COMMIT/

WS-VLAM Workflow Management System and its Applications

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Lunch meeting, Netherlands eScience Center, Amsterdam 2013

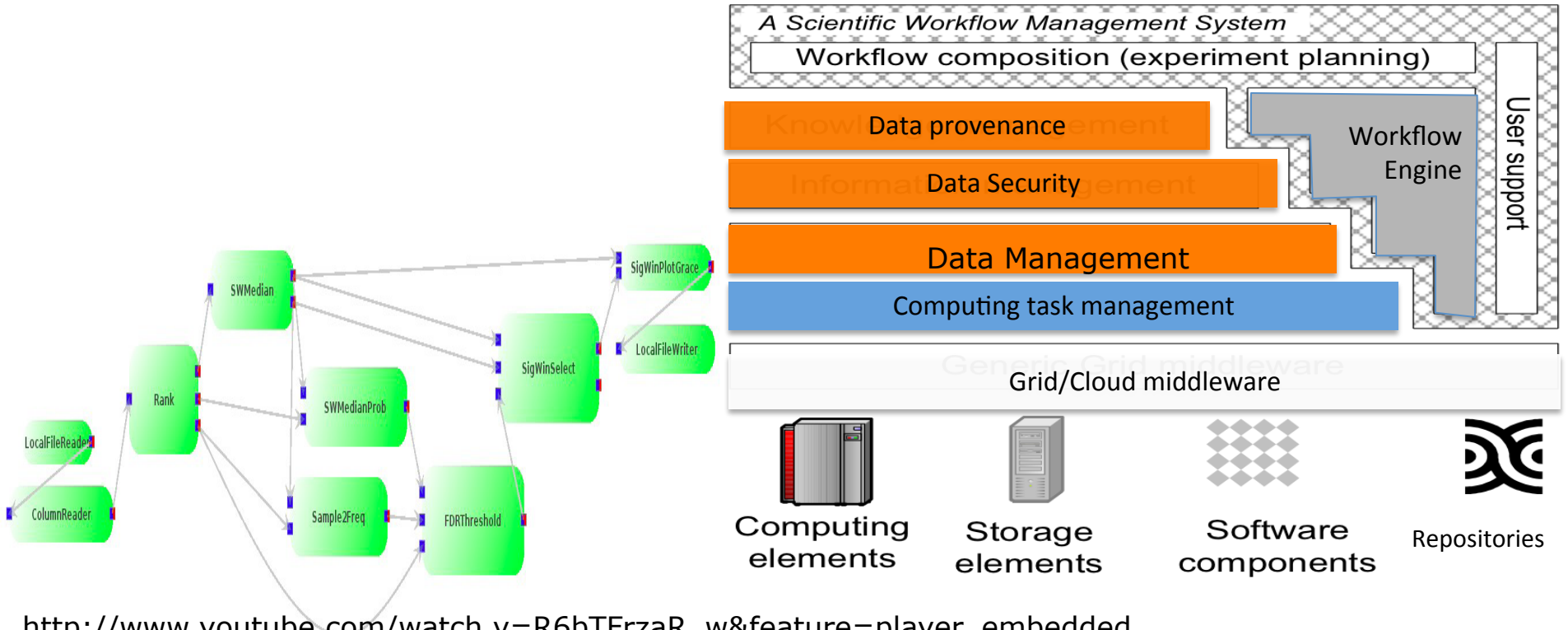
System and Network Engineering

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
- Computing in the browser
- Conclusions

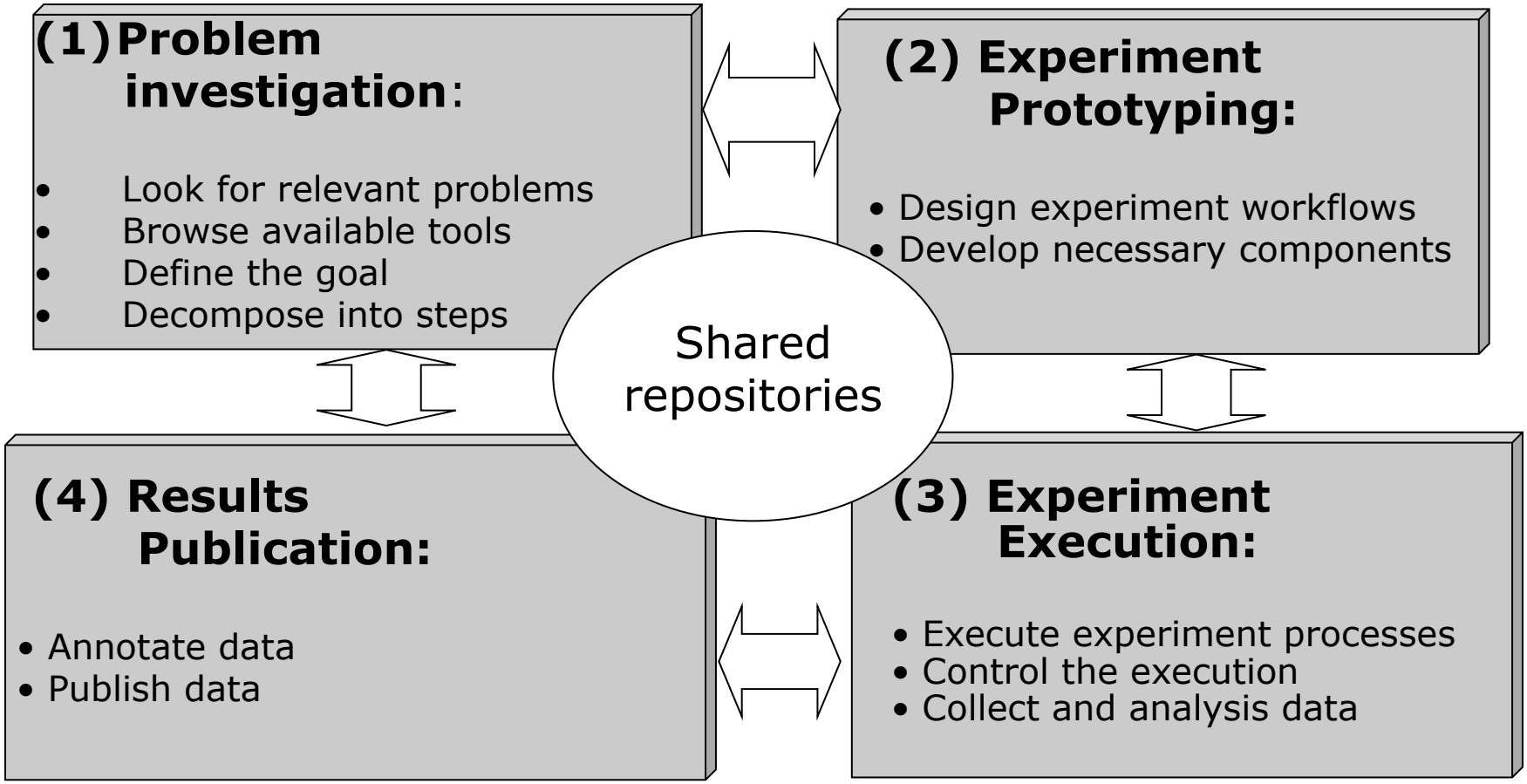
Workflow Management Systems

Workflow management system **coordinates the execution** of a scientific applications on a set of **computing distributed resources**



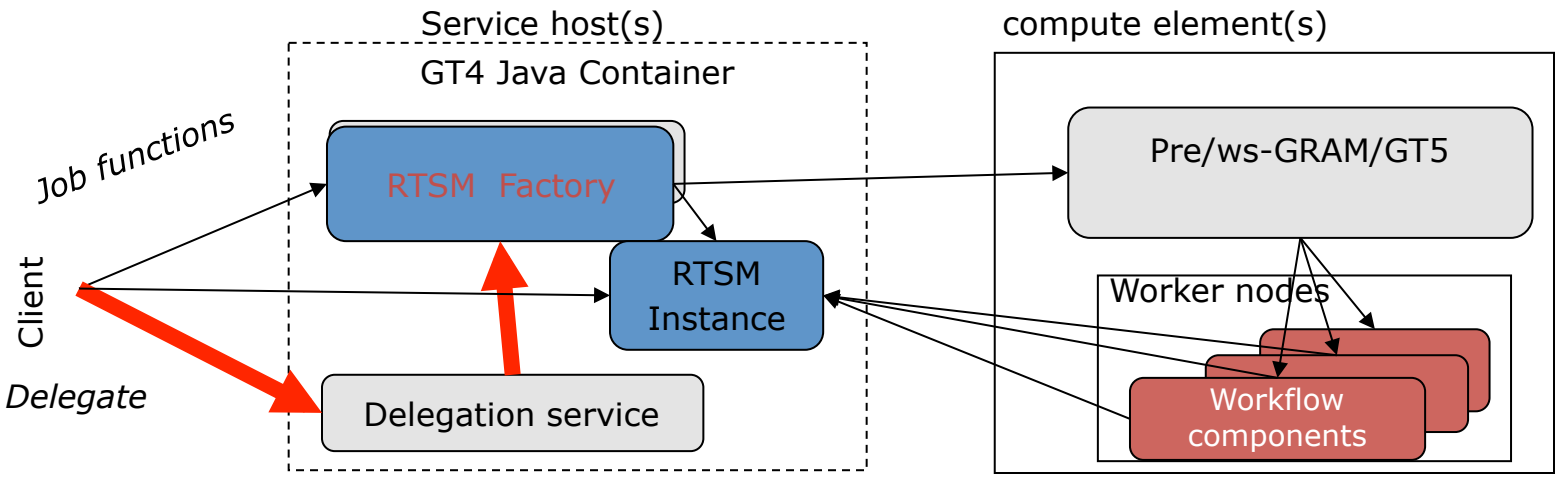
http://www.youtube.com/watch v=R6bTFrzaR_w&feature=player_embedded

