

vl·e



virtual laboratory for e-science

# VL-e Med, VL-fMRI and all that

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vl·e

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# Overview

- VL-e, VL-e Medical
- Use Case: Functional MRI
  - Introduction
  - Virtual Lab for fMRI
    - Approach
    - Implementation
- Final Remarks



# Virtual Lab for e-Science

## *Towards a new Science Paradigm*

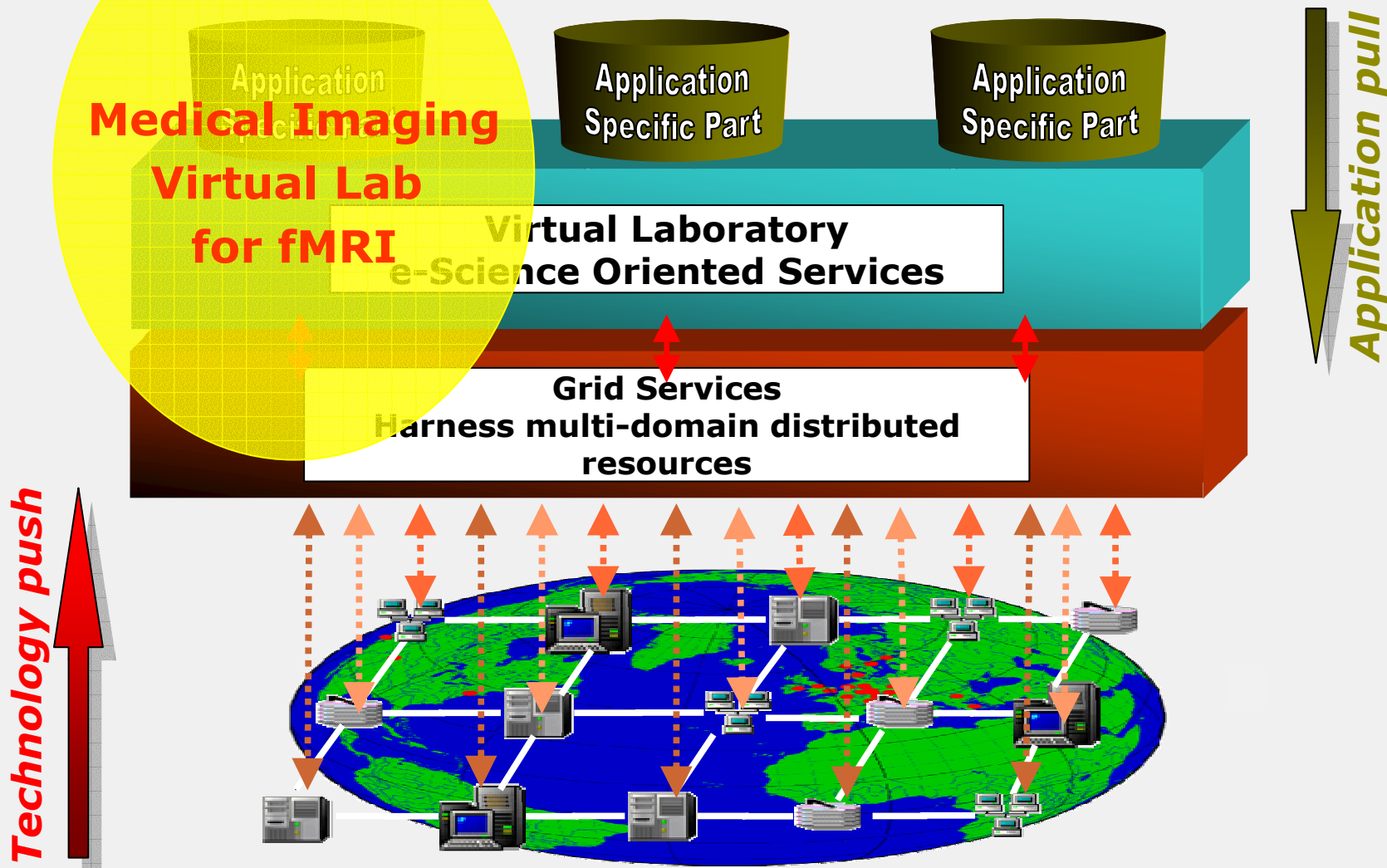
**Project Director**  
**Prof. Dr. L.O. Hertzberger**

This work is supported by a BSIK grant of the  
Dutch Ministry of Education, Culture and Science (OC&W)  
and is part of the ICT innovation programme of the  
Dutch Ministry of Economic Affairs (EZ)

# VL-e

- Goal
  - “bridge the gap between the technology push of the high performance networking and the Grid and the application pull of a wide range of scientific experimental applications”
- Approach
  - Provide infrastructure
  - Facilitate expertise exchange (grid technology and application domain)
  - Development of e-Science applications

# VL-e Approach



- The meaning of “e” in **e-Science** is...
  - electronic
  - enhanced



# *Enhancement in Medical Imaging?*

- Data Storage
  - Large capacity, long-term
- Data Analysis
  - Computation capacity (latency, throughput)
  - Software interoperability
- Data Access
  - Remote access (dispersed organizations)
  - Collaboration
  - Security (patient data)
- Data Logistics and Management
  - Heterogeneous and dispersed systems
  - Workflow management



# VL-e Medical Subprogram

- Goal:
  - Develop grid-enabled problem-solving environments to *enhance* advanced clinical and research in medical imaging
- Activities
  - High performance image analysis
  - Workflow
  - Visualization
  - Virtual Lab for fMRI

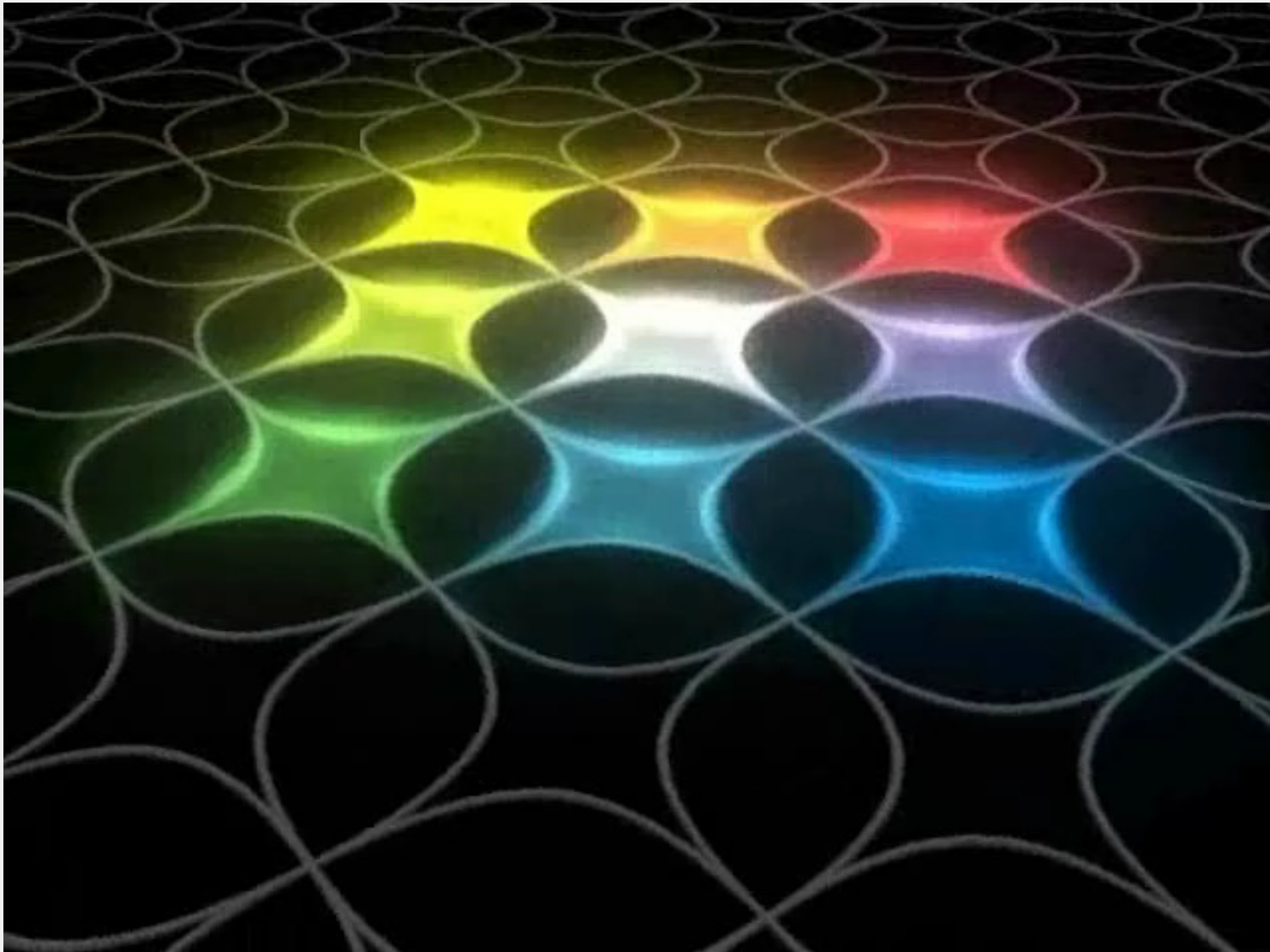


# Overview

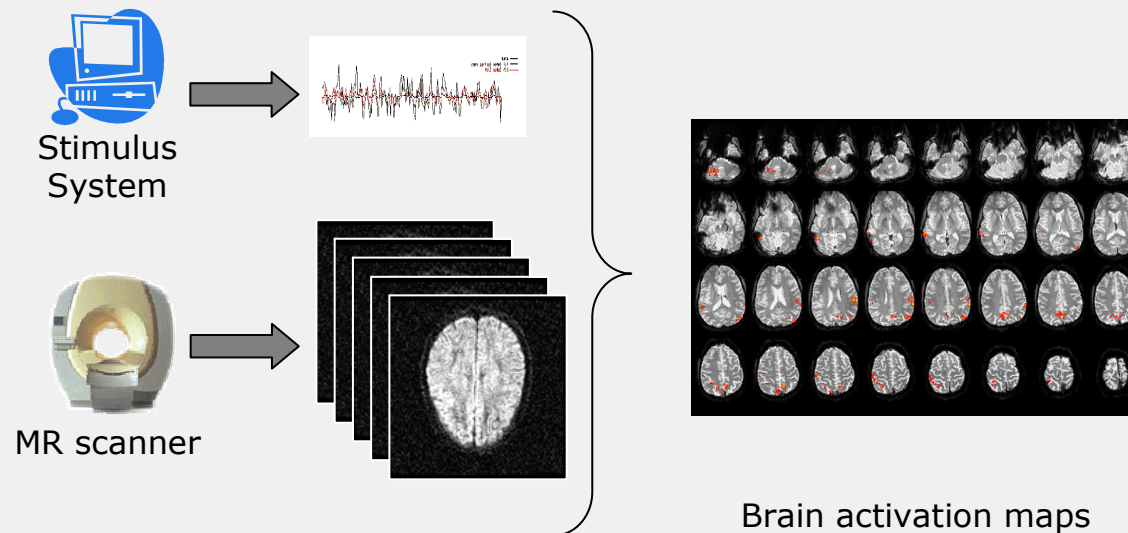
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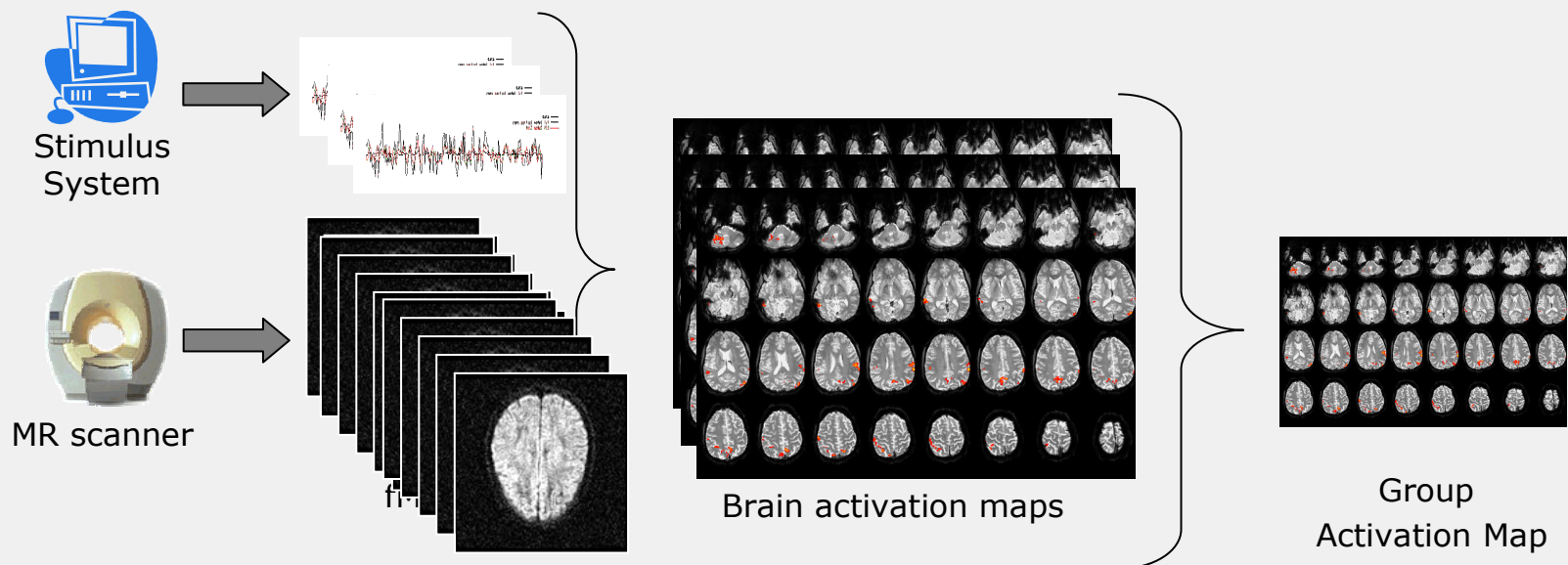
# Functional Imaging of the Brain with fMRI



