vl-e

virtual laboratory for e-science

VL-e eScience Framework: from design to sharing

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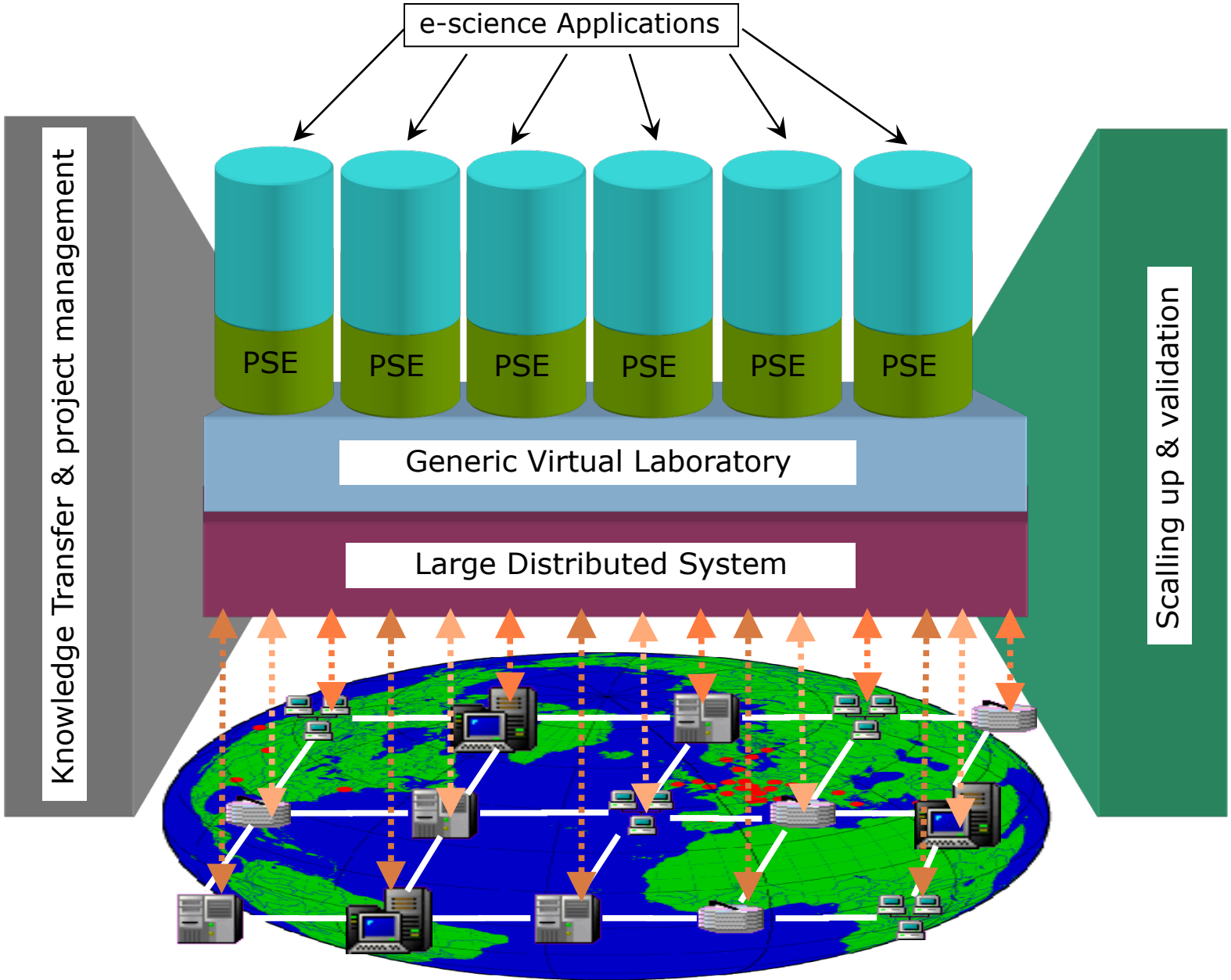
e-science Applications
Knowledge Transfer & project management
PSE
PSE
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PSE
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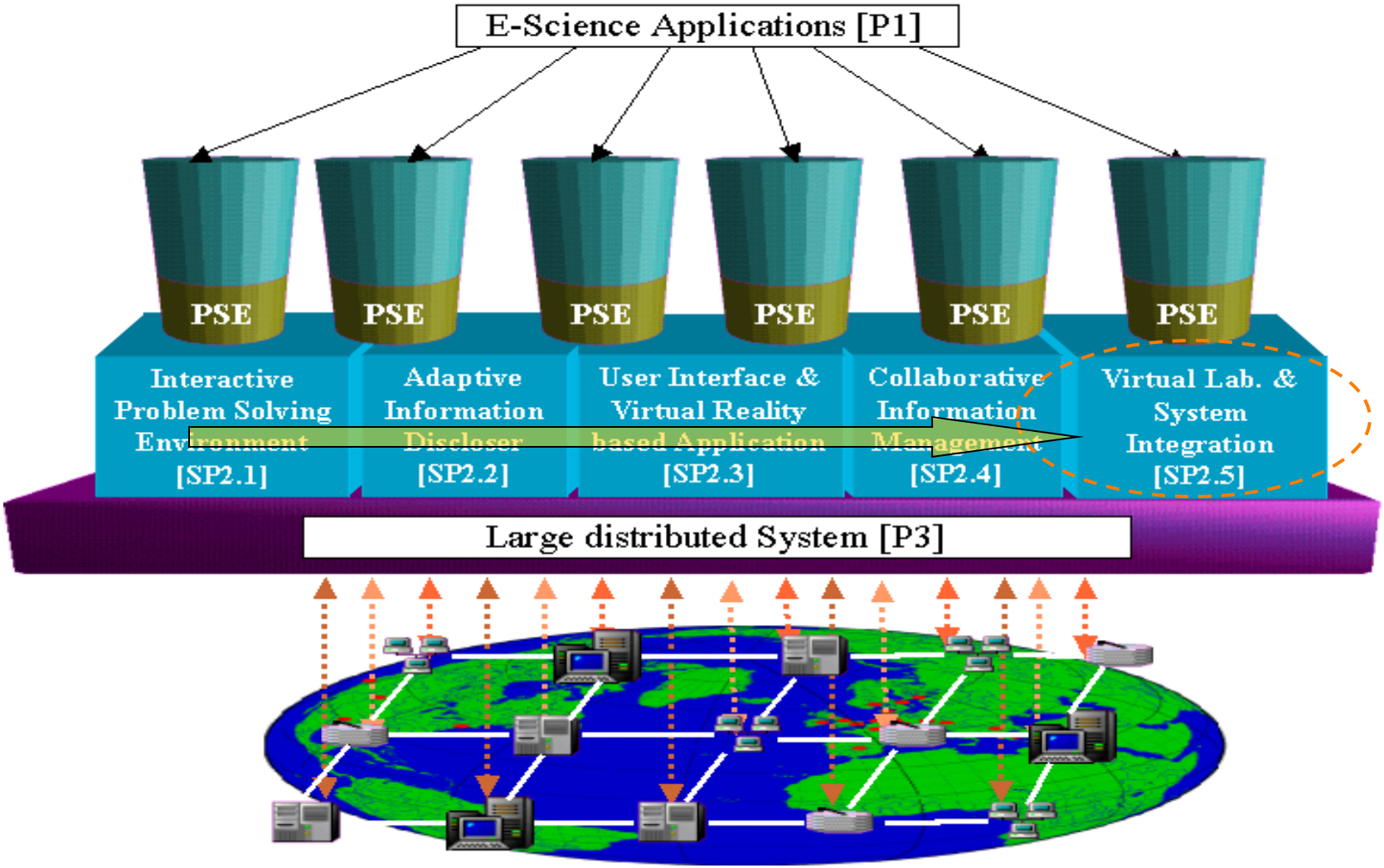
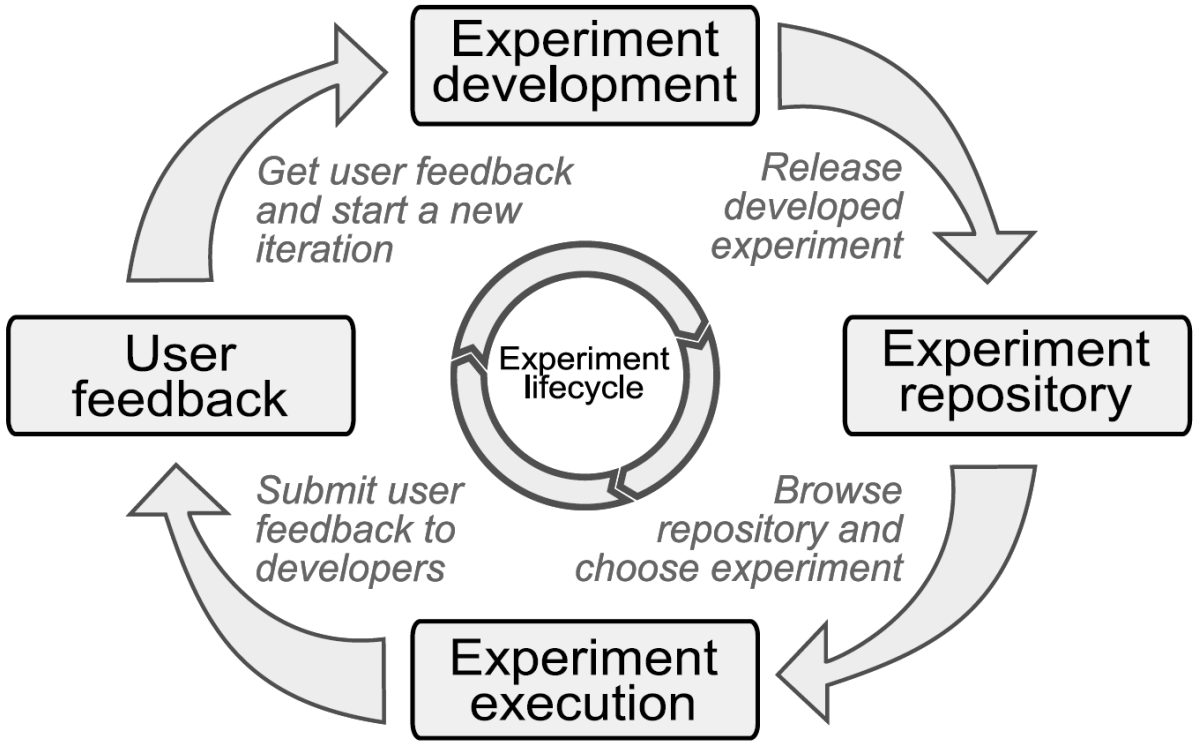
PSE
Generic Virtual Laboratory
Large Distributed System
Scalling up & validation