Life Cycle of a Scientific Experiment



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/AUGUSTInternet Computing, IEEE, vol.15, no.4, pp.39-47, July-Aug. 2011 doi: 10.1109/MIC.2011.87*

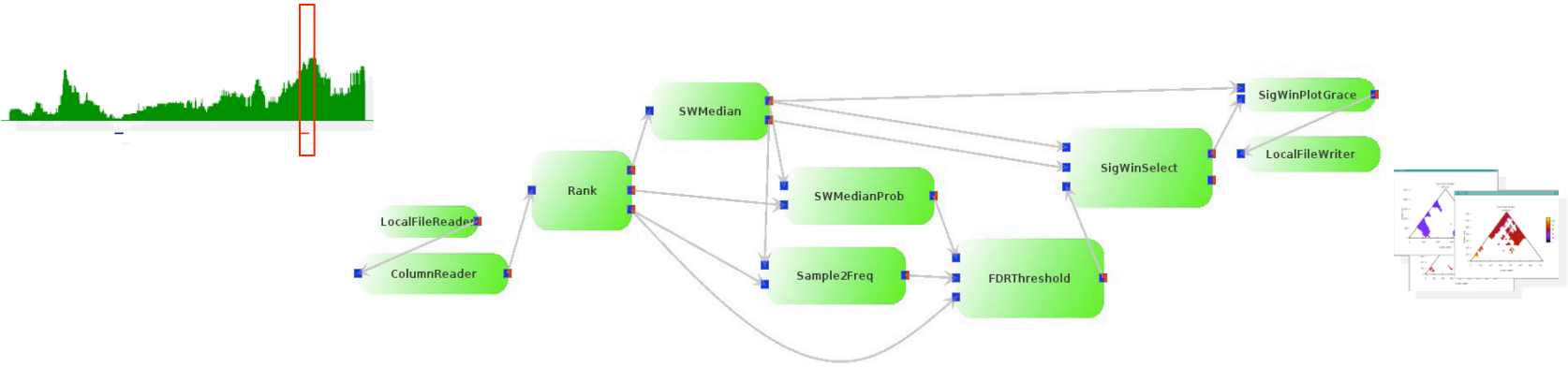
WS-VLAM Engine: Architecture (1st generation)



- Target: stream-based Applications
  - Engine **co-allocates** all workflow components
- Communication: time **coupled**
  - Assumes components are running
  - Simultaneously
  - Synchronized p2p

WS-VLAM Features

- Provide **streaming** facilities between applications executed on resource geographically distributed.
- **Composition** and the execution of **hierarchical** workflows.
- **Remote** graphical output.
- **Detach/attach** capability for long running workflows.
- Provides a **monitoring** facilities based on the WS-notification.
- Provides **workflow farming** possibilities.



DNA curvature of the *Escherichia Coli* chromosome

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.

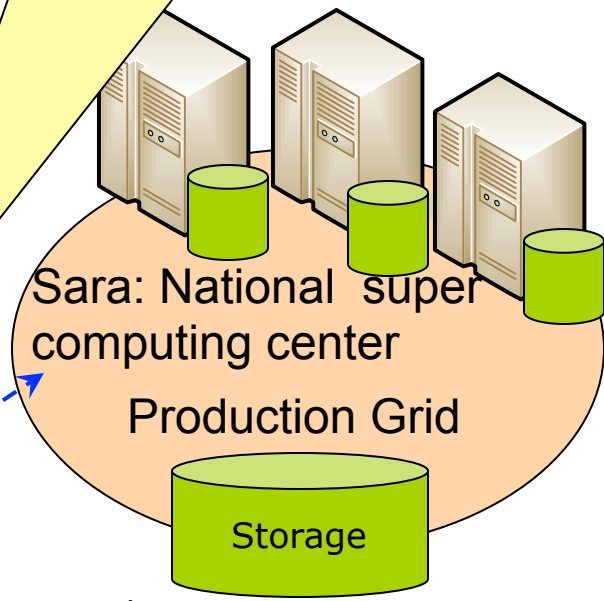
More features: http://staff.science.uva.nl/~gvlam/wsvlam/demos/wsvlam-about.html

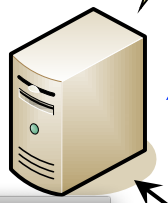
Easy Deployment

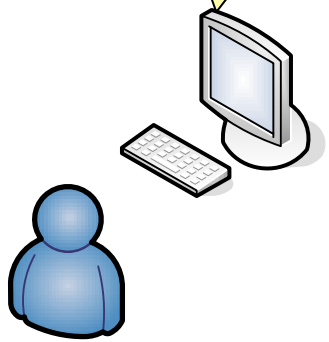
WSRF Services (2 services)
- WS-VLAM engine
- workflow component repository

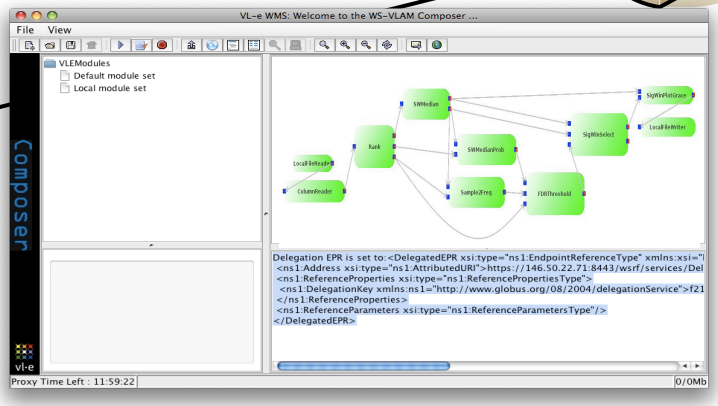
Workflow composer (java Web Start)
- WS-VLAM composer
- VBrowser
- Semantic tools

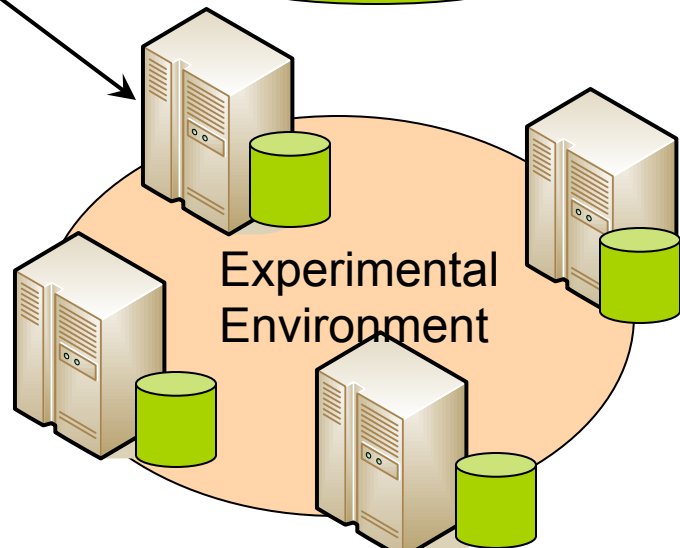
SAW: **S**emantic **A**nnotation for **W**orkflow
CLAMP: **C**onnecting **LA**nguage for **M**odules & **P**rograms
HAMMER: **H**ybrid-b**A**sed **M**atch**M**aker for e-Science **R**esources





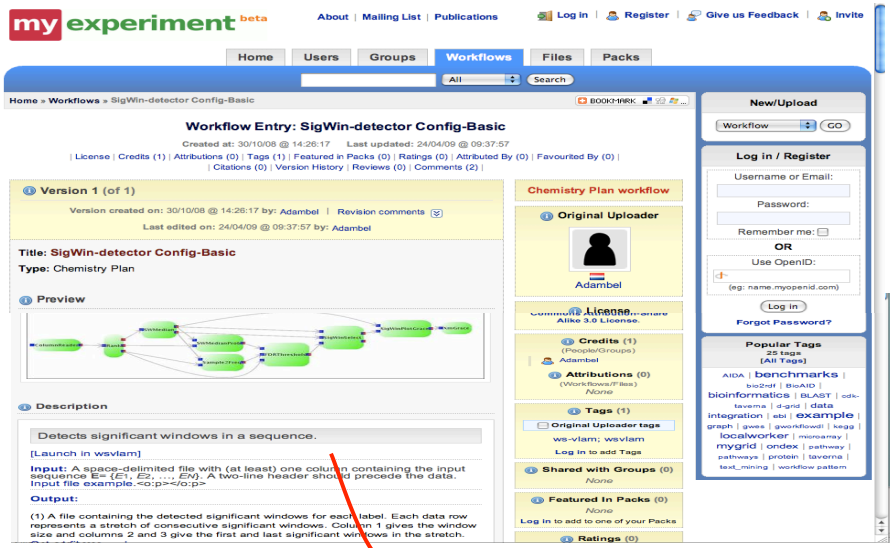




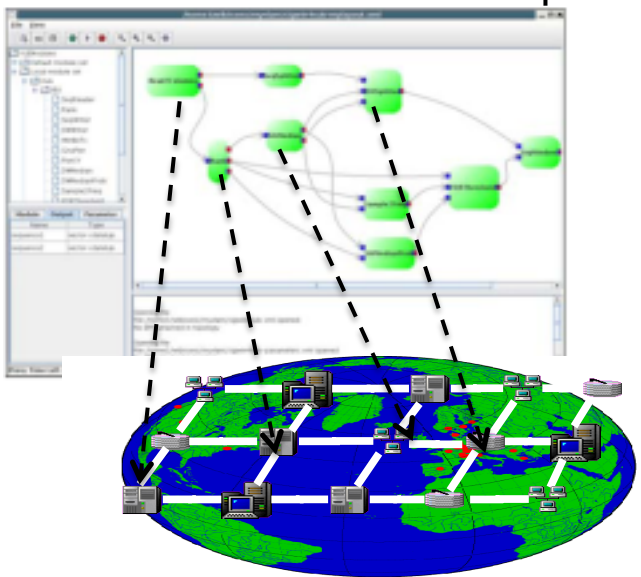


Workflow Sharing and re-usability

- Workflow engine may be invoked form other systems like
  - Taverna, Kepler, Pgrade
- Workflow may be made available to entire community
  - using Web 2.0 approach