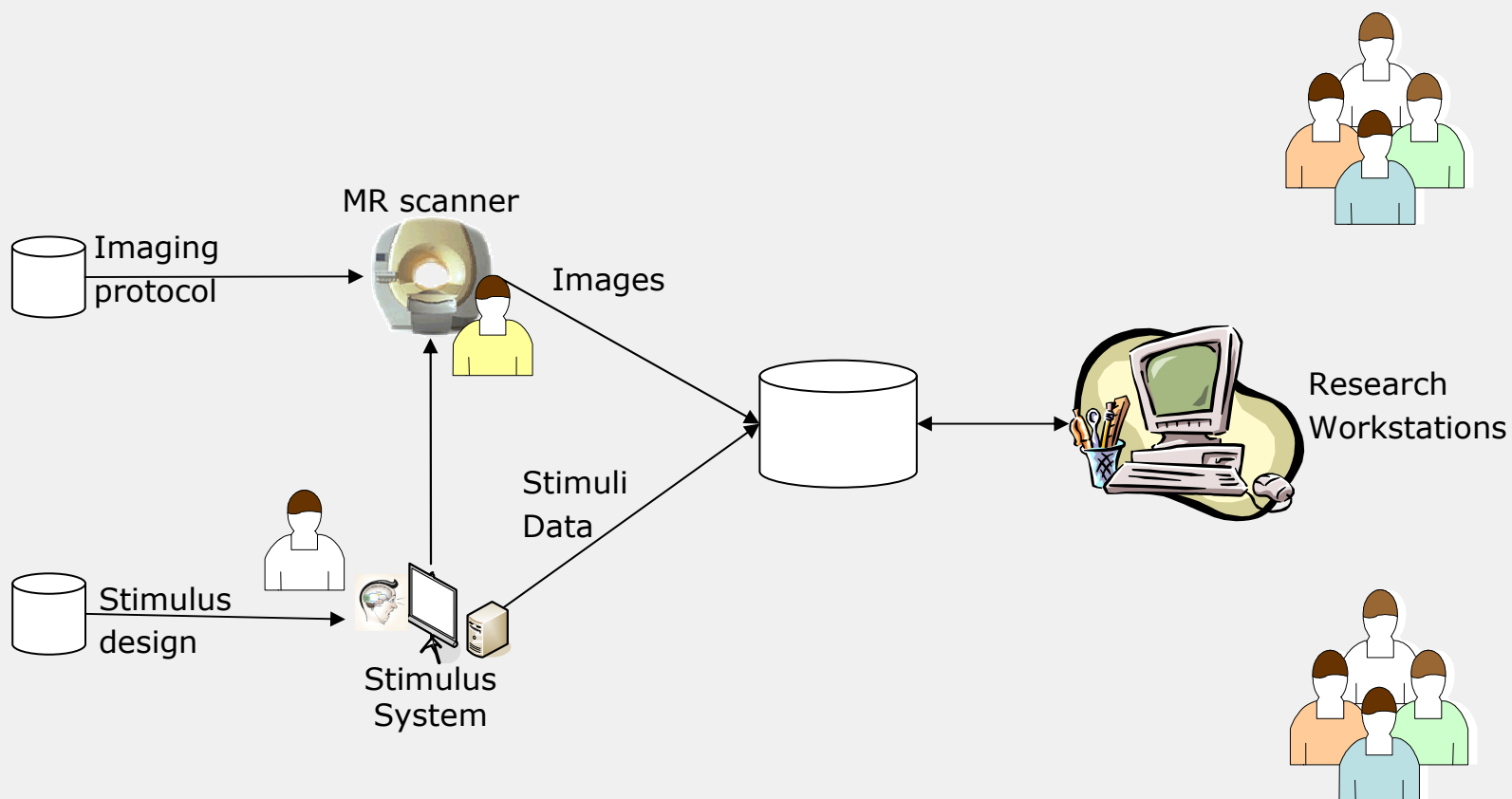
# fMRI: Individuals



# fMRI: Group Studies



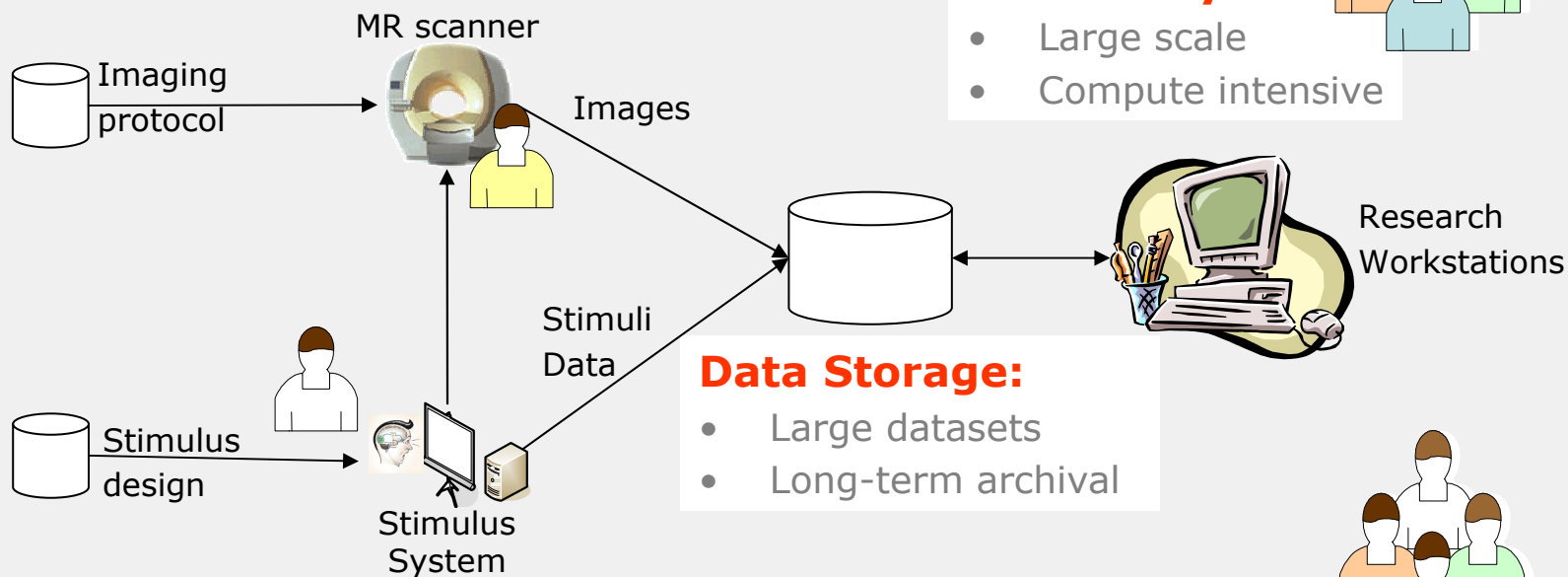
# Data Management in fMRI



# Data Management in fMRI

## Data Acquisition:

- Dispersed equipments
- Data privacy



## Data Analysis:

- Large scale
- Compute intensive

## Data Storage:

- Large datasets
- Long-term archival

## Data Access:

- Collaboration
- Dispersed

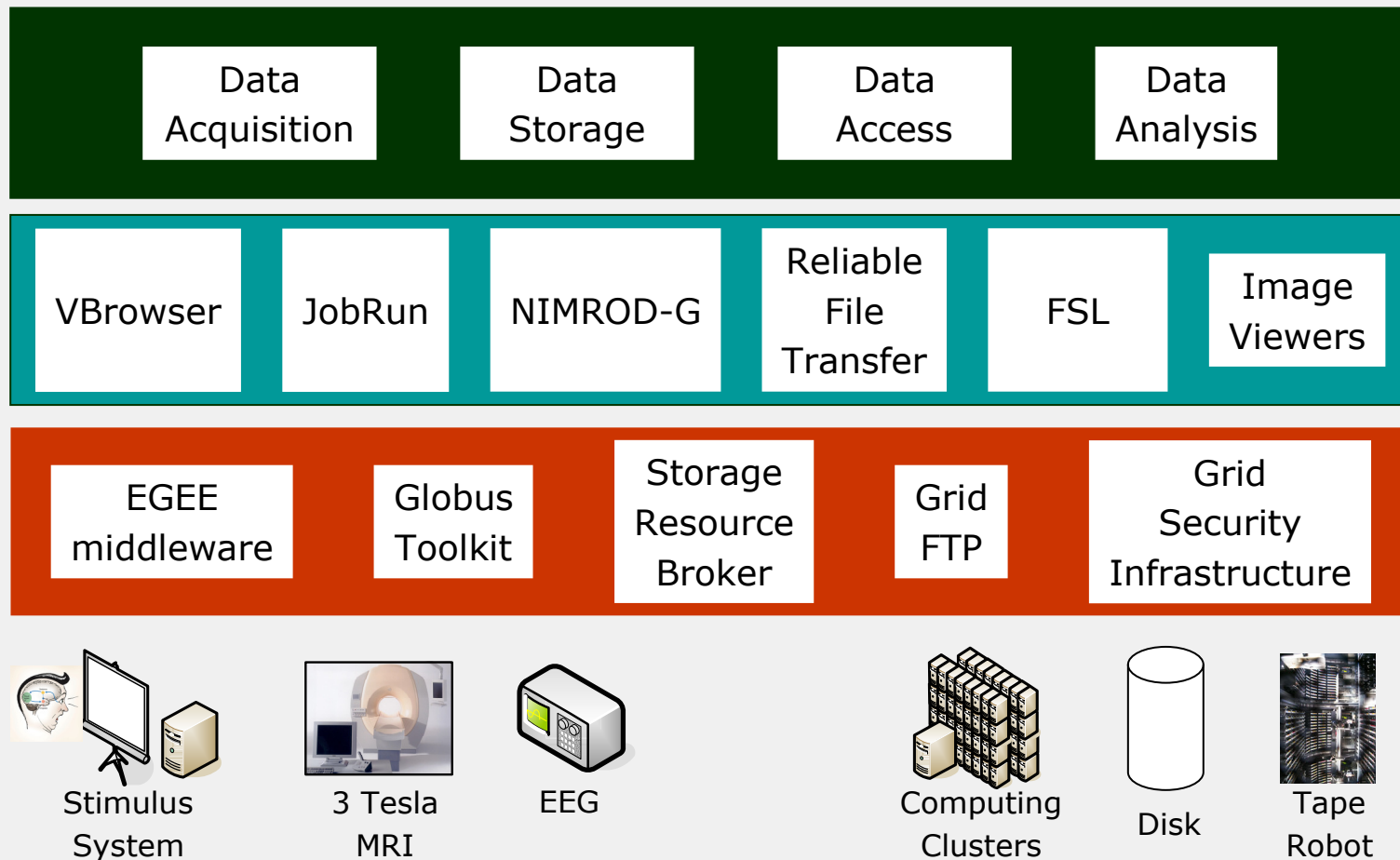
# Overview

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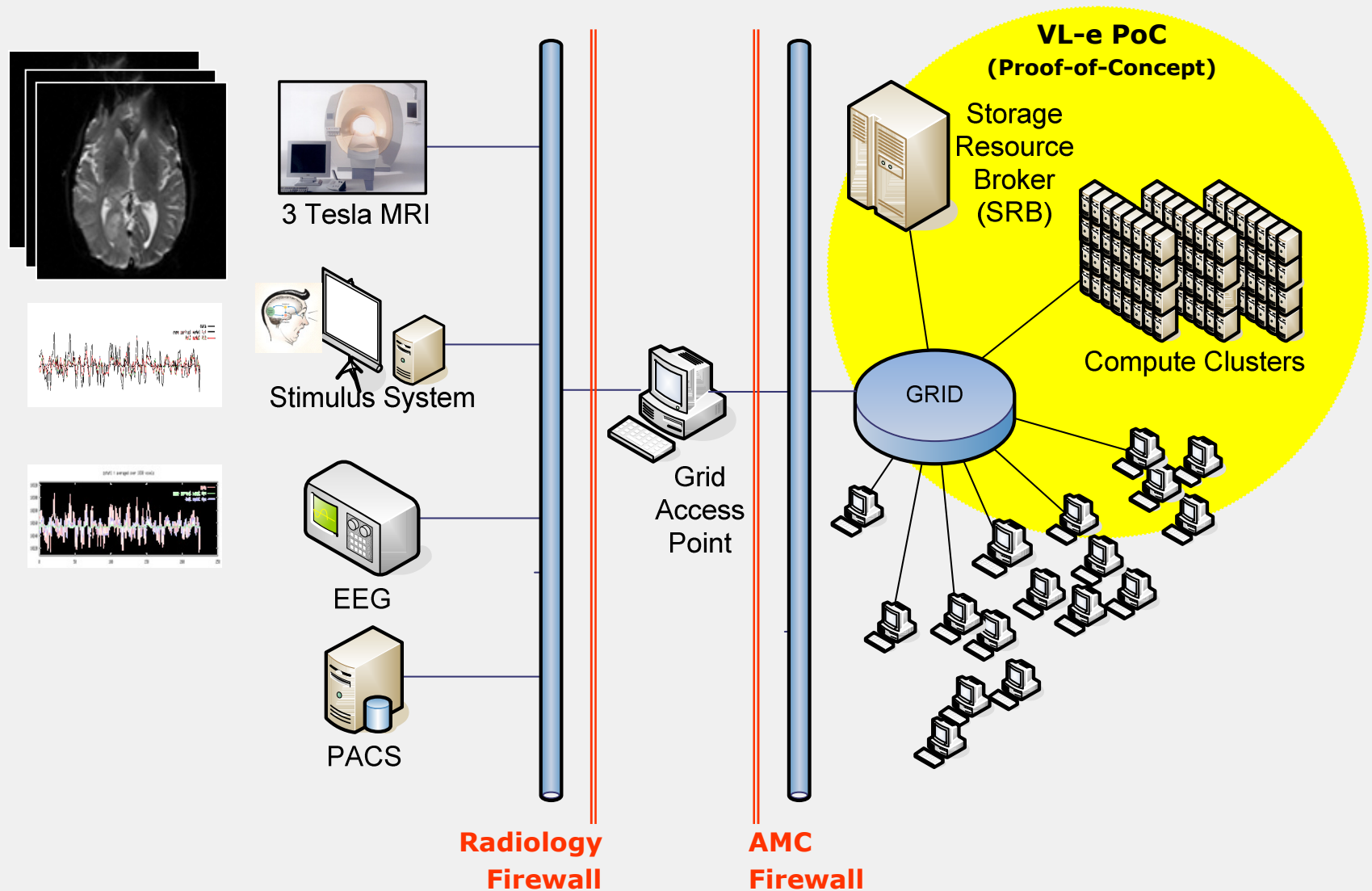




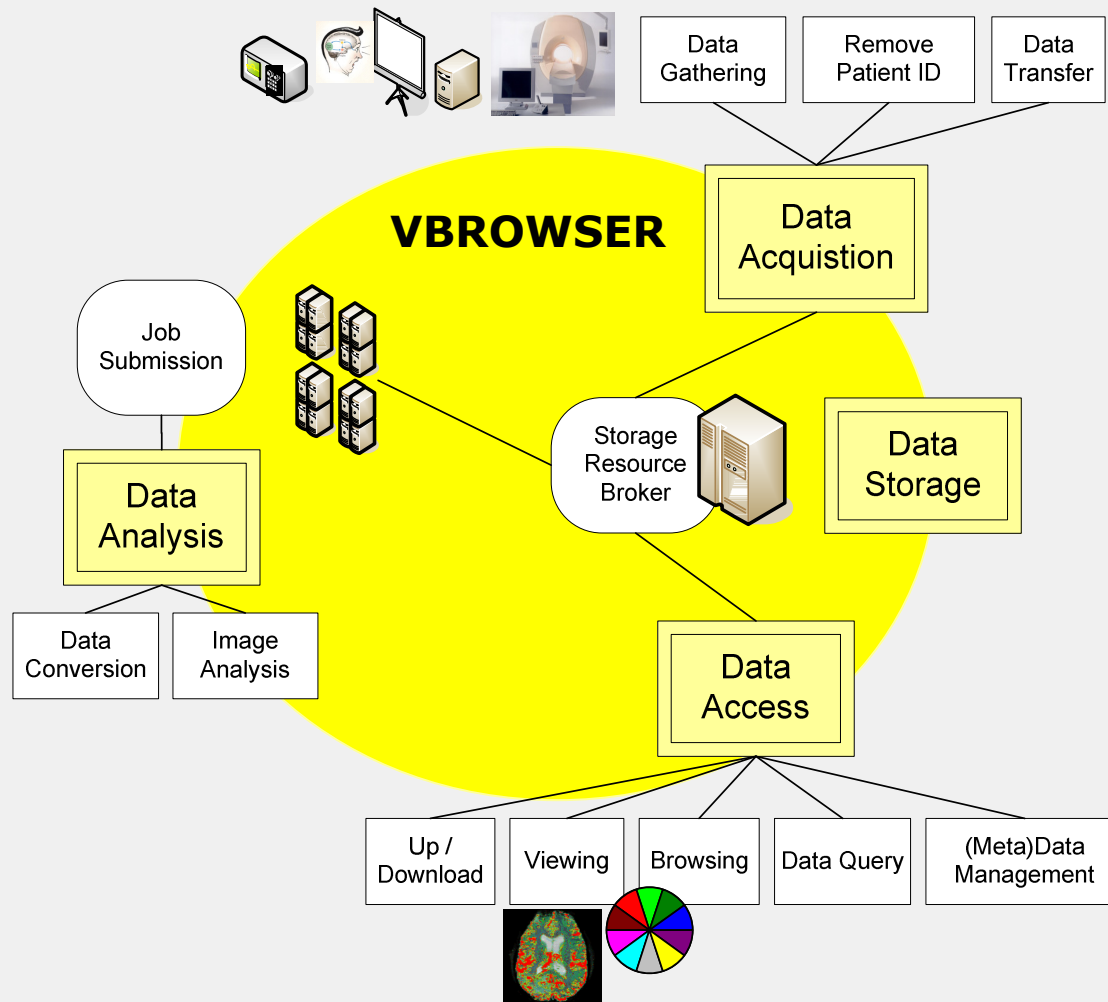
# Virtual Lab for fMRI



# VL-fMRI: Resources



# VL-fMRI: Services



# Virtual Resource Browser

*Contrib: Piter de Boer (IvI,UvA)*

- Interactive GUI for resource browsing
- Access to virtual (grid-enabled) resources
- MIME-type enabled
- Built on VL-e Toolkit (VLET)
- Plug-ins
- Multi-platform (Java)



# Data Acquisition

The screenshot displays a Grid environment interface. On the left, a 'Resource' panel lists available resources: MyVLe: ///, /home/silvia, MySRB, GFTP AMC-UI, 3TMRI, ui.matrix, RFTS AMC-UI, nimrod, lvi, sftp lvi, and thuis. The main area features an 'IconsPanel' with icons for these resources, some highlighted with red and green circles. To the right of the icons, the text 'SARA' is in red and 'AMC' is in green. Below the icons is a 'TablePanel' containing a table with the following data:

icon	type	name	sche...	hostname	path
	Link	/home/silvia	file		/home/silvia
	Server	MySRB	srb	mu2.matrix.sara.nl	/~
	Server	GFTP AMC-UI	gftp	grid-ui01.amc.nl	/~
	Server	3TMRI	sftp	145.117.194.143	/home/export
	Server	ui.matrix	sftp	ui.matrix.sara.nl	/~
	Server	RFTS AMC-UI	rfts	grid-ui01.amc.nl	
	Server	nimrod	sftp	nimrod.vl-e.nl	/~
	Server	lvi	sftp	remote.science.uv...	/~
	Server	thuis	sftp	ns.tacta.nl	/~
	Link	localhost: /	file		/

