

vl·e



virtual laboratory for e·science



An Approach to build an e-Science framework

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Institute of Informatics
University of Amsterdam

Conference of the High Performance Computers' Users, Zakopane Poland March 9-11 2011

UvA



UNIVERSITEIT VAN AMSTERDAM

Outline

- VL-e project
- Mission & Strategy
- Infrastructure
- Workflow an approach to model experiments
- Successful stories
- Rollout
- Follow-up

“Information has become the fuel of our knowledge society, and our ability to digest, understand and share it will determine scientific, economic and social progress”

Mission and strategy

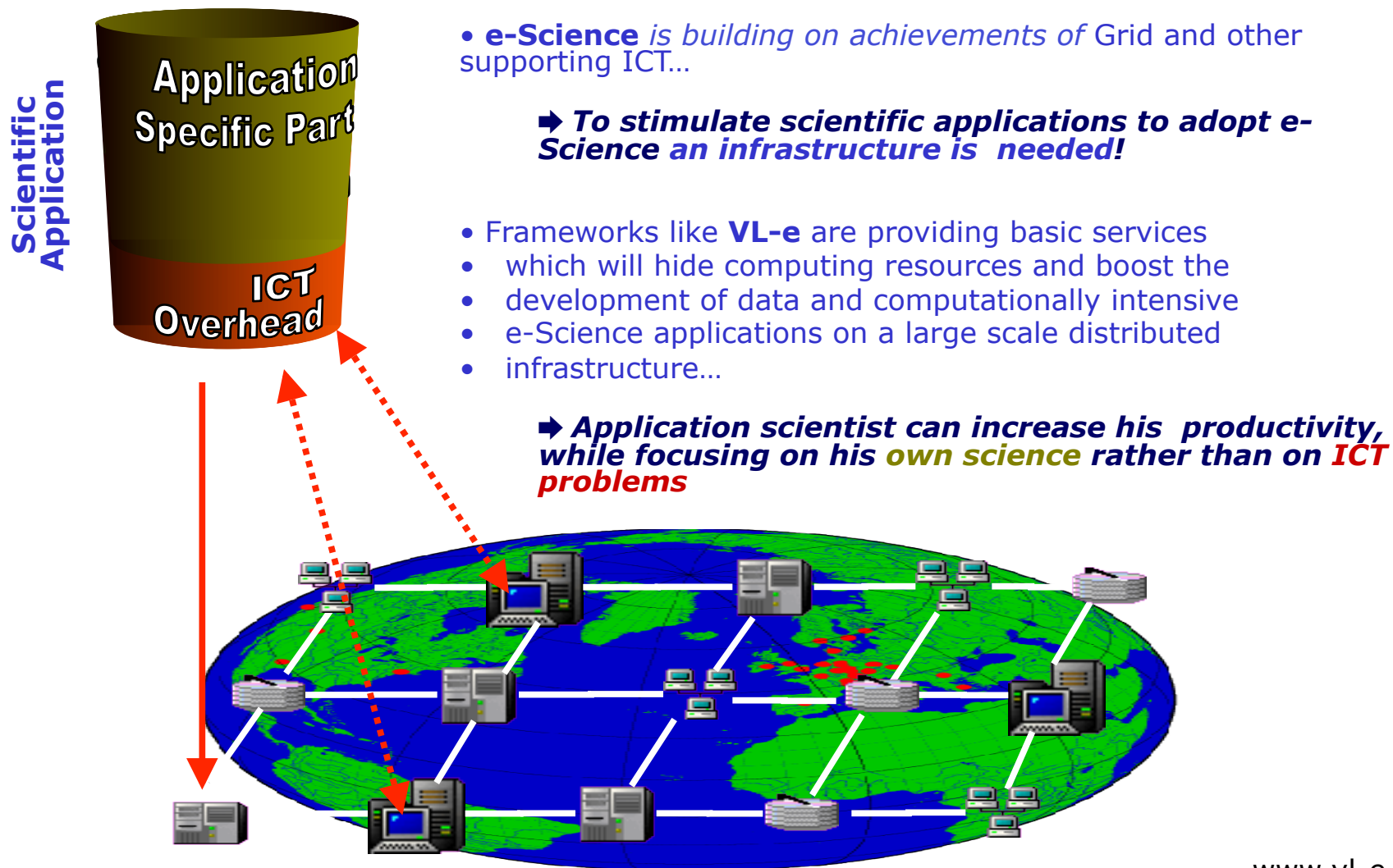
Mission

To boost e-Science by creating an e-Science environment and carrying out research on methodologies.

Strategy

To carry out concerted research along the **complete e-Science technology chain**, ranging from applications to networking, focusing on new methodologies and re-usable components.

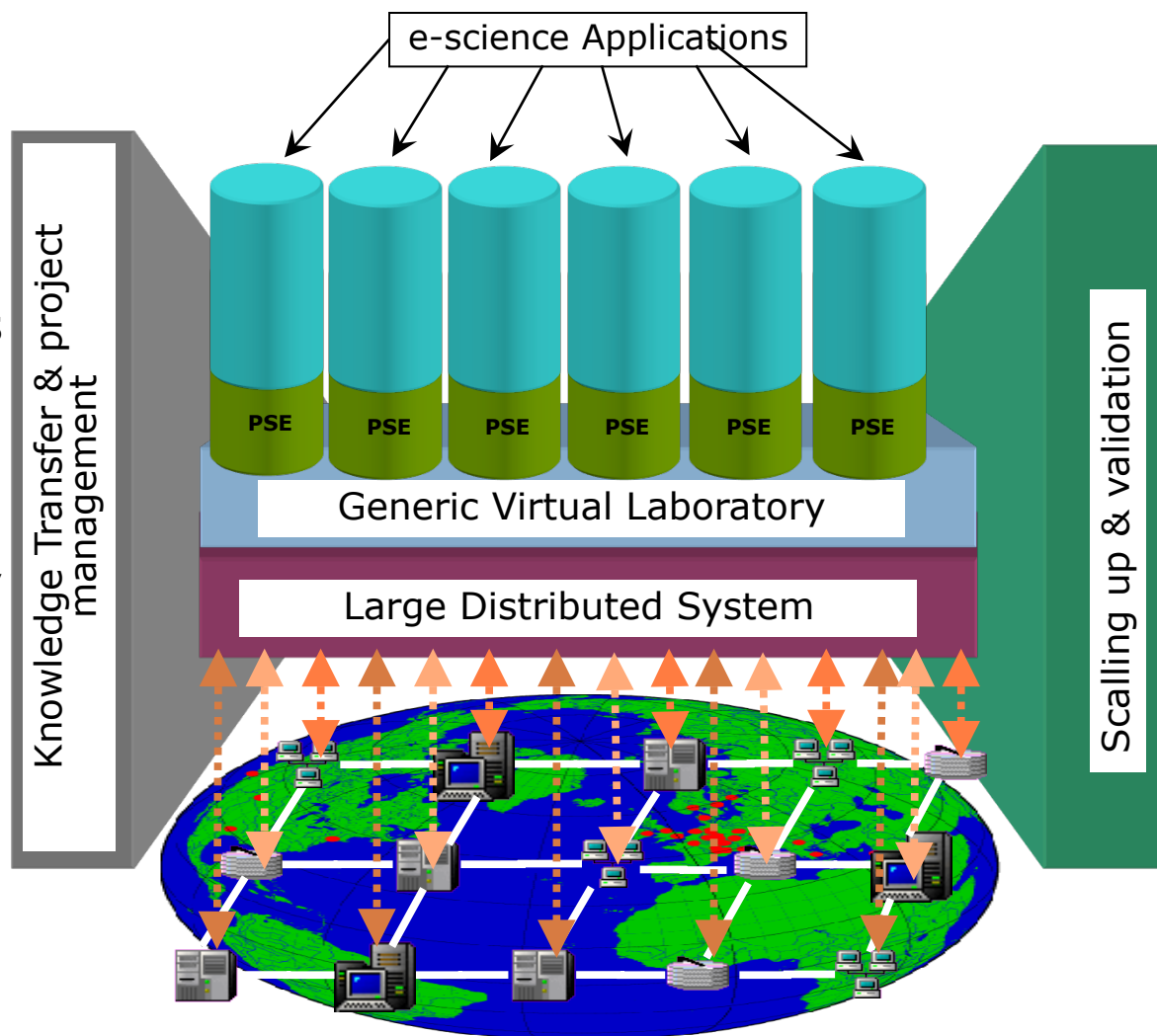
Mission and strategy



Mission and strategy

To achieve its mission the VL-e project has set itself the following aims:

- create scientific prototypes of application-specific e-Science environments,
- develop a methodology for re-usable ICT components,
- **scaling up** & validating in 'real-life applications',
- build up and **transfer knowledge** on effectively realising application-specific e-Science environments.



Project organization

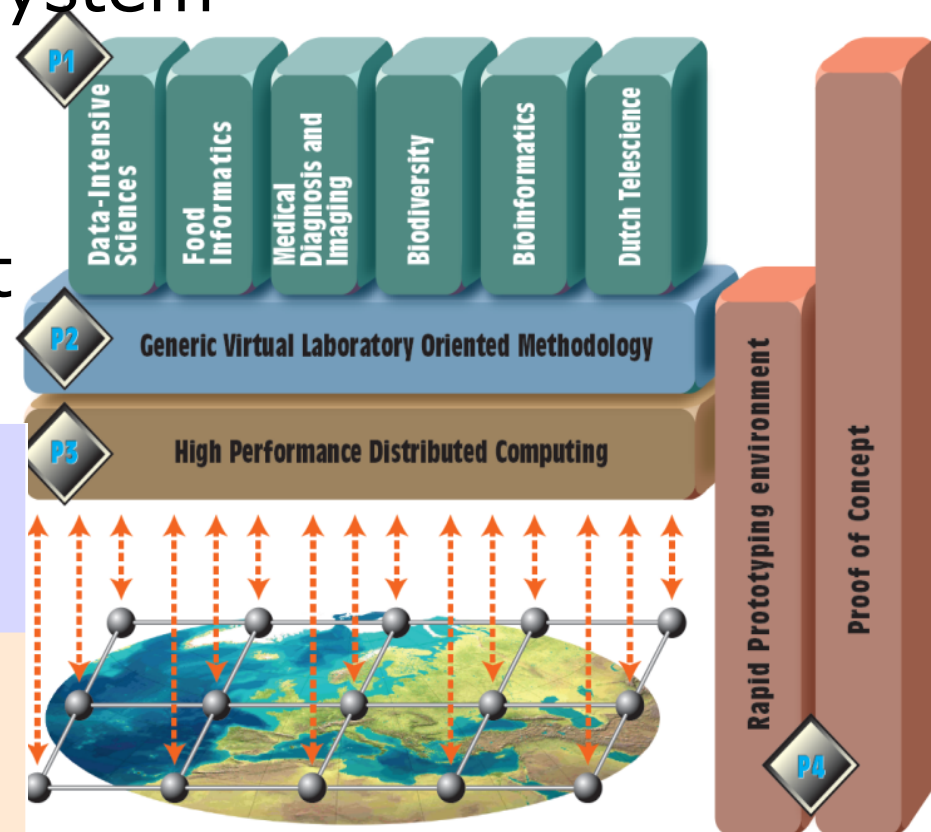
- Getting everybody onboard: Scientific domain, Application developers, middleware developers, system administrators
- Getting the right Infrastructure at the right time

vl-e facts

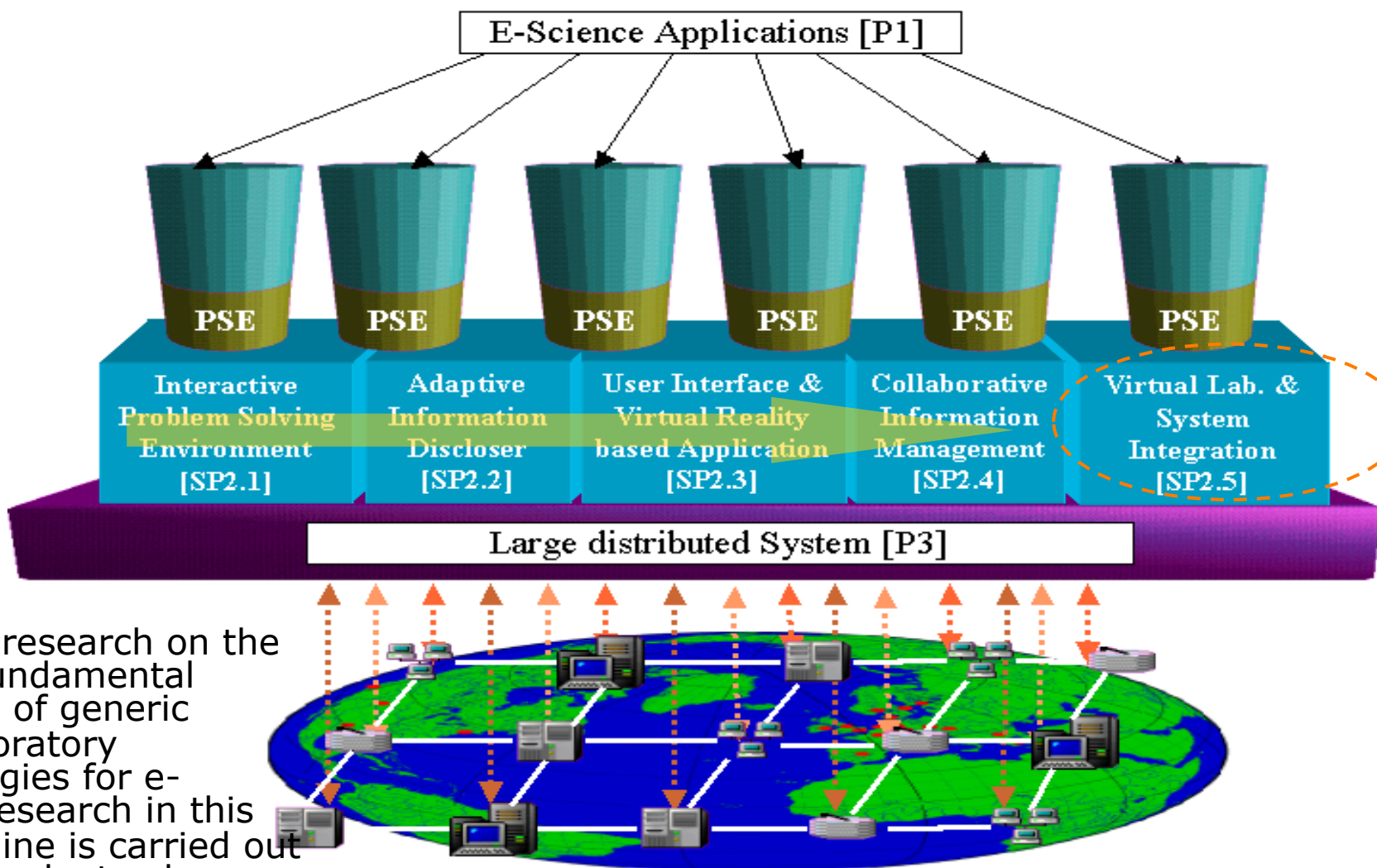
budget 40 M, period 2004-2008
 more than 20 consortium partners from industry and academia
 director: prof. dr. L.O. Hertzberger
 website: <http://www.vl-e.nl>

consortium partners

A&F Wageningen, AMC, CWI, DSM, Friesland Foods, FEI, FOM AMOLF, NBIC, Nikhef, IBM, LogicaCMG, Philips Research, Philips Medical, SARA, Top Institute Food and Nutrition, TNO Kwaliteit van Leven, TU Delft, Unilever, UvA-IBED, UvA-IvI, UvA-SILS, VU, VUmc, WTCW