WS-VLAM composer

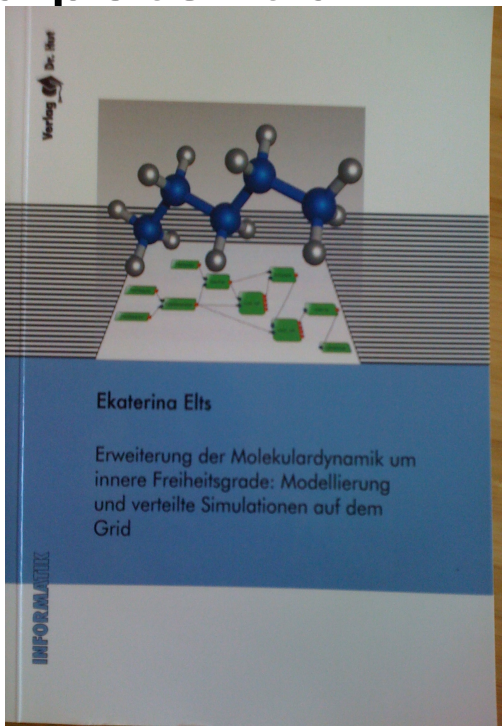


Comparing to other Workflow Management Systems

- WS-VLAM was studied by Elts and Bungartz in 2010 from the Institute of informatics of the Technical university of Munich as a potential platform for a PhD work

Grid-Workflow-Management-Systeme fur die Ausfuhrung wissenschaftlicher Prozessablaufe
Ekaterina Elts, Hans-Joachim Bungartz

http://staff.science.uva.nl/~gvlam/wsvlam/Publications/workflow_review_Elts.pdf



WS-VLAM Comparing to other Workflow Management Systems

	Open Source	Universalität	Middleware	GUI	Legacy Code	Komponenten-bibliothek	Komponenten-entwicklung	Parameter Studium
Taverna	ja	nein	-	gut	mit SOAPLAB	umfangreich	N/A	Liste
Triana	ja	ja	GT4 durch Java-GAT	gut	ja	umfangreich	Java	Liste
WS-PGrade	nein	ja	GT2/4, gLite LCG2	gut	mit GEMLCA	-	-	Liste,Bereich, Random, aus Eingangs-datei
WS-VLAM	ja	ja	GT2, GT4	gut	ja	umfangreich	Java, Python C++	Liste, Bereich
Kepler	ja	ja	GT2	gut	ja	sehr umfangreich	Java	via Nimrod
ASKALON	nein	ja	GT2, GT4	gut	muss als Service adaptiert wer-den	-	-	beliebig kom-pliziertes, mittels ZEN-Direktiven
ICENI	ja	ja	Condor, GT2, SGE	beschränkt	ja	nicht umfangreich	Java	Liste
Pegasus	ja	ja	Condor, GT2/3/4	beschränkt	beschränkt	nicht umfangreich	N/A	beschränkt
GWES	ja,aber nicht GUI	ja	GT4, pure Web-Services	beschränkt	ja	kein	kein	beschränkt
Karajan	ja	ja	GT2, GT4	beschränkt	ja	kein	kein	Liste, Bereich, Hashmap
g-Eclipse	ja	ja	gLite, GRIA, GT2	gut	ja	JSDL-Dateien	JSDL-Dateien	nein
UNICORE	ja	ja	UNICORE	gut	ja	JSDL-Dateien	JSDL-Dateien	Liste, beschränkt

Tabelle 1: WMS Übersicht

by Ekaterina Elts TUMunchen

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UNICORE	ja	ja	UNICORE	gut	ja	JSDL-Dateien	JSDL-Dateien	Liste, beschränkt

Tabelle 1: WMS Übersicht

by Ekaterina Elts TUMunchen

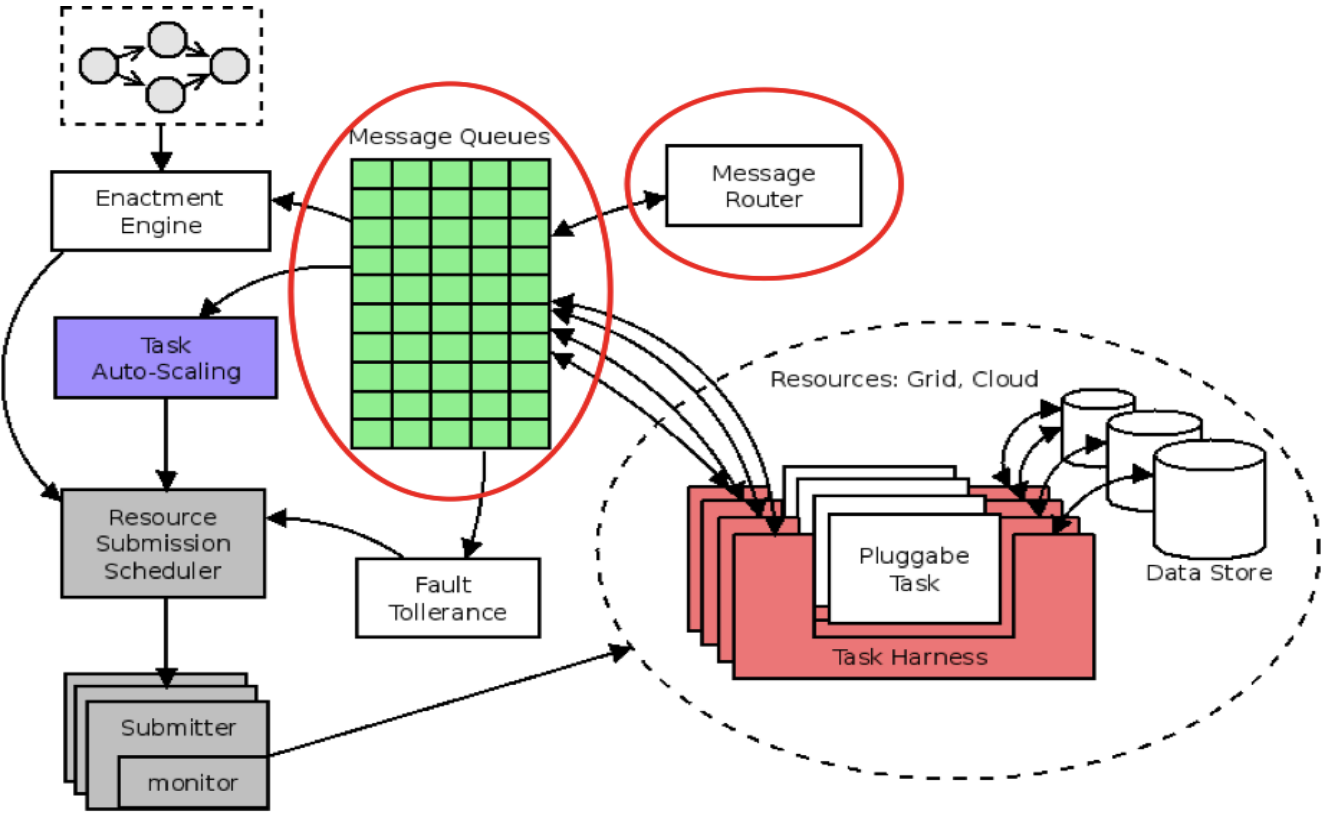
WS-VLAM Engine: architecture (2nd generation)

- Target: loosely couple applications
  - 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

WS-VLAM Engine: Architecture (2nd generation)

Data driven Workflow coordination



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

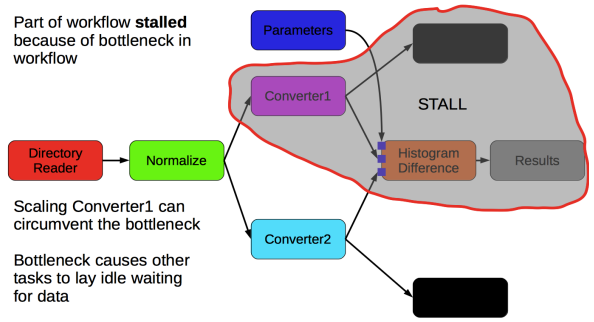
Reginald Cushing, Spiros Koulouzis, Adam S. Z. Belloum, Marian Bubak, **Prediction-based Auto-scaling of Scientific Workflows**, MGC'2011, December 12th, 2011, Lisbon, Portugal

Farming with WS-VLAM

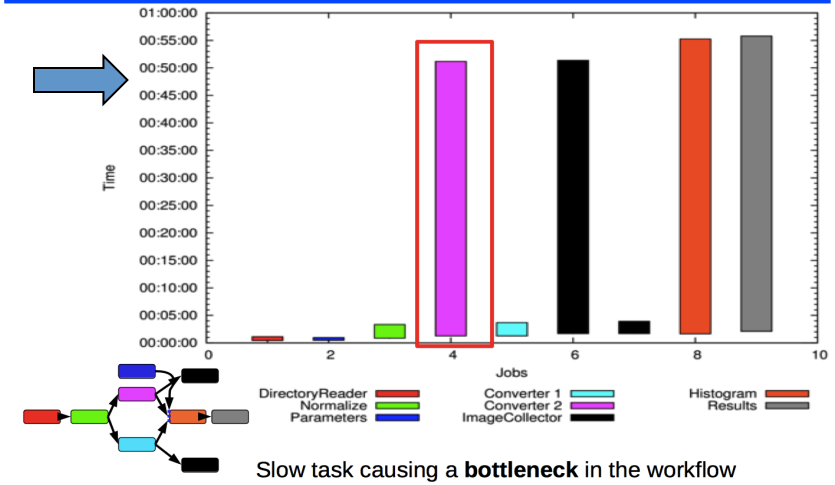
- Task farming: **task** replication
  - parameter sweep application,
  - DNA Sequencing,
  - Monte Carlo,
  - …
- Implements 3 types of farming:
  - Auto Farming: the number of tasks/services to run is proportional to the load
  - One-to-One Farming: A task replicated for every message received.
  - Fixed Farming: user defined farming.