# Data Acquisition: 3.0 Tesla MRI

VBrowser[0]:sftp://3tftp@145.117.194.143/home/export

Location: sftp://3tftp@145.117.194.143/home/export

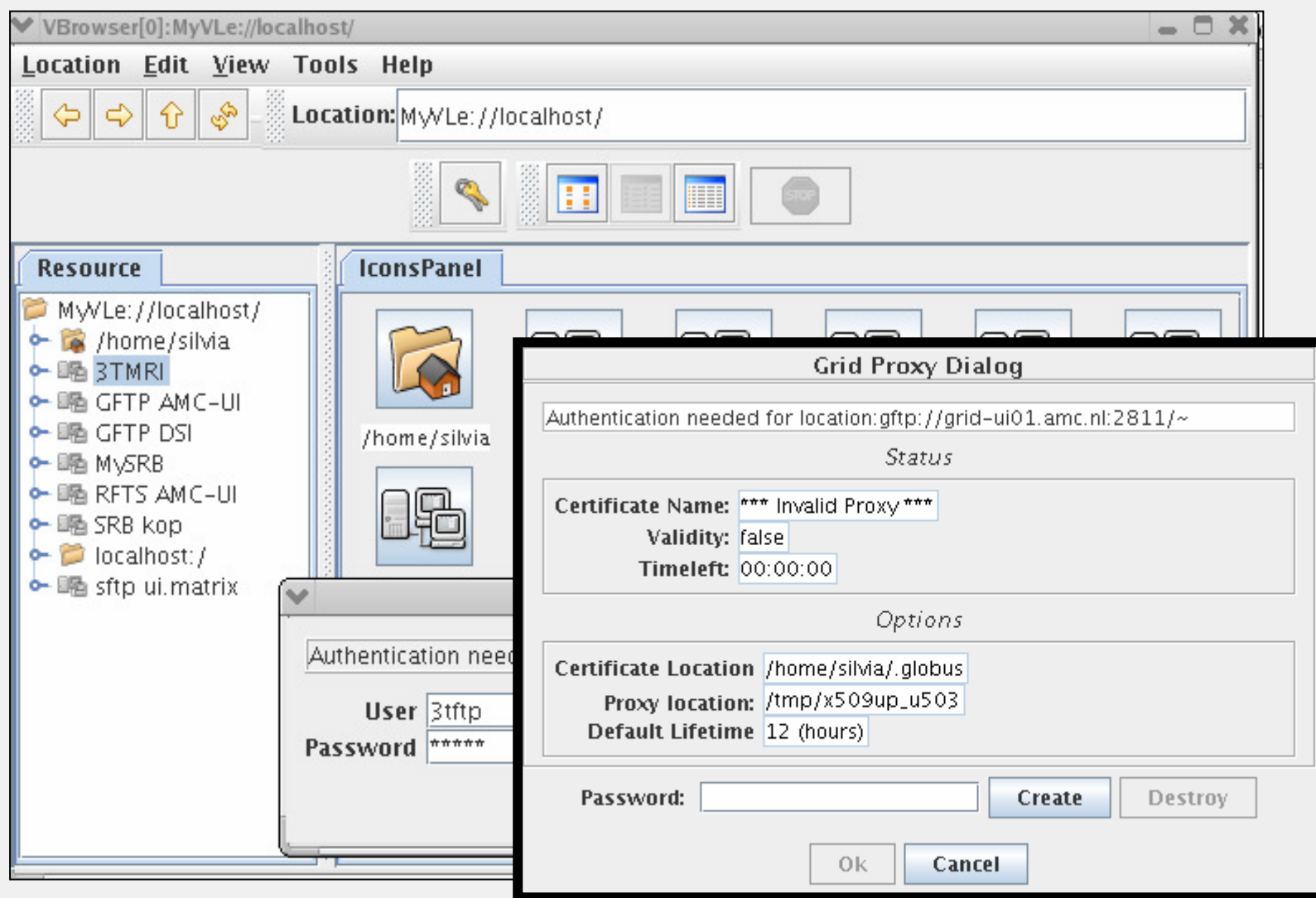
Resource

- MyVLe: //localhost/
  - /home/silvia
    - 3TMRI
      - C
        - My Music
        - My Pictures
        - My eBooks
        - als\_spectra
        - 010170\_3\_1.PAR
        - 010170\_3\_1.REC
        - 010170\_4\_1.PAR
        - 010170\_4\_1.REC
        - 010170\_5\_1.PAR
        - 010170\_5\_1.REC
        - 010170\_5\_2.PAR
        - 010170\_5\_2.REC
        - 010170\_6\_1.PAR
        - 010170\_6\_1.REC
        - 010175T1\_4\_1.PAR
        - ALLEMAN\_ACT.SDAT
        - ALLEMAN\_ACT.SPAPAR
        - ALLEMAN\_REF.SDAT
        - ALLEMAN\_REF.SPAPAR
        - BESSELINK\_6\_1.PAR
        - BESSELINK\_6\_1.REC
        - BESSELINK\_6\_2.PAR
        - BESSELINK\_6\_2.REC
        - BRANDSMA\_LEVER1...

TablePanel

icon	name	type	length	modificationTime	MimeType	per...
dir	My eBooks	Dir	0	2005 Jun 22 12:56:04 (...)	application/...	d-...
dir	My Music	Dir	0	2005 Aug 23 17:32:17 (...)	application/...	d-...
dir	als_spectra	Dir	0	Jul 21 19:11:09 (MEST)	application/...	d-...
dir	C	Dir	0	Sep 06 14:03:06 (MEST)	application/...	dr...
dir	My Pictures	Dir	0	Aug 28 12:00:25 (MEST)	application/...	d-...
file	PPAYSO1_4_1.PAR	File	222745	Aug 22 15:07:08 (MEST)	application/...	----
file	PPAYSO1_4_1.REC	File	9011200	Aug 22 15:07:08 (MEST)	application/...	----
file	PPAYSO1_3_1.REC	File	9011200	Aug 22 15:07:21 (MEST)	application/...	----
file	PPAYSO1_3_1.PAR	File	222745	Aug 22 15:07:21 (MEST)	application/...	----
file	PPAYSO1_2_1.REC	File	31457280	Aug 22 15:07:23 (MEST)	application/...	----
file	PPAYSO1_2_1.PAR	File	16832	Aug 22 15:07:23 (MEST)	application/...	----
file	PPAYSO1_1_1.PAR	File	6635	Aug 22 15:07:23 (MEST)	application/...	----
file	PPAYSO1_1_1.REC	File	1179648	Aug 22 15:07:23 (MEST)	application/...	----
file	PPADRIENNE1_4_1.PAR	File	222751	Aug 23 13:48:31 (MEST)	application/...	----
file	PPADRIENNE1_4_1.REC	File	9011200	Aug 23 13:48:31 (MEST)	application/...	----
file	PPADRIENNE1_3_1.PAR	File	16838	Aug 23 13:48:32 (MEST)	application/...	----
file	PPADRIENNE1_3_1.REC	File	31457280	Aug 23 13:48:32 (MEST)	application/...	----
file	PPADRIENNE1_1_1.REC	File	1179648	Aug 23 13:48:33 (MEST)	application/...	----
file	PPADRIENNE1_1_1.PAR	File	6643	Aug 23 13:48:33 (MEST)	application/...	----
file	PPADRIENNE1_5_1.REC	File	9011200	Aug 23 13:55:56 (MEST)	application/...	----
file	PPADRIENNE1_5_1.PAR	File	222751	Aug 23 13:55:56 (MEST)	application/...	----
file	PPADRIENNE1_6_1.REC	File	2883584	Aug 23 13:57:51 (MEST)	application/...	----
file	PPADRIENNE1_6_1.PAR	File	9223	Aug 23 13:57:51 (MEST)	application/...	----
file	HOEKENRICHE_12_2.REC	File	0	Aug 24 09:31:56 (MEST)	application/...	----
file	HOEKENRICHE_12_2.PAR	File	4849	Aug 24 09:31:56 (MEST)	application/...	----
file	HOEKENRICHE_12_1.REC	File	5242880	Aug 24 09:31:58 (MEST)	application/...	----
file	HOEKENRICHE_12_1.PAR	File	36765	Aug 24 09:31:58 (MEST)	application/...	----
file	HOEKENRICHE_11_1.REC	File	9175040	Aug 24 09:32:01 (MEST)	application/...	----

# User Authentication



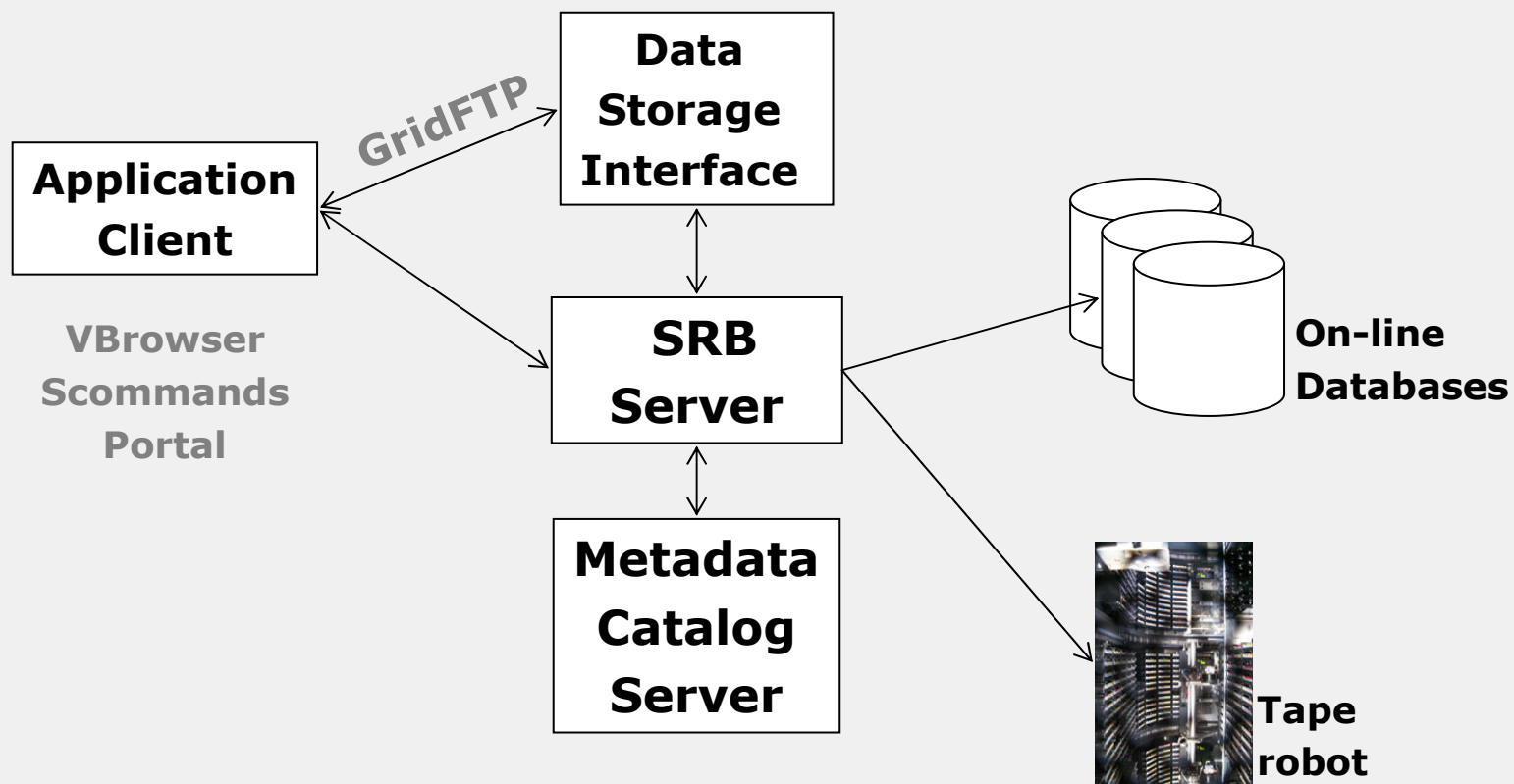


# Data Storage

- SDSC Storage Resource Broker (SRB)
  - single file hierarchy for data distributed across heterogeneous storage systems in multiple organizations.
  - supports the management, collaboration, controlled sharing, publication, replication, transfer, and preservation of distributed data.
- In VL-e PoC
  - SRB server hosted by SARA
  - On-line storage
  - Near-line storage (tape)