The virtual Laboratory layer

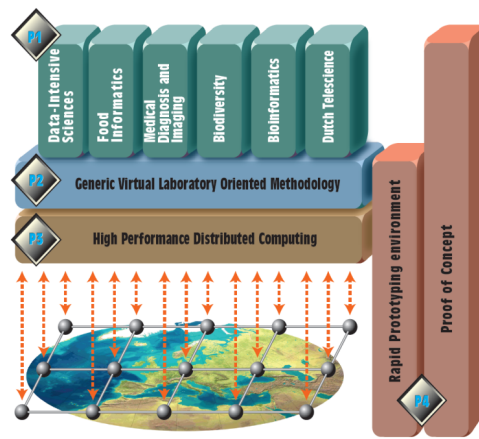


addresses research on the required fundamental knowledge of generic virtual laboratory methodologies for e-Science. Research in this programs line is carried out in 5 independent sub-programs

Rapid prototyping Environment

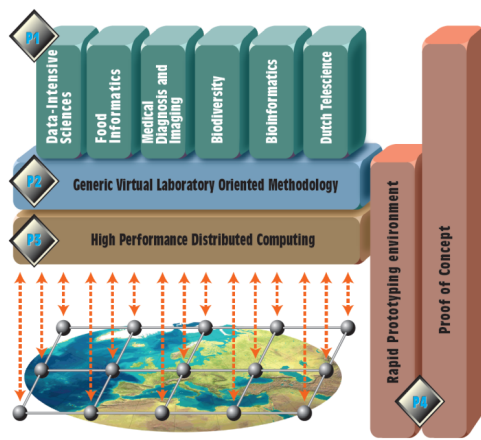
DAS3 cluster is composed of 5 clusters located at:

- University of Amsterdam (**28** nodes), Multimedia lab in UvA (**41** nodes),
- Vrije University (**79** nodes),
- Technical University in Delft (**64** nodes),
- Leiden Institute of Advanced Computer Science (**23** nodes)



VL-e PoC Environment

- The PoC infrastructure consists of a wide variety of resources and access points, including:
 - large computer clusters
 - storage space in near-line tape storage,
 - all accessible via grid and data management tools



The PoC infrastructure hosted by the National super computing Center SARA



VL-e PoC environment

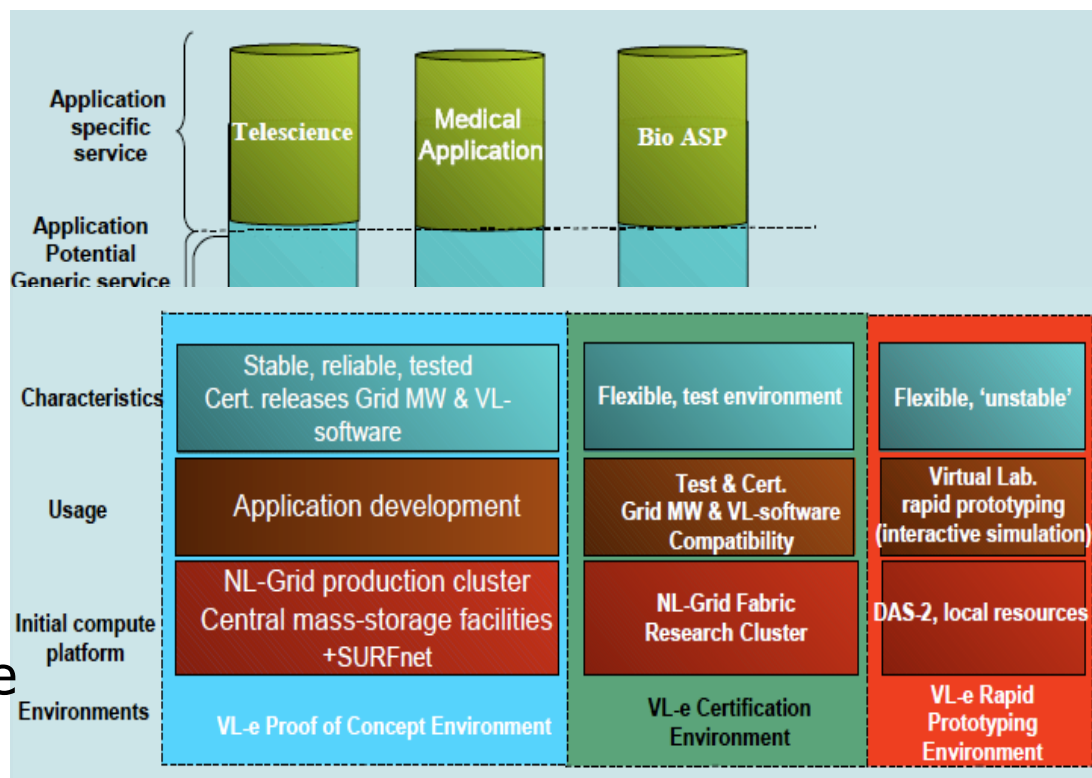
- NL-Grid production cluster (SARA)
 - ✓ 36 dual 3 GHz Intel Xeon nodes
 - ✓ 1 Tbyte storage
 - ✓ Gigabit Ethernet interconnect
 - ✓ Stable production environment
 - Access node
 - Resource brokering
 - Information services
- Tape library with capacity of 1.2 PByte
 - ✓ Accessible as storage element (SE) through the Dutch National Supercomputing Facility 'TERAS/ASTER'



From Rapid Prototyping to PoC

The stability of the PoC is maintained for the benefit of the applications.

- Rigorous software engineering and testing are implemented on a dedicated “**certification test-bed**”,
- where the release candidates for the next version of the PoC are evaluated.
- Release to the PoC at large is scheduled at fixed regular intervals

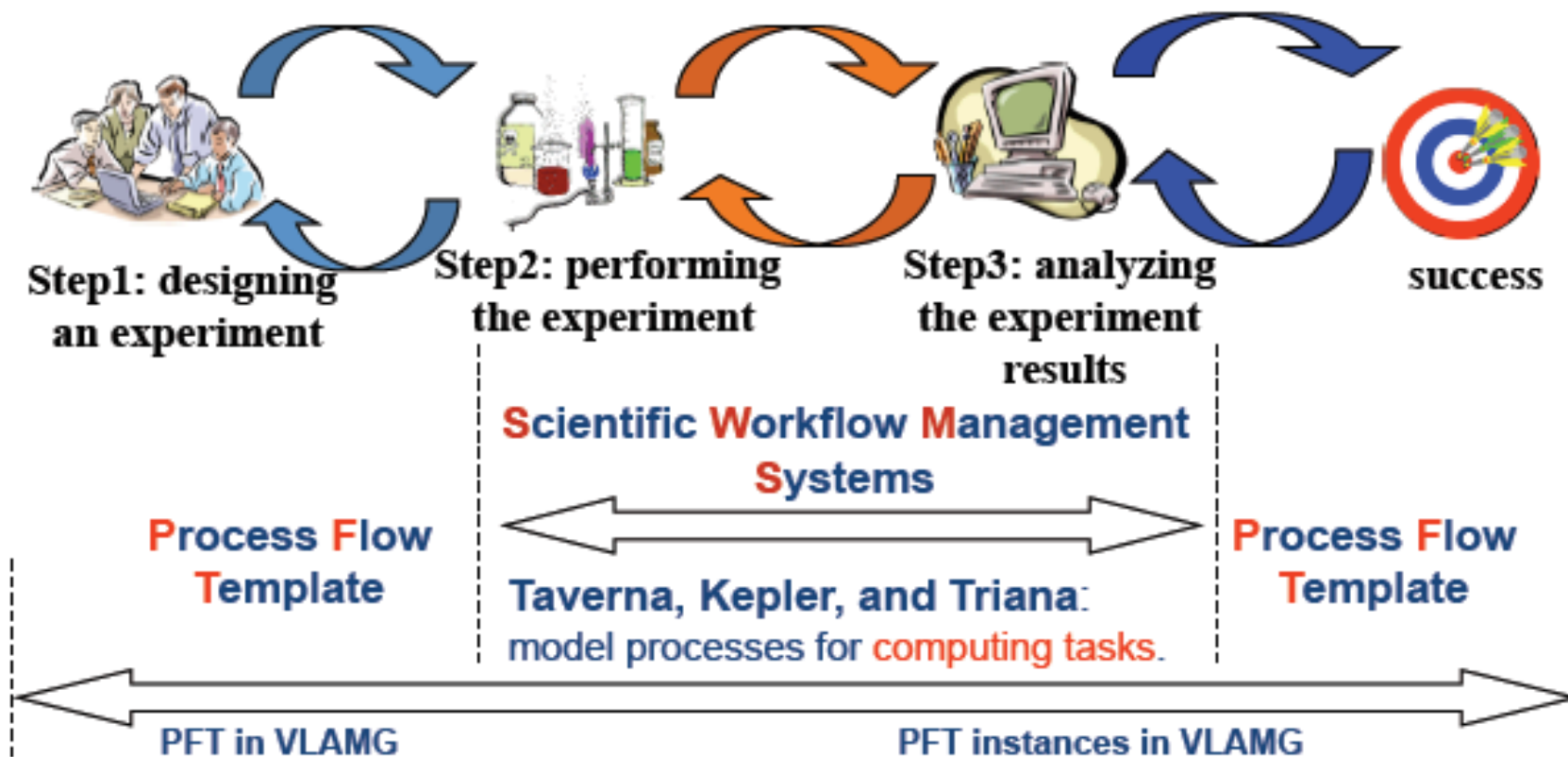


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Let us Start with an UvA-Slide: Virtual Laboratory for eScience

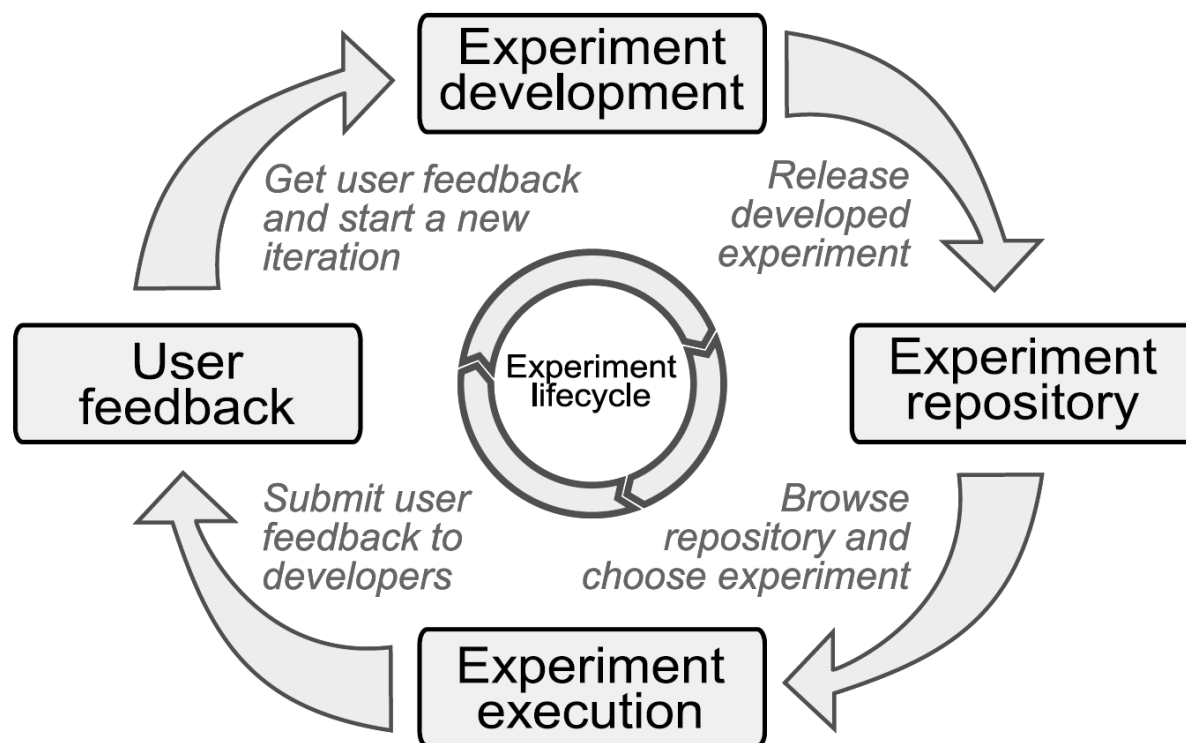


In VL-e: model both computing tasks and **human activity based processes**, and model them from the perspective of an entire lifecycle. It tries to support