Farming and Auto-scaling of Workflows

Use Case

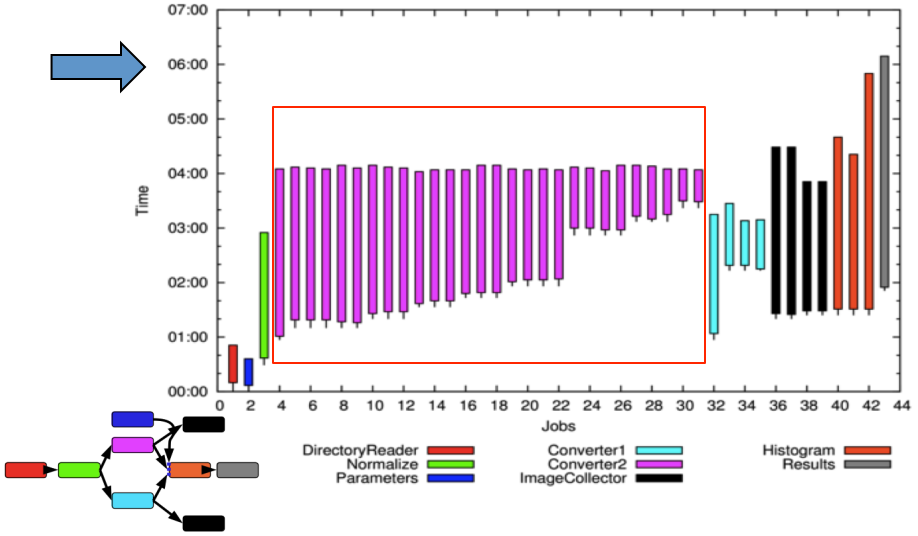


Workflow Without Scaling



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

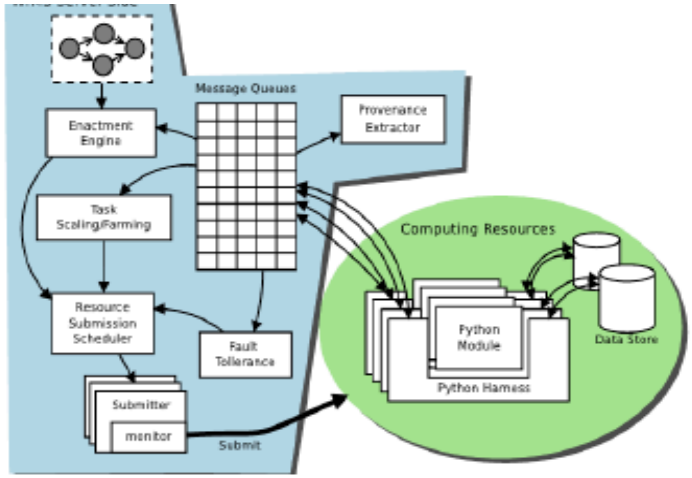
Workflow execution with Scaling



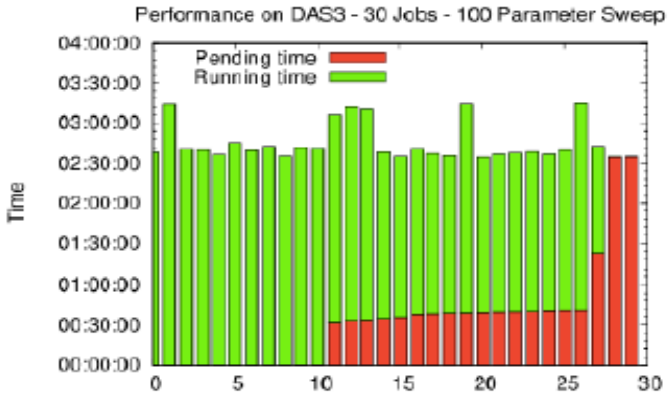
Reginald Cushing, Spiros Koulouzis, Adam S. Z. Belloum, Marian Bubak, **Prediction-based Auto-scaling of Scientific Workflows**, Proceedings of the 9th International Workshop on Middleware for Grids, Clouds and e-Science, ACM/IFIP/USENIX December 12th, 2011, Lisbon, Portugal

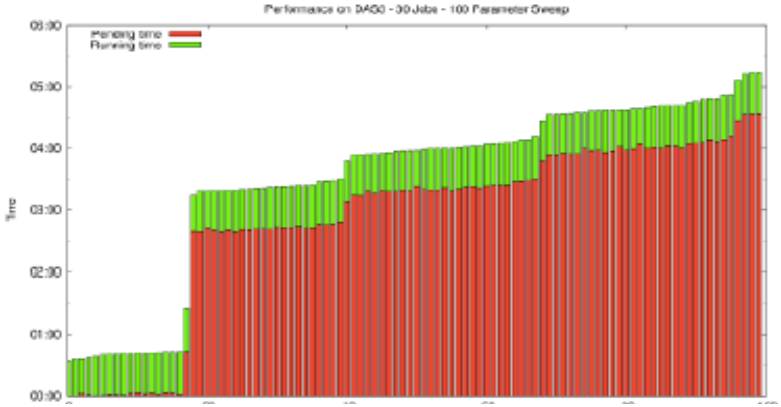
Workflow as a Service (WFaaS)

Reduce Scheduling Overhead



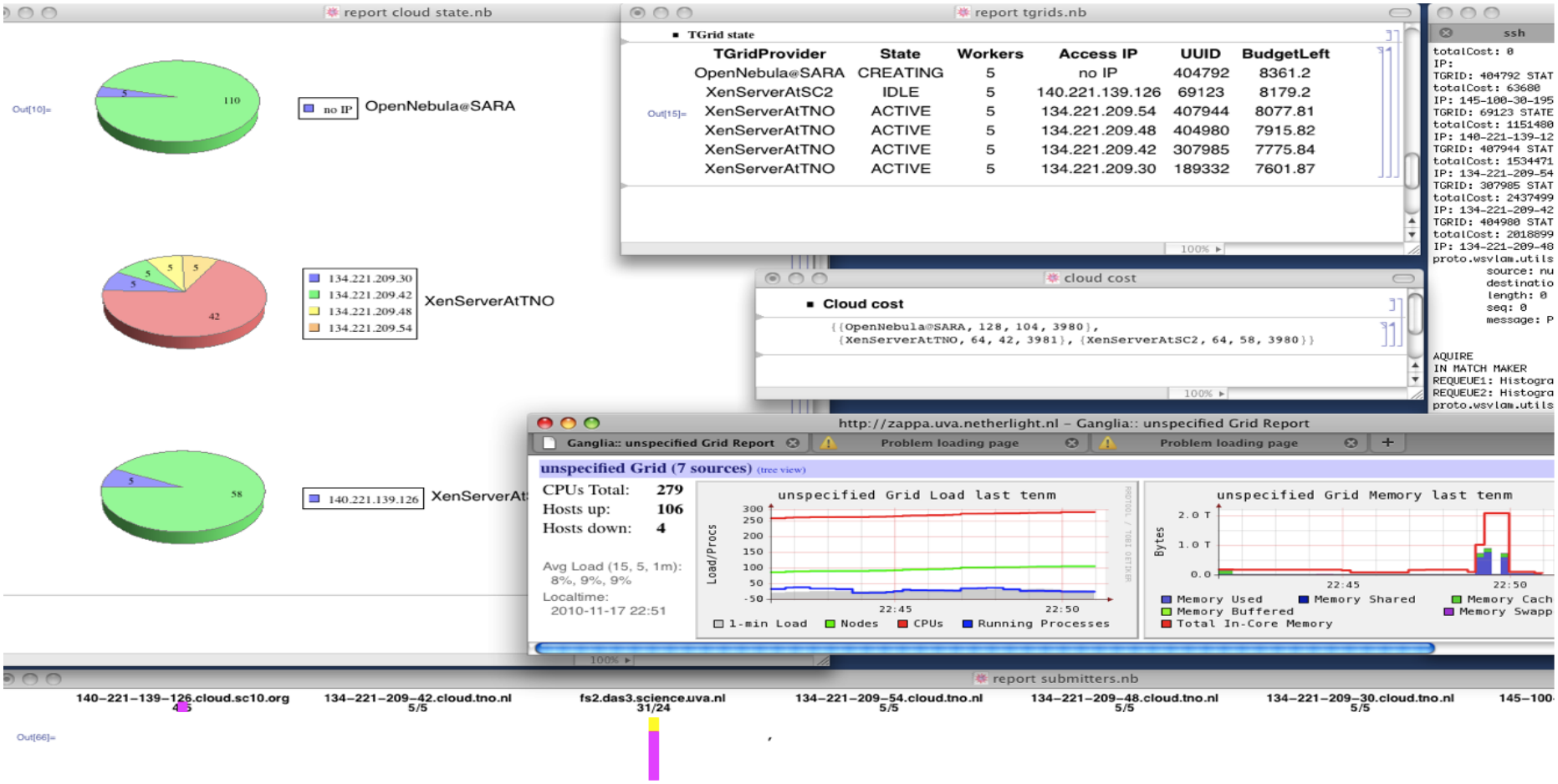
- We describe the notion of a workflow as a service WFaaS
- Once a workflow is initiated onto the resources it can stay alive and data is continuously fed to it for processing
- Workflow becomes a stream processor
- Reduces scheduling overhead