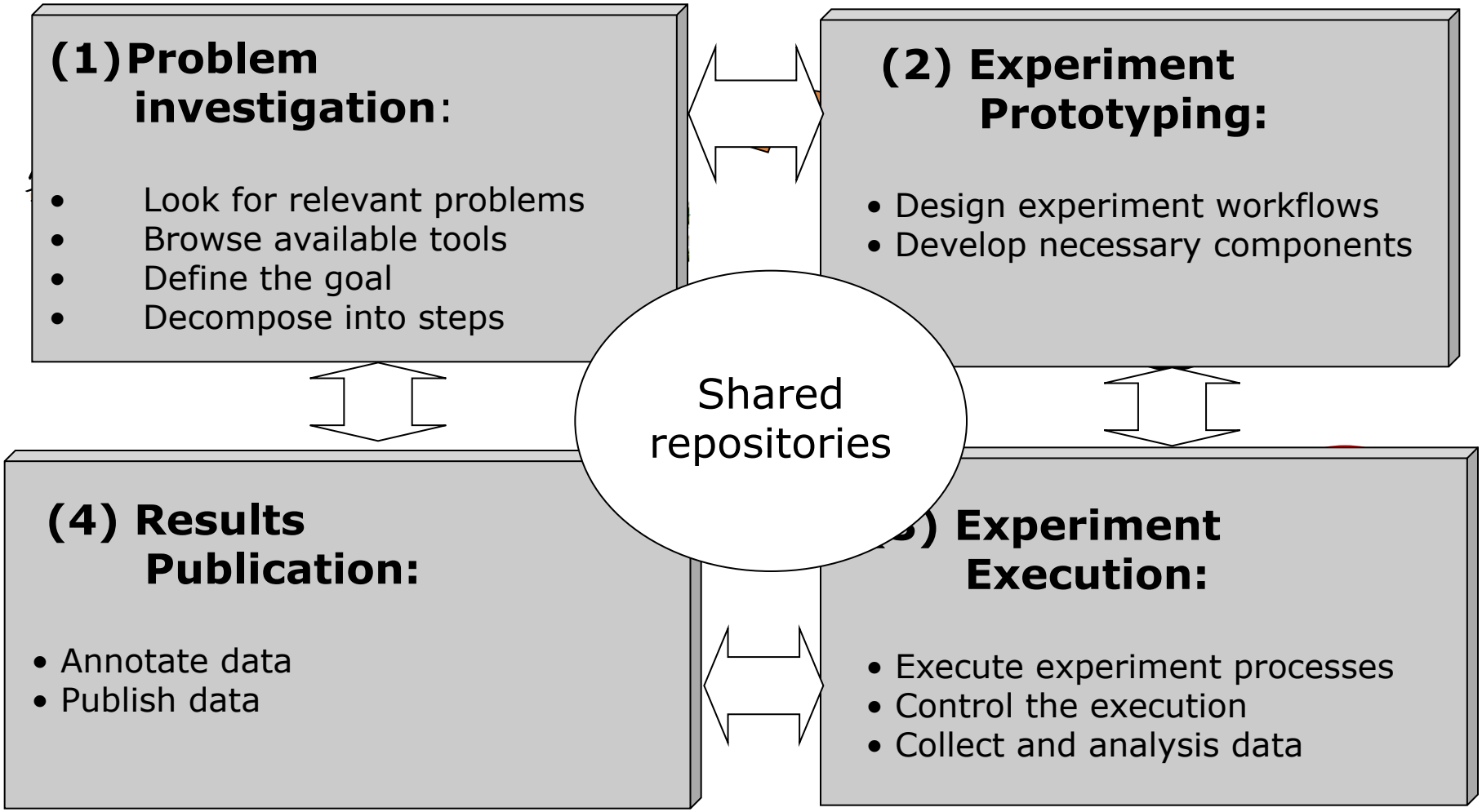

E-Science Applications [P1]
PSE
PSE
PSE
PSE
PSE
PSE
Interactive Problem Solving Environment [SP2.1]
Adaptive Information Discloser [SP2.2]
User Interface & Virtual Reality based Application [SP2.3]
Collaborative Information Management [SP2.4]
Virtual Lab. & System Integration [SP2.5]
Large distributed System [P3]

Experiment Lifecycle

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



Complex Scientific experiments model



Objective

- The Objective of this work is to address the research issues related to building an e-Science Framework which will support scientists to share their knowledge and to perform specific experiments on grid resources

Keywords:

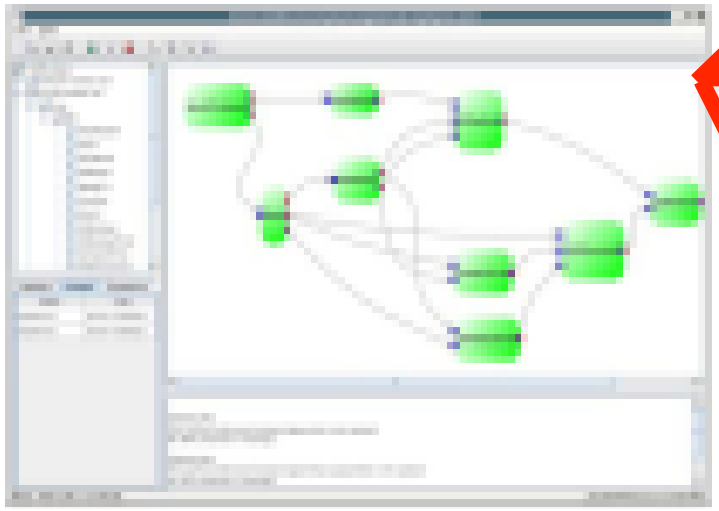
- Grid, Scientific workflow, SOA, provenance, interoperability

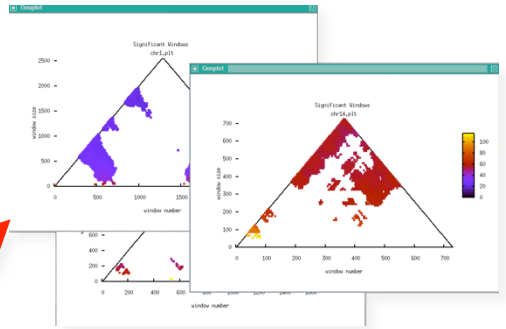
WS-VLAM e-Studio

- So far it is **simple program**, used to start the different **tools developed** in the VL-e project by the *Virtual Laboratory and system integration* group