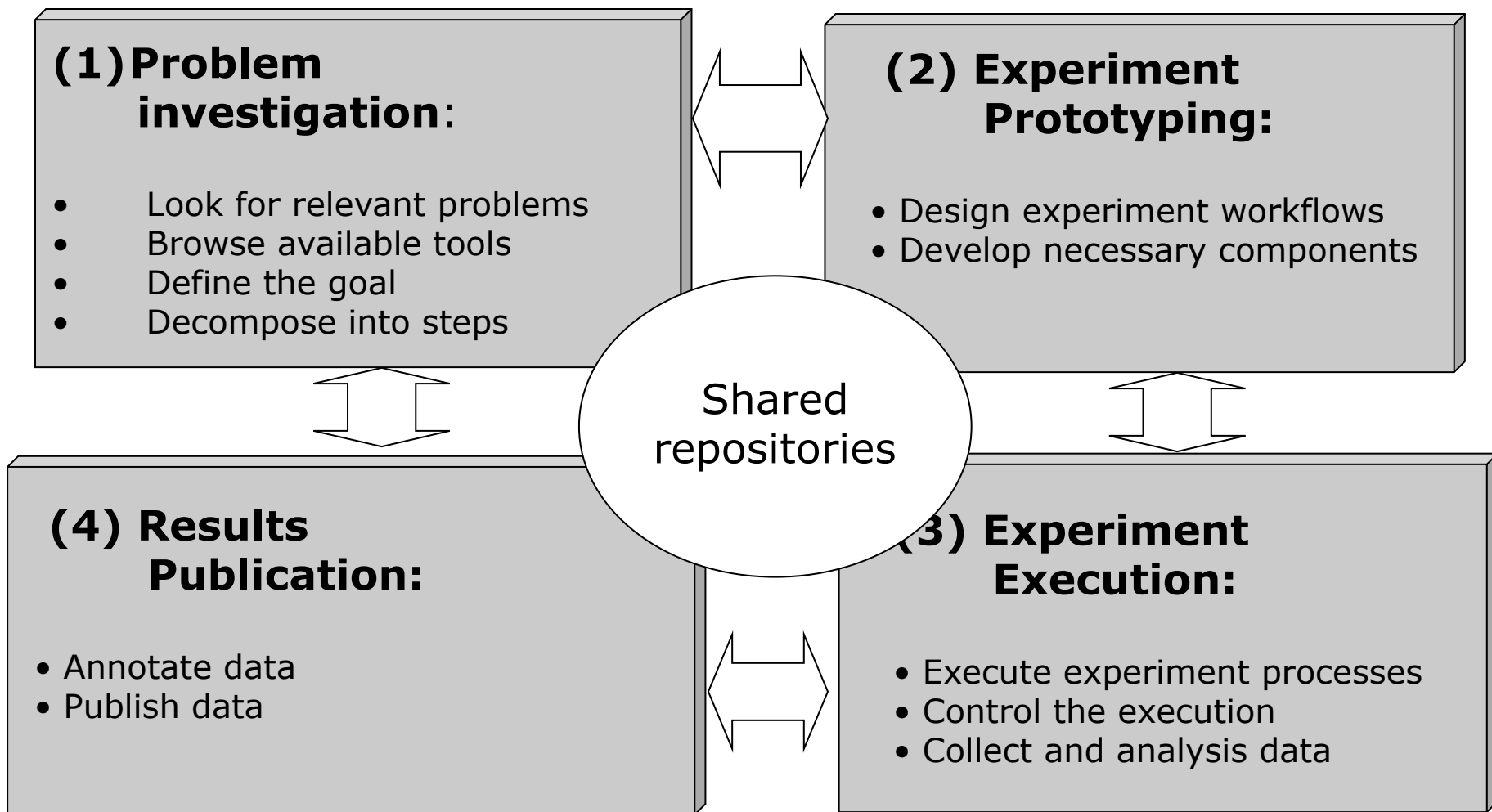
- Collaboration in different stages
- Information sharing
- Reuse of experiment

Experiment Lifecycle

- *Experiment Pipeline* - a collaborative planning and execution process that may create a new experiment

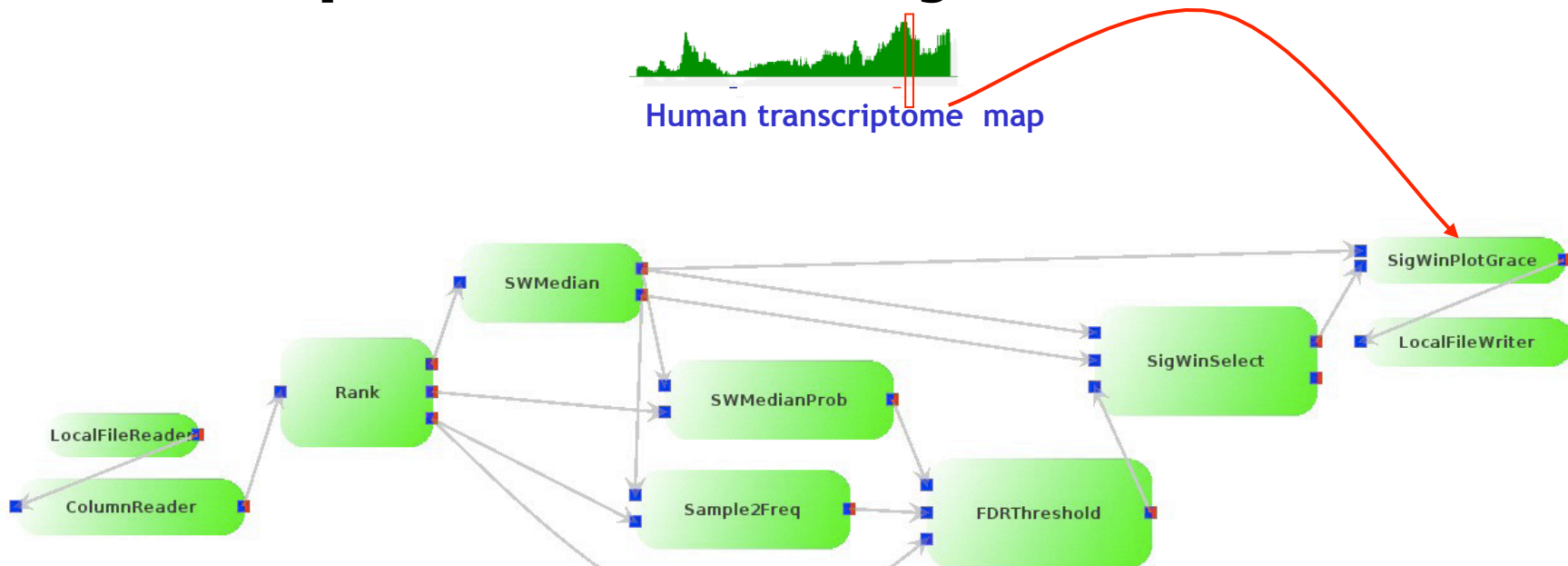


Complex Scientific experiments model



Workflow

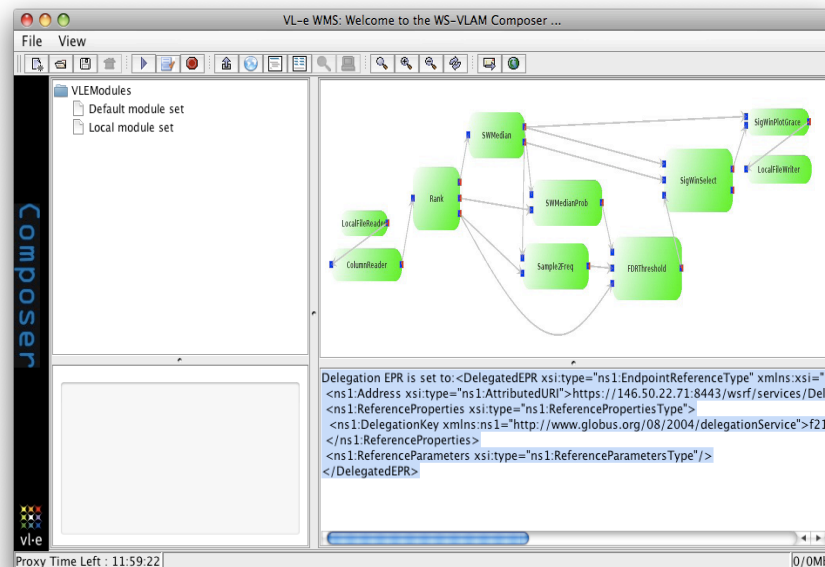
- A workflow is a model to represent a **reliably repeatable** sequence of operations/tasks by showing **explicitly** the **interdependencies** among them.



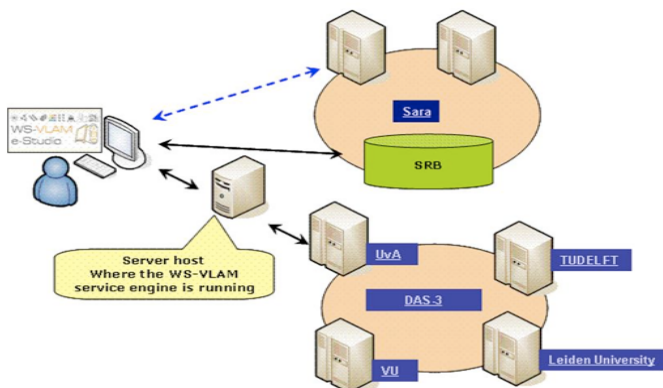
SigWin-Detector workflow has been developed in the VL-e project to detect ridges in for instance a Gene Expression sequence or Human transcriptome map

Workflow management system

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

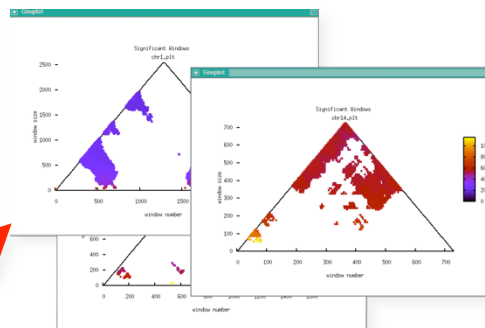
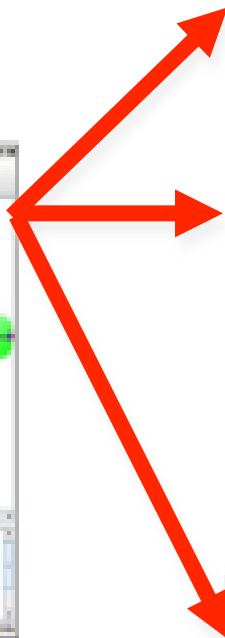
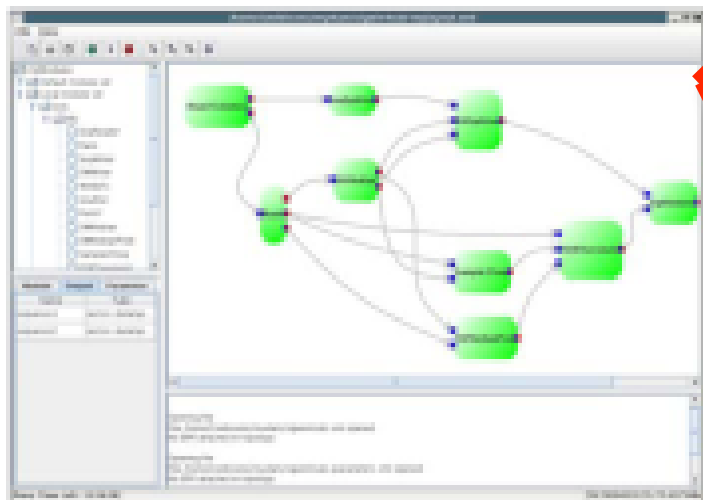


The user interface of the WS-VLAM a workflow management system developed in the VL-e project to execute application workflow on geographically distributed computing resources

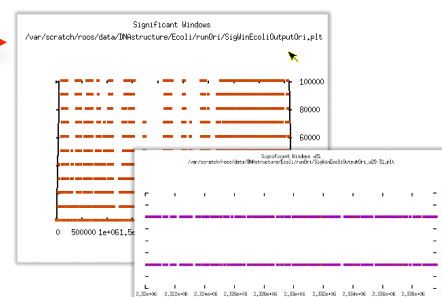


The Application Workflow ...

