Z. Belloum, V. Korkhov, D. Vasyunin, M.T. Bubak, C. Leguy
ECMLS'12, June 18, 2012, Delft, *Workflow as a Service: An Approach to Workflow Farming*, The Netherlands

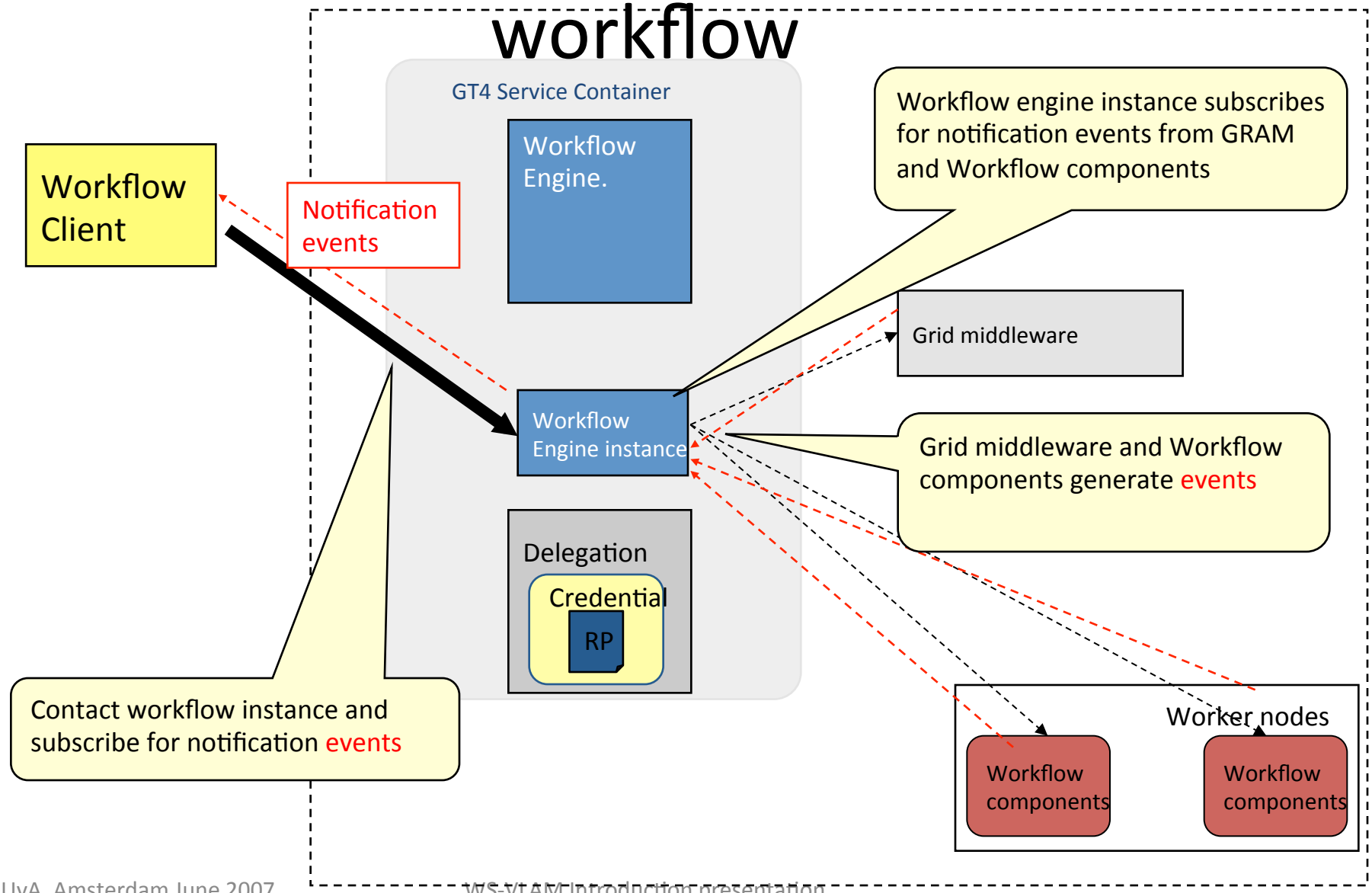
Step1: Create Delegated Credential



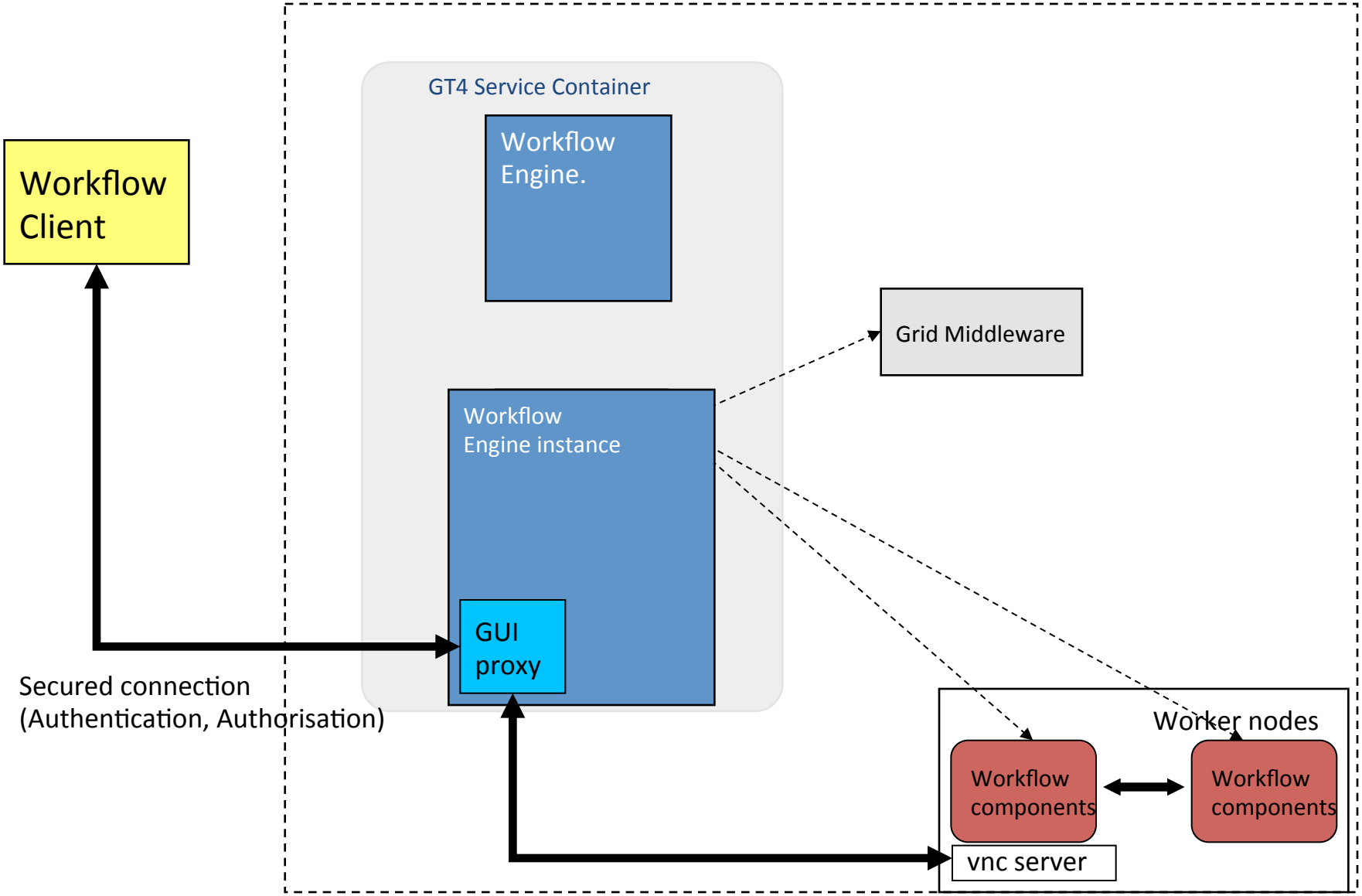
Step 2: instantiates the workflow components