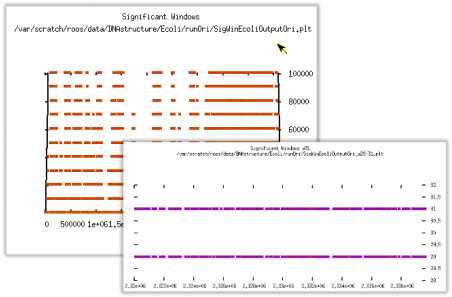
The Application Workflow …

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

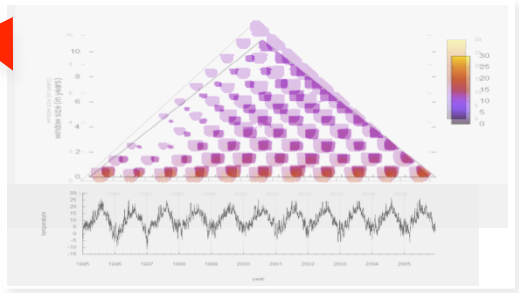




Human transcriptome map



DNA curvature of the *Escherichia coli* chromosome

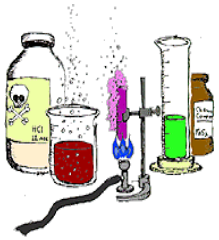


Temperature in Amsterdam

(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**-Science **R**esources
    - Web Service Harvester (RPC Style WSDL)

designing the experiment



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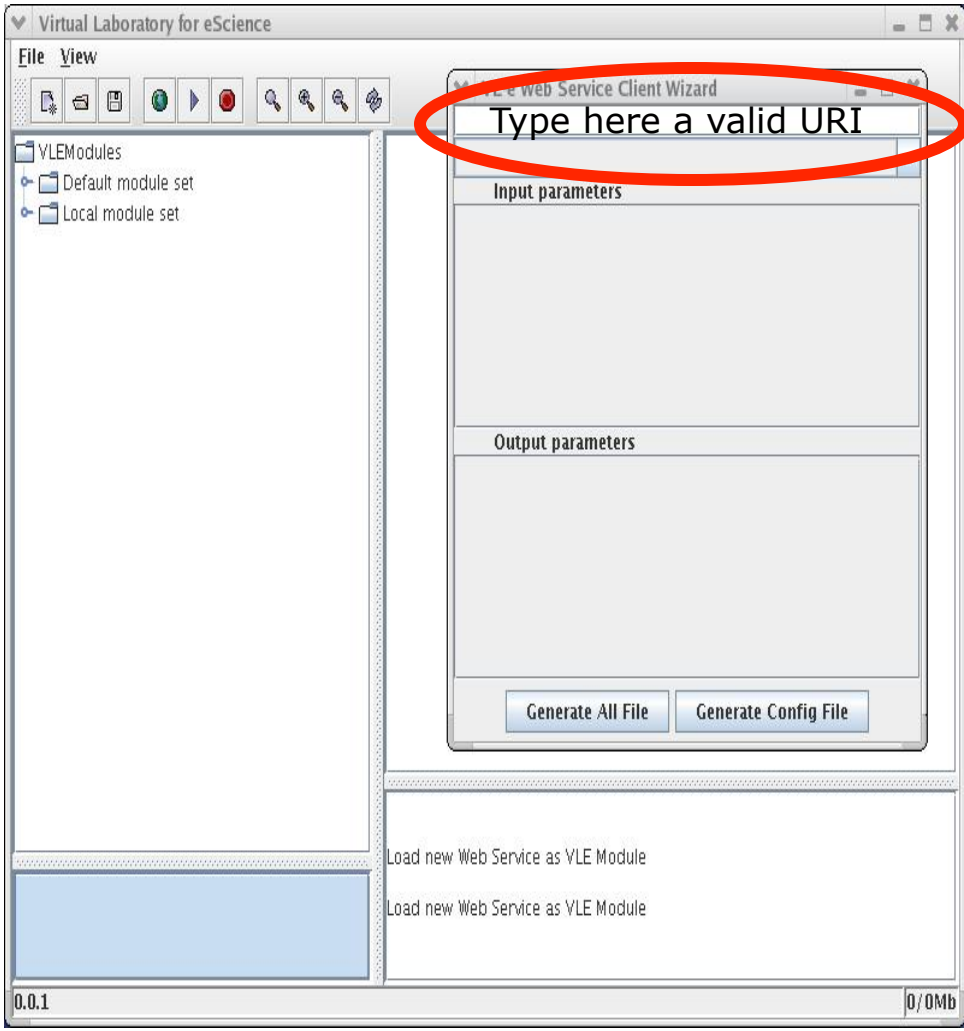
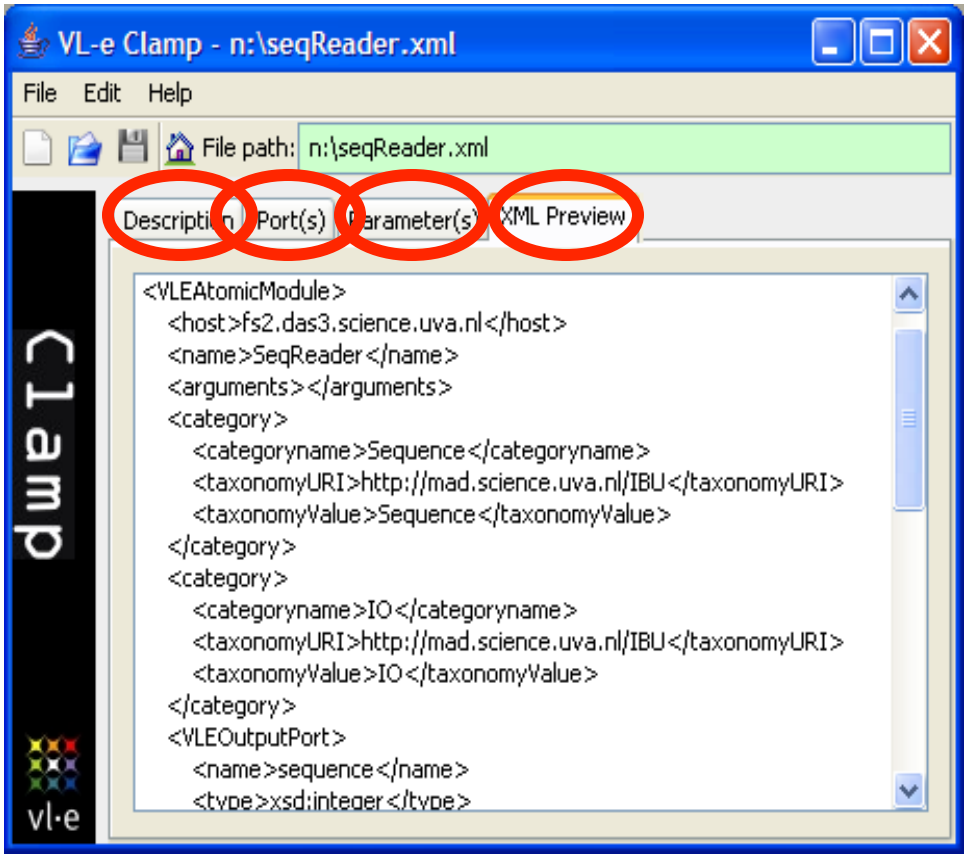


