A View from the Application Front: Virtual Lab for Functional MRI

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Overview

- VL-e
- VL-e Medical Use Case
  - Introduction: Functional MRI
  - Virtual Lab for fMRI
    - Approach
    - Implementation: Data Facilities
    - Implementation: Compute Facilities
- 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)

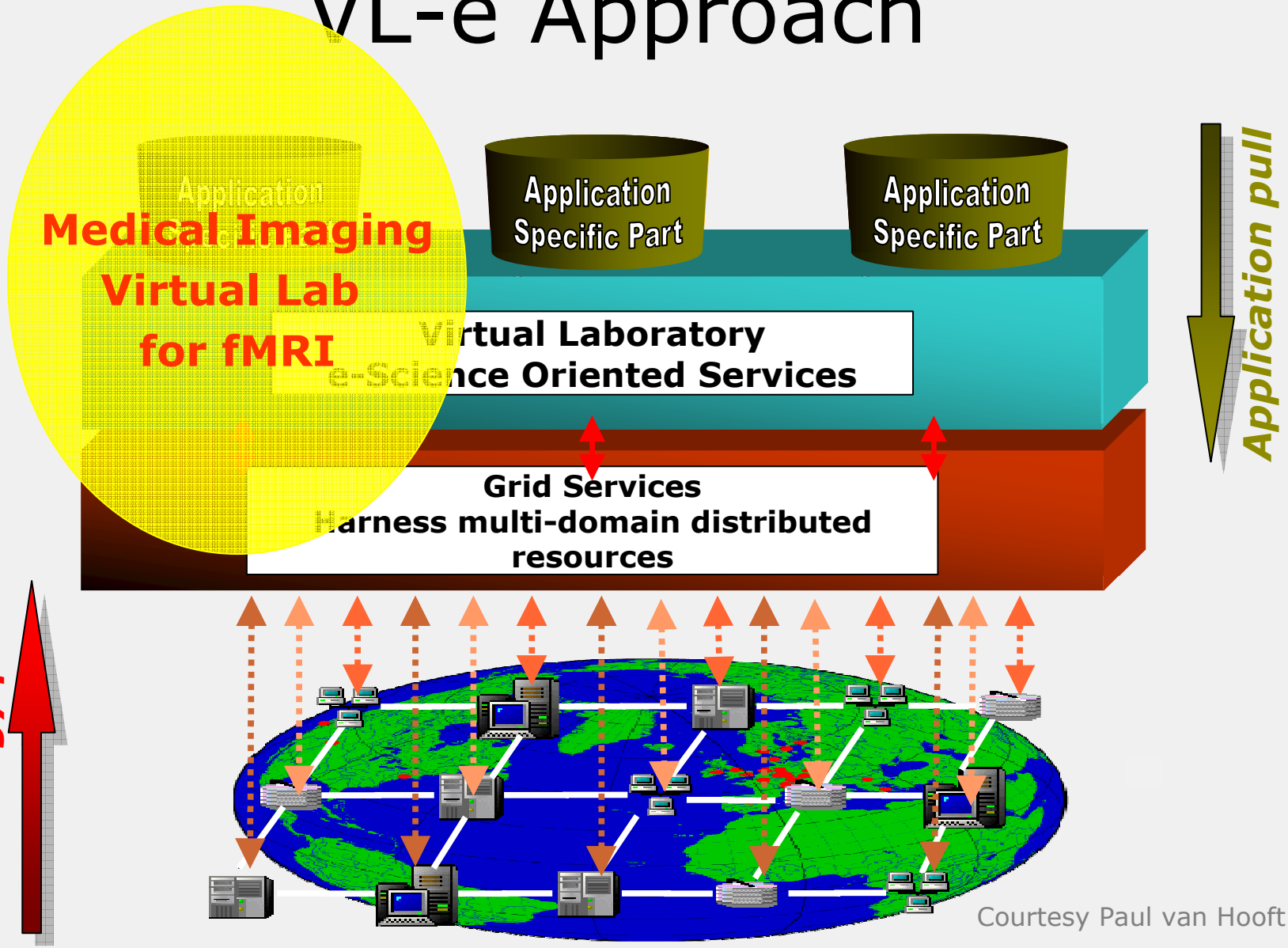
VL-e

- 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

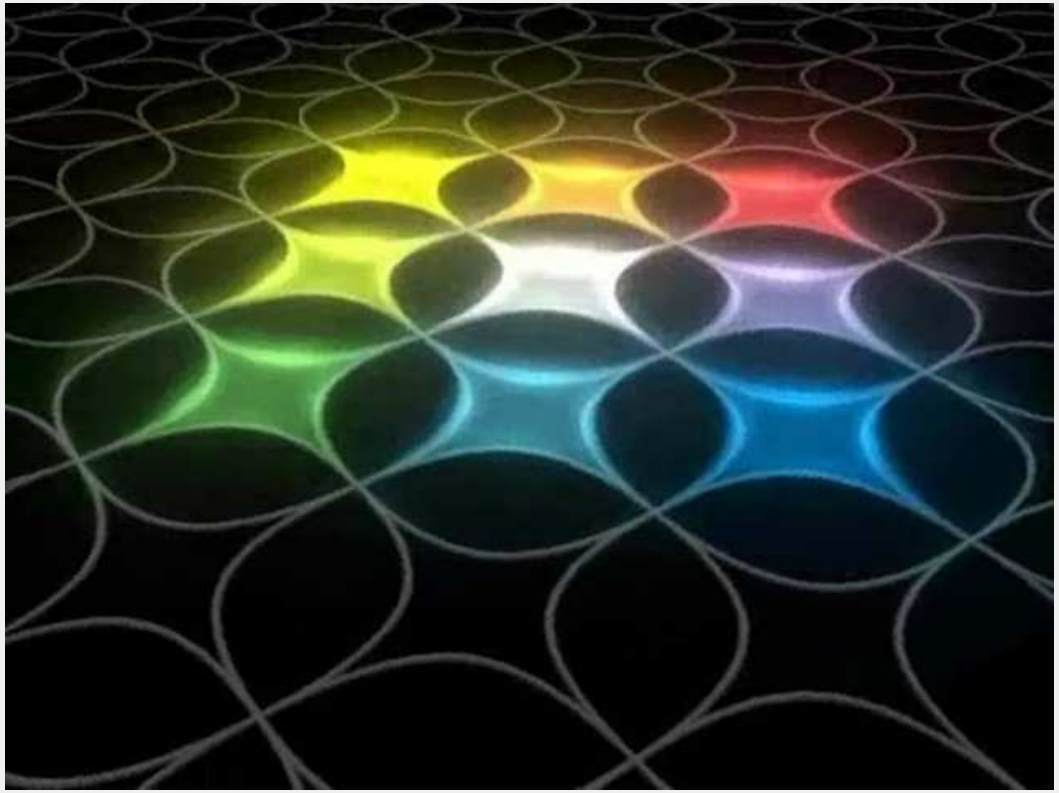
VL-e Approach



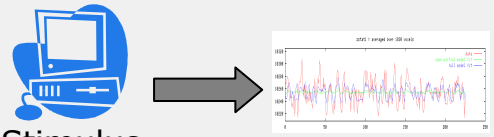
Courtesy Paul van Hooft

Functional Imaging of the Brain with fMRI

See video in http://www.vl-e.com (outreach)