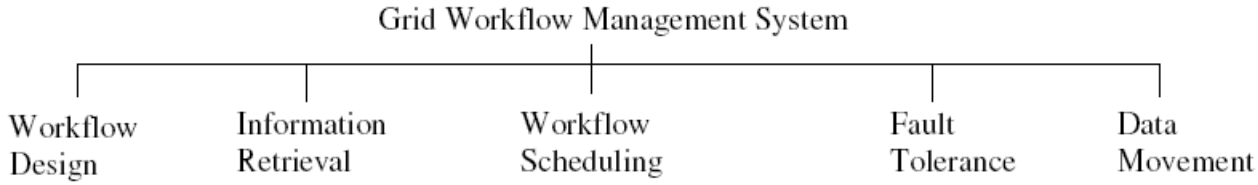
Step3: monitors the application workflow



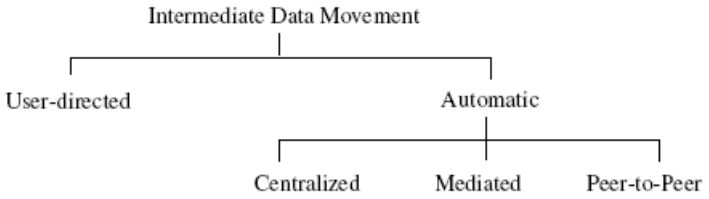
Workflow components with graphical output



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

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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?

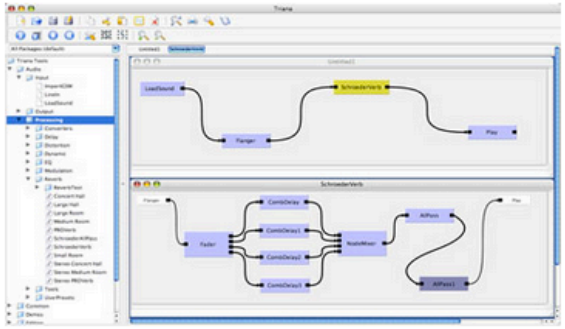
An open source problem solving environment developed at Cardiff University that combines an intuitive visual interface with powerful data analysis tools. Already used by scientists for a range of tasks, such as signal, text and image processing, Triana includes a large library of pre-written analysis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

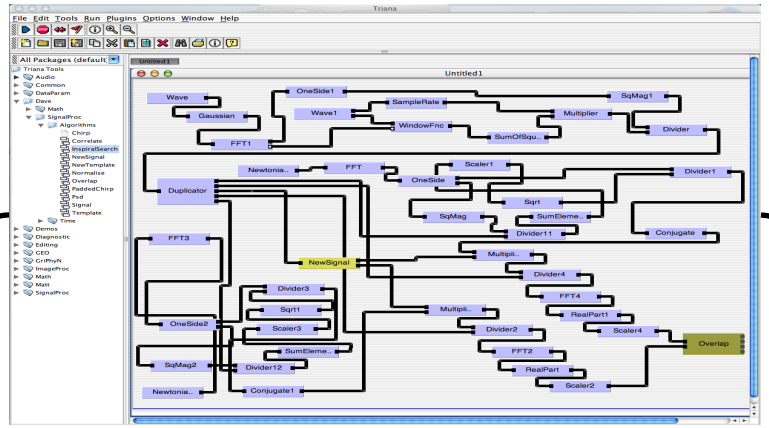
What does it look like?