# SRB @ VL-e PoC



# Reliable File Transfer (GT4) Service

*Contrib: Ketan Maheshwari (IvI,UvA)*

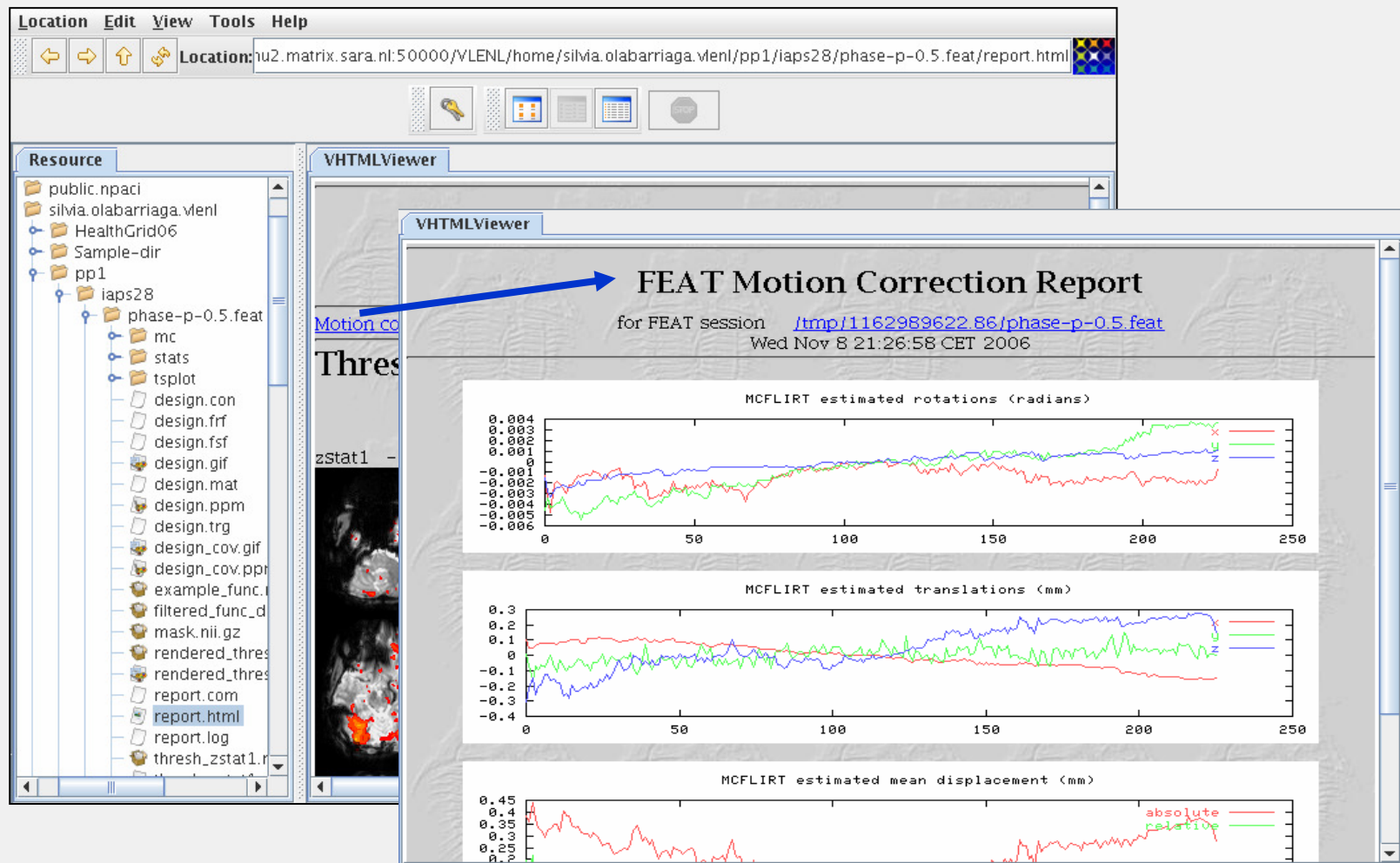
The screenshot displays the VL-fMRI Storage interface. On the left, a 'Resource' tree shows a hierarchy of folders and files. The 'TablePanel' on the right contains a 'PropertyViewer' with fields for 'icon', 'name', 'sourceFilename', and 'sourceHostname'. A 'Resource Event Message' dialog box is open in the foreground, displaying the following text:

```

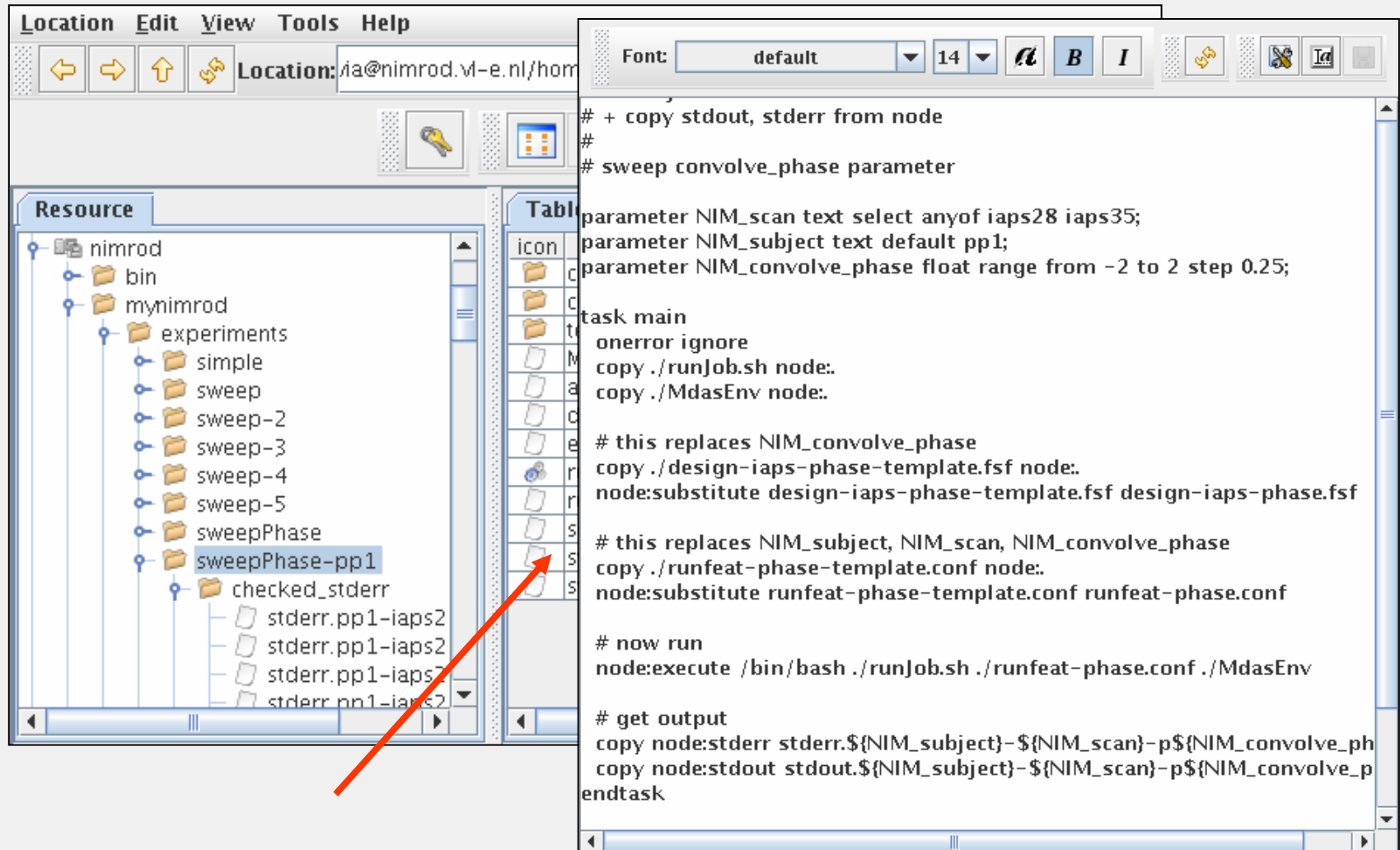
=== Finished RFT Transfer ===
Transfer key = 46
Overall Status = Done
--- Transfer[0]---
- source    = gsiftp://grid-ui01.amc.nl:2811/home/silvia/Transfer/
- destination = gsiftp://kop.nikhef.nl:2811/VLENL/home/silvia.olabarriaga.menl/Transfer/
- nr. attempts = null
- status    = null
  
```

The dialog box has an 'OK' button at the bottom right.

# Data Access



# Data Access (2)



The screenshot shows a file manager window on the left and a text editor on the right. The file manager displays a directory tree for 'nimrod' with subdirectories like 'bin', 'mynimrod', 'experiments', and 'sweepPhase-pp1'. A red arrow points from the 'sweepPhase-pp1' directory to the text editor. The text editor contains a workflow script with the following content:

```

# + copy stdout, stderr from node
#
# sweep convolve_phase parameter
parameter NIM_scan text select anyof iaps28 iaps35;
parameter NIM_subject text default pp1;
parameter NIM_convolve_phase float range from -2 to 2 step 0.25;

task main
onerror ignore
copy ./runJob.sh node:
copy ./MdasEnv node:

# this replaces NIM_convolve_phase
copy ./design-iaps-phase-template.fsf node:
node:substitute design-iaps-phase-template.fsf design-iaps-phase.fsf

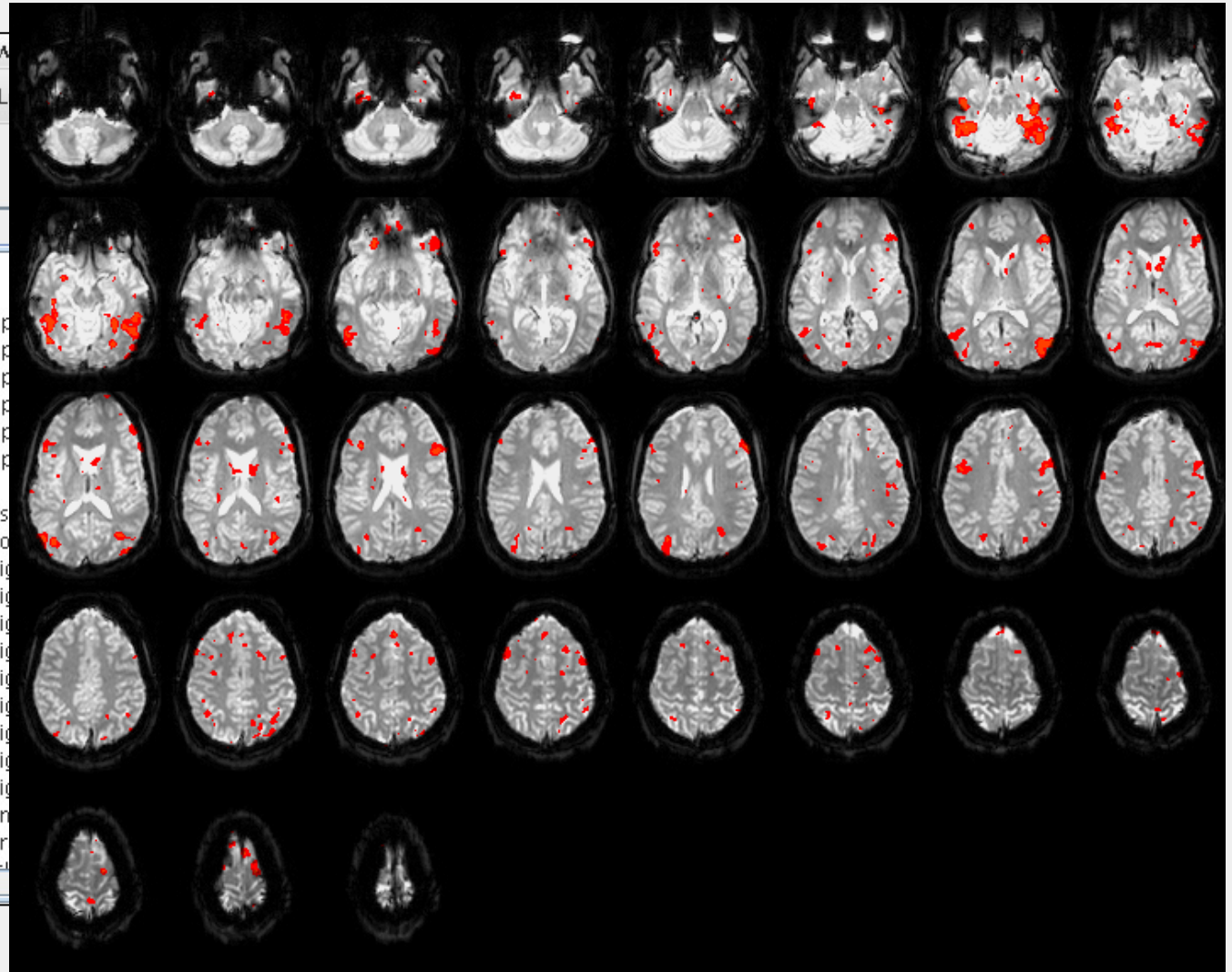
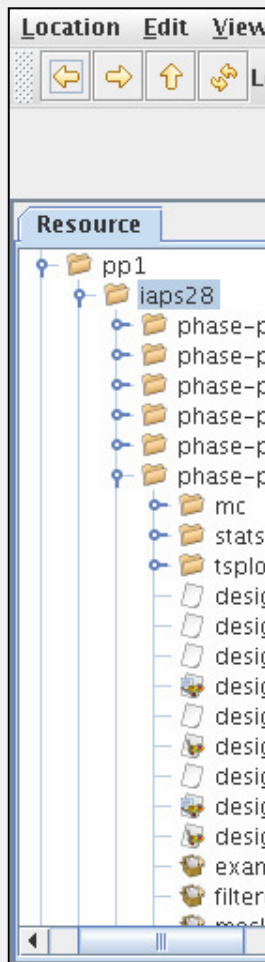
# this replaces NIM_subject, NIM_scan, NIM_convolve_phase
copy ./runfeat-phase-template.conf node:
node:substitute runfeat-phase-template.conf runfeat-phase.conf

# now run
node:execute /bin/bash ./runJob.sh ./runfeat-phase.conf ./MdasEnv

# get output
copy node:stderr stderr.${NIM_subject}-${NIM_scan}-p${NIM_convolve_ph
copy node:stdout stdout.${NIM_subject}-${NIM_scan}-p${NIM_convolve_p
endtask

