



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

Adam Belloum Institute of Informatics University of Amsterdam a.s.z.belloum@uva.nl

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**UNIVERSITEIT VAN AMSTERDAM** 





# Outline

- Introduction
- Life cycle of e-Science Workflow
- Different approaches to workflow scheduling
  - Workflow Process Modeling & Management In Grid/Cloud
  - Workflow and Web services (intrusive/non intrusive)
- Provenance









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Computational Science

- Objective of the group
  - address the research issues related to building an e-Science framework which enables scientist to share, use knowledge add use geographically distributed resources (grids, clouds)
- Keywords:
  - Grid, Scientific workflow, SOA, provenance, interoperability

**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







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# 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

# 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.



# List of applications developed using WS-VLAM

<ul> <li>siaWin detector</li> </ul>	[Micro-Array Dept-UvA]
Affymetrix Permutation	[Micro-Array Dept-UvA]
• Omnimatch	[UU/Leiden]
<ul> <li>wave propagation</li> </ul>	[TUE]
• Blast	[AMC ]
<ul> <li>gut microbiota</li> </ul>	[CWI]
<ul> <li>Smart Infrastructure</li> </ul>	[SNE-UvA]
<ul> <li>Dynamic network control</li> </ul>	[SNE-UvA]
<ul> <li>GridSFEA,</li> </ul>	[TU Munchen]

More applications www.science.uva.nl/~gvlam/wsvlam/Applications

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APPLIED SCIENCI

#### Let us Start with an UvA-Slide: Virtual Laboratory for eScience





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#### Complex Scientific experiments model



**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





# Targets

- **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?

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# A WSRF enabled workflow engine



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



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# WS-VLAM Engine: architecture (1/2)







#### WS-VLAM Engine: architecture (2/2)







# Sequence-diagram







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# Sequence-diagram















# Model of computation

- Model of computation: stream-based process network.
  - Engine **co-allocates** all workflows.
  - Components waste time idling.
  - Co-allocation difficult.
- Communication: time **coupled** 
  - Assumes components are running
  - Simultaneously
  - Synchronized p2p
  - Fixed TCP/IP



#### **WS-VLAM** communication library



Fig. 1. Run-Time System Architecture.

V. Korkhov et al. VLAM-G: Interactive data driven workflow engine for Grid-enabled resources, Scientific Programming 15 (2007) 173–188 173 IOS Press



# WS-VLAM communication library

- Data transfer rate as a function of the data block size (average of 10 measurements per each data-block
- with the deviation not exceeding 5 percent)



Fig. 7. Average performance of the RTS library on WAN compared with standard Globus data transfer tool.

V. Korkhov et al. VLAM-G: Interactive data driven workflow engine for Grid-enabled resources, Scientific Programming 15 (2007) 173–188 173 IOS Press





# Model of computation

- Model of computation: dataflow network
  - components scheduled depending on data
  - components **only activated** when data is available
  - no need for co-allocation
- Communication: time decouples
  - messaging communication system.
  - components not synchronized
  - communication not strictly TCP/IP



# Additional features-Farming

- Task farming: task replication.
- Increases data consumption and production.
- Implements 3 types of farming:
  - Auto Farming: The engine decides on farm size depending on port load.
  - One-to-One Farming: A task replicated for every message received.
  - Fixed Farming: Statically defined.
- Allows parameter sweep studies.
- A task becomes a parameter engine







Reginald Cushing, Spiros Koulouzis, Adam S. Z. Belloum, Marian Bubak, **Prediction-based Auto**scaling of Scientific Workflows, 7th IEEE International Conference on e-Science, December 2011, Stockholm, Sweden





#### System Overview



Loosely coupled modules revolving around a message broker

Reginald Cushing, Spiros Koulouzis, Adam S. Z. Belloum, Marian Bubak, **Prediction-based Auto-scaling** of Scientific Workflows, Proceedings of the 9th International Workshop on Middleware for Grids, Clouds and e-Science, ACM/IFIP/USENIX December 12th, 2011, Lisbon, Portugal





#### **Enactment Engine**



Dataflow engine (**top-level** scheduler) based on Freefluo<sup>§</sup>

Models workflows as dataflow graphs

Vertices are tasks while edges are dependencies(data

Tasks have **ports** to simulate data channels

Dataflow model dictates that **only** tasks which have input are scheduled for execution.