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

Resource on-demand for Applications with Hard Deadline (Urgent Computing)



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

Outline

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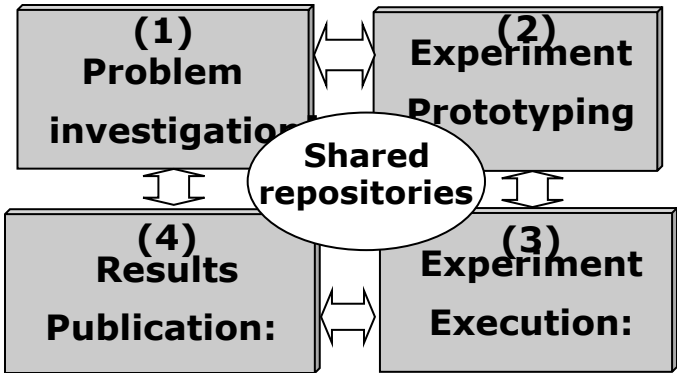
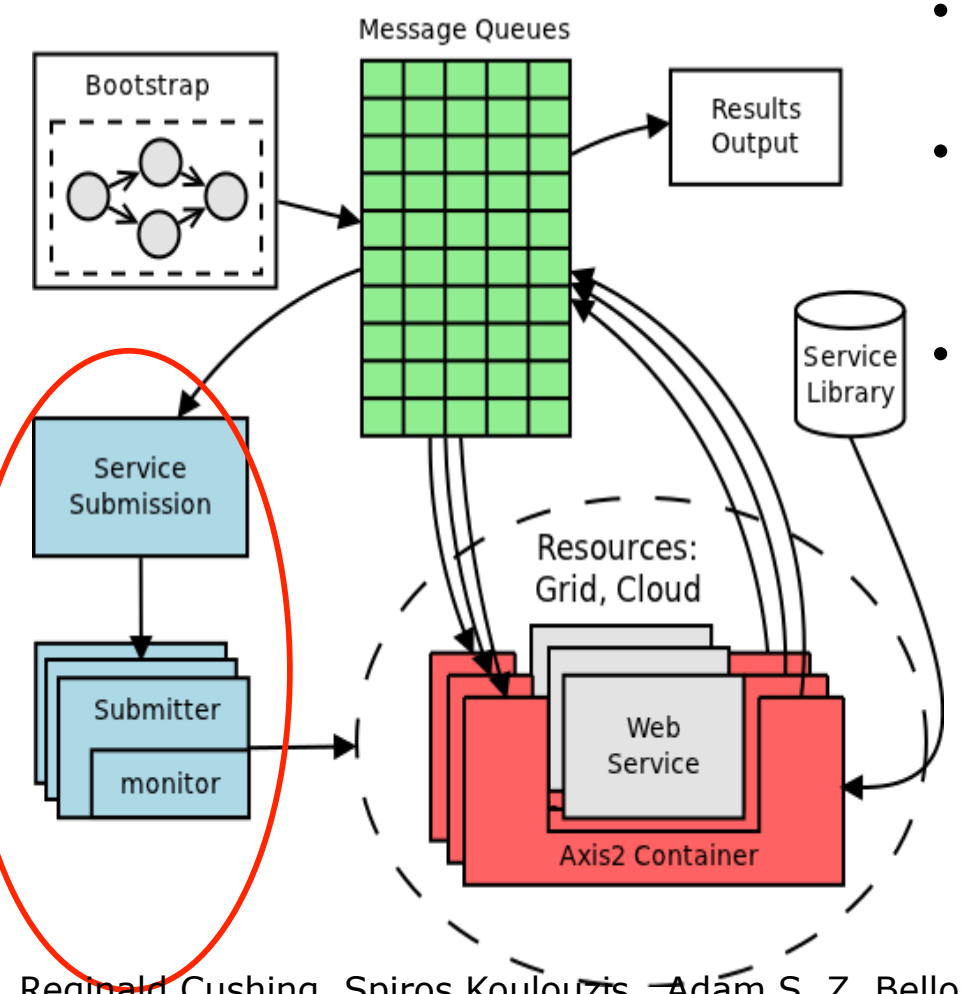


Web Services in eScience with WS-VLAM

- 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 or being overload*

***Scale up** the number of Web service to keep up with the incoming load*

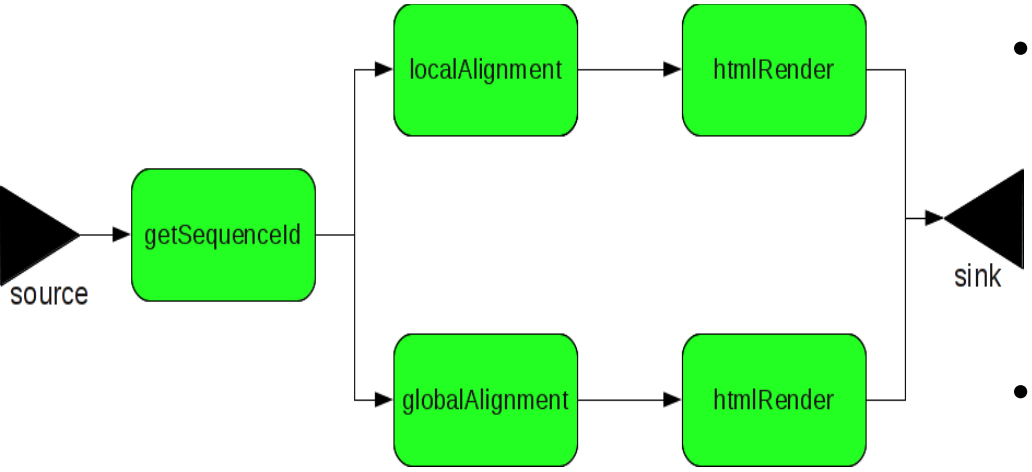
Scaling up the number of Web services



- Tasks/Jobs can be **queued** on the runqueue.
- 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 (Condor, ibis, …)

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

Sequence Alignment Use Case

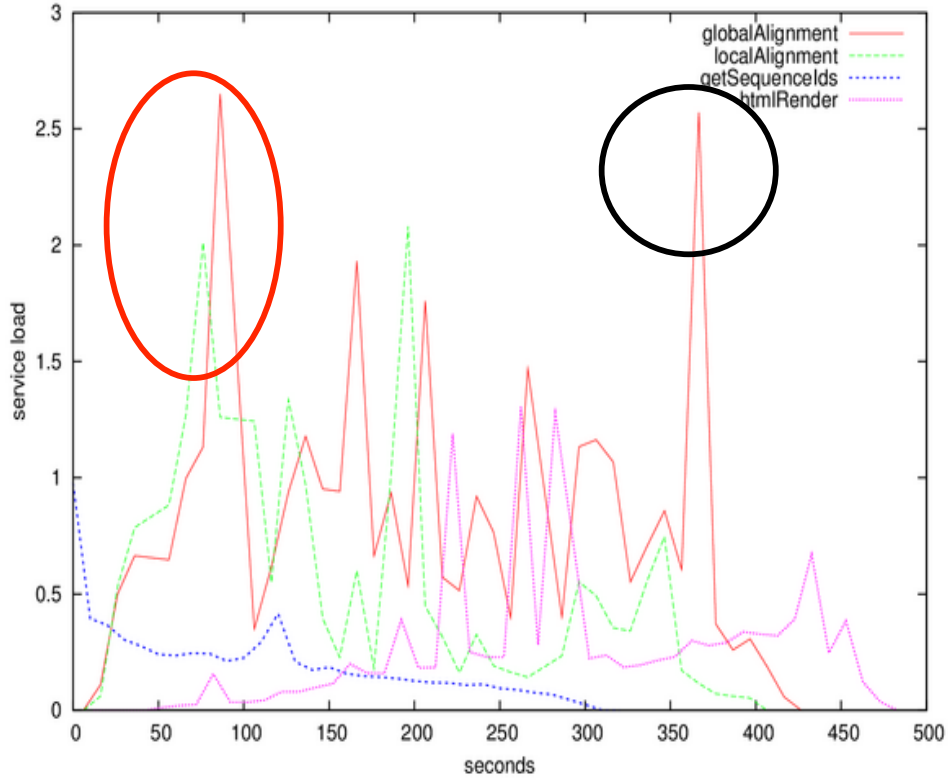


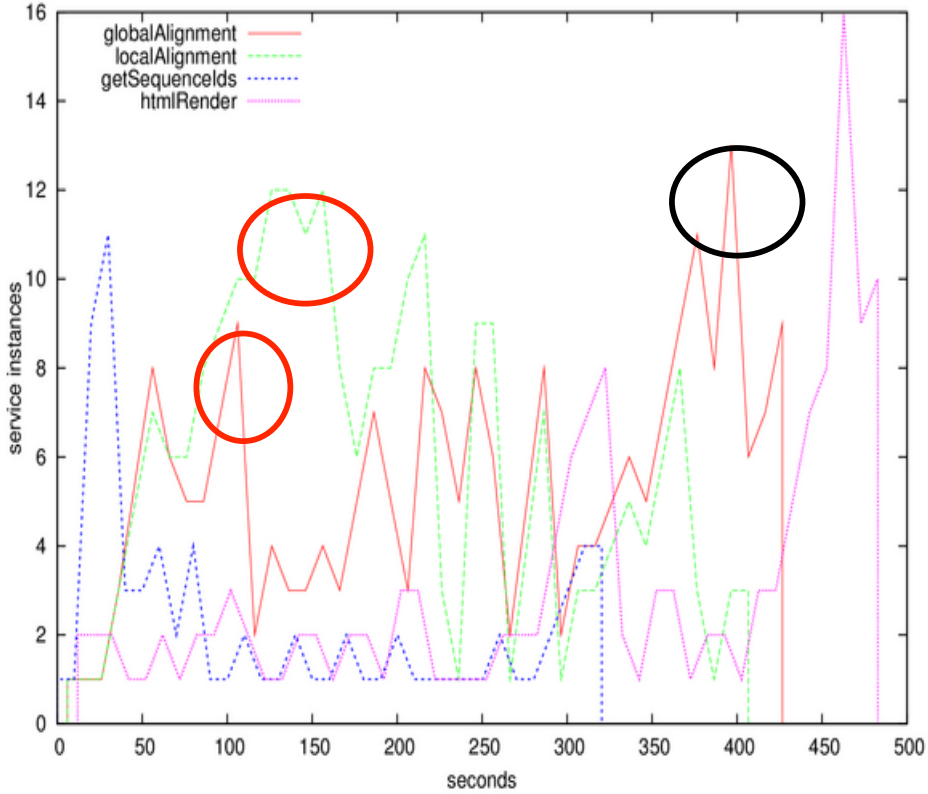
- Workflow with 2 pipelines. The pipelines perform sequence alignments using data from UniProtKB
- Each pipeline performs 22500 alignments i.e. 45100 total alignments in all