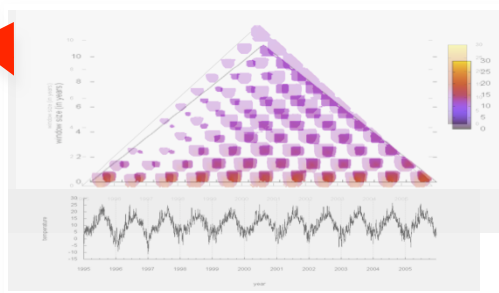
Developed in the context of the
Ridge-O-grammer Application use case
by Micro-array department UvA



Human
transcriptome
map



DNA curvature
of the
Escherichia coli
chromosome



Temperature in
Amsterdam

(1) Problem investigation

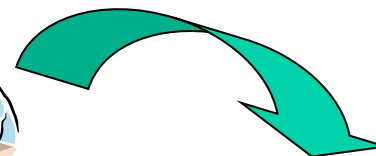
- Tools to improve **re-usability**, and **share of expertise**. These tools should allow:

- Advanced **search capabilities**

- HAMMER: **H**ybrid-b**A**sed **M**atch-**M**aker for **E**-**S**cience **R**esources
- Web Service Harvester (RPC Style WSDL)

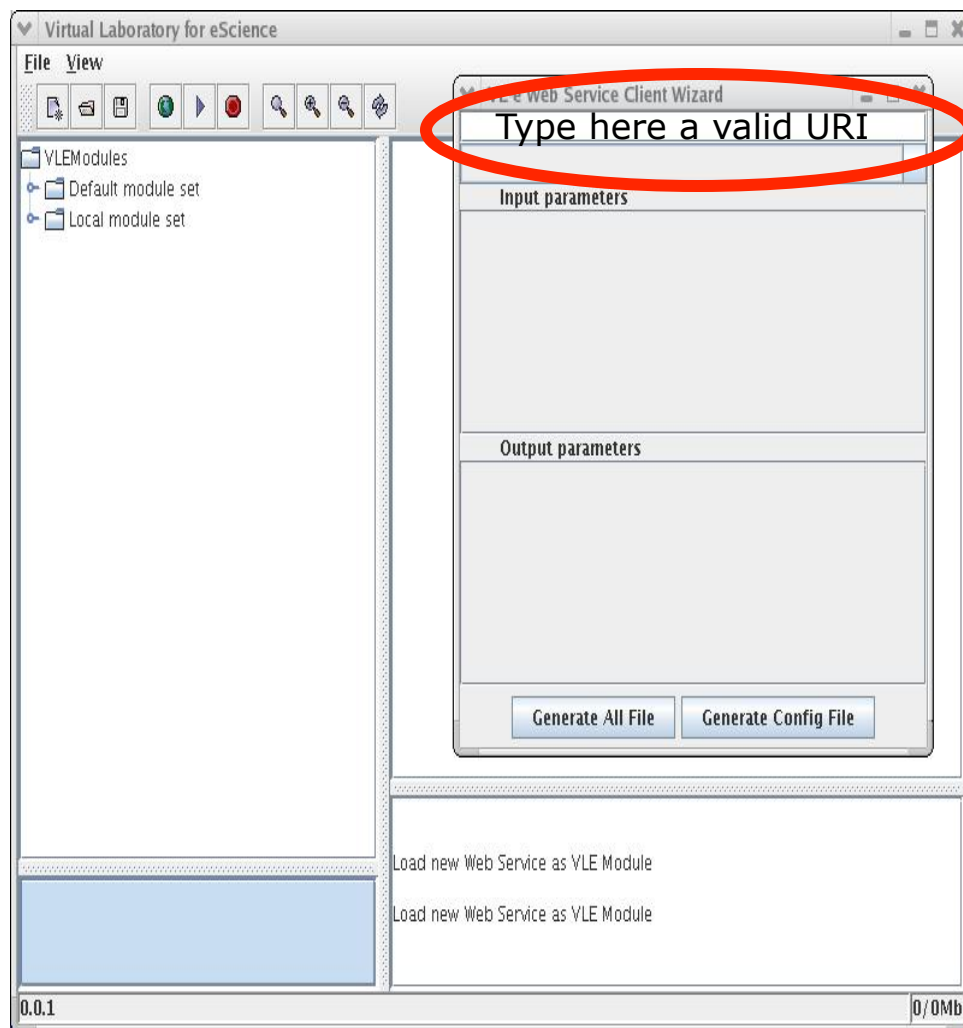


designing the experiment



(1) Problem investigation

- Tools to improve **re-usability**, and **share of expertise**. These tools should allow:
 - Advanced **search capabilities**
 - HAMMER: **H**ybrid-**b**Ased **M**atch-**M**aker for **E**-Science **R**esources
 - Web Service Harvester (RPC Style WSDL)



(1) Problem investigation

- Tools to design **new components**. These tools should allow:
 - **Speedup** and **simplify** the design of the new components
 - CLAMP: **C**onnecting **L**anguage for **M**odules and **P**rograms

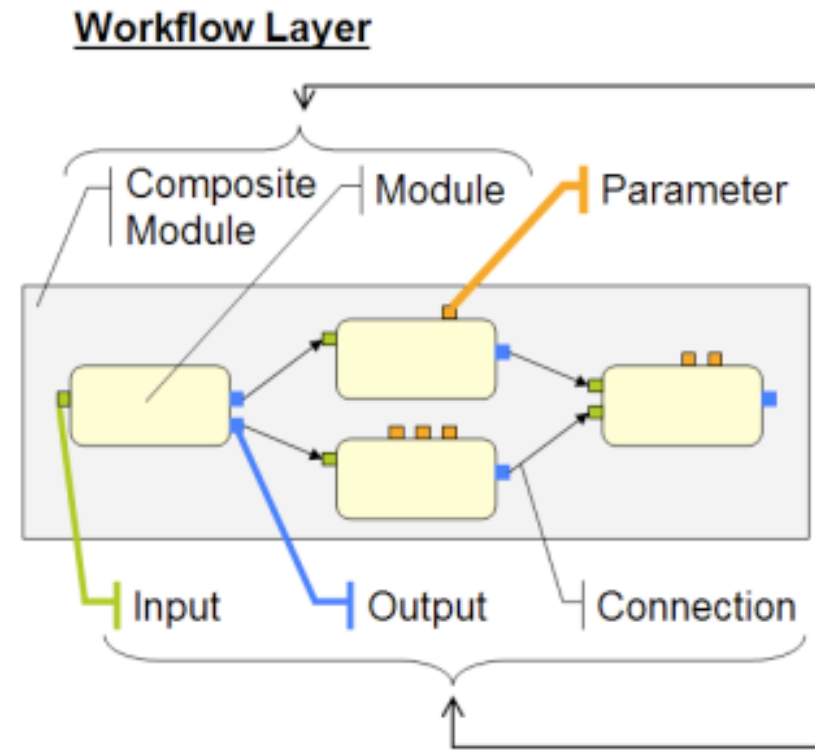


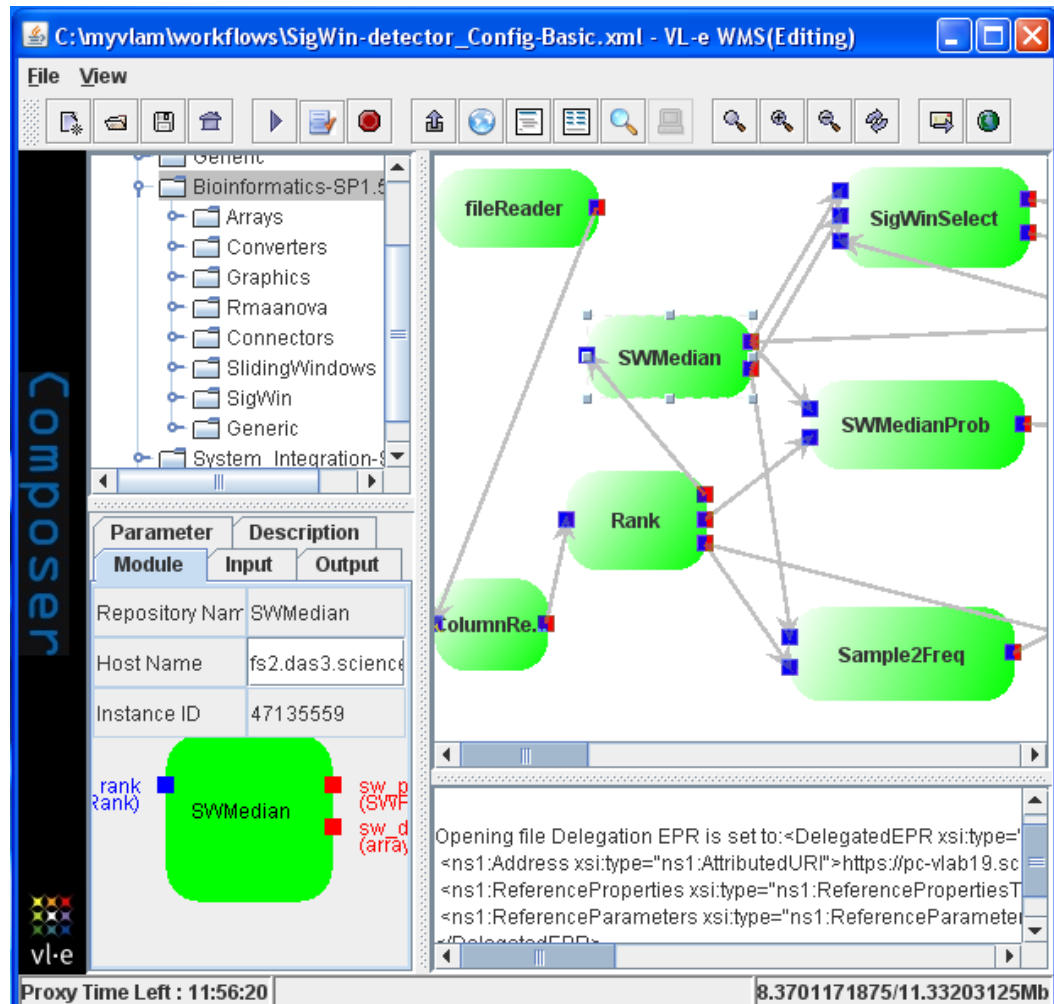
Figure B. Layers of workf

(2) Experiment Prototyping

Grid Enabled workflow management system

- Tools to **speedup** and **simplify** building prototypes. These tools should allow:

- **Combine** existing software components
- **Seamless access** to computational and storage resources.



Composer

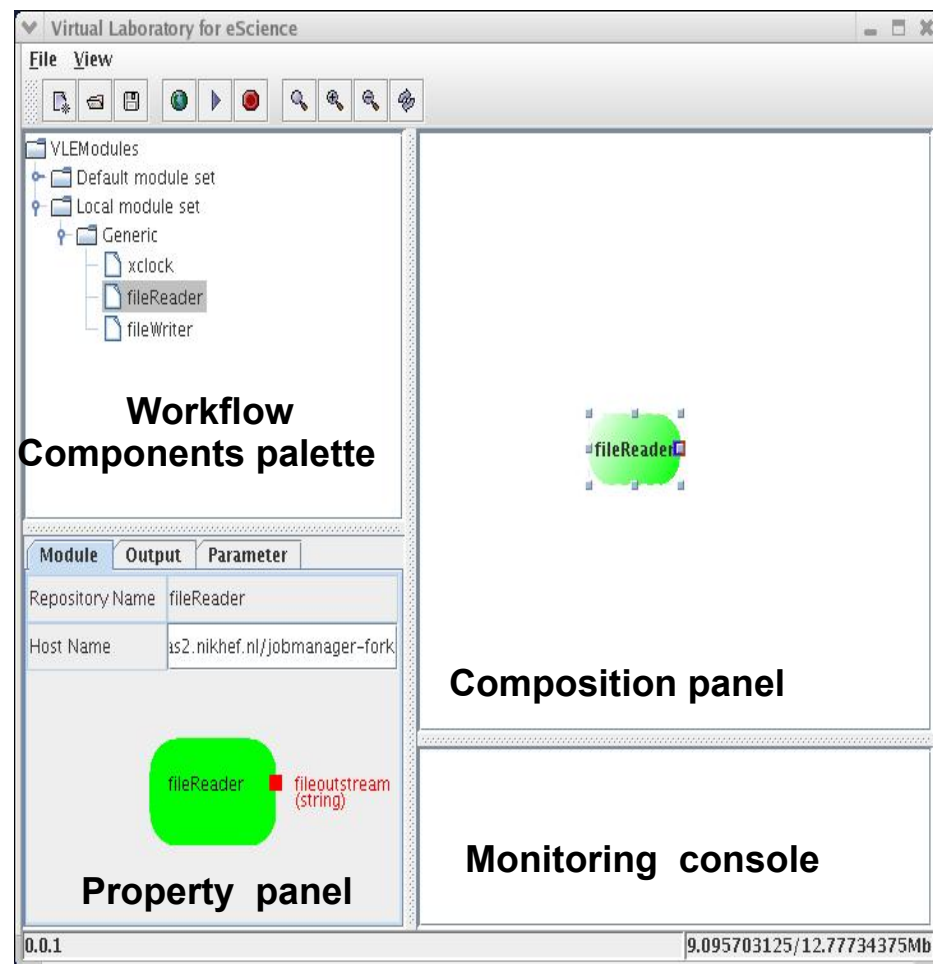
Parameter	Description	
Module	Input	Output
Repository Name	SWMedian	
Host Name	fs2.das3.science	
Instance ID	47135559	
rank	rank	rank
	SWMedian	SW_p (SWF) SW_d (arfa)

Proxy Time Left : 11:56:20 | 8.3701171875/11.33203125Mb

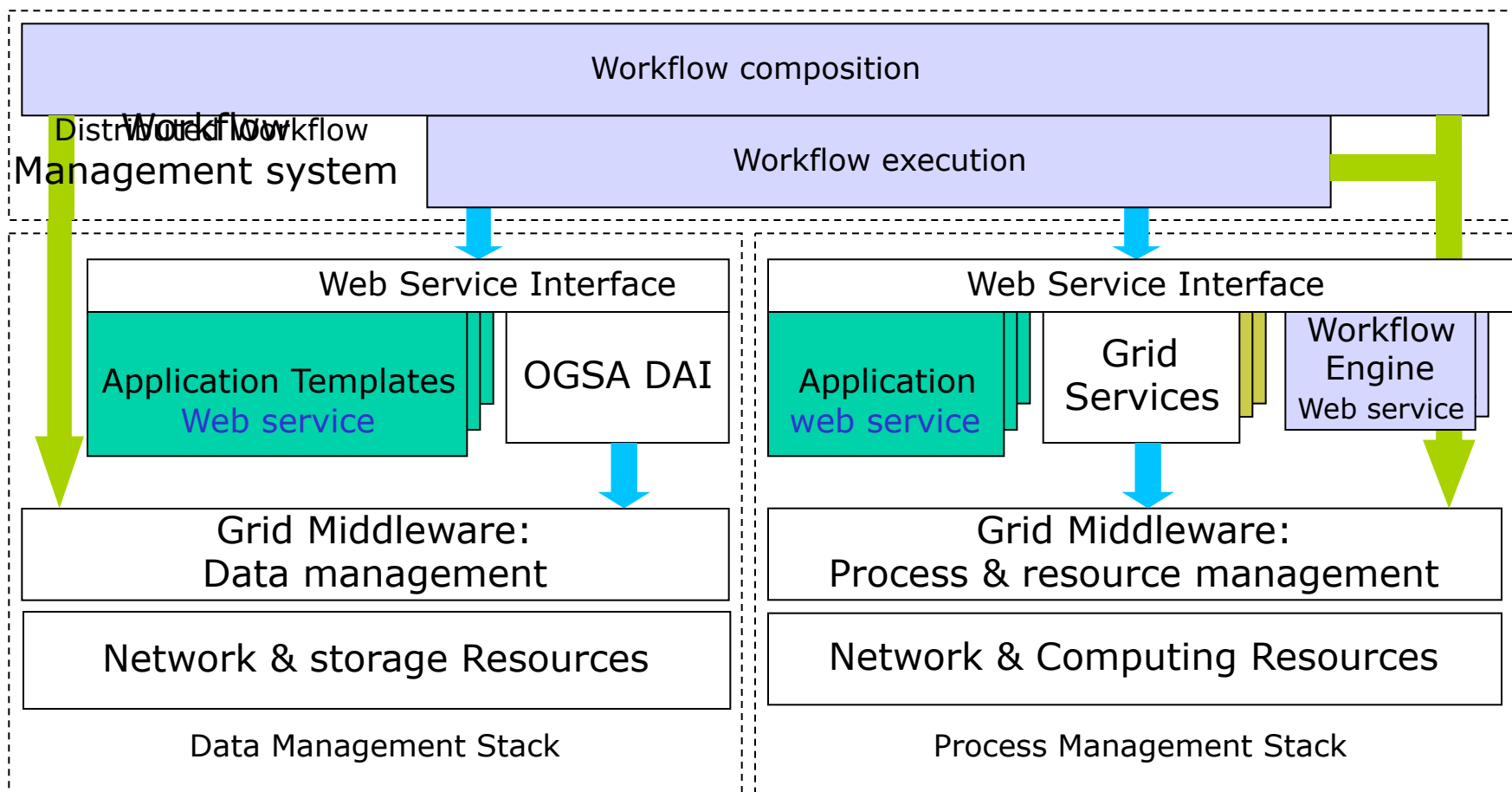
(2) Experiment Prototyping

Grid Enabled workflow management system

- For Application developers
 - API for JAVA, C/C++, PYTHON,
 - Data Streaming capabilities
- End-users (**scientists**)
 - Workflow monitoring
 - Drag-and-drop composition
 - Hierarchical workflow creation
 - User in the loop
 - Detach/re-attach capability