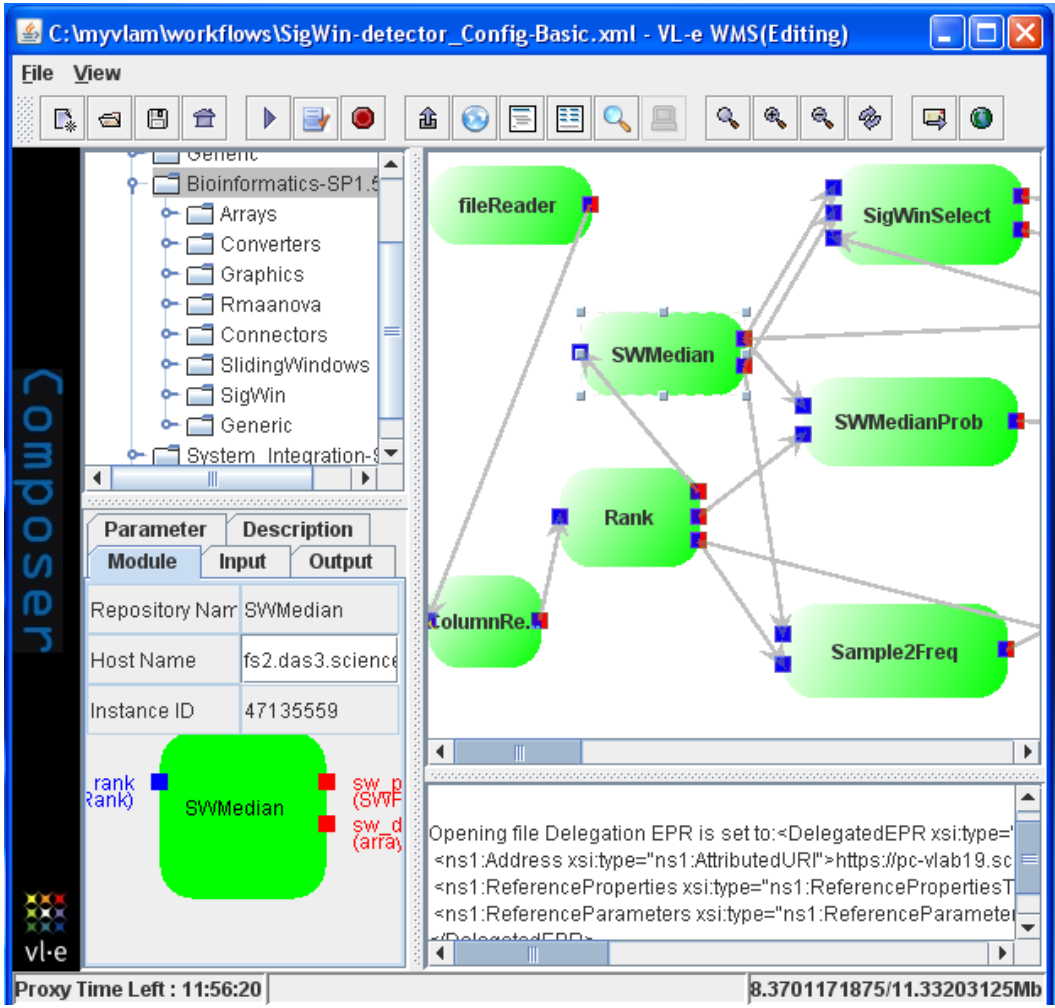
(1) Problem investigation

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



(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.

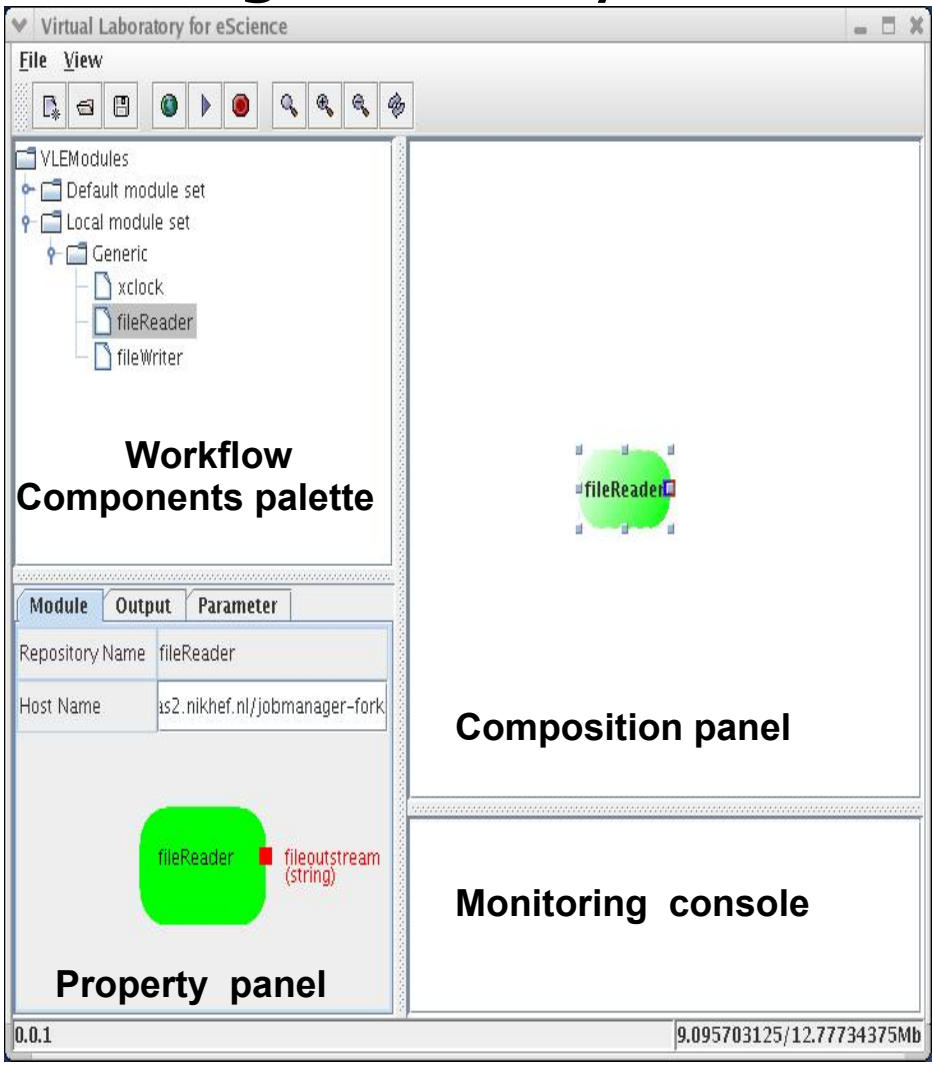


http://staff.science.uva.nl/~gvlam/wsvlam

(2) Experiment Prototyping
Grid Enabled workflow management system

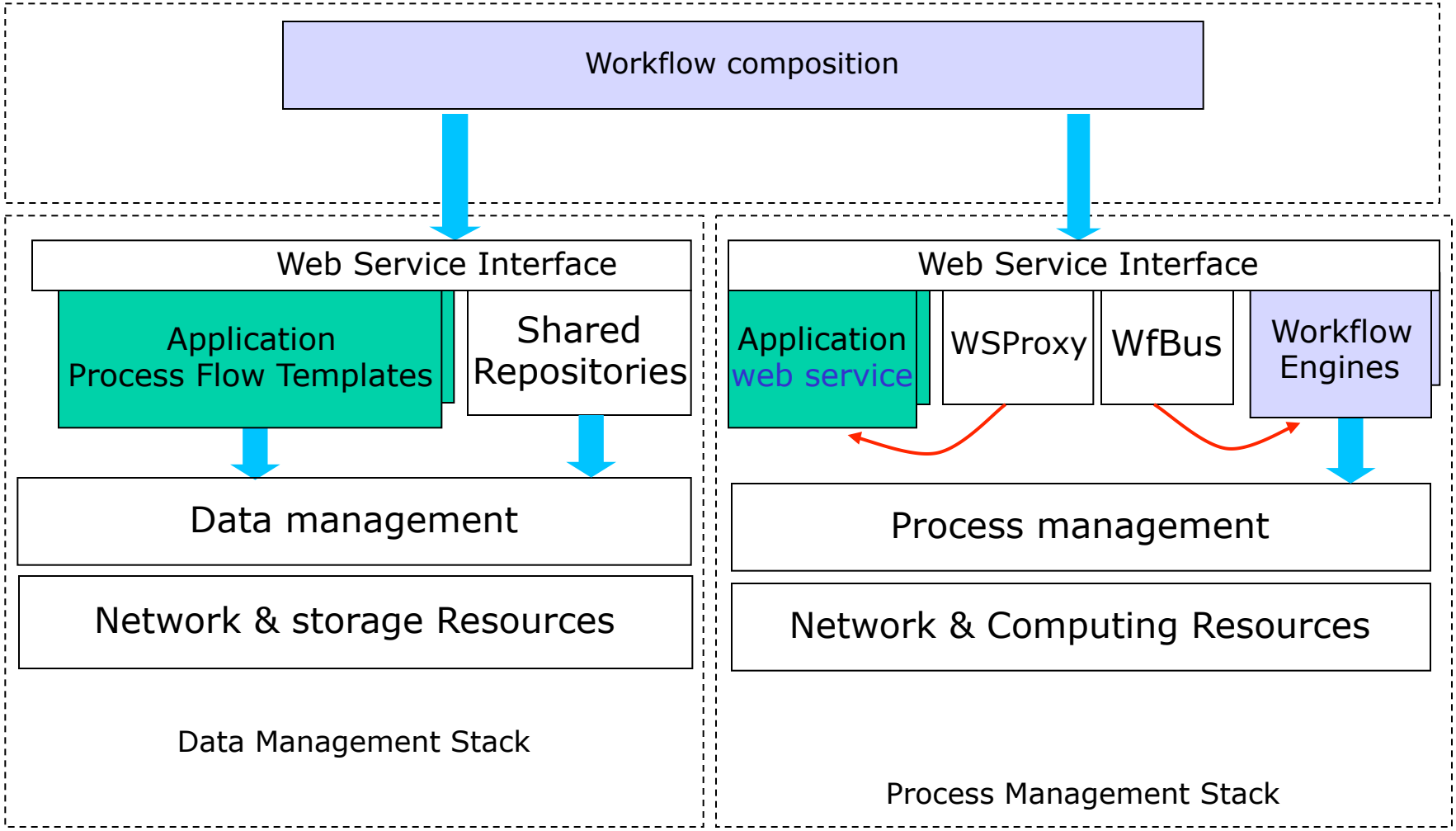
- For Application developers
  - API for JAVA, C/C++, PYTHON,
  - Data Streaming capabilities