```

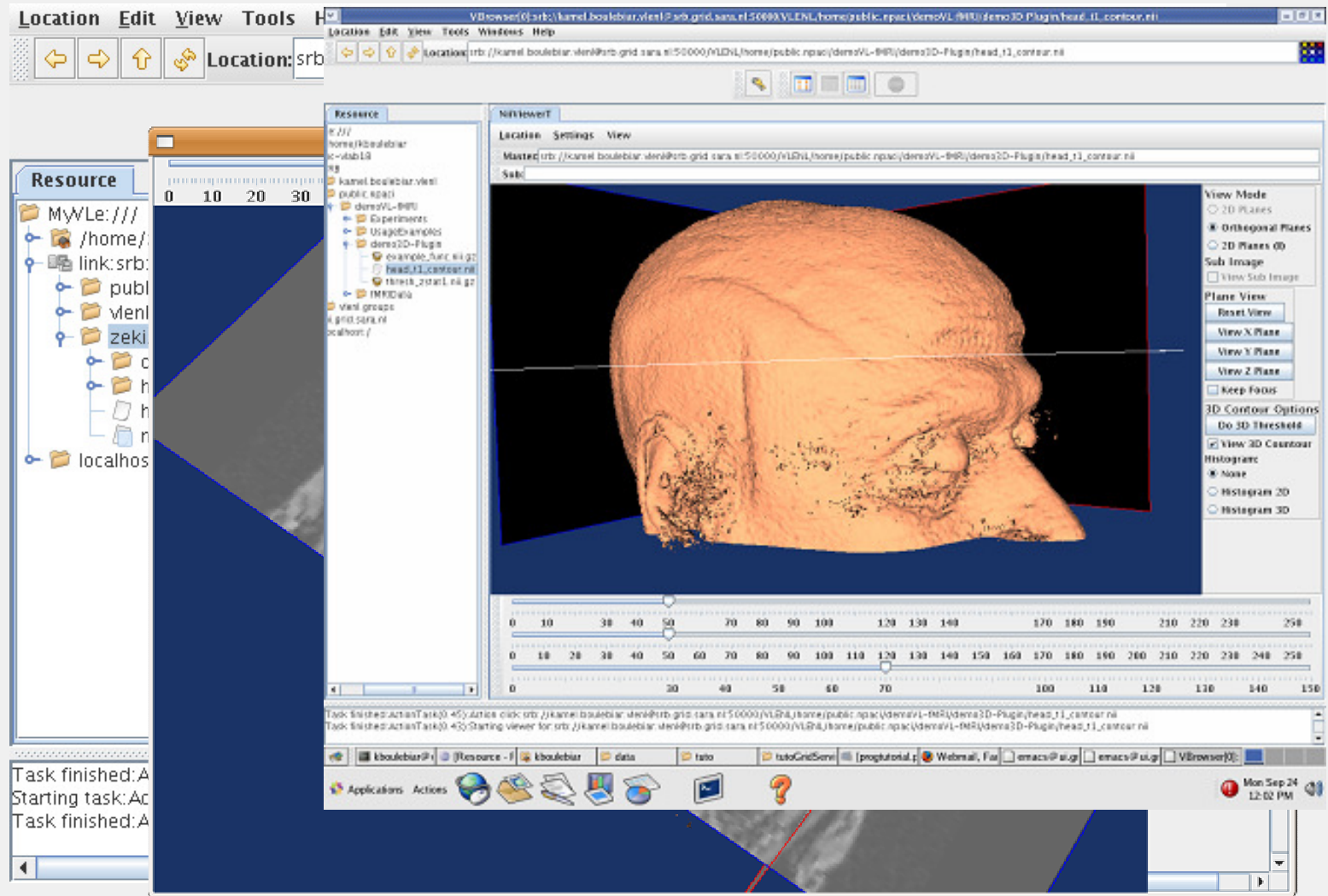
# Data Access (3)





# Data Access (4)

*Contrib: Abdullah Ozsoy (IvI, UvA)*

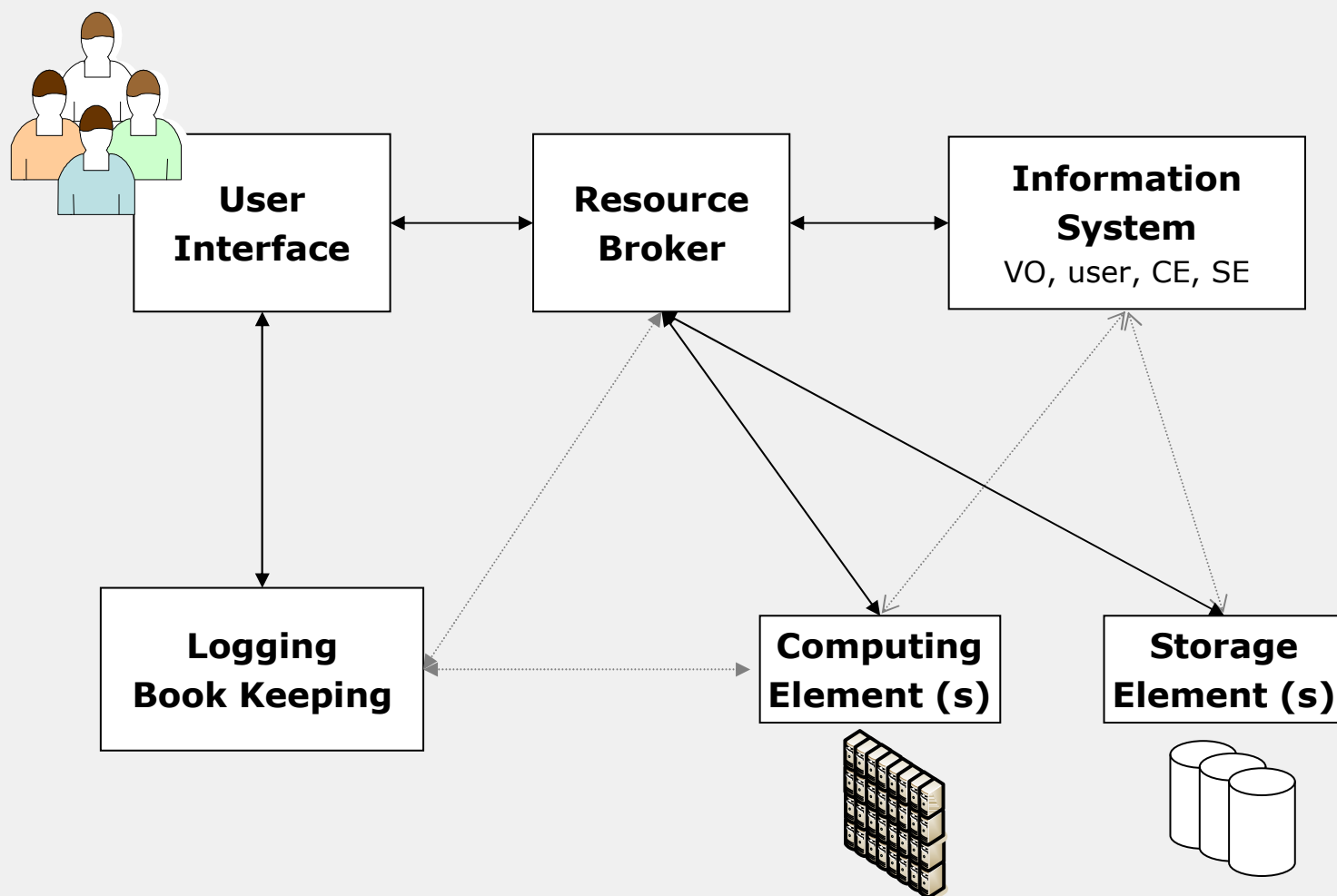


# Data Analysis

- Computing clusters
  - SARA, NIKHEF, AMC
  - many others: BIGGrid, DAS-3
- Standard software installation
  - VL-e PoC
  - Includes imaging packages (VTK,ITK,FSL)
- Various middleware
  - EGEE
  - Experiment managers (NIMROD, custom)