Triana, the GAT and the GAP

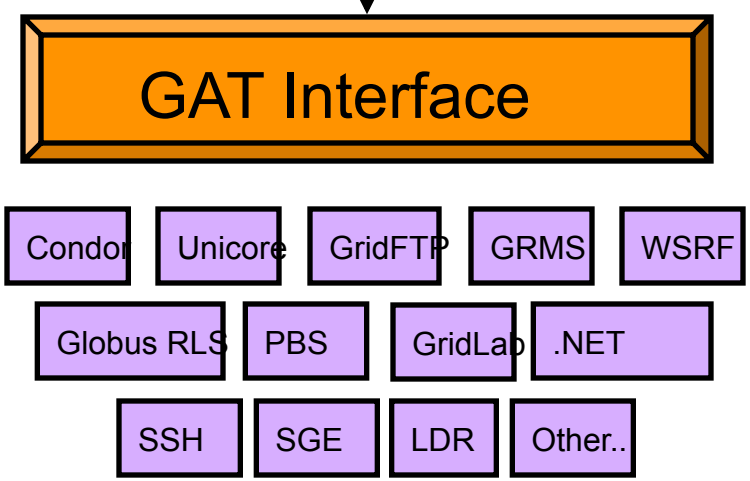
Grid Computing:

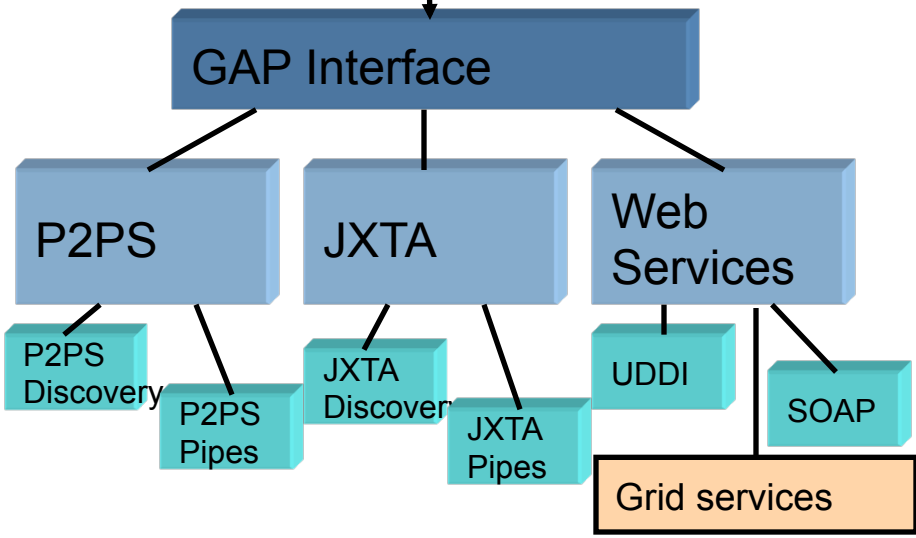
Job Submission, data services On top of a number of Grid Middleware



Service Based Computing:

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





Component Based Workflow Description: Kepler

user developer

you are here: home

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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, Kepl tists, analysts, and computer programmers create, execute, and share models and analyses across a broad range of scientific and engineering disciplines. Kepler of formats, locally and over the internet, and is an effective environment for integrating disparate software components, such as merging "R" scripts with compiled distributed execution of models. Using Kepler's graphical user interface, users simply select and then connect pertinent analytical components and data sources to executable representation of the steps required to generate results. The Kepler software helps users share and reuse data, workflows, and components developed address common needs.