- End-users (**scientists**)
  - Workflow monitoring
  - Drag-and-drop composition
  - Hierarchical workflow creation
  - User in the loop
  - Detach/re-attach capability



Tutorials for both developers and End-users are available at
http://www.science.uva.nl/~gvlam/wsvlam/Documentation

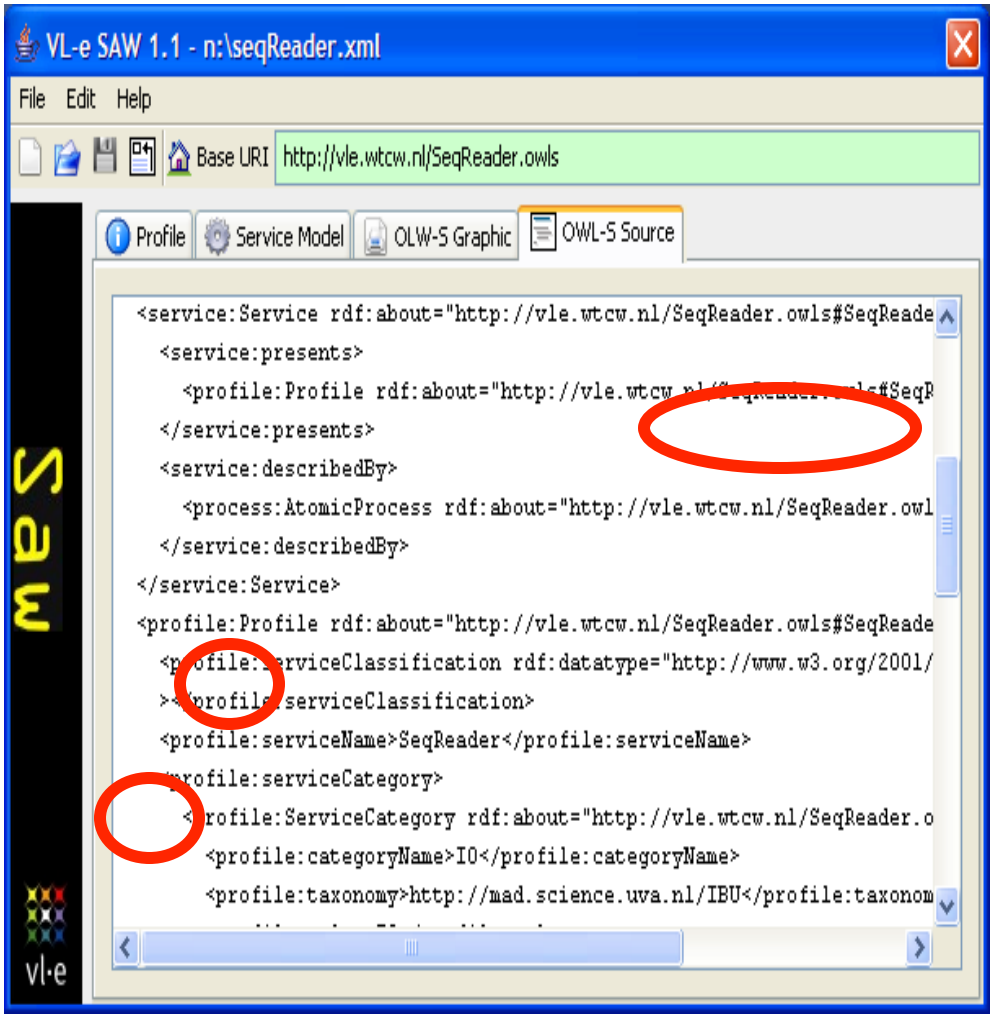
A WSRF enabled workflow engine



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

(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**A**sed **M**atch-**M**aker for **E**-Science Resources



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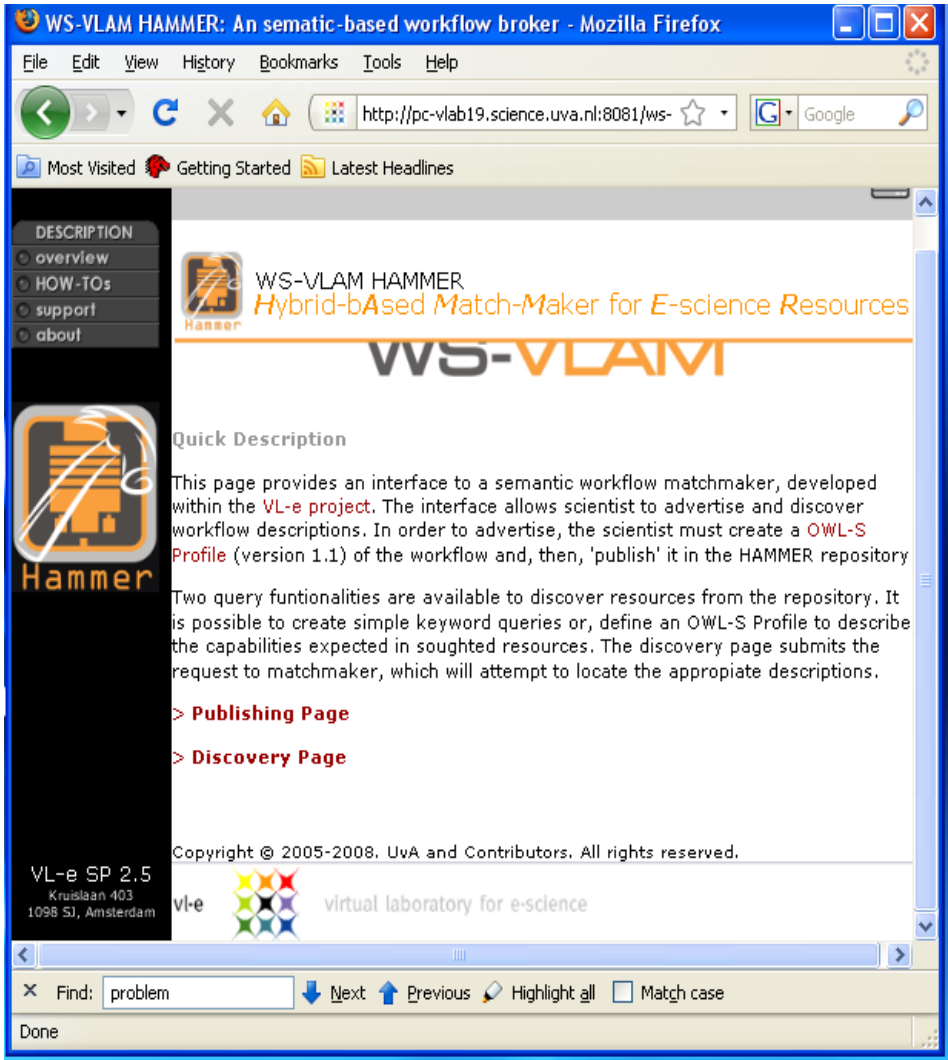
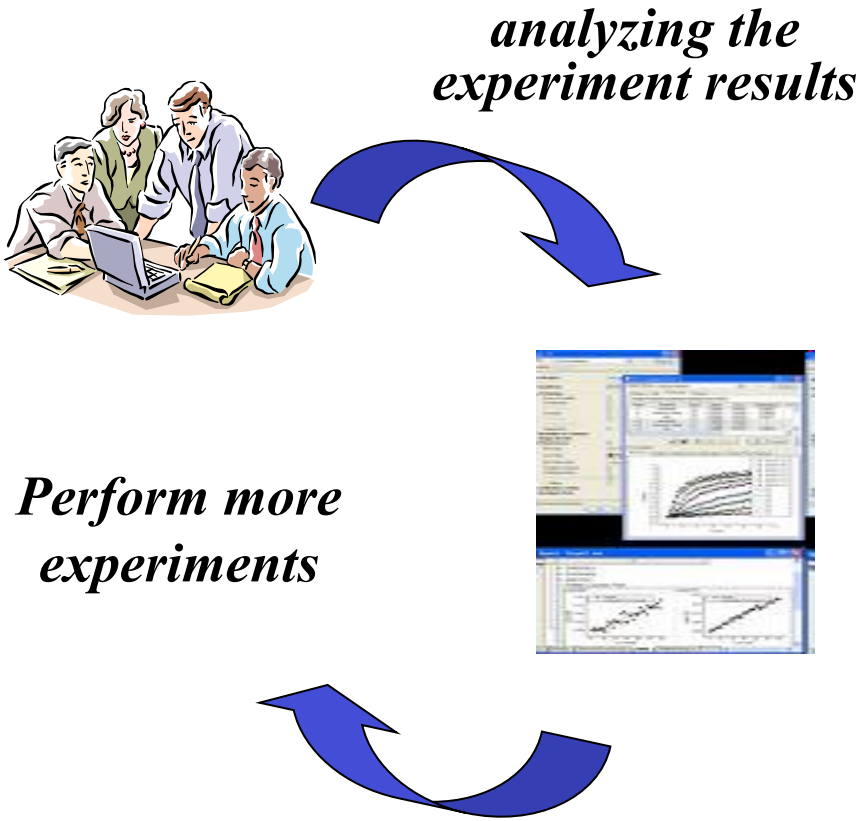