A WSRF enabled workflow engine



(2) Experiment Prototyping Semantic tools

- Tools to improve **sharing** and **re-usability**. These tools should allow:

- **Annotate** and **publish** the designed experiment prototype

- SAW: Semantic Annotation for Workflow and workflow components
- HAMMER: **H**ybrid-**b**Ased **M**atch-**M**aker for **E**-Science Resources

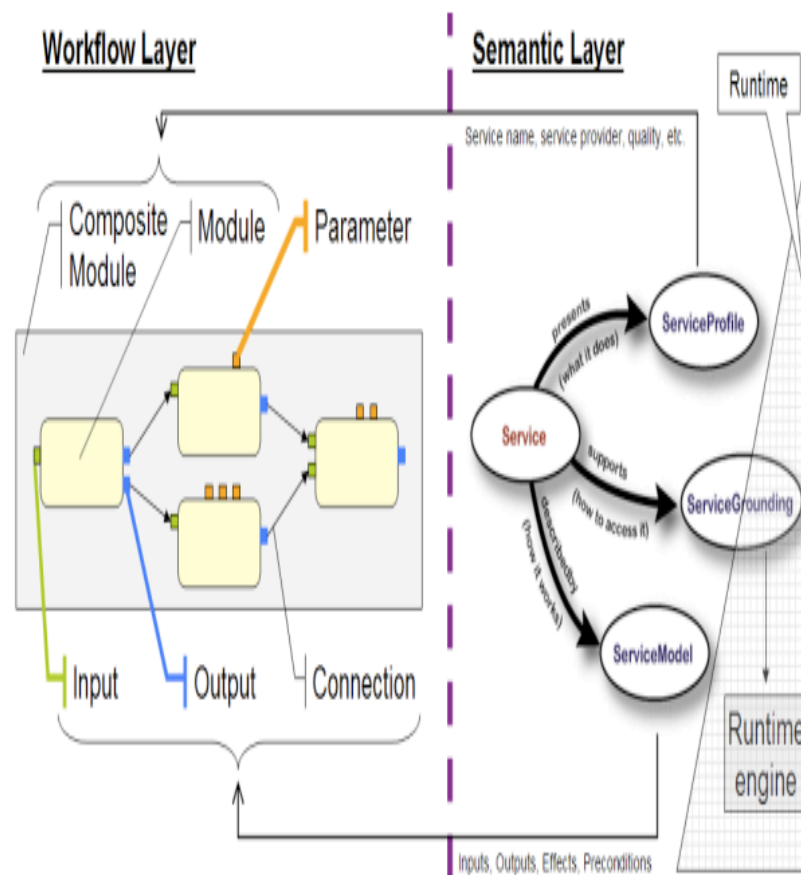


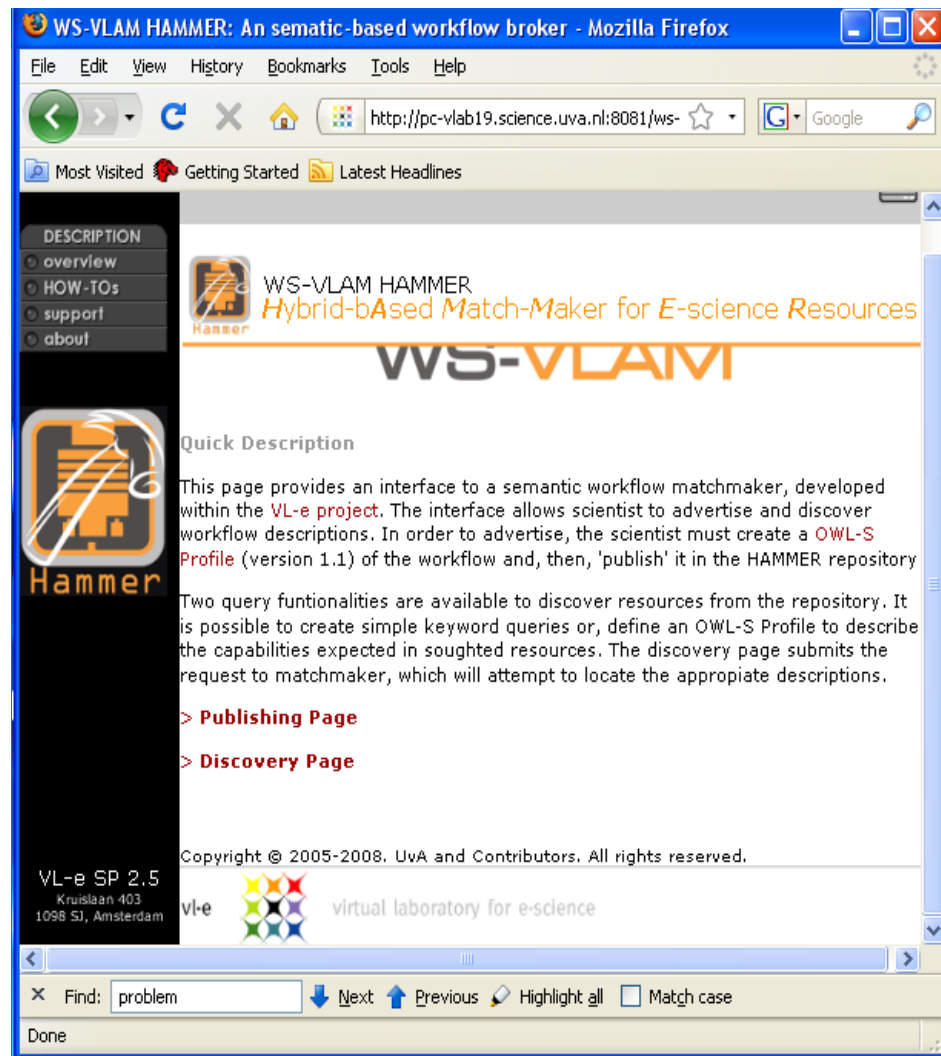
Figure B. Layers of workflow descriptions.

(2) Experiment Prototyping Publishing tools

- Tools to improve **sharing** and **re-usability**. These tools should allow:

- **Annotate** and **publish** the designed experiment prototype

- SAW: Semantic Annotation for Workflow and workflow components
- HAMMER: **Hybrid-bA**sed **Match-Maker** for **E**-Science Resources



WS-VLAM HAMMER: An semantic-based workflow broker - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://pc-vlab19.science.uva.nl:8081/ws-

Most Visited Getting Started Latest Headlines

DESCRIPTION

- overview
- HOW-TOs
- support
- about

Hammer

WS-VLAM HAMMER
Hybrid-bAased Match-Maker for E-science Resources

WS-VLAM

Quick Description

This page provides an interface to a semantic workflow matchmaker, developed within the VL-e project. The interface allows scientist to advertise and discover workflow descriptions. In order to advertise, the scientist must create a OWL-S Profile (version 1.1) of the workflow and, then, 'publish' it in the HAMMER repository

Two query functionalities are available to discover resources from the repository. It is possible to create simple keyword queries or, define an OWL-S Profile to describe the capabilities expected in soughted resources. The discovery page submits the request to matchmaker, which will attempt to locate the appropriate descriptions.

> Publishing Page

> Discovery Page

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VL-e SP 2.5
Kruislaan 403
1098 SJ, Amsterdam

vl-e virtual laboratory for e-science

Find: problem Next Previous Highlight all Match case

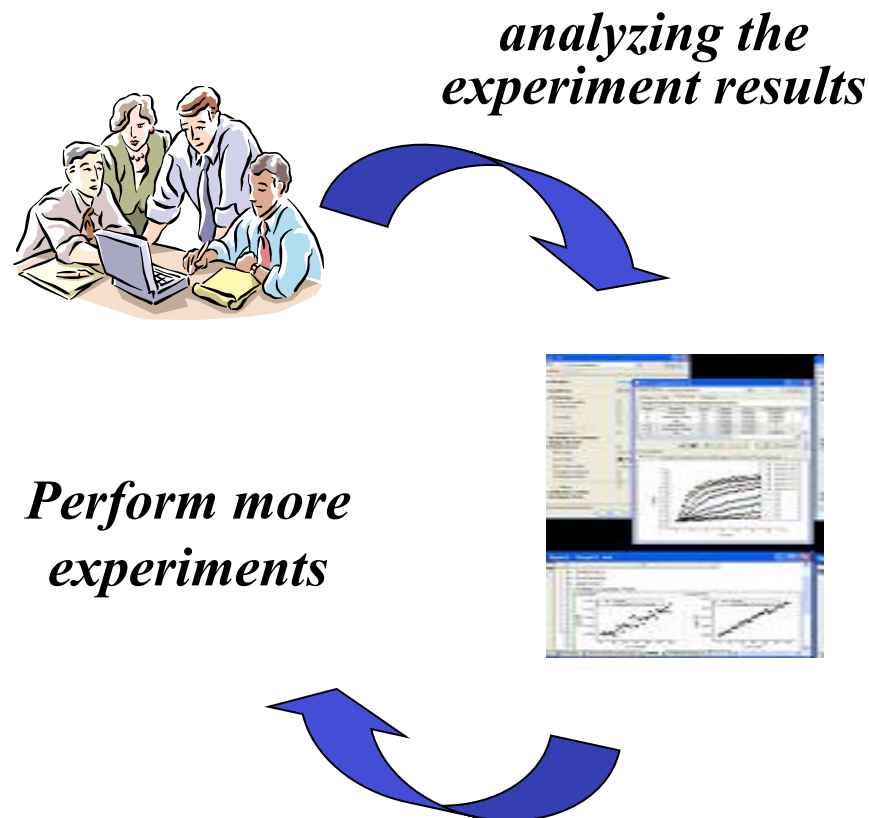
Done

<http://elab.science.uva.nl:8081/ws-hammer/>

(3) Experiment Execution Virtual resource Browser

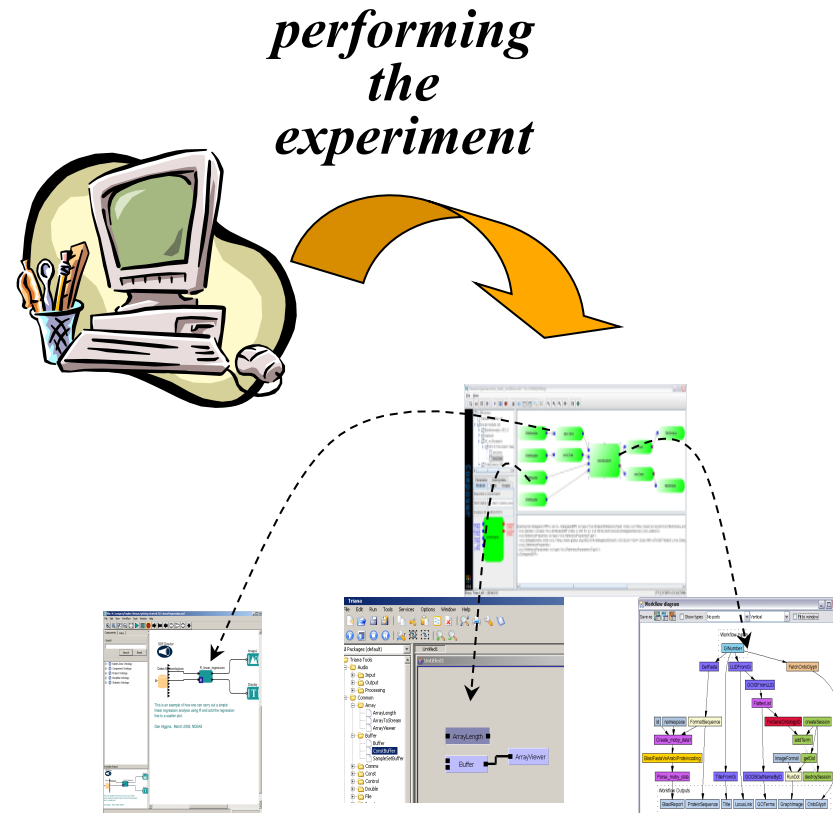
- Tools with **intuitive interface** allowing end users (Scientists):

- **Find** results: access resources to manipulate data
- **Re-start** experiment and monitor its execution



(3) Experiment Execution VLE-WFBus

- Tools to **improve interoperability** among various execution platforms.
 - Recognize different workflow descriptions.
 - Coordinate the execution of workflows, and monitor their execution.