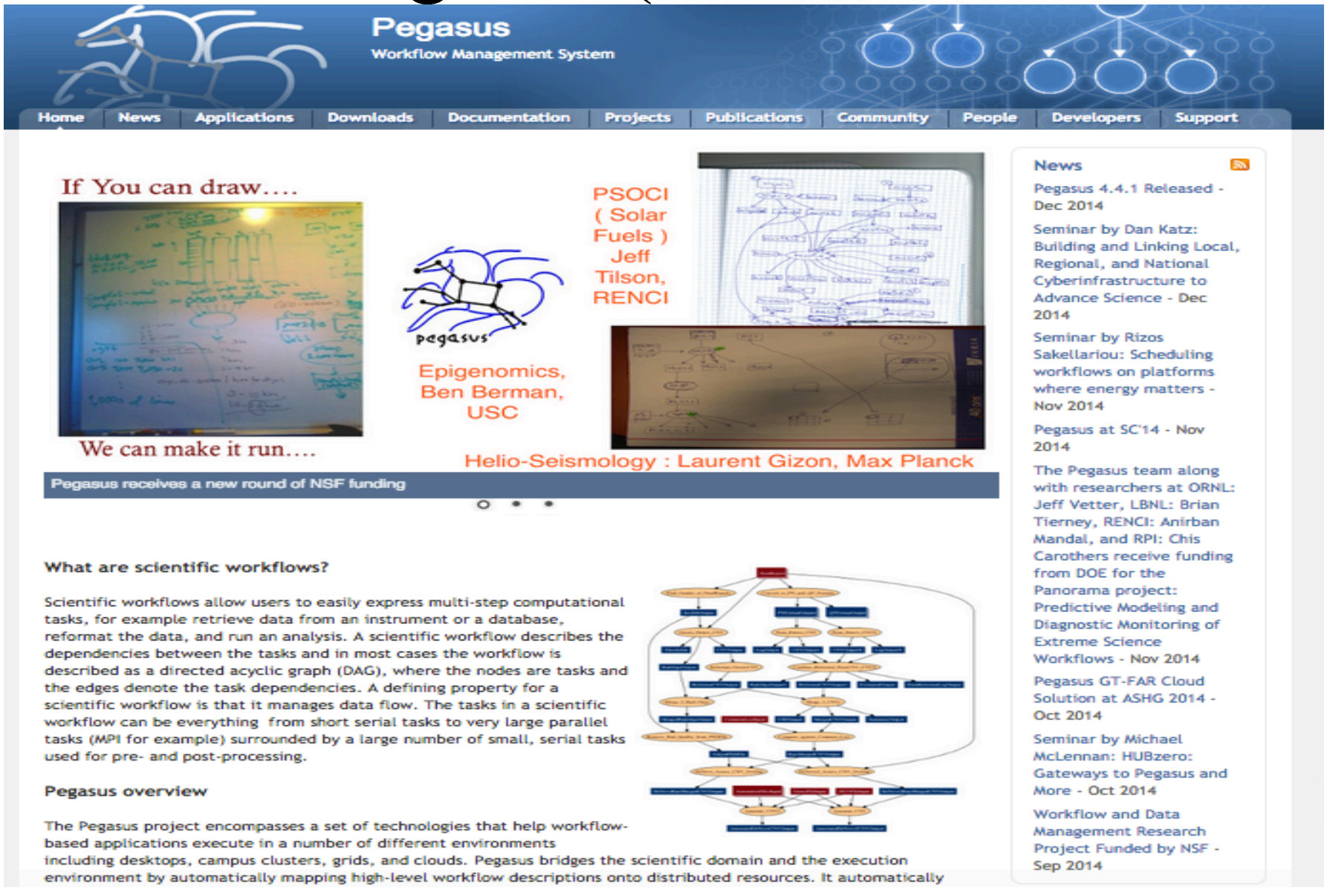
The Kepler software is developed and maintained by the cross-project Kepler collaboration, which is led by a team consisting of several of the key institutions that Santa Barbara, and UC San Diego. Primary responsibility for achieving the goals of the Kepler Project reside with the Leadership Team, which works to assure the l 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 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 we

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 K 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

Pegasus (GriPhyN)



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*

- 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.

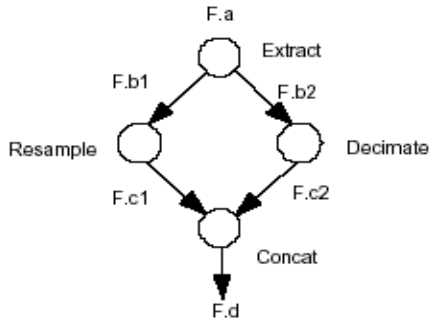


Figure 1.2. An example abstract workflow.