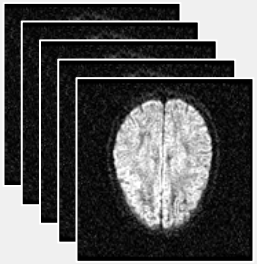


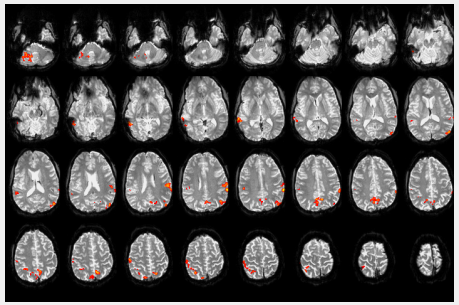
fMRI: Individuals



Stimulus System

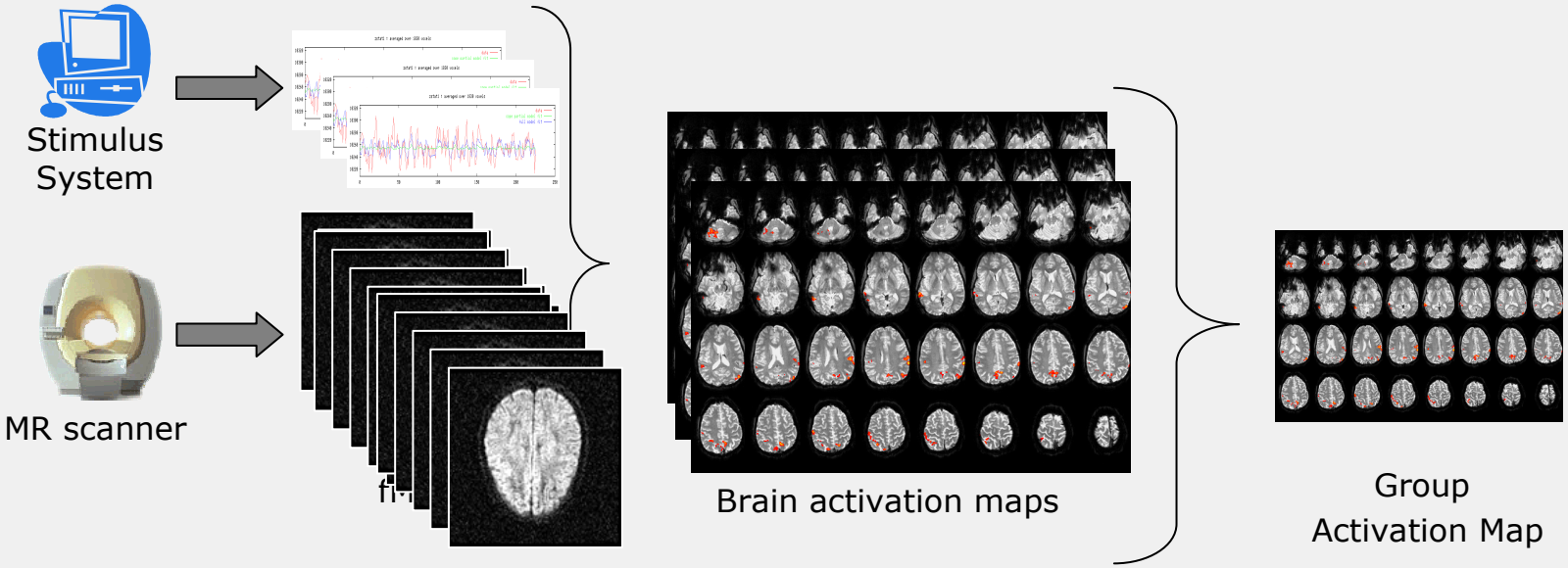
MR scanner



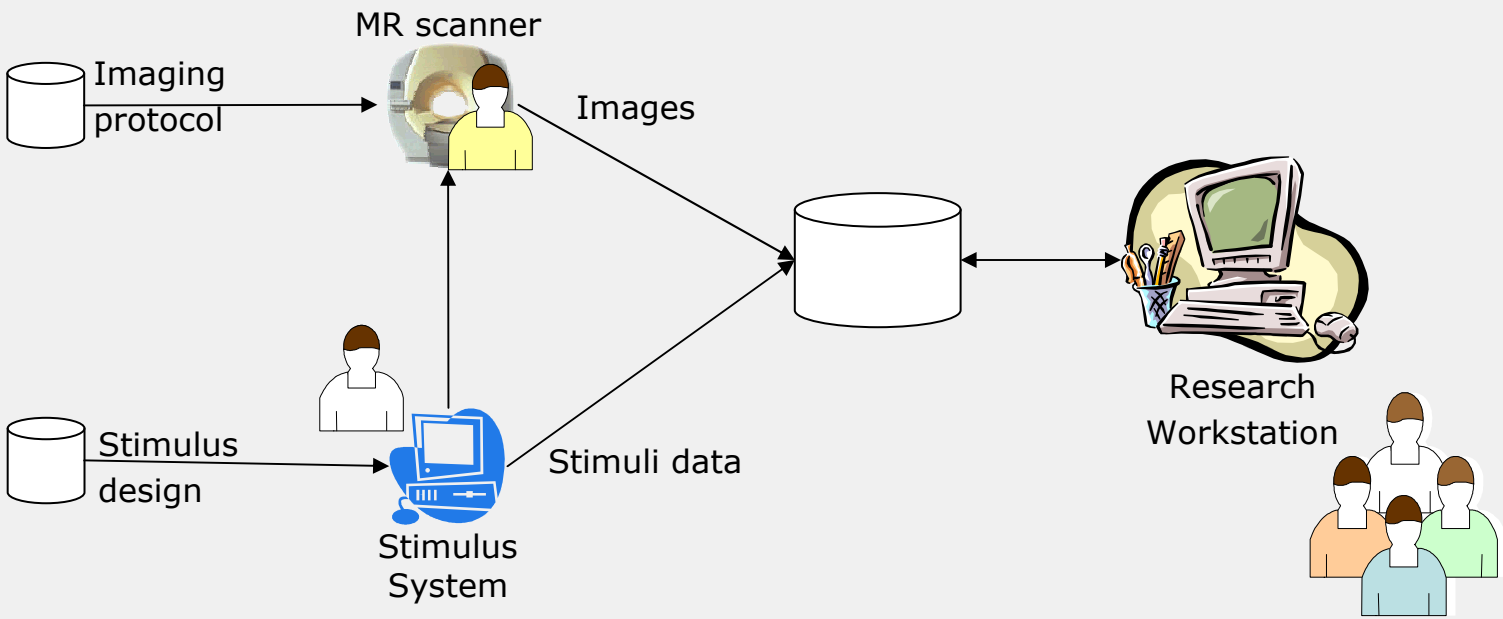


Brain activation maps

fMRI: Group Studies

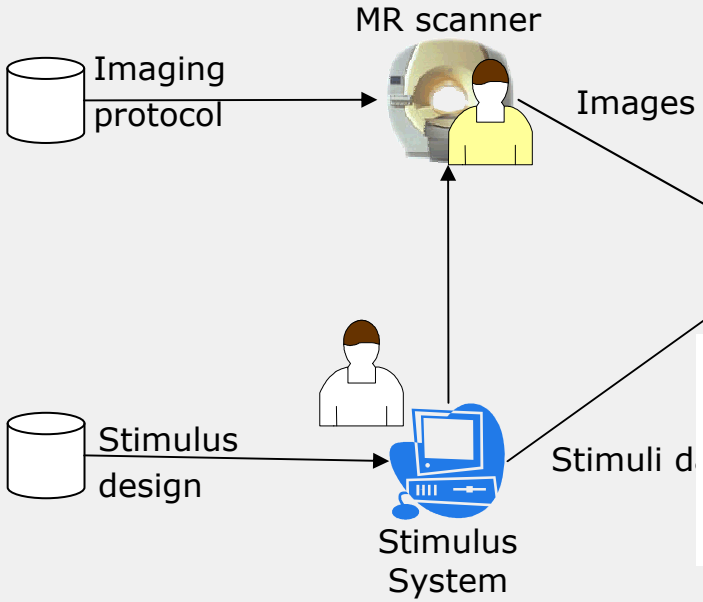


fMRI: Image Analysis Workflow

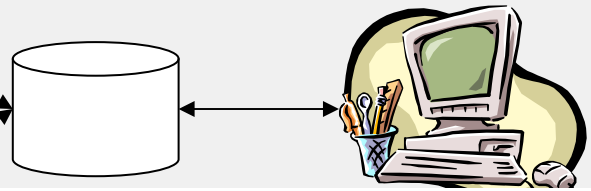


fMRI: Problems

Data Acquisition:
- Complex experiments
- Dispersed equipments



Data Analysis:
- Large scale
- Computation-demanding
- Interactive response



Data Storage:
- Large, many data instances
- Heterogeneous data types
- Confidential data

Shared Access to Data:
- Multiple centres
- Many users, diff access rights
- Long-term archival