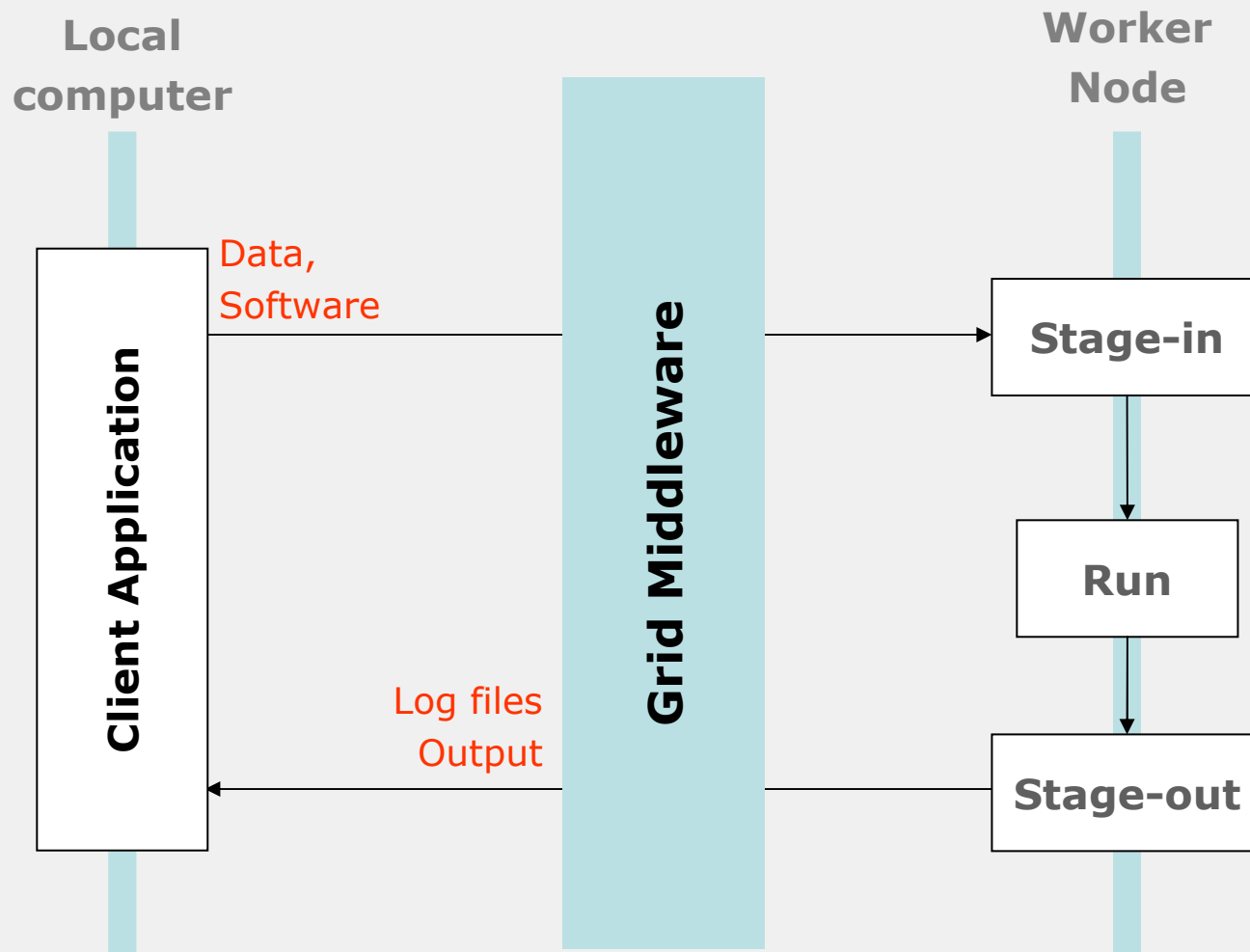
# Computing @ VL-e PoC EGEE Middleware





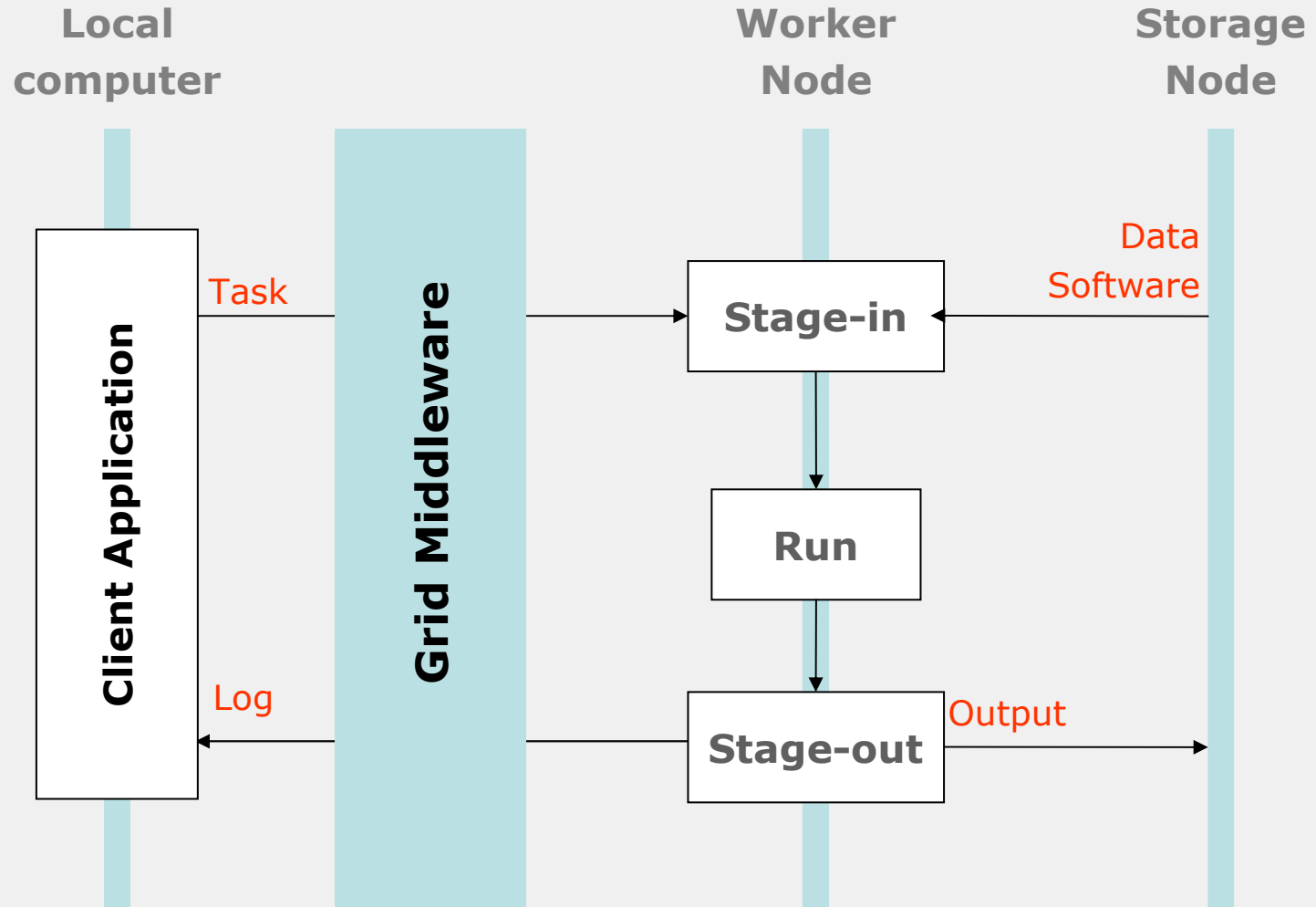
# Computing Jobs on the Grid

## Local storage



# Computing Jobs on the Grid

## External storage



# jobrun Package

- bash script
- Features:
  - SRB as file system
  - Error checking
  - Configurable
- Usage
  - `jobrun.sh <job-config> <SRB-config>`

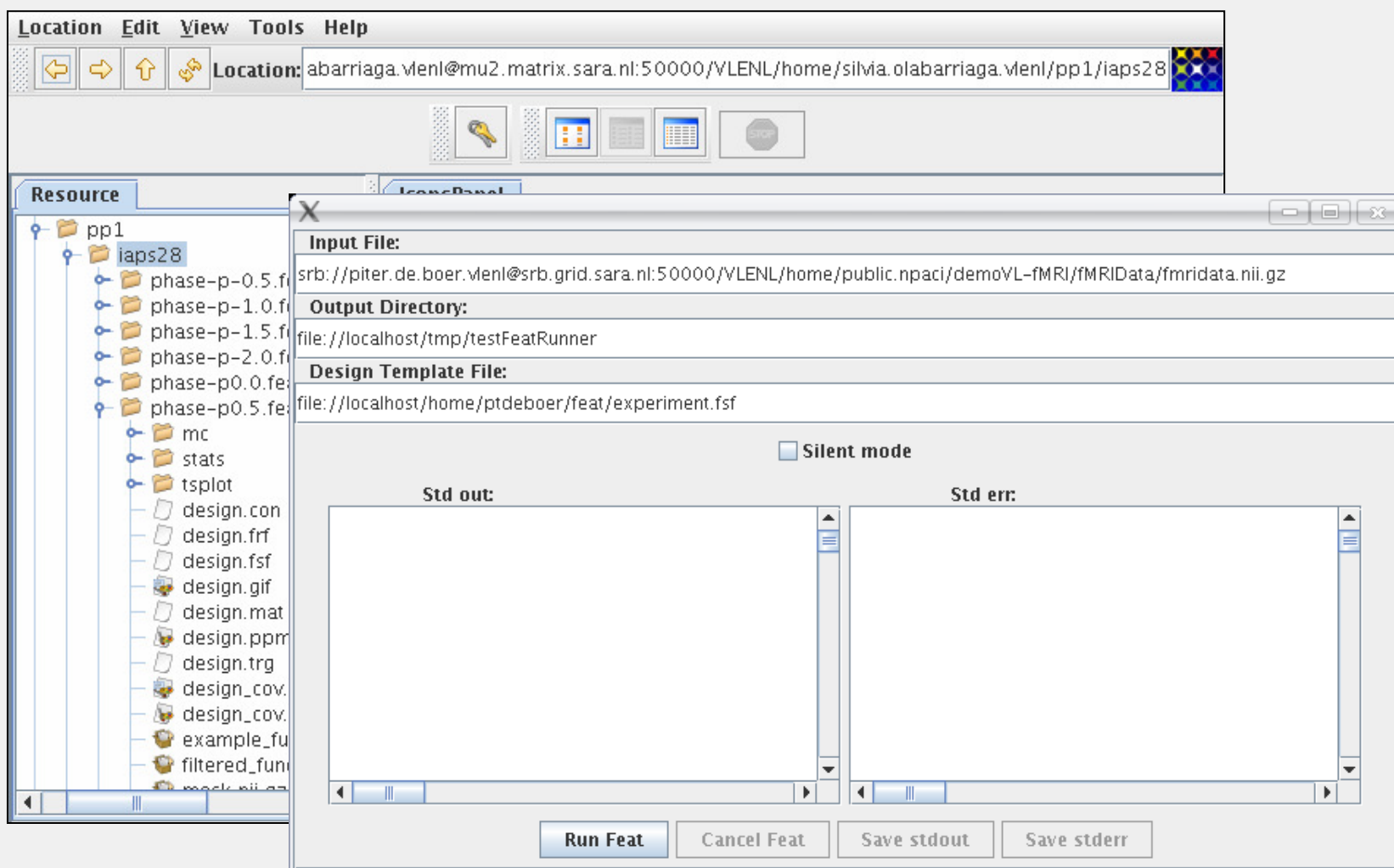
# jobrun: Submission

- *edg-job-submit job.jdl*

```
Executable = "runJob.sh";  
Arguments  = "testJob.conf MdasEnv";  
StdOutput  = "std.out";  
StdError   = "std.err";  
OutputSandbox = {"std.out" , "std.err" };  
InputSandbox  = {"runJob.sh", "testJob.conf" , "MdasEnv" };  
Requirements  = Member("nl.vl-e.poc-release-1.0", \  
    other.GlueHostApplicationSoftwareRunTimeEnvironment);
```

# fMRI Analysis Jobs: *feat* wrapper

*Contrib: Kamel Boulebiar (IvI, UvA)*



# Experiment Manager

- Facilitates data and job management of large experiments
  - Parameter and image sweeps
- with facilities for
  - Distribution of jobs on resources
  - Monitoring
- Example:
  - NIMROD (Monash University, Australia)

# Experiment Plan

parameters

stage in

run task

stage out

```

Font: default 14
# + copy stdout, stderr from node
#
# sweep convolve_phase parameter

parameter NIM_scan text select anyof iaps28 iaps35;
parameter NIM_subject text default pp1;
parameter NIM_convolve_phase float range from -2 to 2 step 0.25;

task main
  onerror ignore
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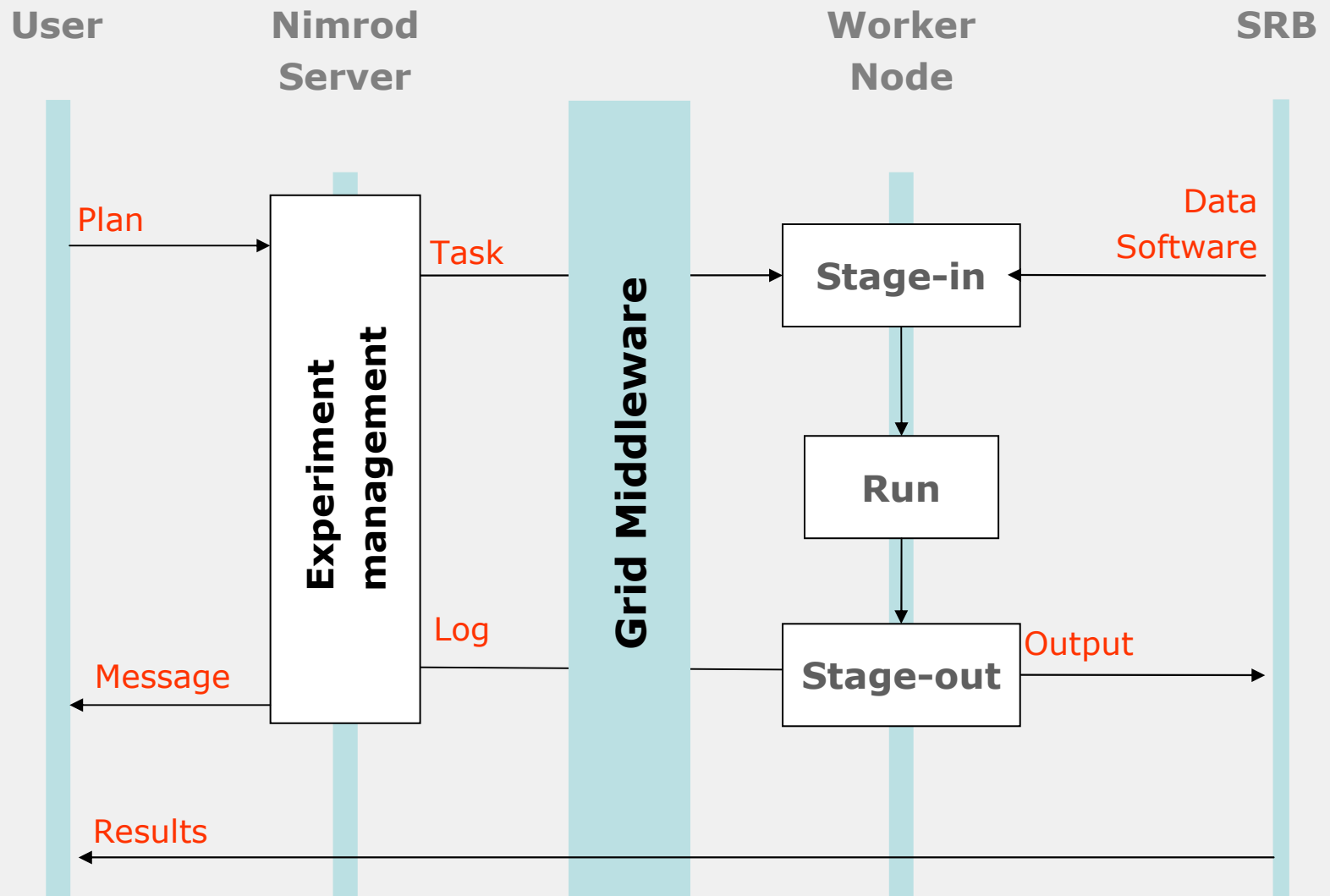
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  node:substitute runfeat-phase-template.conf runfeat-phase.conf

  # now run
  node:execute /bin/bash ./runJob.sh ./runfeat-phase.conf ./MdasEnv

  # get output
  copy node:stderr stderr.${NIM_subject}-${NIM_scan}-p${NIM_convolve_ph
  copy node:stdout stdout.${NIM_subject}-${NIM_scan}-p${NIM_convolve_p
endtask