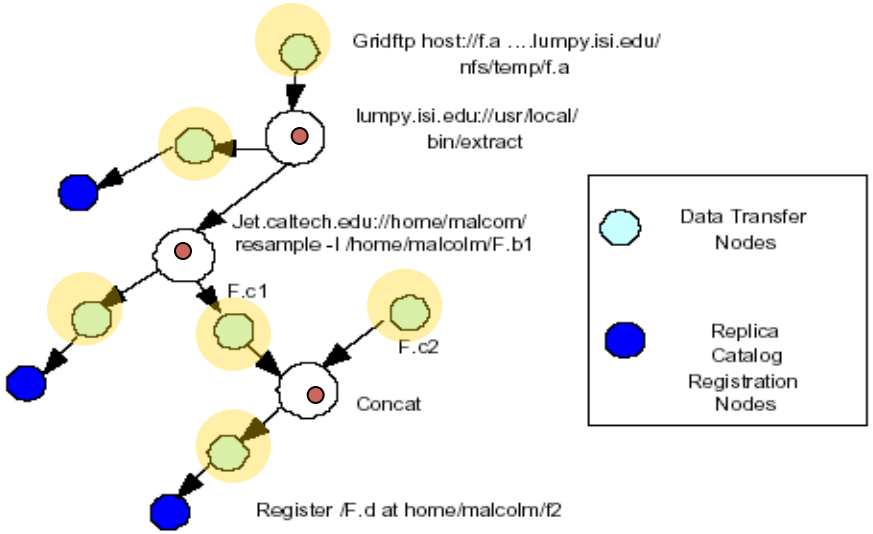


Figure 1.3. An example reduced, concrete workflow.

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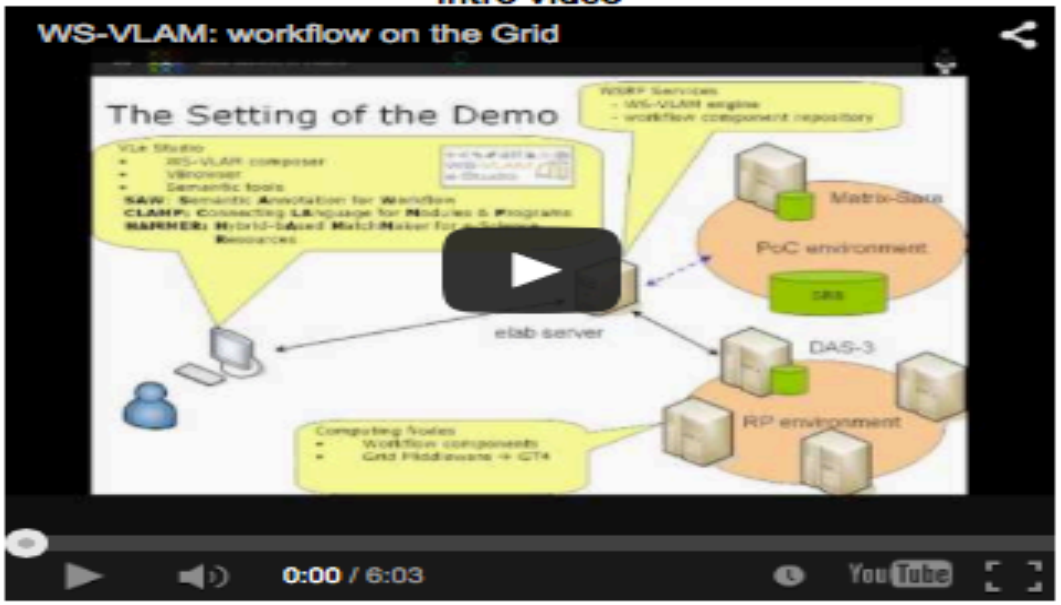
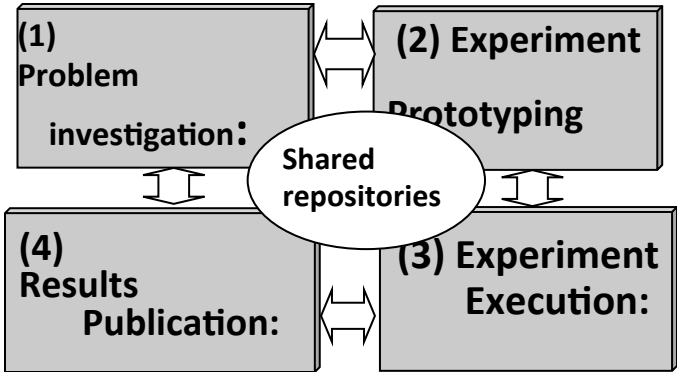
Intro video