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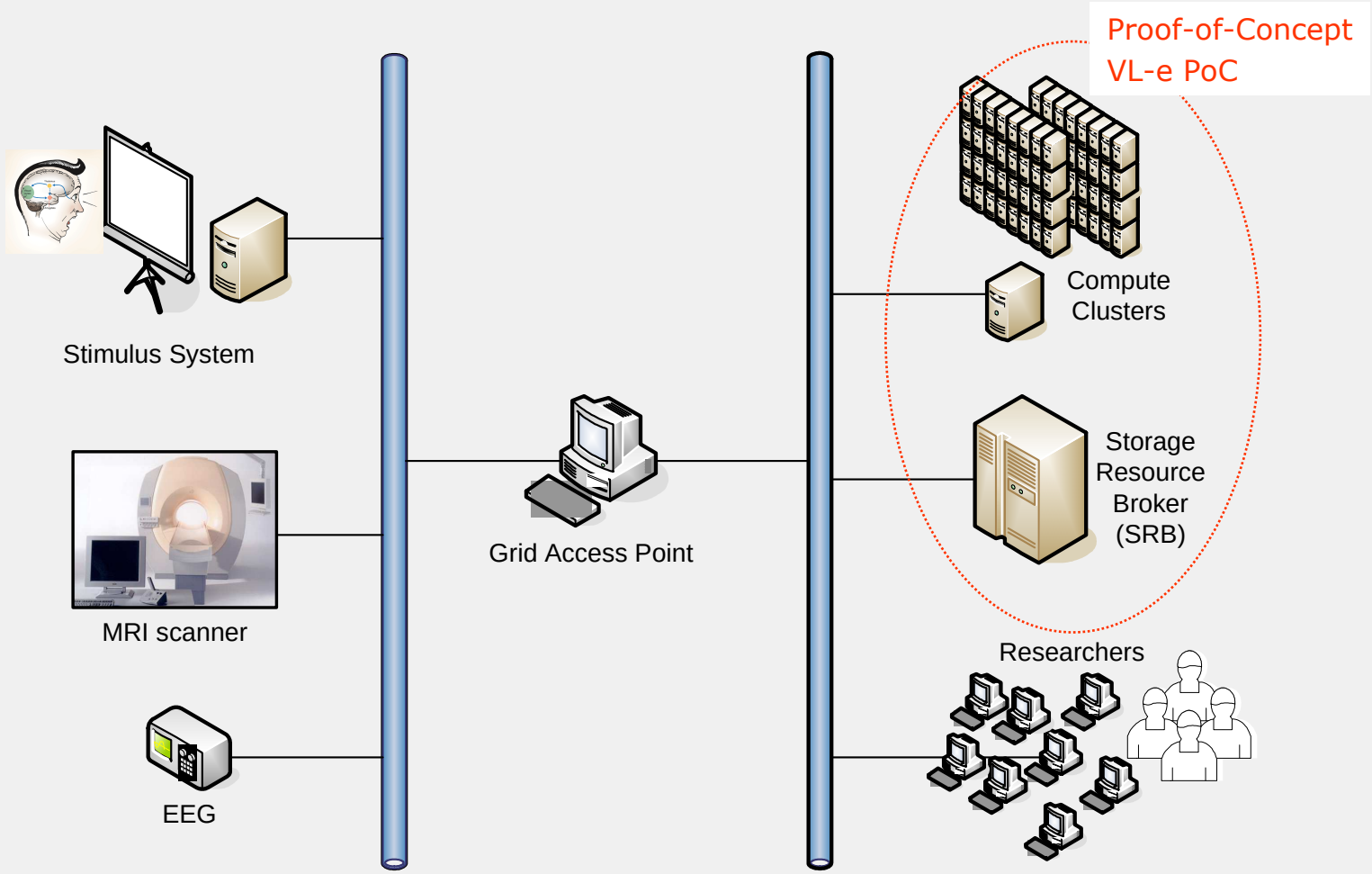
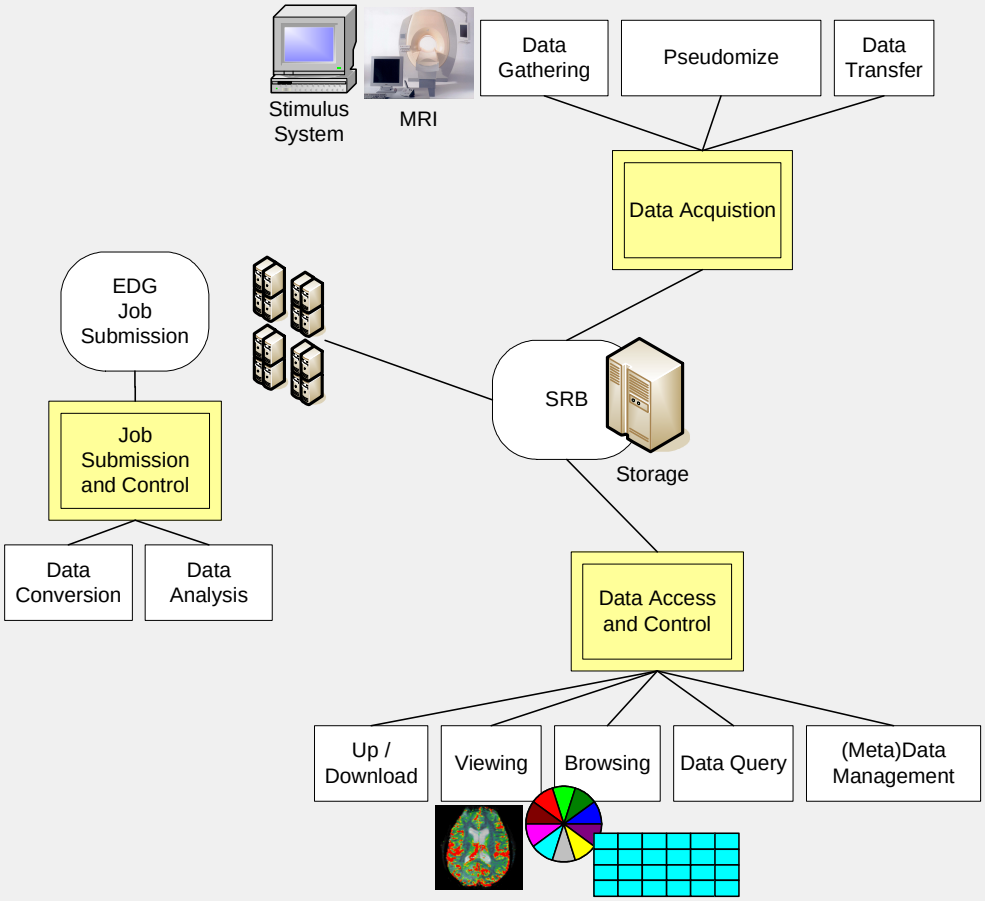
Virtual Lab for fMRI: VL-fMRI

- Goals
  - Facilitate data gathering after acquisition
  - Facilitate storage and archival of large amounts of data
  - Provide remote and controlled access to data
  - Increase computation throughput (HPC resources)
  - Facilitate data retrieval (metadata)
  - Facilitate logistics (workflow automation)
  - Be usable (by non-IT specialists)