```

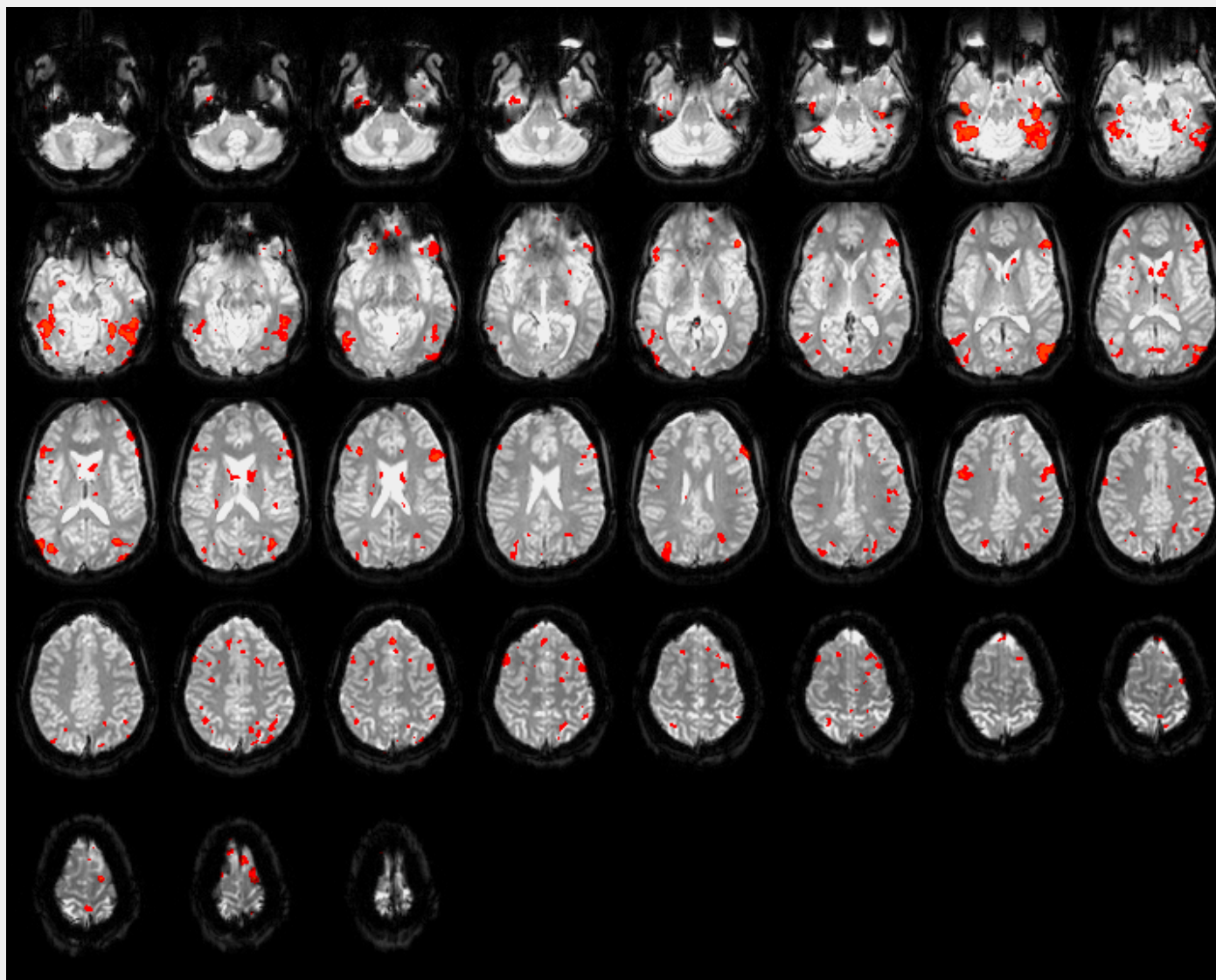
# Large Experiments on the Grid





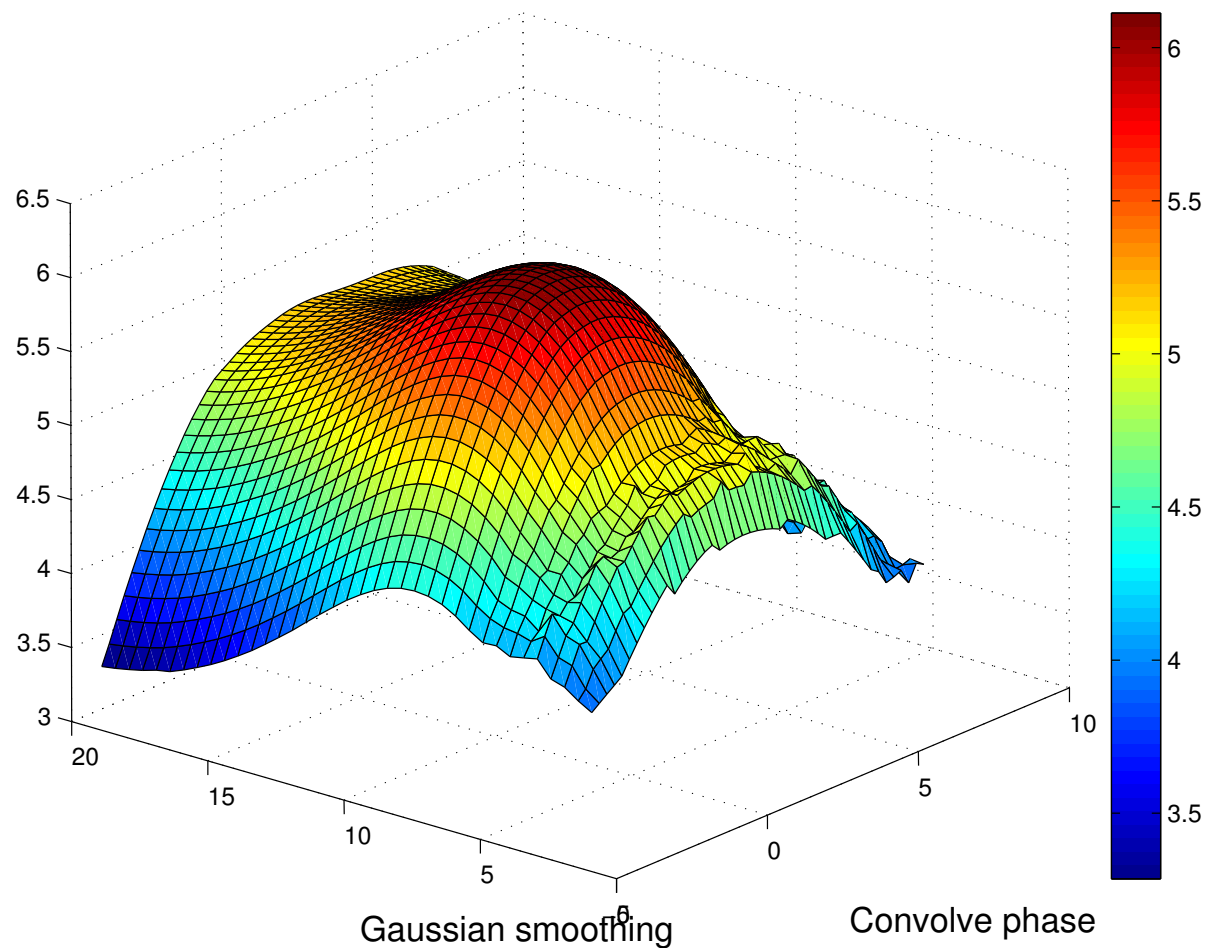
# 1-D Parameter Sweep

22 scans, 17 values, 374 jobs, 420h CPU



## 2-D Parameter Sweep

1 scan, 1665 jobs, ~555h CPU



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# Current Status

- GAP at AMC
- Feat analysis from VBrowser
- New experiment manager under development
- Added value for clinical research?
- More info
  - [www.science.uva.nl/~silvia/vlfmri](http://www.science.uva.nl/~silvia/vlfmri)

# Final Remarks

- No “rocket science”, no “free lunch” ...
  - Evolving technology and requirements
  - Evolving/unstable/poorly documented infrastructure
  - Tools with low usability for “end users”
  - Insufficient experts for application development
  - Difficult communication across domains and expertises (informatics, medical)

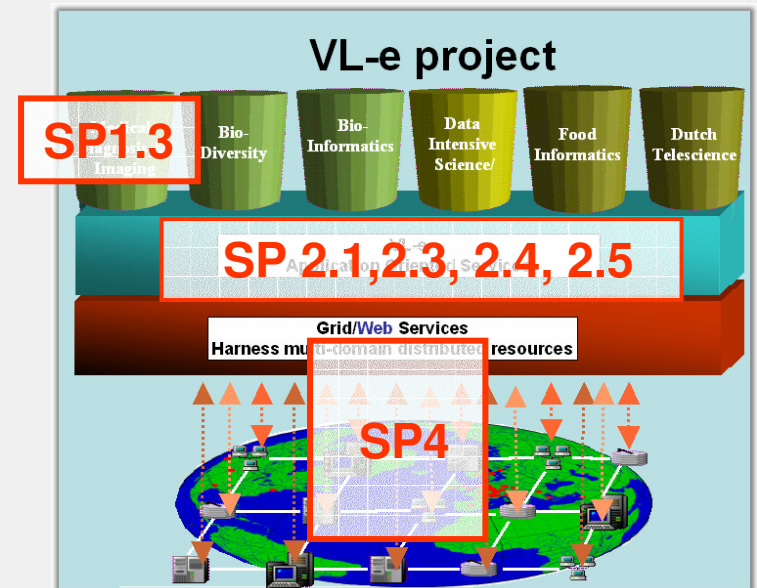
# Conclusions

- “High Energy Physics Experiment” model is not appropriate for all application domains
- Collaboration among experts from various fields is essential for development of grid applications
- VL-e provides the scope for this collaboration



# VL-e Medical & Co

- **AMC (SP1.3)**
  - Aart Nederveen, Matthan Caan, Sanna Gevers, Silvia Olabarriaga
  - Kees Grimbergen, Ard den Heeten, Charles Majoie
- **IvI**
  - Kamel Boulebiar (SP1.3)
  - Piter de Boer, Adam Belloum (SP2.5)
  - Abdullah Ozsoy, Robert Belleman (SP2.1)
  - Breannán Ó Nualláin (SP2.1)
  - Guido van't Noordende, Matthijs Koot (SP2.4)
- **SARA (SP4)**
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  - [grid-support@sara.nl](mailto:grid-support@sara.nl)
- **NIKHEF (SP4)**
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  - [grid-support@nikhef.nl](mailto:grid-support@nikhef.nl)
- **VUMC (SP1.3)**
  - Keith Cover, Bob van Dijk
  - Hugo Vrenken, Frederik Barkov
- **Previous members**
  - K. Maheshwari
  - J. Snel, J. Alkemade
  - A. Bucur, H. Obbink, J. van Leeuwen



# Special Credits

- VBrowser: P. de Boer
- RFTS: K. Maheshwari
- 3D Viewer plug-in: A. Ozsoy
- fMRI analysis plug-in: K. Boulebiar
- GAP installation support: J.J. Keijser
- Clinical data: A. Nederveen
  
- Prof. Dr. Bob Hertzberger

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Dutch Ministry of Education, Culture and Science  
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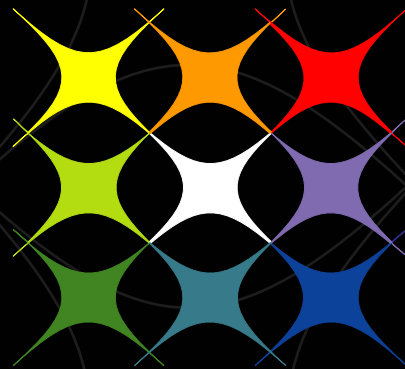


Thanks for your attention!

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vl-e

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