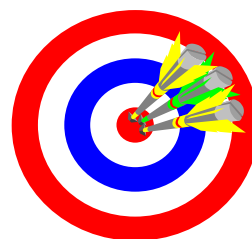


(4) Results Publication

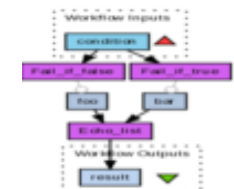
- Tools to improve **share of expertise**.
These tools should allow:

- **Annotate** and **publish** data, workflows, etc

- HAMMER: **H**ybrid-**b**Ased **M**atch-**M**aker for **E**-Science Resources (at the project level)
- MyExperiment: (at the community level)



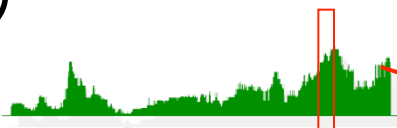
success



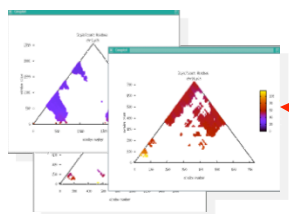
publish

(4) Results Publication

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

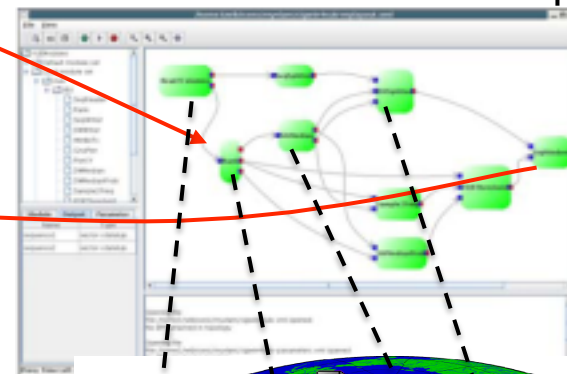


Human transcriptome map



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 Complex eScience

VLe Studio

- WS-VLAM composer
- VBrowser
- Semantic tools



SAW: Semantic Annotation for Workflow

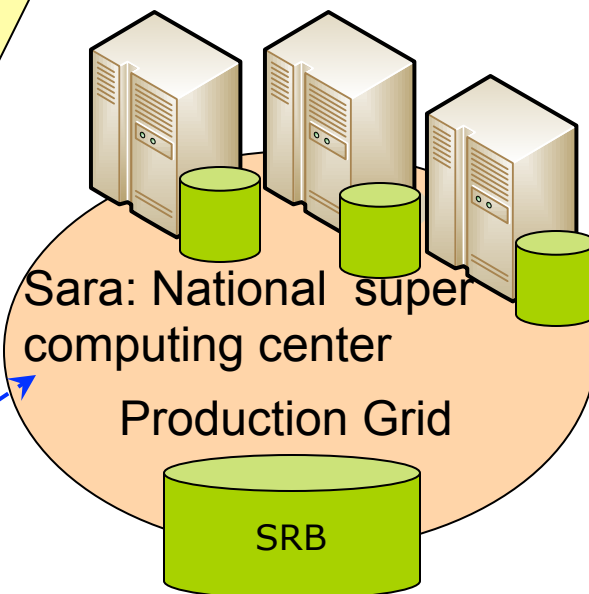
CLAMP: Connecting Language for Modules & Programs

HAMMER: Hybrid-based MatchMaker for e-Science

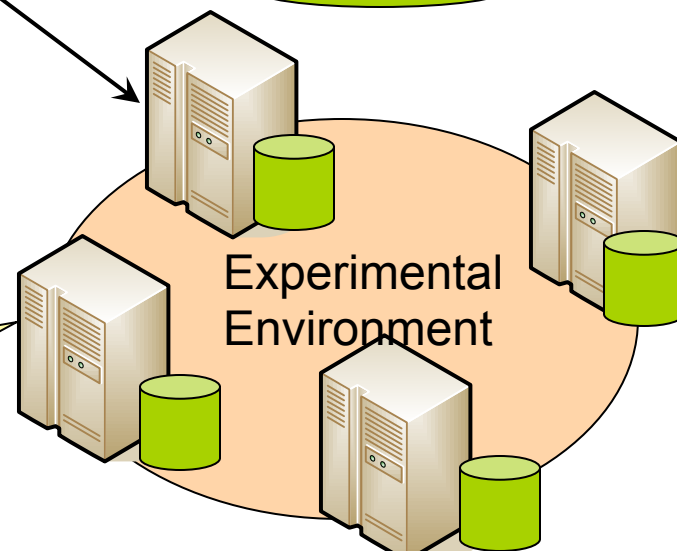
Resources

WSRF Services

- WS-VLAM engine
- workflow component repository

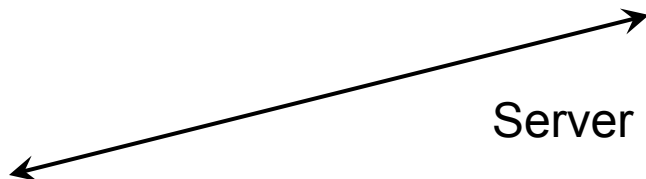
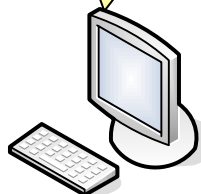
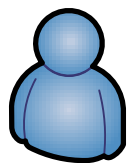


Server host



Computing Nodes

- Workflow components
- Grid Middleware → GT4



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sigWin detector

[developed Micro-Array Dept-UvA]

application that takes a sequence of numbers and a series of window sizes as input and detects all significant windows for each window size using a moving median false discovery rate (mmFDR) procedure.

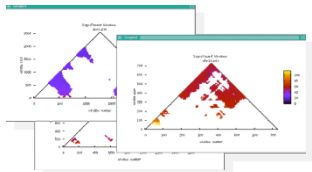
A significant window is a window in the input sequence for which the median value is significantly higher than expected, if assumed that the ordering of the numbers in the input sequence is random.

The results of a SigWin-detector analysis are summarized in a graph called SigWin-map. In the special case that the input sequence is a transcriptome map, the significant windows are called RIDGES and the output graph is called a RIDGEOGRAM.

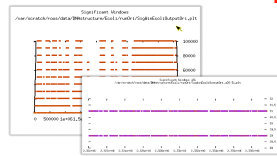
SigWin-detector runs under the WS-VLAM workflow management system.



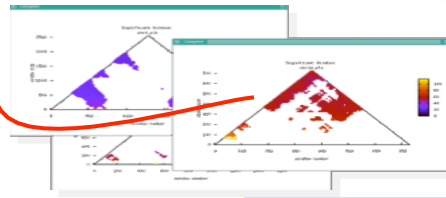
discovered RIDGE



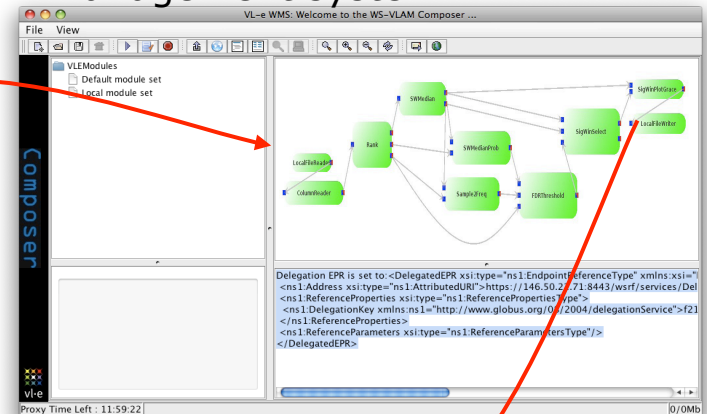
Temperature in Amsterdam



DNA curvature of the *Escherichia Coli* chromosome



Human transcriptome map



VLAM composer window

Ridgeogramer

Affymetrix Permutation-based Probe Level Estimation

[developed Micro-Array Dept-UvA]

Goal: Because of its cost, microarray experiments are frequently designed using a relatively small number of biological or technical replicates. This can result in low statistical power when the number of differentially expressed genes is inferred.

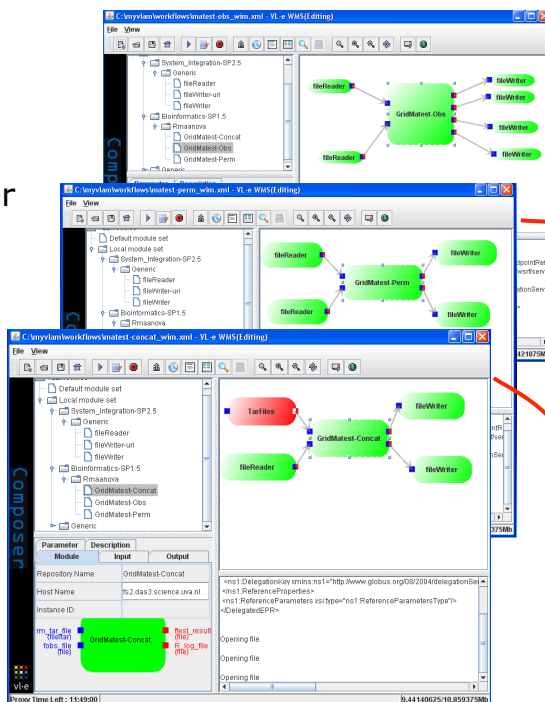
This work investigates whether the statistical power of Affymetrix experiments can be increased, without the need to increase the number of hybridizations.

Permutation tests are computationally intensive (**1000 permutations** per gene). For large experiments, the in-built feature of running R/MAANOVA in a single cluster may not be enough.

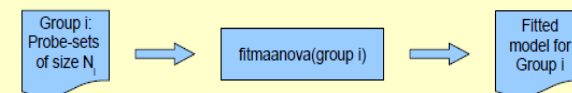
Plan: In Affymetrix microarrays, specific genes and transcripts are reported by different short oligonucleotide sequences or probes. Gene expression is generally estimated in a two-step procedure

The proposed approach skips certain steps and use the individual probe values as input in a gene specific mixed effect ANOVA model.

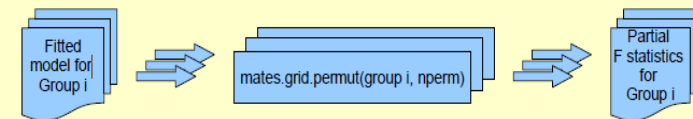
In this new approach, Probe appears as a factor nested into the factor *Chip*.



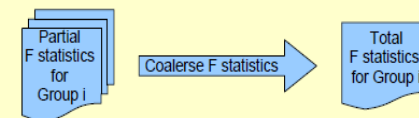
Step 1: Fit model



Step 2: Farm permutations (P jobs \times M permutations = total number of permutations)



Step 3: Coalesce F statistics

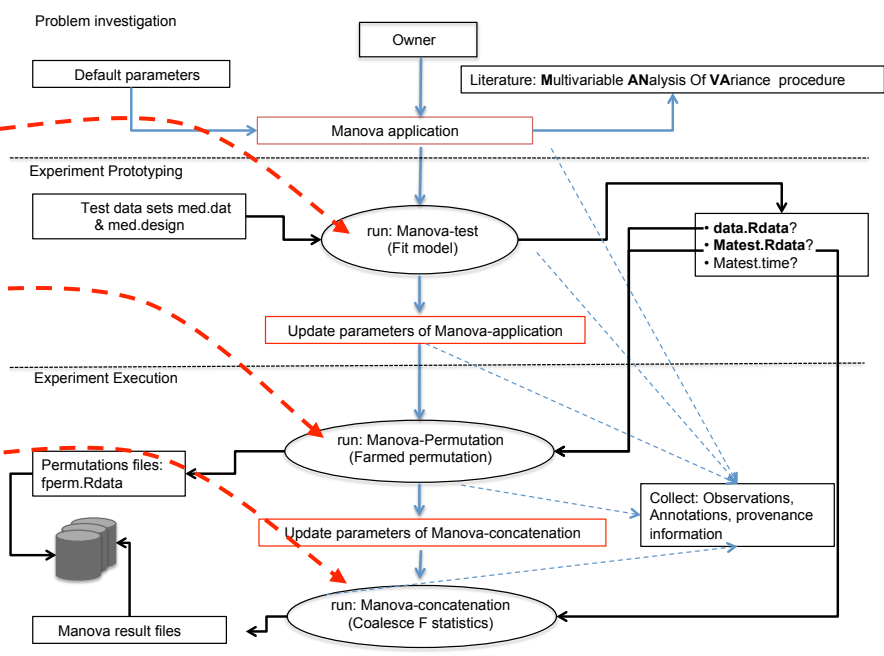




The screenshots show the Composer workflow editor with three different workflow configurations:

- Top screenshot (obs):** Shows a workflow with 'GridMatest-Obs' as the central module, connected to 'FileReader' and 'FileWriter' modules.
- Middle screenshot (perm):** Shows a workflow with 'GridMatest-Perm' as the central module, connected to 'FileReader' and 'FileWriter' modules.
- Bottom screenshot (concat):** Shows a workflow with 'GridMatest-Concat' as the central module, connected to 'FileReader' and 'FileWriter' modules. Below the workflow, a table lists parameters for the 'GridMatest-Concat' module.