<sup>§</sup>http://freefluo.sourceforge.net





#### Message Broker



Message broker plays a pivotal role in the system

Message broker acts as a data buffer

Communicating tasks are **time decoupled** 

Through queue sharing we can achieve scaling

Tasks **communicate** through messaging where messages contain **references** to actual data





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# Submission System



Pluggable schedulers (**bottomlevel**) for task match-making

Submitters (drivers) abstract actual resources such as cluster, grid, cloud

Scheduler matches a task to a submitter

Submitter does actual task/job submission



# Task Harnessing



Task harness is a **late binding**, **pilot-job** mechanism

A harness is submitted which will **pull** the actual job

The harness separates data transport from scientific logic

Better control of tasks





#### Task Auto-scaling



Messages between tasks are monitored

Queued data and mean data processing time are used to calculate **task load** 

Auto-scaling **replicates** a particular task to ameliorate the task load

Replicated tasks (*clones*) **partition** data by sharing same input message queues





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# Scaling Concepts



Data organized in atomic parcels(messages)









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# Scaling Concepts



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




## Auto-scaling steps

## Calculate data processing rate for designated port

$$proc(ip_{t_k}) = \frac{size(C_{ip.t_k})}{\sum_{j=2}^{n} mit_{ip.t_k}(m_{j-1}, m_j)}$$





# Auto scaling steps

## Calculate data processing rate for designated port







# Auto scaling steps

## Calculate data processing rate for designated port

$$proc(ip_{t_k}) = \frac{size(C_{ip.t_k})}{\sum_{j=2}^{n} mit_{ip.t_k}(m_{j-1}, m_j)}$$

Predict processing time for queued data

$$pred(ip_{t_k}) = size(Q_{ip.t_k}) \times proc(ip_{t_k})$$





# Auto-scaling Steps

## Calculate data processing rate for designated port

 $proc(ip_{t_k}) = \frac{size(C_{ip.t_k})}{\sum_{j=2}^{n} mit_{ip.t_k}(m_{j-1}, m_j)}$ Predict processing time for queued data  $pred(ip_{t_k}) = size(Q_{ip.t_k}) \times proc(ip_{t_k})$ Data size of queued data





# Auto-scaling Steps

#### Calculate data processing rate for designated port

$$proc(ip_{t_k}) = \frac{size(C_{ip.t_k})}{\sum_{j=2}^{n} mit_{ip.t_k}(m_{j-1}, m_j)}$$

Predict processing time for queued data

$$pred(ip_{t_k}) = size(Q_{ip.t_k}) \times proc(ip_{t_k})$$

Calculate needed replicated instances

$$repl(t_k) = \frac{pred(ip_{t_k})}{t_k^{st}}$$





# Auto-scaling Steps

### Calculate data processing rate for designated port

$$proc(ip_{t_k}) = \frac{size(C_{ip.t_k})}{\sum_{j=2}^{n} mit_{ip.t_k}(m_{j-1}, m_j)}$$

Predict processing time for queued data

$$pred(ip_{t_k}) = size(Q_{ip.t_k}) \times proc(ip_{t_k})$$
Calculate needed replicated instances
$$repl(t_k) = \underbrace{pred(ip_{t_k})}_{t_k^{st}}$$
Time Quantum for task



# Auto-scaling Steps (summary)

- Each task **port** is monitored to calculate the data **processing rate**
- Data is parceled in messages. Tasks consume messages
- Using the mean data processing rate and the amount of data queued on the port we extrapolate the proc. time for all data
- Based on the current resource we can estimate how many clones are needed to process all data within a time quantum
- Clones are submitted in **bursts** so not to flood resources
- Port is **continuously** monitored and further bursts can be submitted
- Once clones are active, message consumption is faster since clones share same queues