(3) Experiment Execution

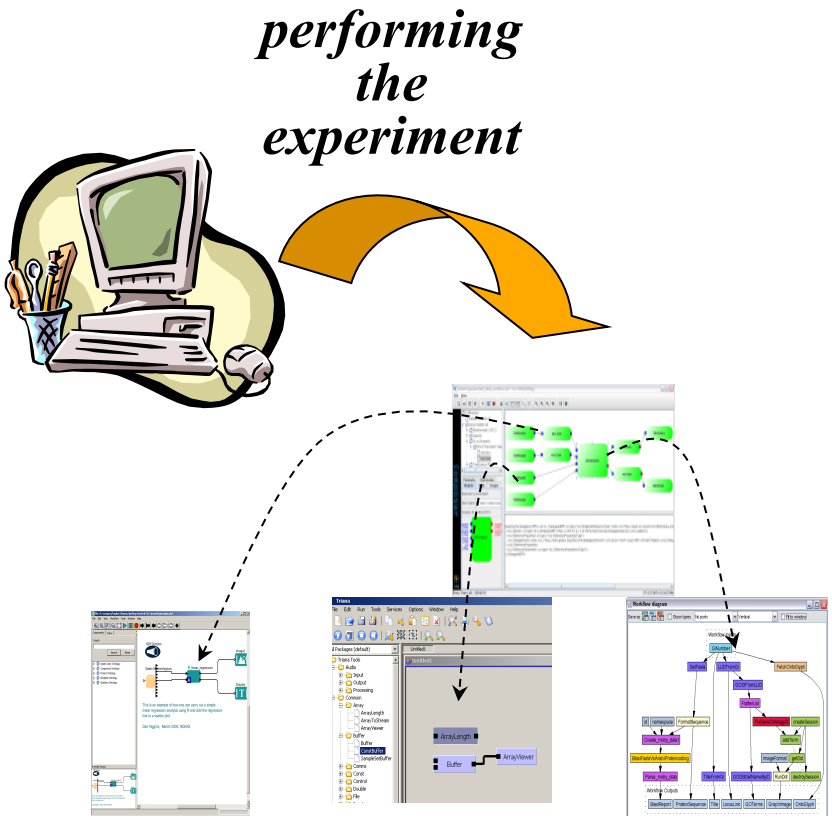
Virtual resource Browser

- Tools with **intuitive interface** allowing end users (Scientists):
  - **Find** results: access resources to manipulate data
  - **Re-start** experiment and monitor its execution



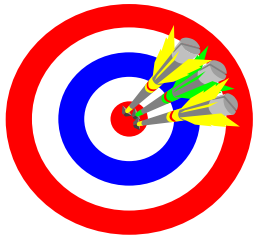
(3) Experiment Execution VLE-WFBus

- 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**A**sed **M**atch-**M**aker for **E**-Science Resources (at the project level)
    - MyExperiment: (at the community level)