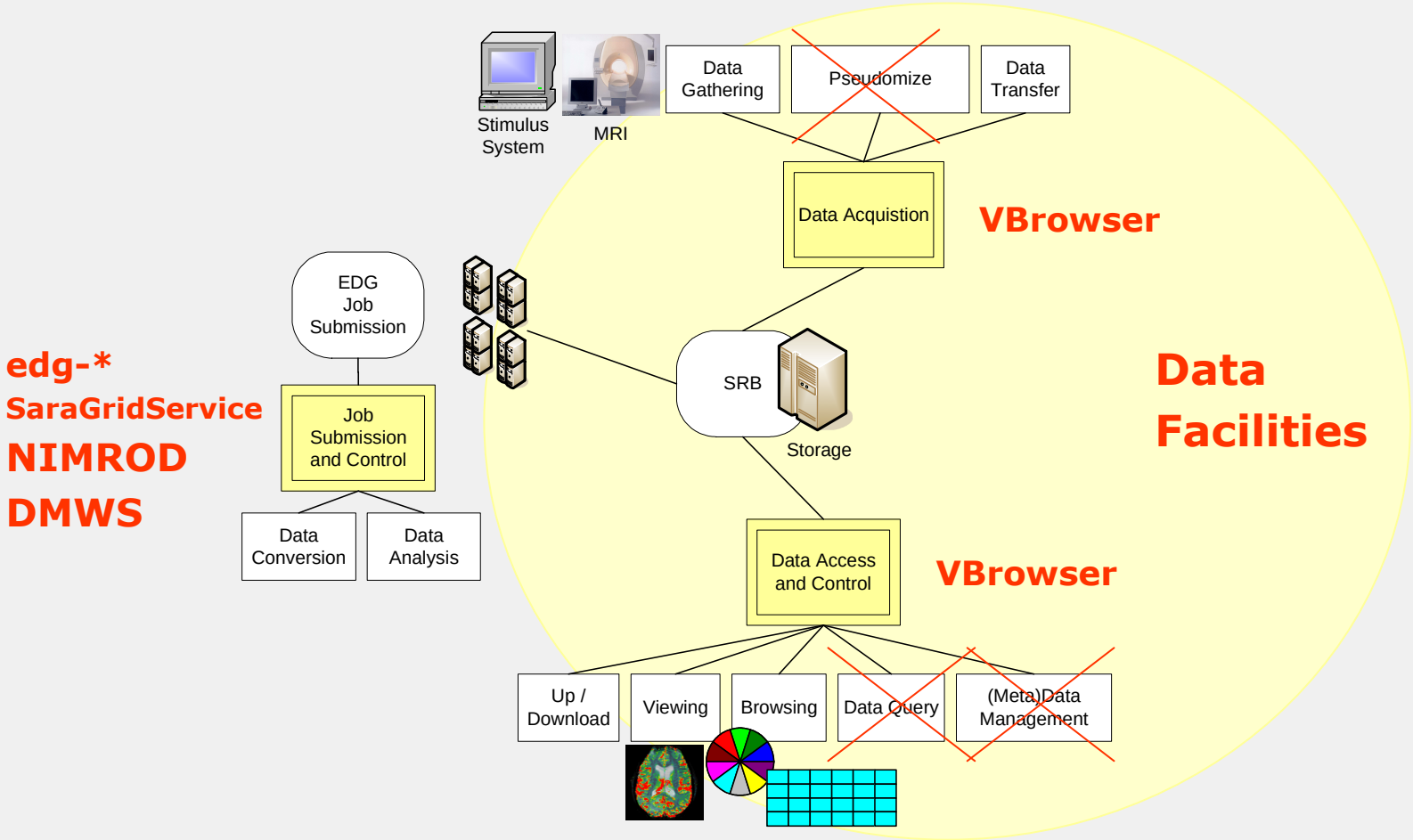
VL-fMRI: Resources



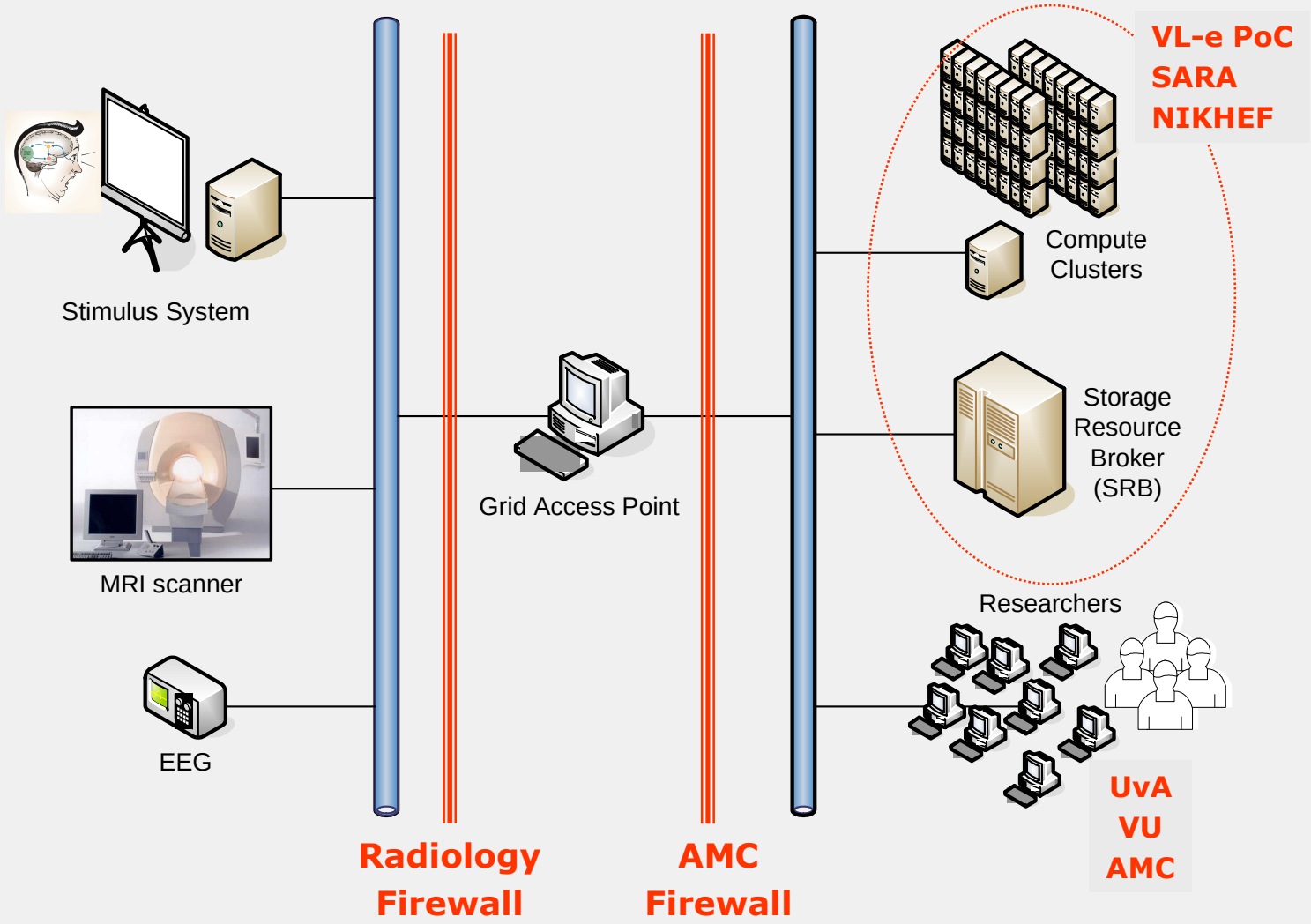
VL-fMRI: Functional Overview



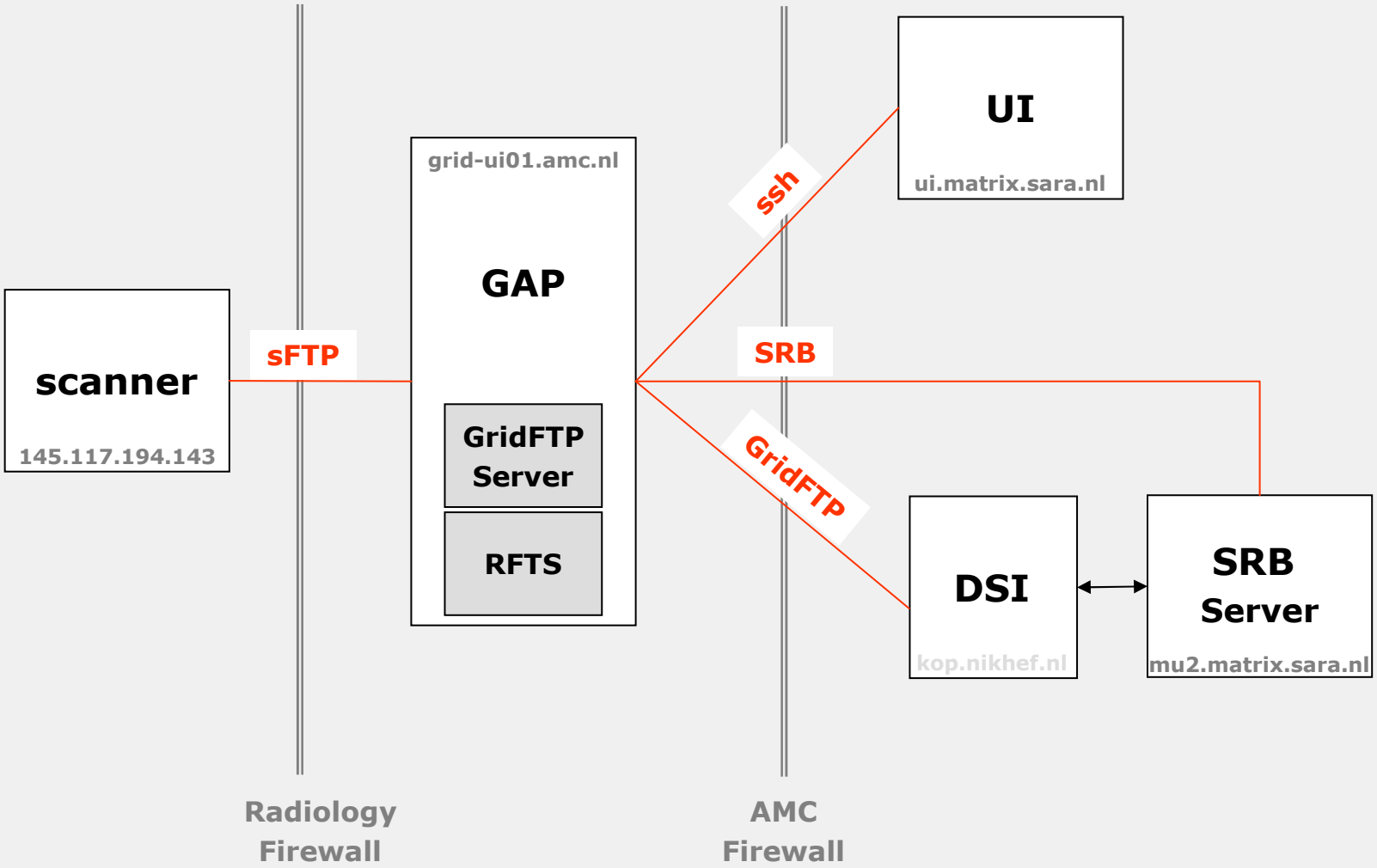
VL-fMRI: Phase 1



Data Facilities



Connectivity



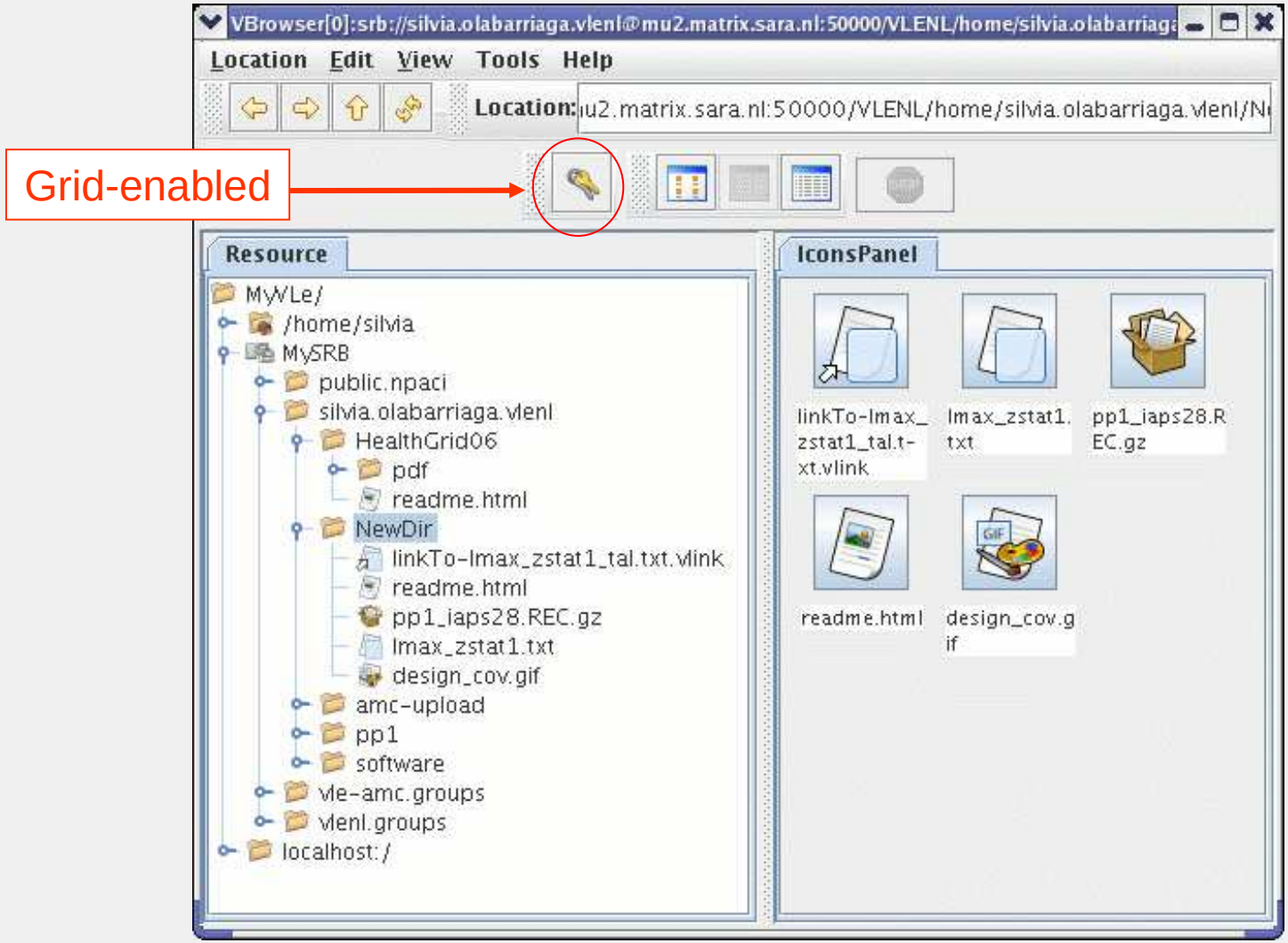
Virtual Resource Browser