- 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

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

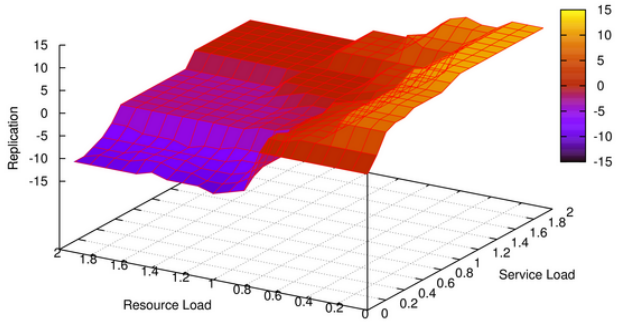
Scale up web services





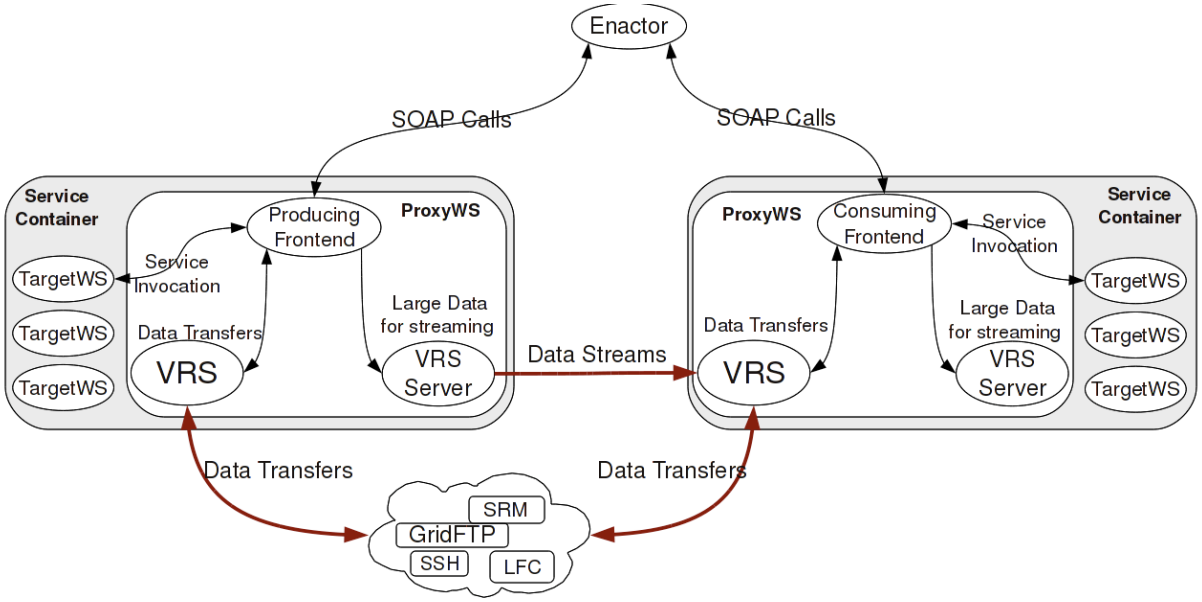
Peaks in load(left) will result in peaks in instances(right).

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



Enabling web services to consume and produce large distributed

- 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**

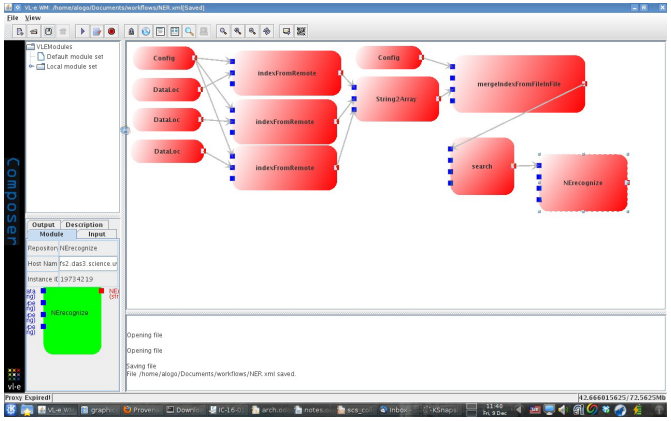


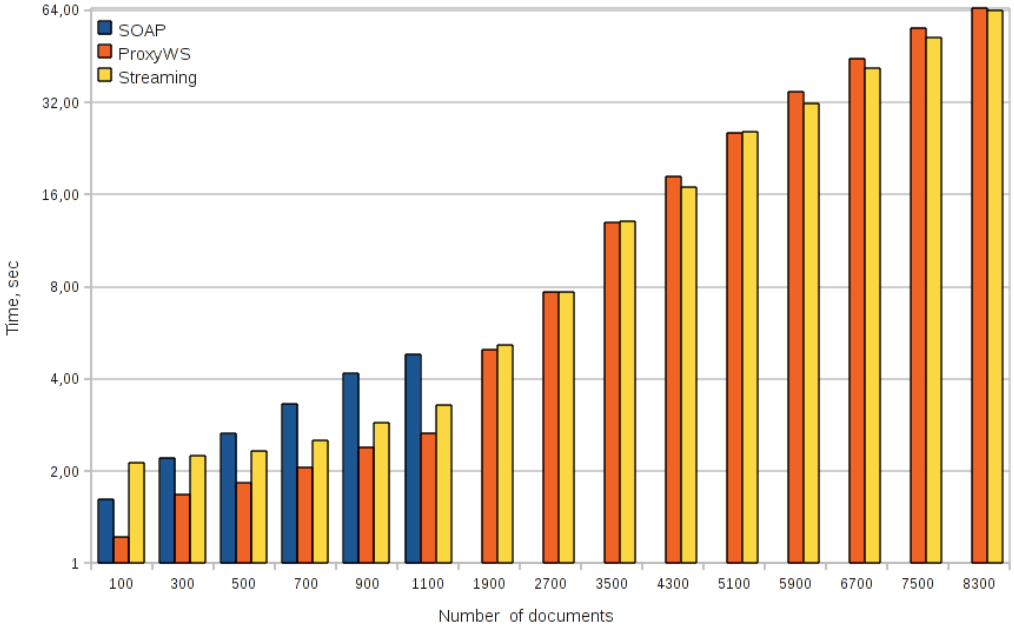
Enabling web services to consume and produce large distributed *datasets Spiros Koulouzis, Reginald Cushing, Konstantinos Karasavvas, Adam Belloum, Marian Bubak to be published JAN/FEB, IEEE Internet Computing, 2012*

Enabling web services to consume and produce large distributed

Indexing Web Services for **Information Retrieval** (NER) are tools that help biologists to identify and retrieve information

- Index 8.4GB of medline documents





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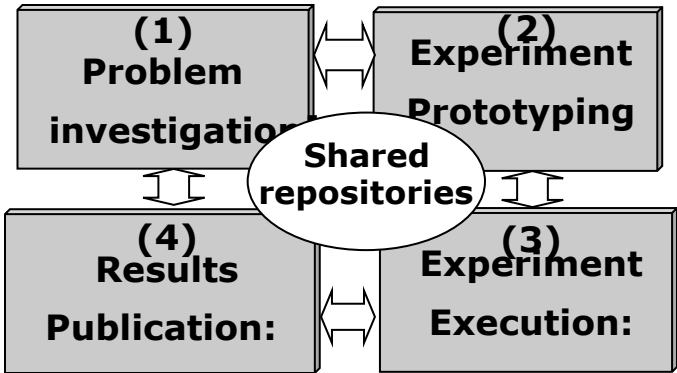


Provenance/ Reproducibility

- "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

History-tracing XML (FH Aachen)

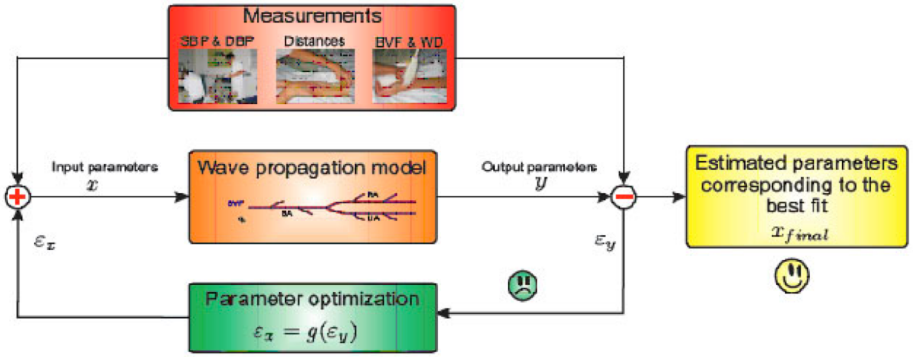
provides data/process provenance following an approach that