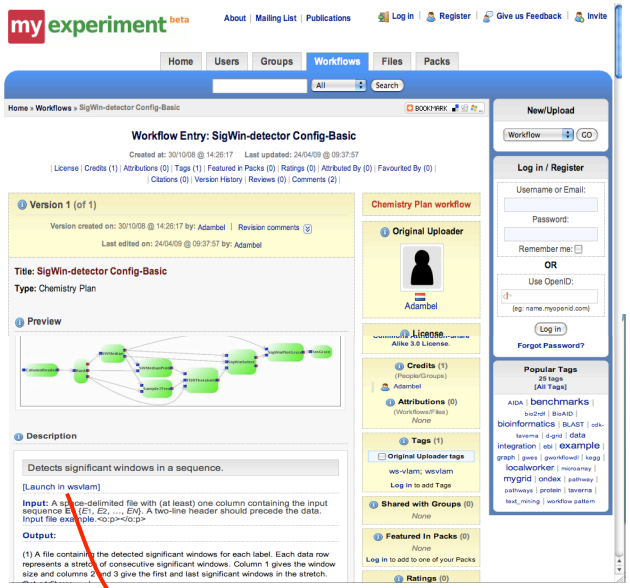
success

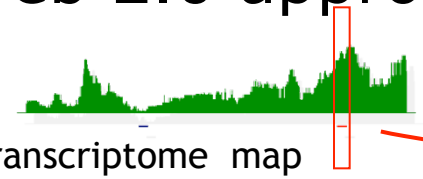
publish

(4) Results Publication

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

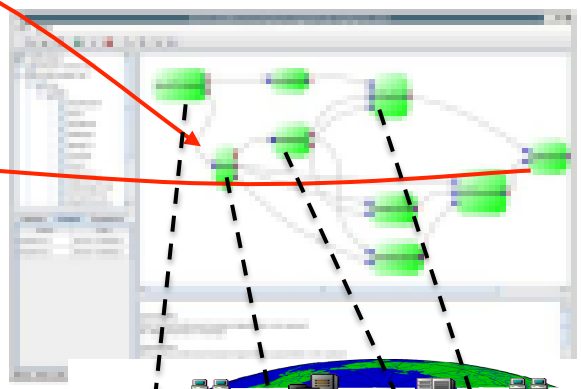
•myexperiment web site

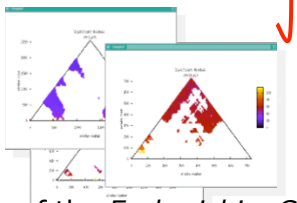




•Human transcriptome map

•WS-VLAM composer





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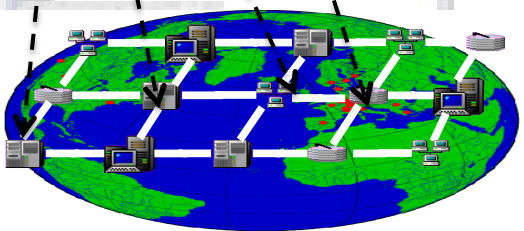
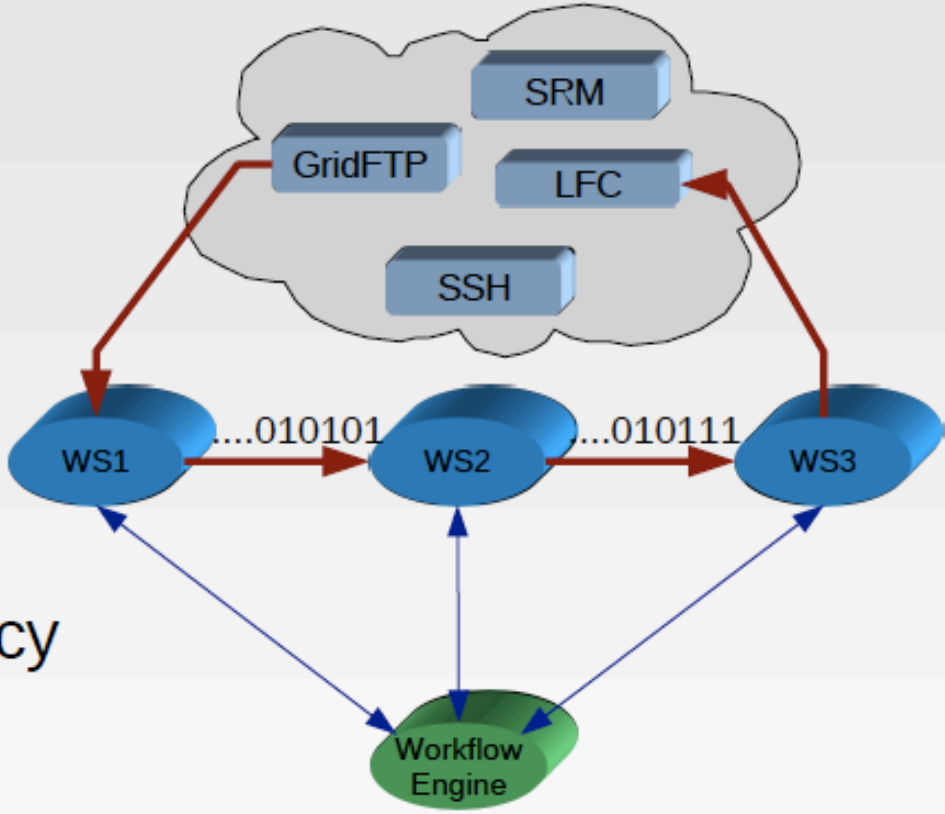


Marcia A Inda, Marinus F van Batenburg, Marco Roos, Adam SZ Belloum, Dmitry Vasunin, Adianto Wibisono, Antoine HC van Kampen and Timo M Breit SigWin-detector: *a Grid-enabled workflow for discovering enriched windows of genomic features related to DNA sequences,* BMC Research Notes 2008,

(*) Web Service and Data centric workflows

- Introduce a new execution model for data driven workflows.
- It will enable e-Science applications to meet increasing data demands.
  - Provide scalable data transports for web services.
  - Bring data to and from legacy web services
  - Develop an API that web services can use.



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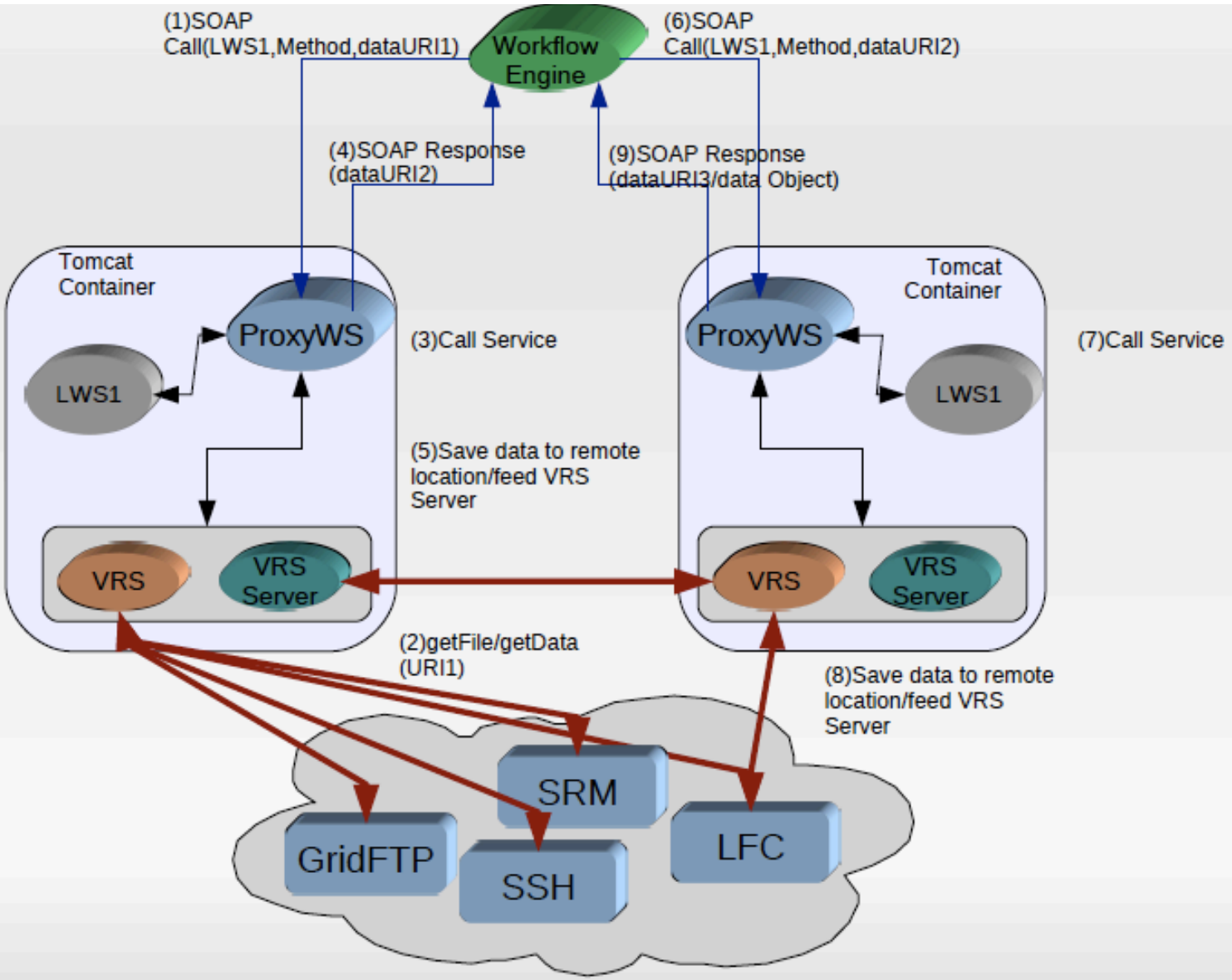

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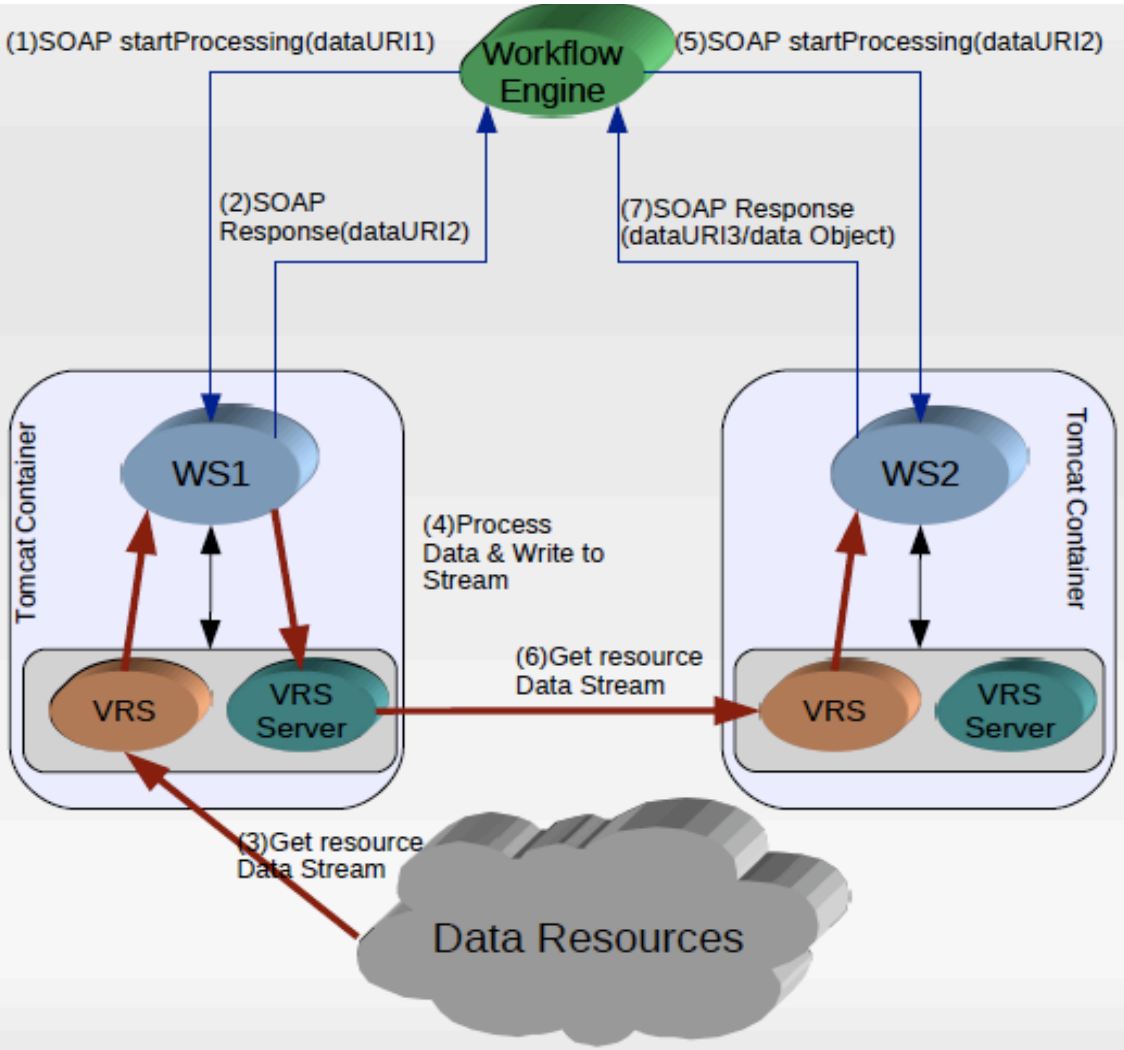