Architect + main developer: Piter de Boer (IvI,UvA)

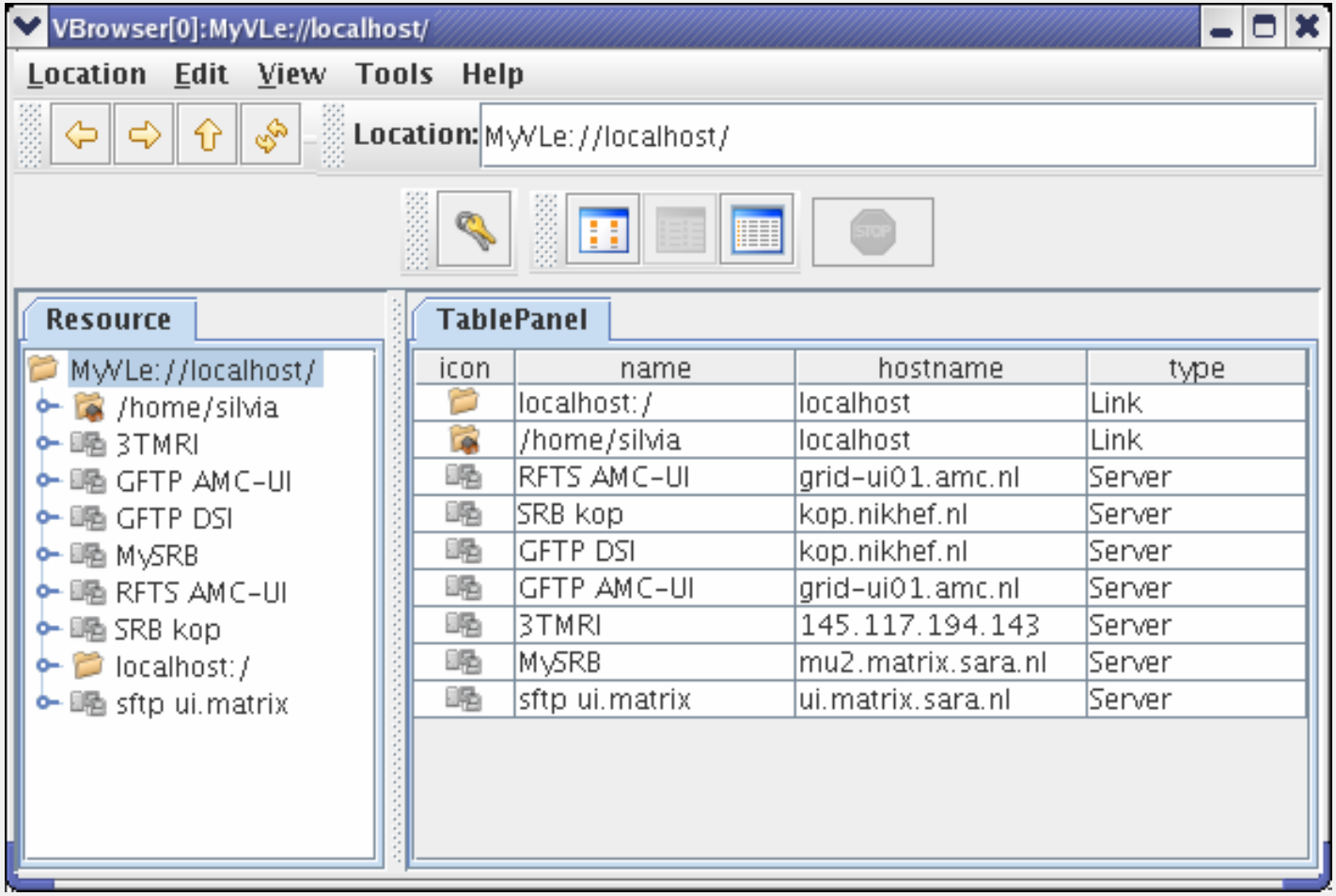
- Interactive GUI for resource browsing
- Access to virtual (grid-enabled) resources
  - Grid: SRB, GridFTP, Secure FTP, RFTS
  - Local: Linux and Windows file systems
- MIME-type enabled
  - Text, 2D images, HTML
- Multi-platform (Java)