#### Queue sharing



Data partitioning using message queues. **Shadow**(gray) queues allow non partitionable data to be received by all clones





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#### Use case



Histogram difference is calculated between color spaces



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### Use case



### Workflow Without Scaling



## Workflow Without Scaling









## Use Case







#### Workflow execution with Scaling







#### Workflow execution with Scaling





# Auto Scaling Task -1





# Auto Scaling Task -2





### Other Scaled Task -1

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# Auto Scaling Task -2

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## Extension to support Cloud resources



Resource on-demand using multiple cloud providers, Super-computing 2010, and SCALE 2012



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# Usage of Web Services in e-science

- 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,
- but any workflow implementation is potentially faced with a *data transport problem*





# Service Submission



- Tasks/Jobs can be queued on the runqueue by any entity. The service submission listens on the runqueue and picks up new tasks to submit
- Resources such as Grid or Cloud are abstracted using submitters plugins
  - Enabling a new resource is a matter of writing its submitter Service Submission performs **matchmaking** between services and resources to run on

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



## Service Container Module



- The service container (Axis2) is the actual task that is submitted to a resource.
- The service container acts as a **pilot-job** mechanism Once active it will pull a web service to host.
- Axis2 is heavily modified to invert web service invocation from passive to active.
- Scaling, orchestration and communication are all handled within the service container



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# Bootstrapping Workflows



- The architecture has no central coordinator to orchestrate a workflow. Hence a workflow is only bootstrapped i.e. submit the starting services. The rest are autonomously scheduled by the service containers on the resources.
- The bootstrap client submits the **first** service and waits for output of the last service.





## **Orchestration Steps**



- 1. Workflow is **bootstrapped** by submitting the workflow entry points onto the queue
- 2. Submission service picks up the queued service and submits to a resource.
- 3. Service container starts executing on a resource
- 4. Service container **pulls** a web service and polls for data to be consumed by the service.
- 5. Service container outputs data to the next service
- 6. Service container queues the next service if none exist



## Service Container - Transport



- Transport handler requests SOAP from message broker queues instead of passively listening for HTTP
- Pull model allows web services to "bypass" firewalls and thus can be deployed within networks
- **Transport Sender** picks up the return SOAP message and sends it to the message broker

# Service Container - Control



- **Message transformer** transforms a SOAP output to SOAP input for other services in the workflow
- The message transformer allow back-to-back service communication





#### Resource management

- Within a single workflow services are **competing** for resources.
- Scaling one service without any regard to the whole workflow may starve parts of the workflow and hamper progress
- It would be ideal to have a mechanism to greedily consume resources if no one is using them but donate back resources once they are requested.

Fuzzy controller tries to do just that.





## **Fuzzy Controller**



- IF taskLoad IS very\_high AND resourceLoad IS very\_low THEN replication IS positive\_aggressive.
- **IF** taskLoad **IS** very\_low **AND** resourceLoad **IS** high **THEN** replication **IS** negative\_aggressive.







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**Fuzzy** Controller

IF taskLoad IS very\_low AND resourceLoad IS high THEN replication **IS** negative\_aggressive.



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# Fuzzy Rule Map



- Service load is based on the amount of data being queued on the service and the time quantum for the service to run
  - The service container **continuously** monitors the **data processing rate** and estimates the computation time needed to process all the queued data within a time frame of the data and the processing time are directly proportionate. This might not be the case for all problems.

The **estimated processing time** and the **time quantum** given by the resource for executing the service are used to **derive** the **service load**. Thus a service load of 2 means that it will take twice as much time as the allocated quantum to process the data.



## Back-to-Back Communication



- Back-2-Back communication allows web services to communicate directly without the need for an intermediate client.
- This is achieved through the message broker which exposes dedicated connections queues.