- 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
- Workflow components can be eventually, electronically signed.

```
<patternMatch>
  <events>
    <PortResolved>provenance data</PortResolved>
    <ConDone>     provenance data     </ConDone>
    ...
  </events>
  <fileReader2>
    <events> ... </events>
    <sign-fileReader2> ... </sign-fileReader2>
  </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 Provenance Framework for workflows**, WORKS 2010, New Orleans, USA, November 2010

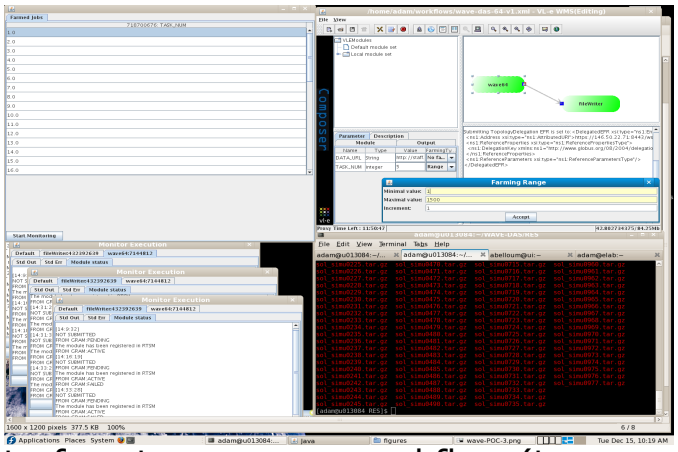
Wave Propagation in Blood Flow



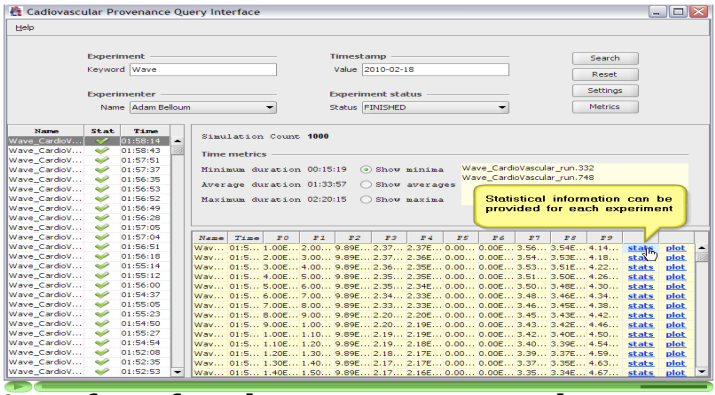
[Biomedical engineering Cardiovascular biomechanics group TUE])

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



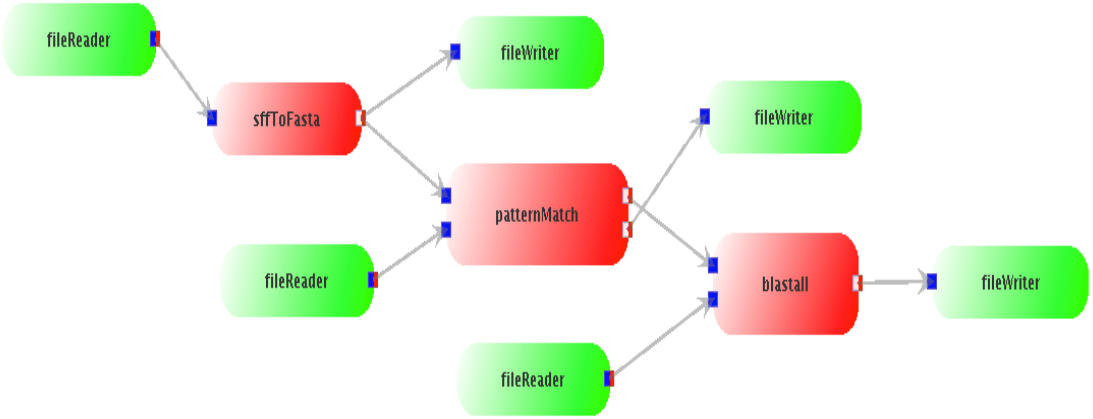
User Interface to compose workflow (top right), monitor the execution of the farmed workflows (top left), and monitor each run separately (bottom left) data



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"*

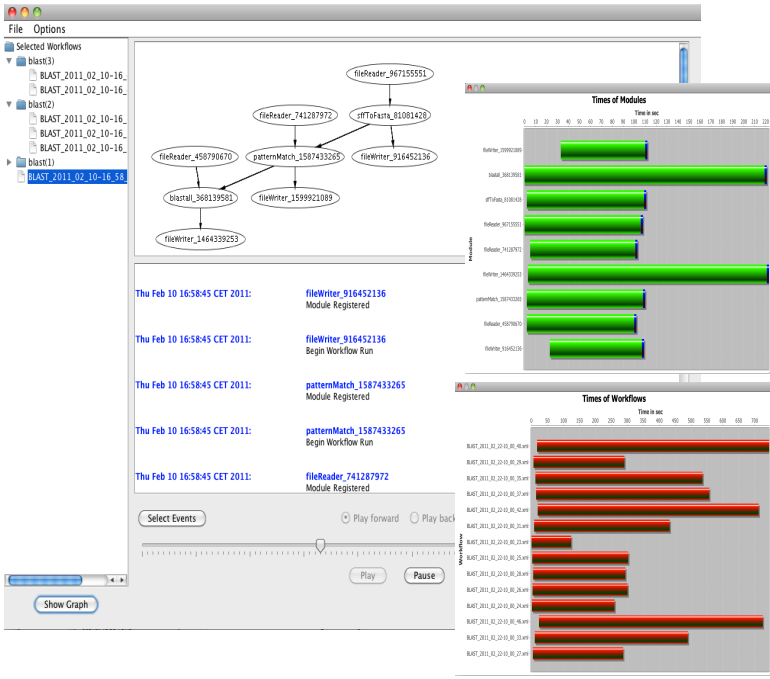
BigGrid project 2009, presented EGI/ BigGrid technical forum 2010

Alignment of DNA Sequence (Blast)



[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.



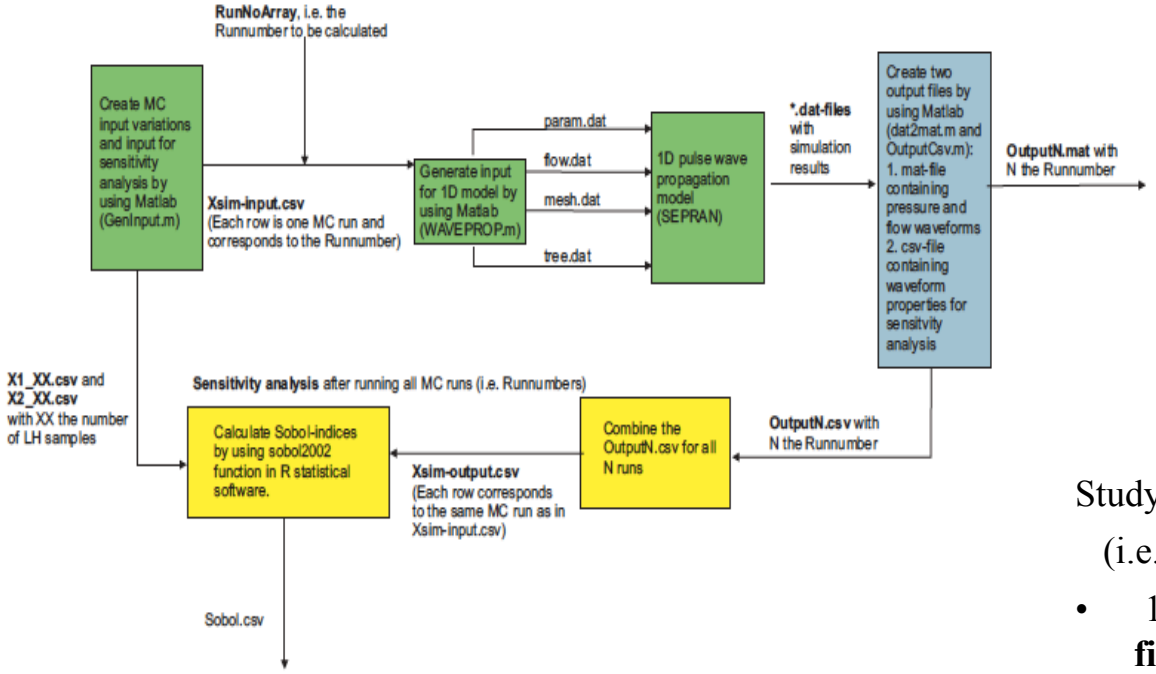
For Each workflow run

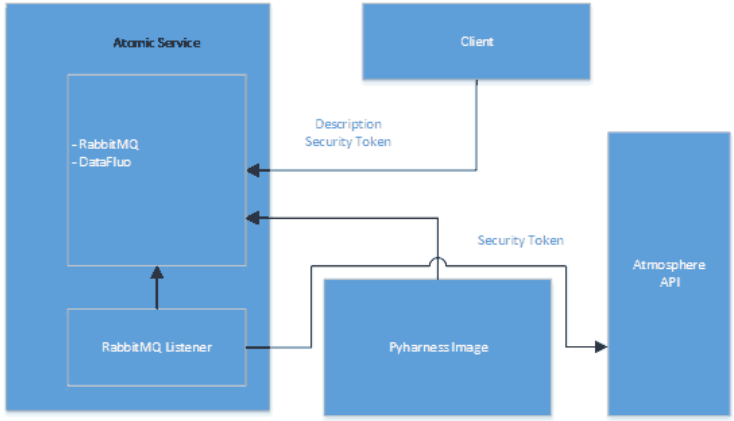
- The provenance data is collected an stored following the XML-tracing system
- User interface allows to reproduce events that occurred at runtime (replay mode)
- User Interface can be customized (User can select the events to track)
- User Interface show resource usage

on-going work UvA-AMC-fh-aachen

Sensitivity Analysis of Cardiovascular Models

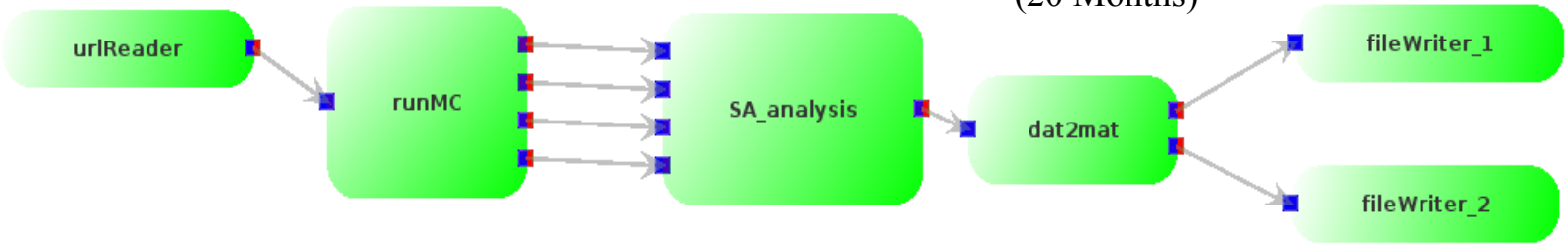
FP7 Project VPH-Share " Virtual Physiological Human: Sharing for Healthcare"





Study covers: **164 patient-specific input parameters** (i.e. vessel diameter and length),

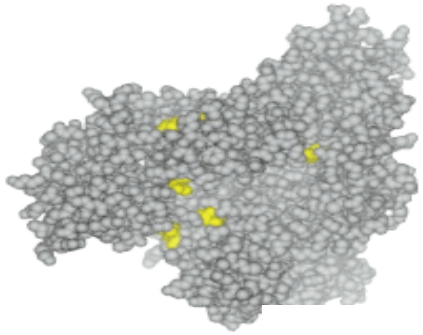
- 1494000 Monte Carlo runs are needed for **this first analysis**.
- Expected execution time on a PC 14.525 hours (20 Months)

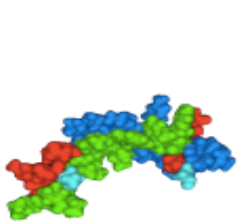


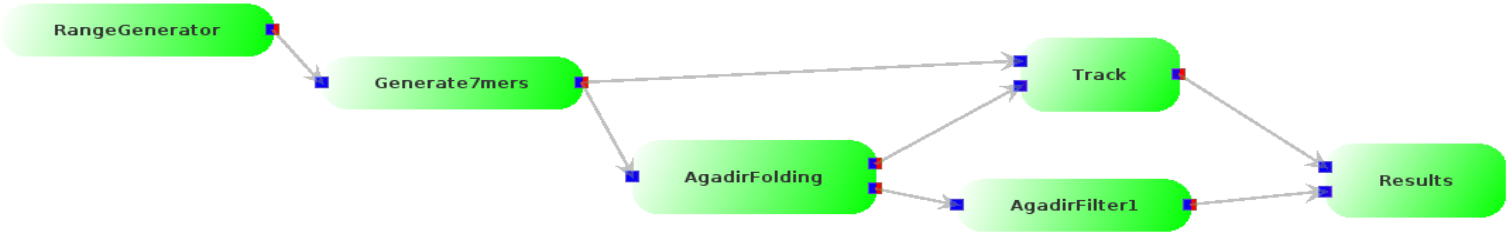
Protein Folding

Sequenomics: Mapping protein folding across sequence space

sequence length	possible sequences
2	4.0E+02