VBrowser

http://www.science.uva.nl/~gvlam/vlet/

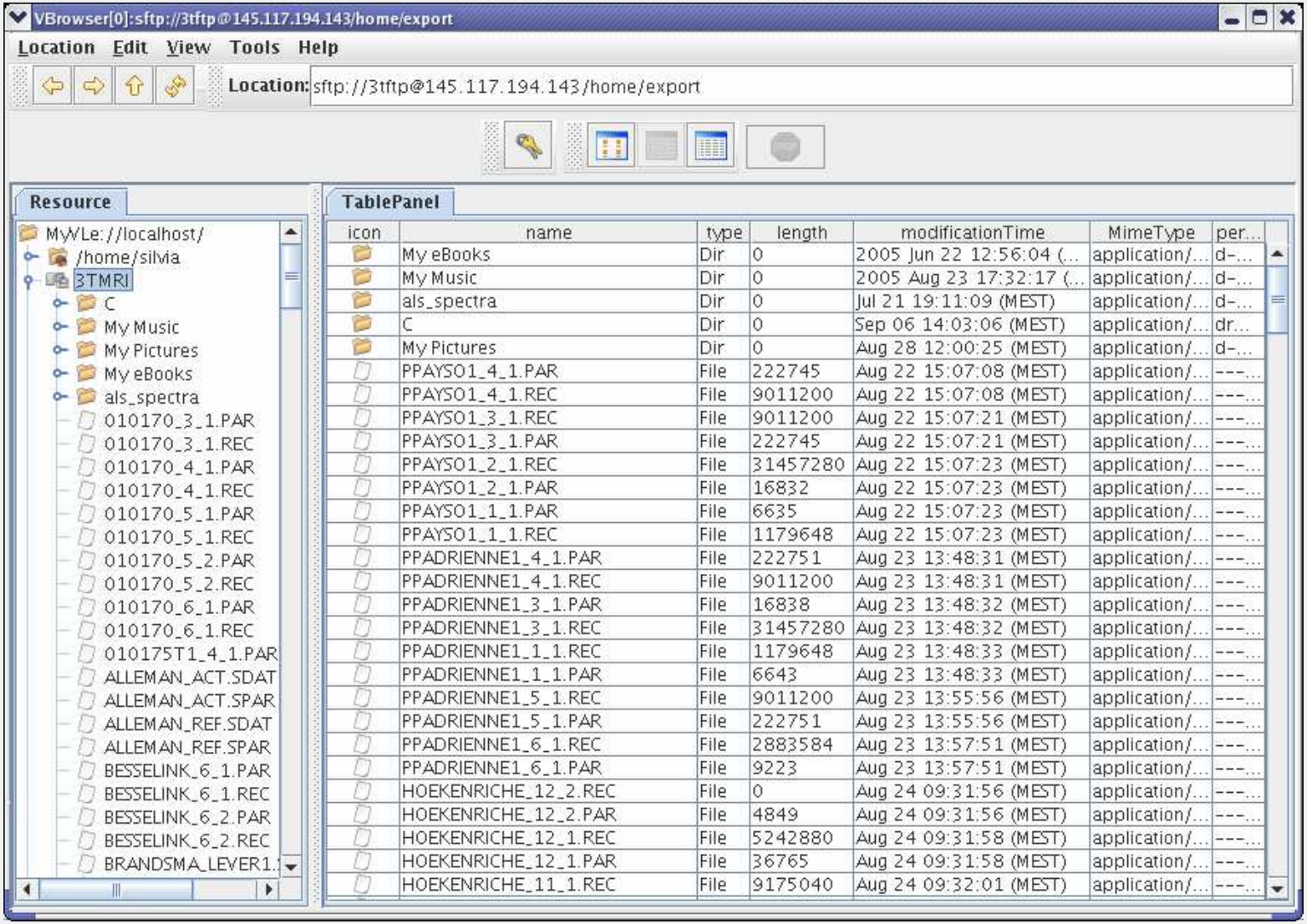


Virtual Resources



User Authentication

Access to 3T MRI Scanner



icon	name	type	length	modificationTime	MimeType	per...
	My eBooks	Dir	0	2005 Jun 22 12:56:04 (...	application/...	d-...
	My Music	Dir	0	2005 Aug 23 17:32:17 (...	application/...	d-...
	als_spectra	Dir	0	Jul 21 19:11:09 (MEST)	application/...	d-...
	C	Dir	0	Sep 06 14:03:06 (MEST)	application/...	dr...
	My Pictures	Dir	0	Aug 28 12:00:25 (MEST)	application/...	d-...
	PPAYSO1_4_1.PAR	File	222745	Aug 22 15:07:08 (MEST)	application/...	---...
	PPAYSO1_4_1.REC	File	9011200	Aug 22 15:07:08 (MEST)	application/...	---...
	PPAYSO1_3_1.REC	File	9011200	Aug 22 15:07:21 (MEST)	application/...	---...