Module	Description	Input	Output
Repository Name	GridMatest-Concat		
Host Name	ps2.daa3.science.univ.nl		
Instance ID			
FileReader		med.dat	
FileWriter			med.design

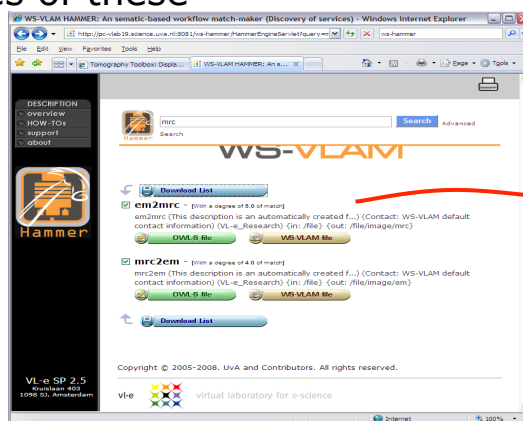


Use of Omnimatch for template matching of 3D electron microscopy reconstructions

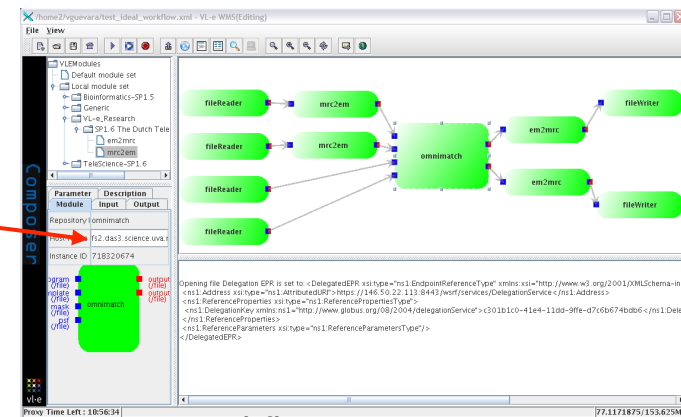
[Application developed UU/Leiden]

Goal. Omnimatch allows to locate specific templates in 3D electron microscopic reconstructions (tomograms) of biological samples. This is useful either to draw specific structures (for examples tubules in a cell) in a tomogram or to compute averages of these specific structures.

Prototype: create a workflow which collects data file stored on geographically distributed storage. Stage them on the targeted computing resource. And execute the Omnimatch software. The output of the experiment is stored on permanent storage systems specified by the end-users.



Online repository of workflow components

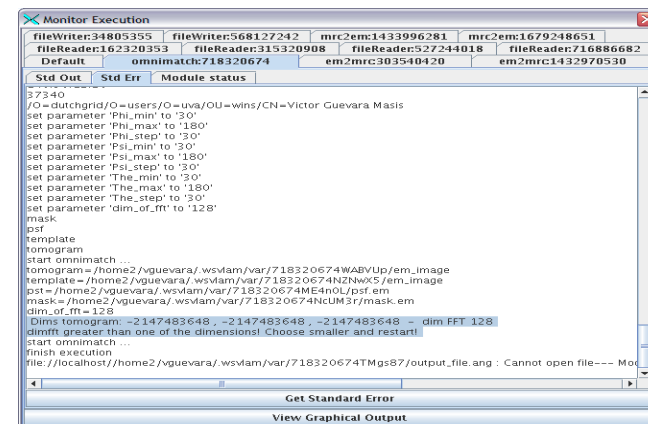


workflow composer

Monitoring: The Omnimatch workflow can be remotely monitored at both workflow level and component level. Workflow components developed for this experiment are stored in a shared repository and can be downloaded

Workflow components can be semantically annotated to enhance the search phase

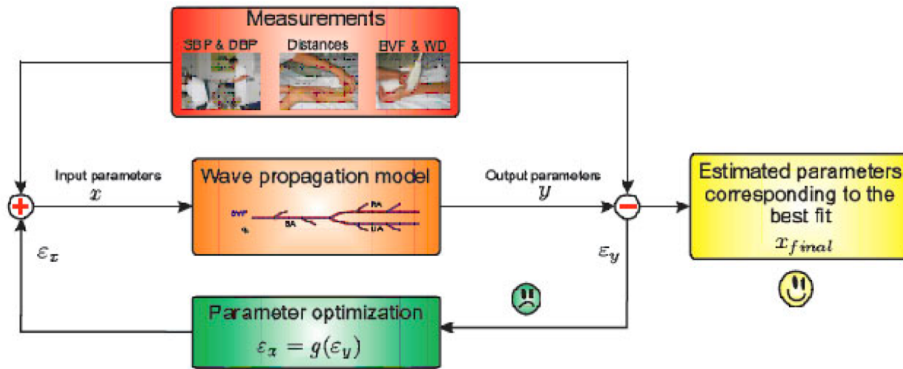
At run time workflow components are deployed on the target host and executed. Std input, std output, std error, and any graphical output can be retrieved and displayed on the end-user



workflow monitoring interface

wave propagation model applications

[Biomedical engineering Cardiovascular biomechanics group TUE]

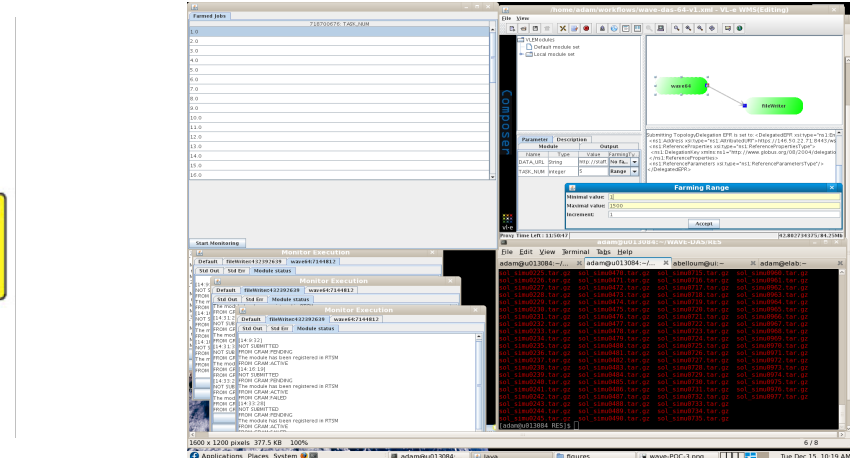


wave propagation model of blood flow in large vessels using an approximate velocity profile function:

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

EGI/BigGrid technical forum 2010

C. Leguy, Bosboom, F.N.V.D Vosse, A.S.Z. Belloum, A. Hoeks "Global sensitivity analysis of a wave propagation model for arm arteries", to be published Journal of Medical Engineering Physics



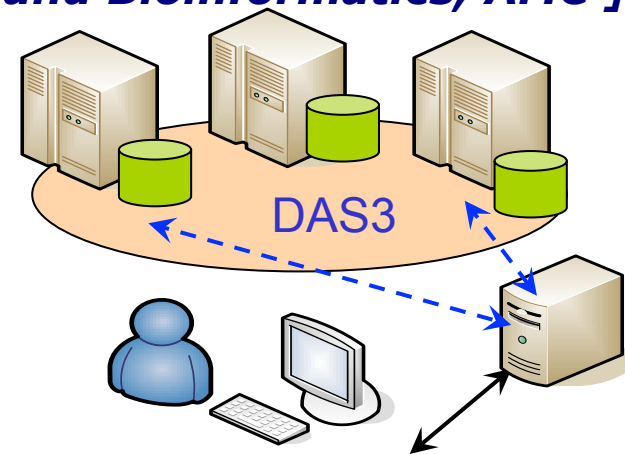
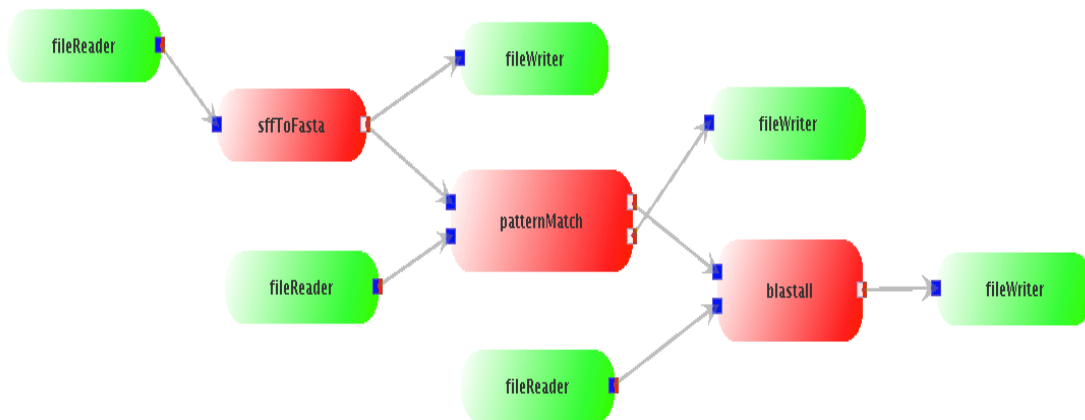
User Interface to compose workflow (top right), monitor the execution of the farmed workflows (top left), and monitor each run separately (bottom left) data

Name	Start	Time	Simulation Count
Wave_CardioV...	01:58:43	01:58:43	1000
Wave_CardioV...	01:57:51	01:57:51	1000
Wave_CardioV...	01:57:37	01:57:37	1000
Wave_CardioV...	01:56:35	01:56:35	1000
Wave_CardioV...	01:56:53	01:56:53	1000
Wave_CardioV...	01:56:52	01:56:52	1000
Wave_CardioV...	01:56:49	01:56:49	1000
Wave_CardioV...	01:56:28	01:56:28	1000
Wave_CardioV...	01:57:05	01:57:05	1000
Wave_CardioV...	01:57:04	01:57:04	1000
Wave_CardioV...	01:56:51	01:56:51	1000
Wave_CardioV...	01:56:18	01:56:18	1000
Wave_CardioV...	01:55:14	01:55:14	1000
Wave_CardioV...	01:55:12	01:55:12	1000
Wave_CardioV...	01:56:00	01:56:00	1000
Wave_CardioV...	01:54:37	01:54:37	1000
Wave_CardioV...	01:55:05	01:55:05	1000
Wave_CardioV...	01:55:23	01:55:23	1000
Wave_CardioV...	01:54:50	01:54:50	1000
Wave_CardioV...	01:55:27	01:55:27	1000
Wave_CardioV...	01:54:54	01:54:54	1000
Wave_CardioV...	01:52:08	01:52:08	1000
Wave_CardioV...	01:52:35	01:52:35	1000
Wave_CardioV...	01:52:53	01:52:53	1000

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, 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.

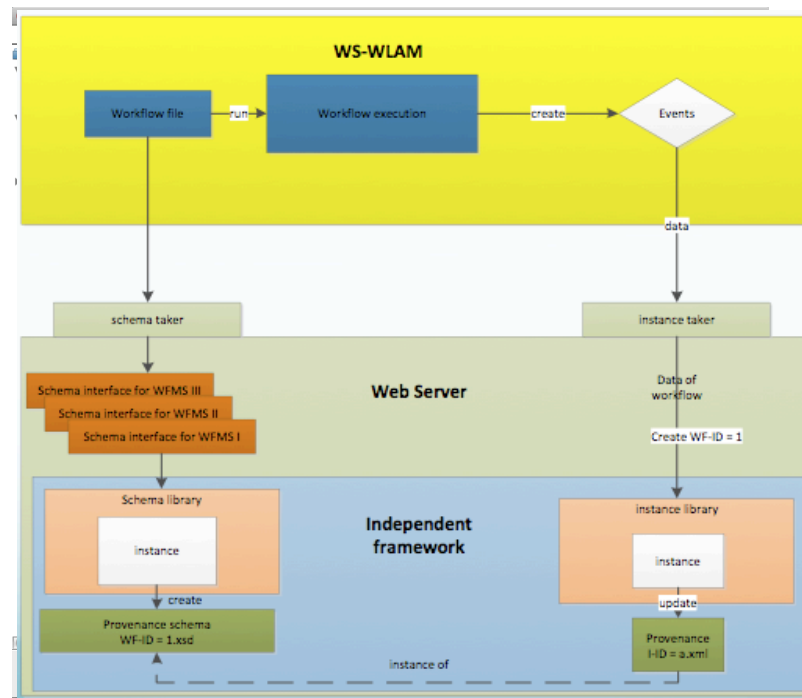
For Each workflow run

The provenance data is collected 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

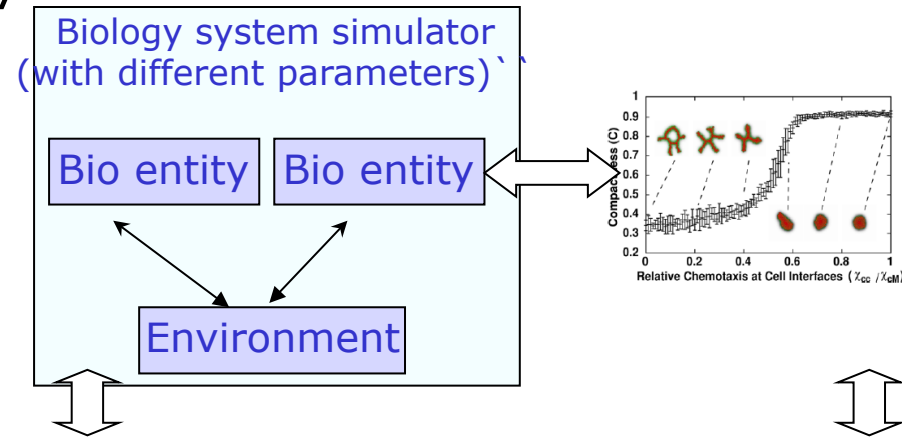


workflow integration in biology model tuning

[system biology group, CWI]

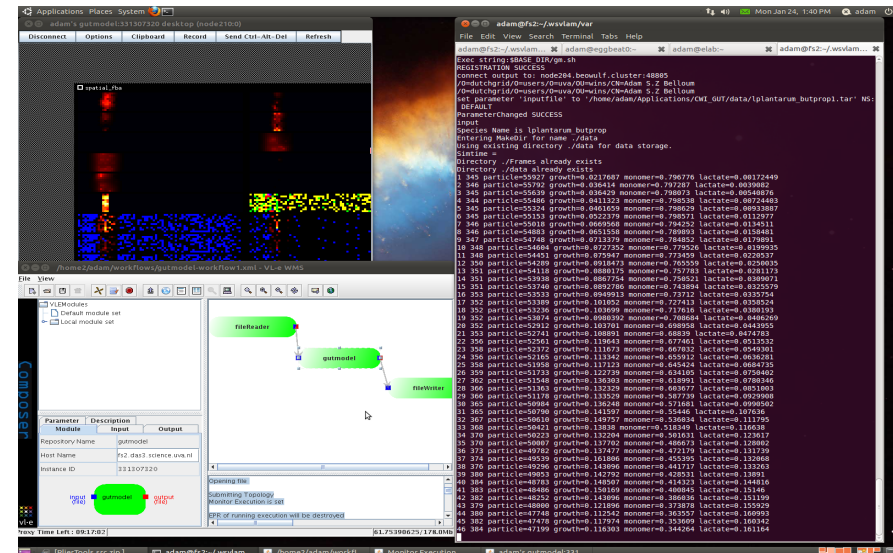
The simulation implements a spatially explicit, computational model of the gut & its micro-biota.