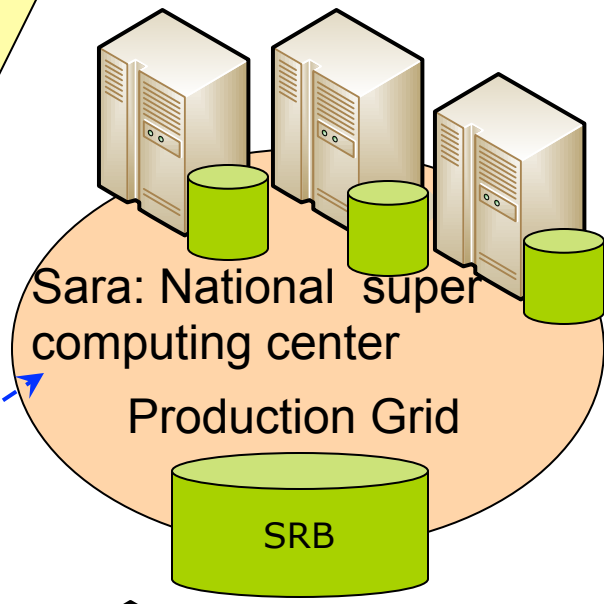
S. Koulouzis, E. Meij, M. S. Marshall, and A. Belloum, ``Enabling data transport between web services through alternative protocols and streaming" eScience, IEEE International Conference on e-Science, vol. 0, pp. 400–401, 2008. 14

Example of Complex eScie

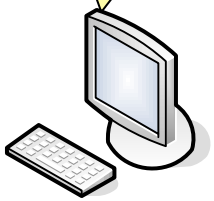
WSRF Services
- WS-VLAM engine
- workflow component repository

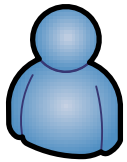
VLe Studio
- WS-VLAM composer
- VBrowser
- Semantic tools

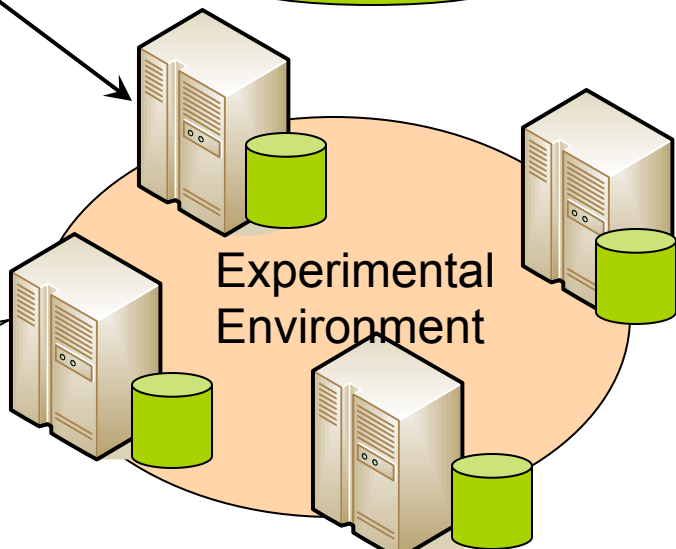
SAW: **S**emantic **A**nnotation for **W**orkflow
CLAMP: Connecting **LA**nguage for **M**odules & **P**rograms
HAMMER: Hybrid-b**A**sed **M**atch**M**aker for e-Science **R**esources



Server host

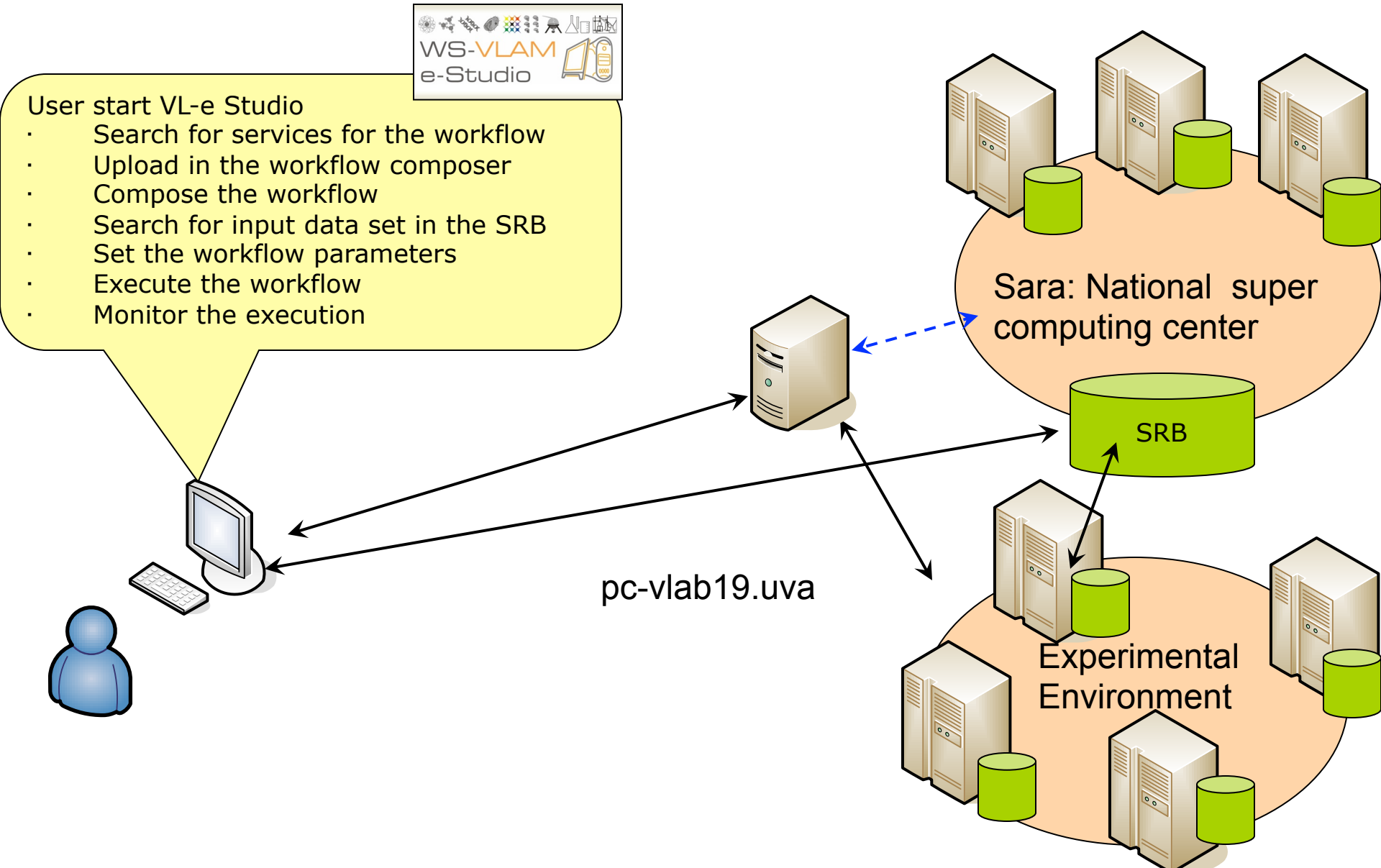






Computing Nodes
- Workflow components
- Grid Middleware → GT4

Example of usage Scenario …



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