3	8.0E+03
4	1.6E+05
5	3.2E+06
6	6.4E+07
7	1.3E+09
8	2.6E+10
12	4.1E+15
40	1.1E+52
80	1.2E+104
160	1.5E+208
300	2.0E+390
320	2.1E+416
1000	1.1E+1301

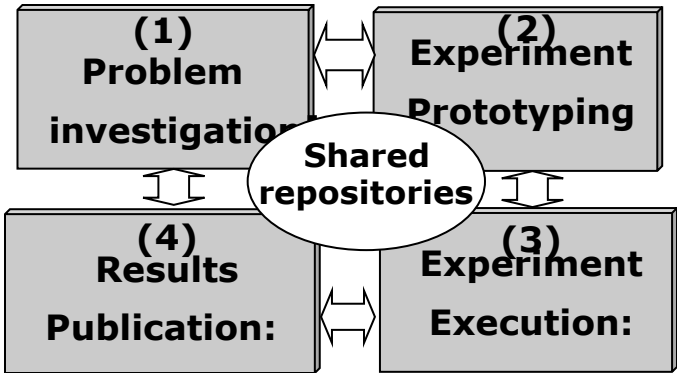






Outline

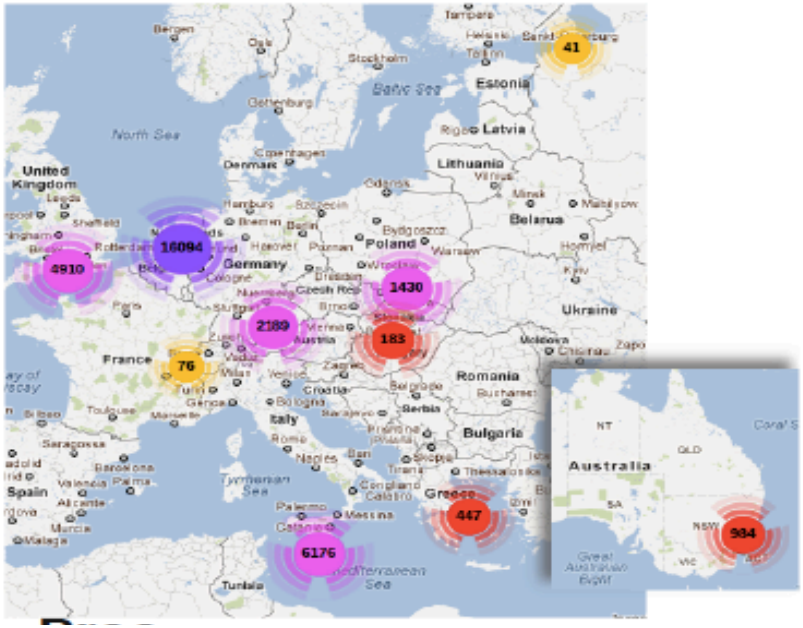
- Introduction
  - Life cycle of e-Science Workflow
- Different approaches to workflow scheduling
  - Workflow Process Modeling & Management In Grid/Cloud
  - Workflow and Web services (intrusive/non intrusive)
- Provenance
- Computing in the browser
- Conclusions



Computing in the Browser (different approach to Grid-desktop)

- **Objectives**
  - Distributed computing using web browsers
- **Features*:***
  - volunteer computing instantly (no third party software installation)
- **How does it work:**
  - Social media mediates the trust between the user and the volunteers asked to join the network.
    - A user with a distributed application uses social media to get colleagues and friends to donate CPU
    - Colleagues and friends join the network by simply opening the shared URL.
    - **Computing starts almost instantly**.

Computing in the Browser

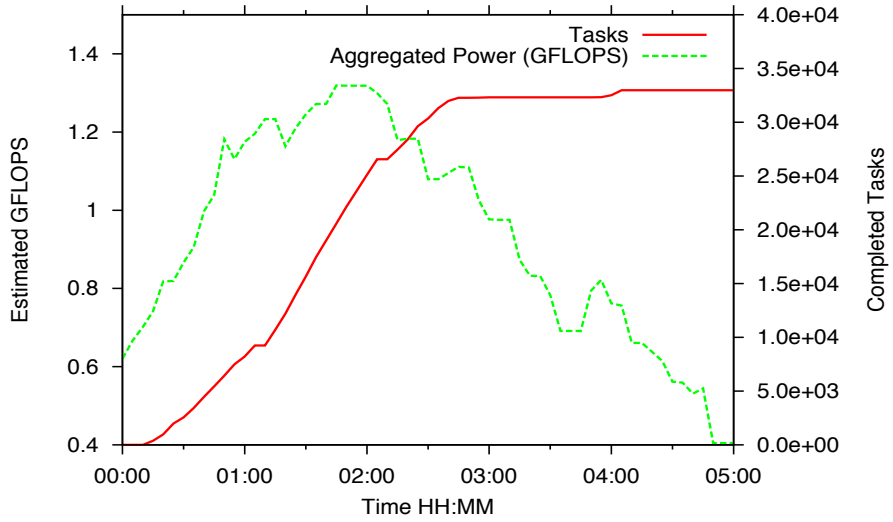


New Web Technologies make JavaScript engines more powerful:

- Web workers
- web socket
- WebGL
- WebCL

Application

- Computing 33,000 bio-informatics tasks on the global cluster of browsers
- Announcing the experiment using social media: via social media tools: twitter, FaceBook, Linkedin, and project mailing lists.
- Volunteers were asked to open the Weevil web page http://elab.lab.uvalight.net/~weevil/ and agree to donate their CPU for 3 hours on Friday December 2011 from 12:00-14:00



Distributed computing on an Ensemble of Browsers, R. Cushing, G.a Putra, S. Koulouzis, A.S.Z Belloum, M.T. Bubak, C. de Laat IEEE Internet Computing, PrePress 10.1109/MIC.2013.3, January 2013

Conclusions

- WS-VLAM has interesting features (farming, automatic scaling, hierarchical workflow, provenance, …) which proved to be interesting for a number scientific applications
- WS-VLAM harnesses various type of computing resources (desktops, Grid, and Cloud resources)
- WS-VLAM has modular design which make easy to adapt/ extend

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