Foreach connection in A.method1.connections
 SOAPTemplate = getTemplate(connection);
 destinationQueue = getDestination(connection);
 newSOAP = transformSOAP(A.method1.output, SOAPTEmplate);
 write(newSOAP, destinationQueue);

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# Autonomous Orchestration



- The service container can query the message broker to deduce if and instance of **B** is running.
- If no instance of B is running, the service container for A submits B to the runqueue.
- Service containers are myopic

Foreach connection in A.method1.connections
 SOAPTemplate = getTemplate(connection);
 destinationQueue = getDestination(connection);
 newSOAP = transformSOAP(A.method1.output, SOAPTEmplate);
 write(newSOAP, destinationQueue);
 If not active(destinationQueue)
 submit( getService(connection) );





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## Use Case



- Workflow with 2 pipelines. The pipelines perform sequence alignments using data from UniProtKB
- Each pipeline performs 22500 alignments i.e. 45100 total alignments in all
- All modules are standard web services which are hosted in the modified Axis2 container
- The alignments where performed using BioJava api
- Source and sink are part of the bootstrapping sequence. Source submits the getSequenceId service while sink waits for output from the htmlRenderer
- The Distributed ASCI Computer 3 (DAS3) was used as the resource pool. www.uniprot.org

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## **Evaluating Auto-Scaling**

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**Running Service instances**


#### Scale up web services

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The fuzzy controllers **scale up** the web services to meet the demands





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#### Scale up web services





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#### Scale down web services





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## Usage of Web Services in e-science

- In service orchestration, all data is passed to the workflow engine before delivered to a consuming WS
- Data transfers are made through SOAP, which is unfit for large data transfers



#### Enabling web services to consume and produce

*large distributed* datasets Spiros Koulouzis, Reginald Cushing, Konstantinos Karasavvas, Adam Belloum, Marian Bubak to be published JAN/FEB, IEEE Internet Computing, 2012



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## ProxyWS

- uses multitude of protocols to transport large data
  - used as an interface for developing WSs able to stream data.
  - Or as enabler for legacy web services to stretch their current potential by referencing data that would otherwise be delivered via SOAP







### Indexing Name Entry Recognition

- AIDA provides a set of components which enable the indexing of text documents in various formats.
- AIDA's Indexer component, called IndexerWS is a WS able to index document with the use of the Streaming library.





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## Results Indexing Web Services for Information Retrieval (Indexing)



**Enabling web services to consume and produce large distributed** datasets Spiros Koulouzis, Reginald Cushing, Konstantinos Karasavvas, Adam Belloum, Marian Bubak to be published JAN/FEB, IEEE Internet Computing, 2012





### Results Indexing Web Services for Information Retrieval (NER)



**Enabling web services to consume and produce large distributed** datasets Spiros Koulouzis, Reginald Cushing, Konstantinos Karasavvas, Adam Belloum, Marian Bubak to be published JAN/FEB, IEEE Internet Computing, 2012



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- 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) 528540

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## 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



- PLIER is an implementation of the OPM 1.1 specifications.
- It's API provides a set of functions to build, store, and share workflow experiments as graphs.
- It also implements an optimal relational database as back-end storage that captures the concepts of the OPM model, using the Java Persistence API (JPA 2.0) and Hibernate.
- In addition, the PLIER API provides specific interfaces, using JDO 3.1, to transform, or serialize, the provenance data into specific formats (e.g. RDF, XML, and DOT).





#### 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

BigGrid project 2009, presented EGI/ BigGrid technical forum 2010



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



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"





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## **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





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### More References

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- 3. A. Belloum, Z. Zhao, and M. Bubak Workflow systems and applications , Future Generation Comp. Syst. 25 (5): 525-527 (2009)
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- Zhiming Zhao, Adam Belloum, Cees De Laat, Pieter Adriaans, Bob Hertzberger Using Jade agent framework to prototype an e-Science workflow bus Authors Cluster Computing and the Grid, 2007. CCGRID 2007



#### http://www.commit-nl.nl/



http://www.science.n/~gvlam/wsvlam/

vl-e http://www.vle.nl/