	PPAYSO1_3_1.PAR	File	222745	Aug 22 15:07:21 (MEST)	application/...	---...
	PPAYSO1_2_1.REC	File	31457280	Aug 22 15:07:23 (MEST)	application/...	---...
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	PPAYSO1_1_1.REC	File	1179648	Aug 22 15:07:23 (MEST)	application/...	---...
	PPADRIENNE1_4_1.PAR	File	222751	Aug 23 13:48:31 (MEST)	application/...	---...
	PPADRIENNE1_4_1.REC	File	9011200	Aug 23 13:48:31 (MEST)	application/...	---...
	PPADRIENNE1_3_1.PAR	File	16838	Aug 23 13:48:32 (MEST)	application/...	---...
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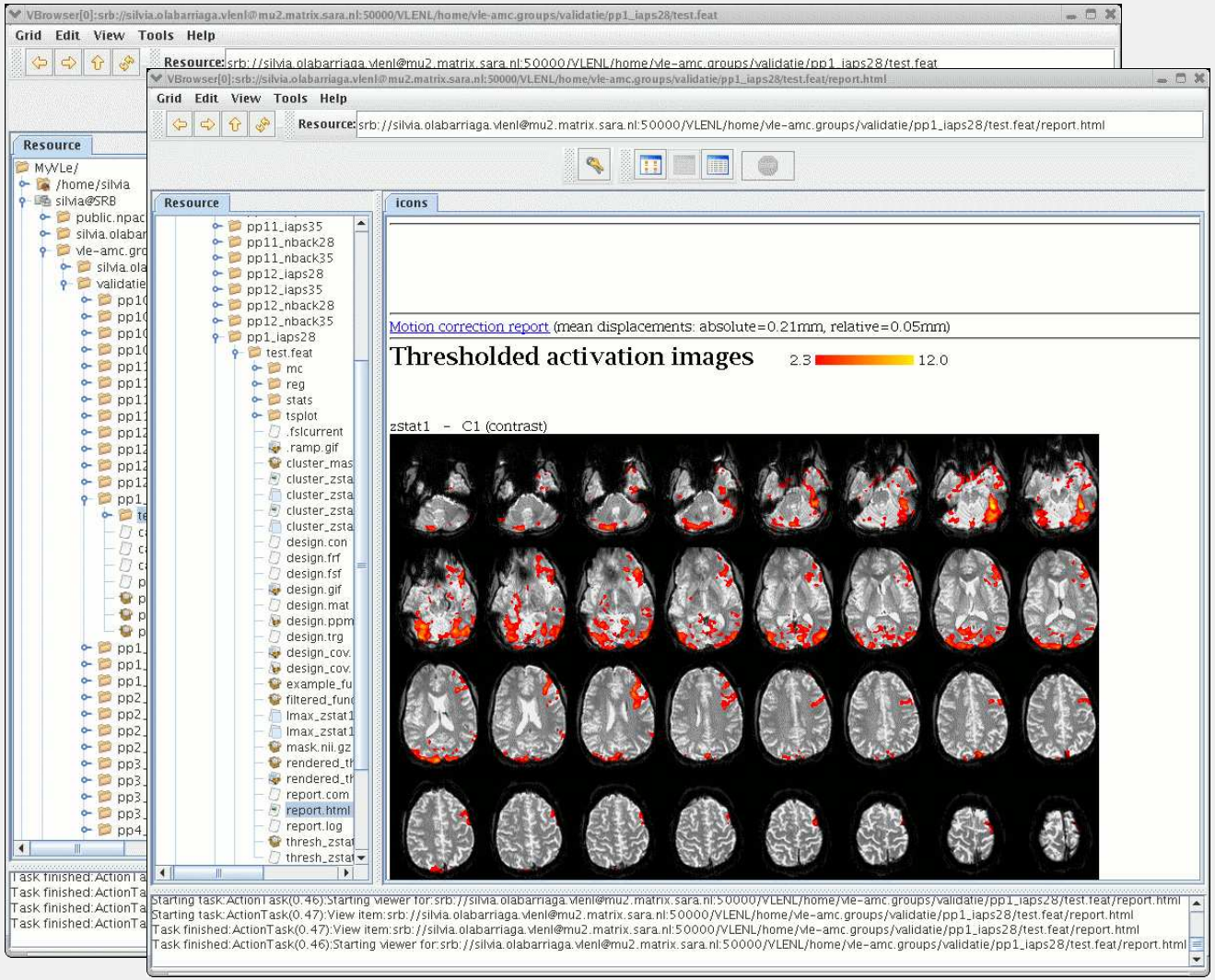
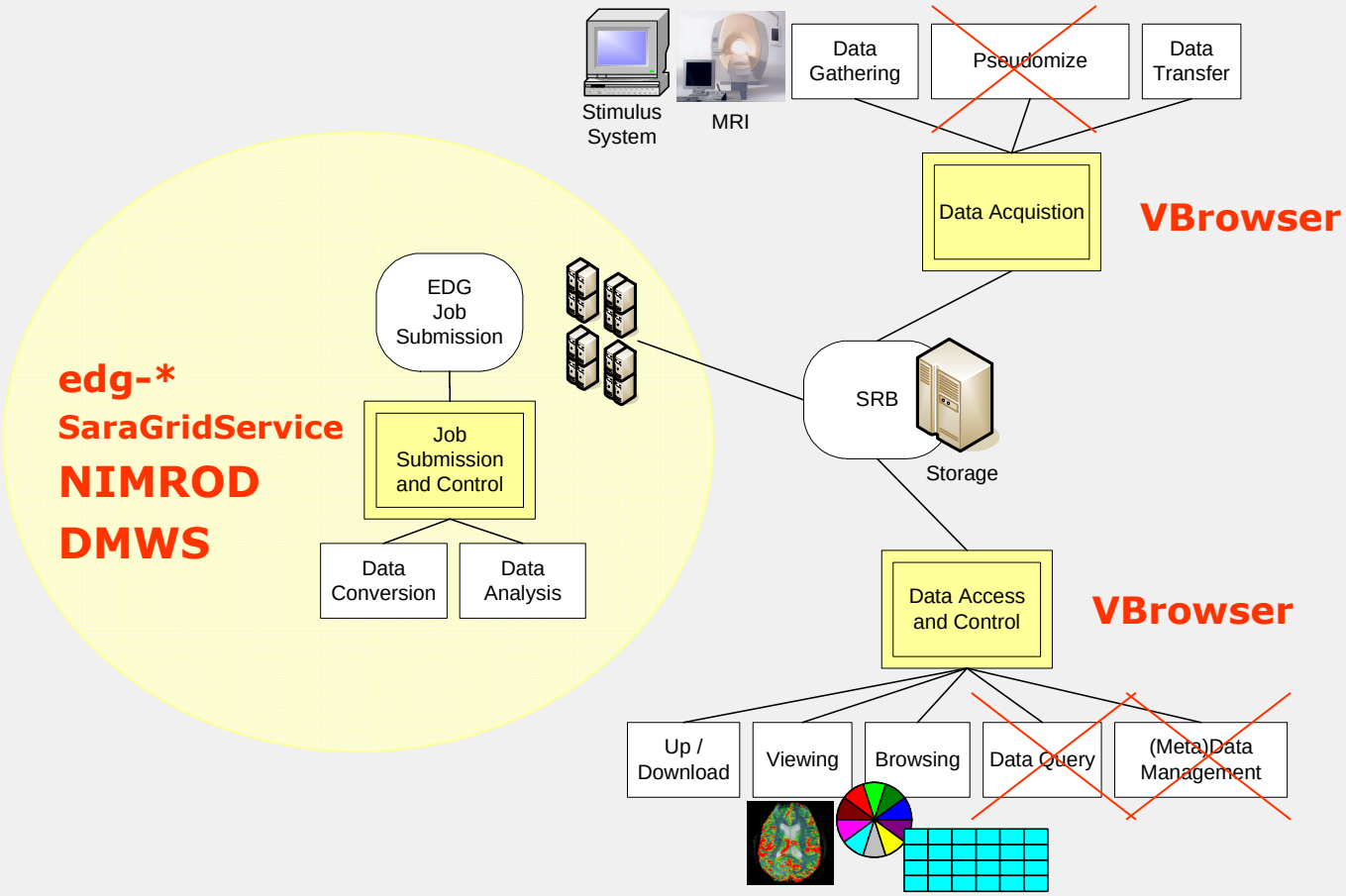
	HOEKENRICHE_11_1.REC	File	9175040	Aug 24 09:32:01 (MEST)	application/...	---...