Given the local environment of cells and cell-specific metabolic network, the growth and uptake rates of metabolites are calculated at each time-step for every cell using a Flux Balance Analysis.



The approach

- The application is modeled as a workflow in WS-VLAM to handle parameter sweep search using bigGrid resources
- User is able to execute, monitor and interact with on-going experiment

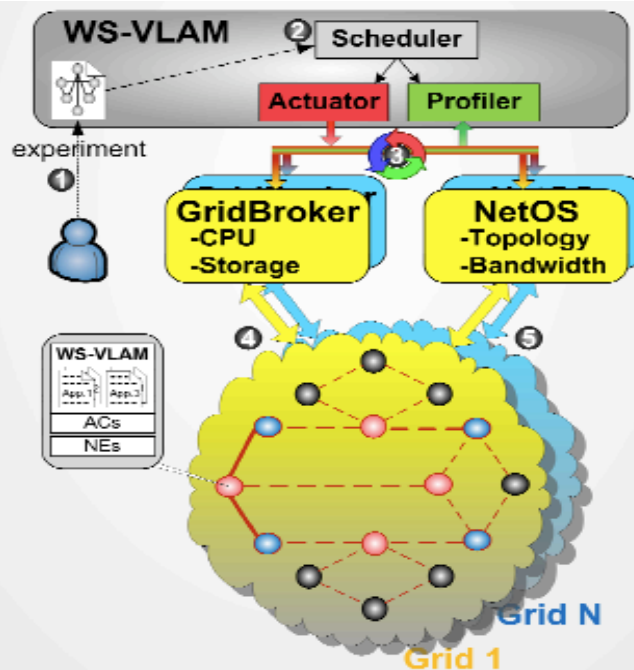


Dynamic network control in distributed computing

[SNE-UvA]

WS-VLAM – workflow execution environment coordinates the execution of distributed Apps

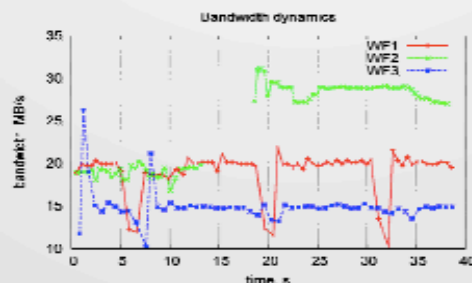
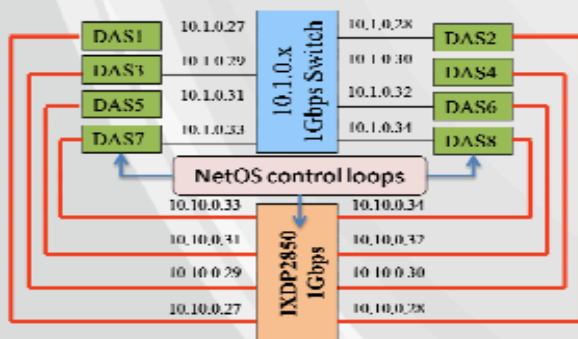
- 1 - **User** deploys an experiment: application & basic infrastructure requirements;
- 2 – **WS-VLAM** maps the experiment using **Actuator** onto available distributed resources as detected by **Profiler**;
- 3 - **Control loops** may occur in which WS-VLAM is a controller to adjust the resources such as to solve the applications demands regardless of the environment changes;



- 4 - **Broker** manages the computational resources;
- 5 - **NetOS** programs the networking infrastructure of distributed system;

Each node:

- supports the applications running under WS-VLAM supervision
- provides the application-specific network services through application-components **ACs** supported by network elements **NEs**.



A testbed showing a distributed system in which nodes are interconnected through 2 networks, as follows:

- a default network uses a shared 1Gbps gigabit switch
- a second network uses a network processor unit programmed to route IP packets at 1Gbps, too.

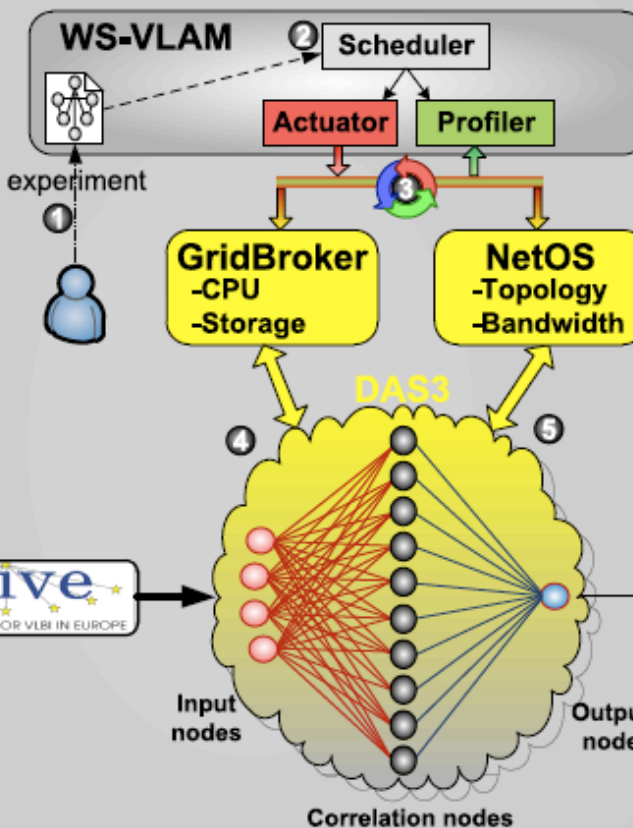
- 1 – WS-VLAM management starts applications and setup the paths one by one on the default network (10.1.0.x);
- 2 – When measured network performance (throughput) decreased below an application threshold, WS-VLAM starts “offloading” the paths from 10.1.0.x network onto 10.10.0.x network;

Smart Infrastructure for VLBI Software Correlation

[SNE-UvA]

WS-VLAM - workflow execution environment coordinates the execution of distributed Apps

- 1 - User deploys an experiment: application & basic infrastructure requirements;
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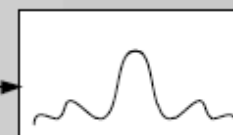


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jive
JOINT INSTITUTE FOR VLBI IN EUROPE

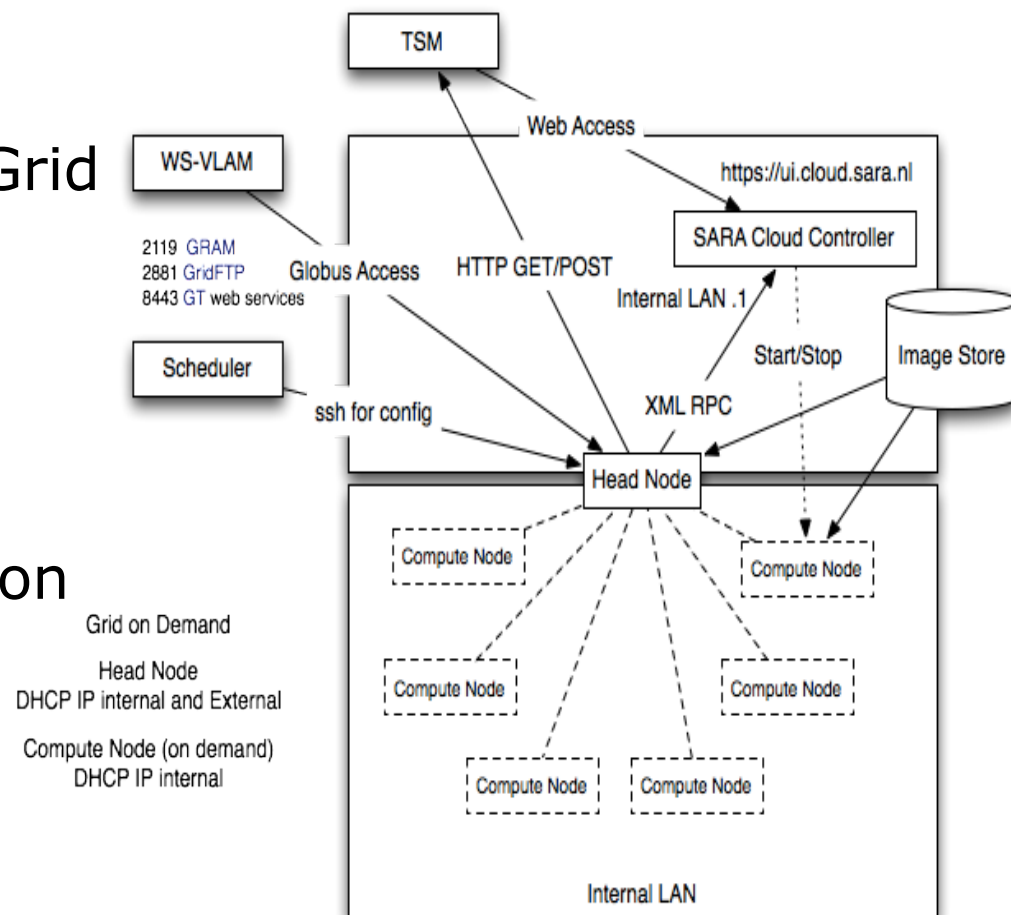


Smart Infrastructure for VLBI Software Correlation

[SNE-UvA]

Grid On-demand for workflow execution

- Workflow execution on Grid and Cloud resources
 - Application urgent computing
 - Runs simultaneously on clusters (DAS-3, TNO Cloud, SARA Cloud, Amazon EC2 Cloud)



List of applications developed using WS-VLAM

- sigWin detector *[Dr. T. Briet Micro-Array Dept-UvA]*
- *Affymetrix Permutation* *[Dr. T. Briet Micro-Array Dept-UvA]*
- *Omnimatch* *[T.P van der Krif UU/Leiden]*
- wave propagation *[Dr. F.N van de Vosse , TUE]*
- Blast *[Dr. S. Olabariga, AMC]*
- gut microbiota *[Dr. F.J. Bruggeman, CWI]*
- Smart Infrastructure *[Prof . C. Delaat SNE-UvA]*
- Dynamic network control *[Prof . C. Delaat SNE-UvA]*

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

publications in international journals and conference proceedings

Project level

- number of publications in int. journals and conference proceedings (**319**)
- number of presentations at int. conferences is (**294**)
- The number of completed PhD theses (**18**).

Sub-program (Virt Lab integration & workflow)

- number of publications (**34**)
- demos: SC, EGEE, EGI, ICT delta.

Other results of the VL-e project



More than one organisation



National Grid Initiatives & European Grid Initiative

- At the national level a grid infrastructure is offered to national and international users by the NGIs. BiG Grid is (de facto) the Dutch NGI.
- The 'European Grid Initiative' coordinates the efforts of the different NGIs and ensures interoperability
- Circa 40 European NGIs, with links to South America and Taiwan
- Headquarter of EGI is at the Science Park in Amsterdam

The follow-up project

COMMIT

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Organization

Contact and Route

ABOUT THE COMMIT PROGRAM

The COMMIT program brings together leading researchers in search engines, parallel computing, databases, interaction in context, embedded systems and knowledge technology.

DOWNLOAD THE PLAN OF THE PROGRAM

The COMMIT program plan can be downloaded [here](#).

OVER HET COMMIT PROGRAMMA

COMMIT is het enig resterende publiekprivate onderzoeksprogramma in de ICT.

Het is groot: er gaat in het totaal 100 M€ in om, waarvan 50 Miljoen subsidie. Er zijn 10 kennisinstellingen en 70 bedrijven bij betrokken. Voorbeelden van deze bedrijven zijn Philips, TNO, Chess Engineering, Thales, ANP, Beeld en Geluid, en vele andere hightech Midden- en Kleinbedrijven.

Doel van COMMIT is het verbreden en versterken van de Nederlandse kennisinfrastructuur in de ICT en bedrijven beter geschikt maken voor de internationale competitie door de beste wetenschappers te verbinden met het hightech bedrijfsleven.

Er zijn 16 projecten, waarin 10 universiteiten, 5 technologische instituten, en ruim 80 Midden- en Kleinbedrijven en grote Nederlandse bedrijven participeren. Ongeveer 10% van het onderzoeksbudget is gereserveerd voor toekomstige projecten die de samenwerking tussen de huidige 16 projecten versterkt.

Het COMMIT programma richt zich op ICT doorbraken voor maatschappelijkeconomische urgente kwestie in health & well-being, science, public safety, en informatie bedrijven.

WHAT'S NEW

The follow-up project

- A work package dedicated to study Workflow **Sharing** and **Reproducibility**
- aims at developing methods enabling workflow sharing and reproducibility of results.
- To enable the sharing of workflows, and make science reproducible, novel methods are needed to enable semantic annotation of workflows and collect provenance information

The follow-up project

- A work package dedicated to study Workflow Process **Modeling & Management**
- investigate the challenging issues in modeling and integrating workflow processes of complex experiments such as:
 - achieving reusability cross multiple workflow management systems,
 - provisioning both computing and network resources required to sustain CPU and data intensive applications workflows

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Thanks to

Current members of the Group

- S. koulouzis (PhD student)
- R. Cushing (PhD student)
- Dmitry Vasunin (programmer)

Former members

- V. guevara (PhD student/Post-doc)
- V. Korkhov (PhD student /Post-doc)
- Z.Zhao (Post-Doc)
- W. Adianto (Programmer)
- M. Torsten (Guest, Ah-aachen)



vl-e



<http://www.vl-e.nl/>

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