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 Deelmana, Dennis Gannonb, Matthew Shields c, Ian Taylor, Future Generation Computer Systems 25 (2009)

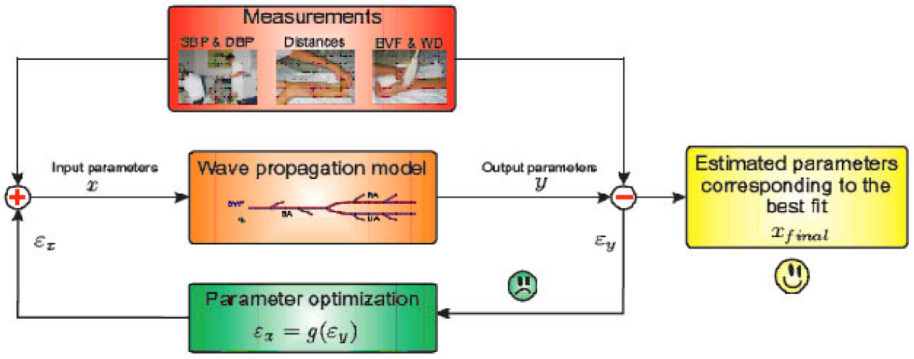
History-tracing XML (FH Aachen)

- 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.

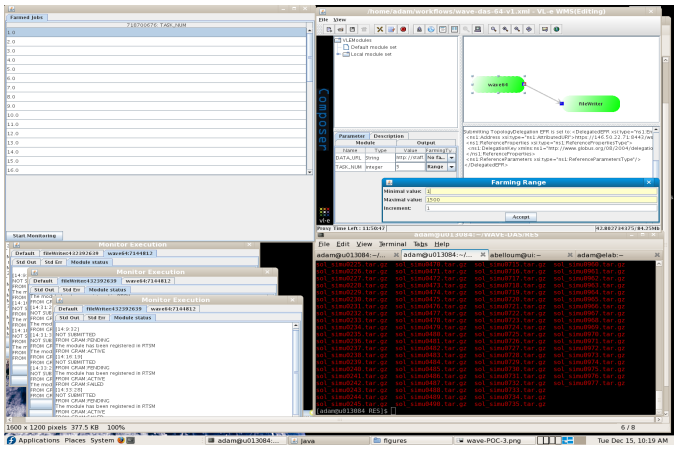
```
<patternMatch>
  <events>
    <PortResolved> provenance
data</PortResolved>
    <ConDone>provenance data
            </ConDone>
    ...
  </events>
  <fileReader2>
    <events> ... </events>
    <sign-fileReader2> ...
          </signfileReader2>
  </fileReader2>
  <sffToFasta>
    Reference
  </sffToFasta>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

M. Gerards, Adam S. Z. Belloum, F. Berritz, V. Snder, S. Skorupa, **A History-tracing XML-base Proveannce Framework for workflows**, WORKS 2010, New Orleans, USA, November 2010

wave propagation model applications



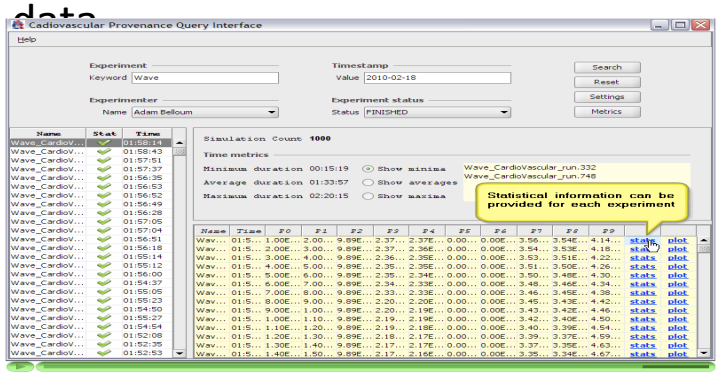
[Biomedical engineering Cardiovascular biomechanics group TUE])



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

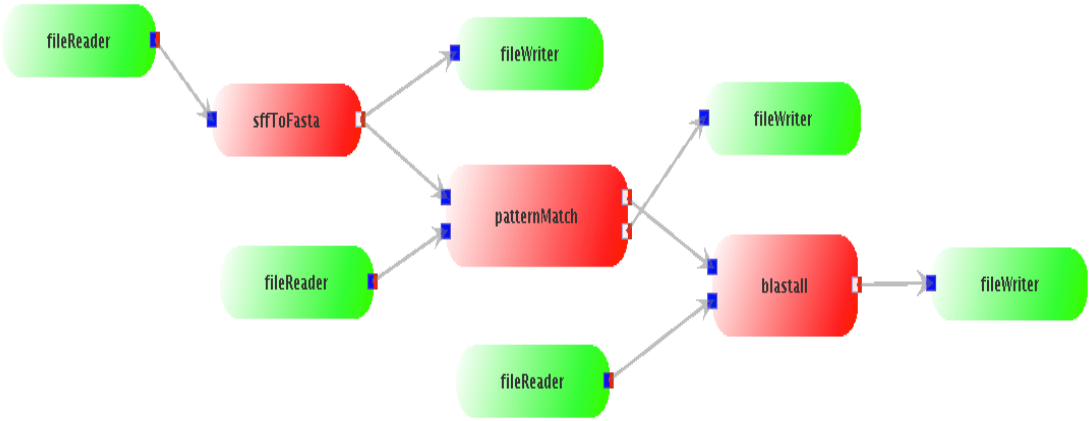
wave propagation model of blood flow in large vessels using an approximate velocity profile function:

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

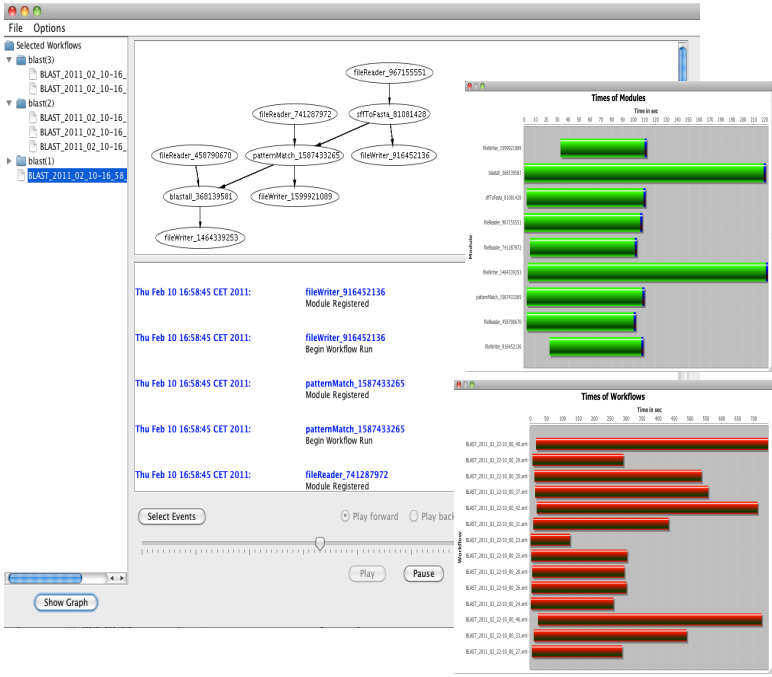


Query interface for the provenance data collected from 3000 simulations of the "*wave propagation model of blood flow in large vessels using an approximate velocity profile function*"

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.

For Each workflow run

The provenance data is collected an 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

on-going work UvA-AMC-fh-aachen

More References

1. A.S.Z. Belloum, V. Korkhov, S Koulouzis, M. A Inda, and M. Bubak *Collaborative e-Science experiments: from scientific workflow to knowledge sharing* JULY/AUGUST, IEEE Internet Computing, 2011
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
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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