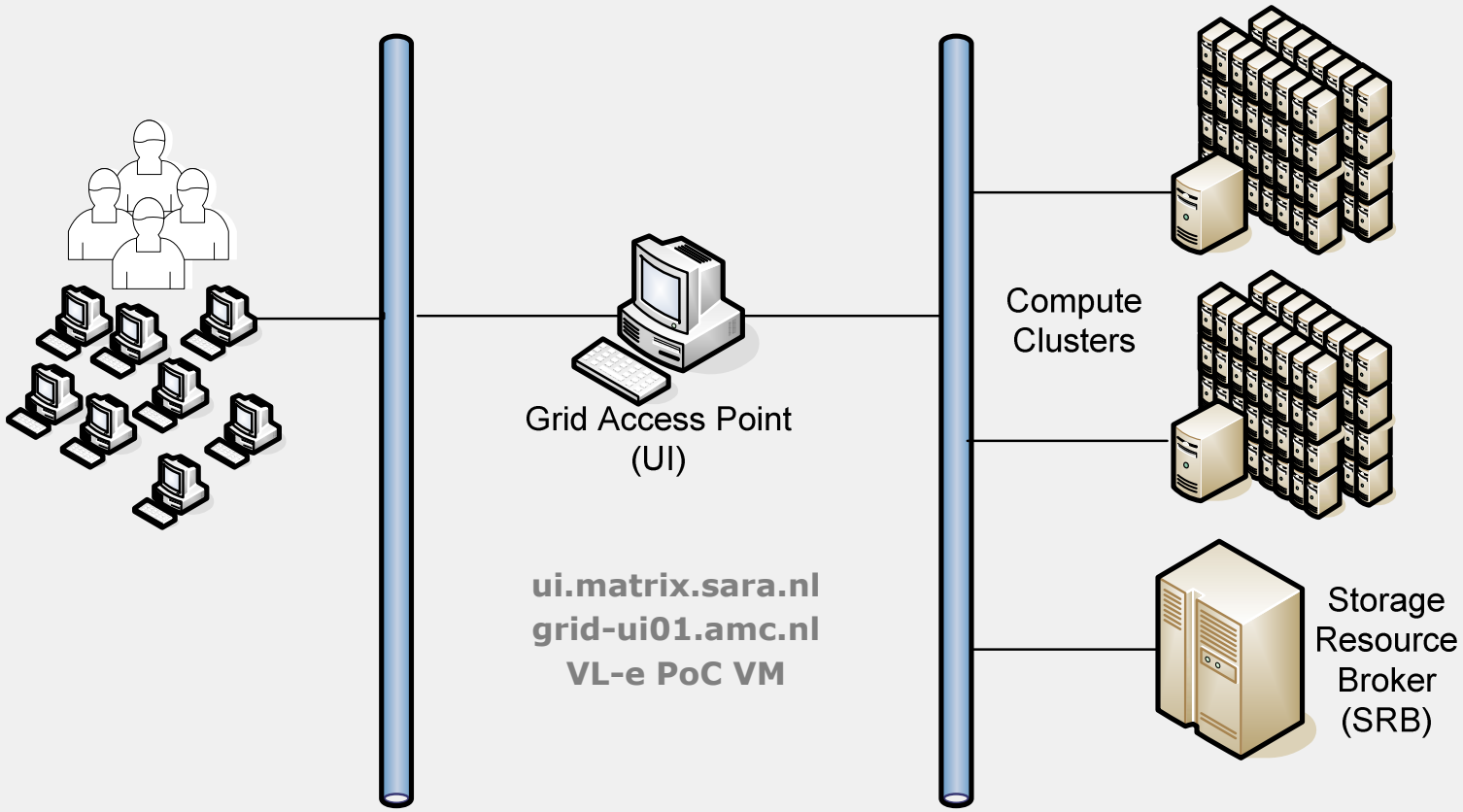
Data Access


Grid Edit View Tools Help
Resource:
Resource
icons
Motion correction report (mean displacements: absolute=0.21mm, relative=0.05mm)
Thresholded activation images
2.3
12.0
zstat1 - C1 (contrast)

VL-fMRI: Phase 1



Compute Facilities



VL-e PoC Installation

Contrib: VL-e SP 4

- General
  - CentOS + LCG + GT4 + SRB clients
- Domain-specific packages
  - FSL, vtk, itk
- For UI and worker nodes
- Identified by Glue attribute

```
Requirements  = Member("nl.vl-e.poc-release-1.0",
   other.GlueHostApplicationSoftwareRunTimeEnvironment);
```

Medical Image Analysis (MIA) Workflow

- Large variety of MIA applications
  - C, matlab, Java (Ibis)
  - Legacy (+ self-developed) code
  - interactive, batch
- Activated from different environments
  - Clinical:
    - automatic (DMWS, AMC)
    - interactive (GAMA, Philips)
  - Research:
    - repetitive, large scale (scripts, NIMROD)

Template: Minimum Workflow

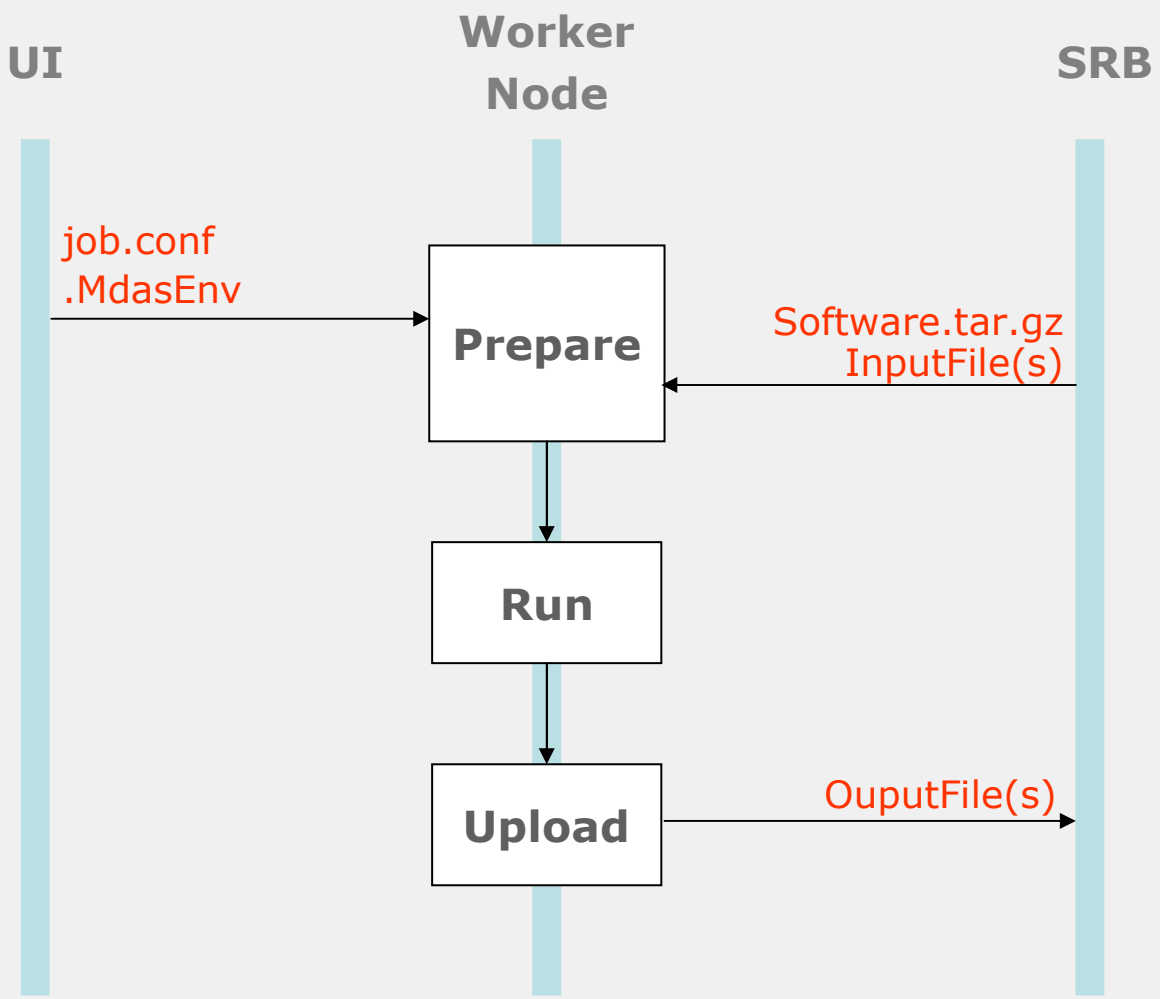
Contrib: Bart Heupers, SARA

- Steps (on worker node):
  - Download software
    - Complementary to VL-e PoC install
  - Download input data
  - Run command
  - Upload results
- Template: **jobrun** package

jobrun Package

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

jobrun: Workflow



jobrun: job configuration

```
srb_software_dir=/VLENL/home/silvia.olabarriaga.vlenl/software
srb_software_archive=DataPrep.tar.gz
export SWDIR=`pwd`/DataPrep
export PATH="${SWDIR}:${PATH}"

srb_data_dir=/VLENL/home/silvia.olabarriaga.vlenl/pp1/iaps28
srb_data_file="image.REC.gz image.PAR"

job_cmd=fMRI_PrepareData.sh
job_args="image image_roi 20 90 5 115 0 35"
job_execs="gunzip rec2analyze.pl avwchfiletype avwroi \
           checkROI.py fMRI_PrepareData.sh"

srb_out_dir=/VLENL/home/silvia.olabarriaga.vlenl/pp1/iaps28
srb_out_file=" "
srb_out_owr_file="image.nii.gz image_roi.nii.gz"
```

jobrun: SRB configuration

- For SRB command-line clients (Scommands)
  - .srb/.MdasEnv

```
mdasCollectionName '/VLENL/home/silvia.olabarriaga.vlenl'
mdasCollectionHome '/VLENL/home/silvia.olabarriaga.vlenl'
mdasDomainName 'vlenl'
mdasDomainHome 'vlenl'
srbUser 'silvia.olabarriaga'
srbHost 'mu2.matrix.sara.nl'
mcatZone 'VLENL'
srbPort '50000'
defaultResource 'vleMatrixStore'
AUTH_SCHEME 'GSI_AUTH'
SERVER_DN '/O=dutchgrid/O=hosts/OU=sara.nl/CN=mu2.matrix.sara.nl'
```

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);
```

Alternatives: Computing Jobs

- Other ways to start (MIA) jobs
  - SaraGridService (Bart Heupers, SARA)
    - Web service
    - Submission from non-grid node
    - Python clients
  - NIMROD (Breanndán Ó Nualláin, IvI-UvA)
    - Management of large number of jobs
    - Parameter sweep, optimization
  - Distributed Workflow Management System (Jeroen Snel, AMC)
    - Automatic after scanning

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Current Status

- GAP at AMC
- VBrowser
  - Basic functionality (Beta release)
- Job execution
  - Scripts (EDG* and Python clients)
  - From ui.matrix, VL-e Poc Virtual Machine
  - NIMROD
- User info
  - http://poc.vl-e.nl/distribution/quickstart.html

Final Remarks

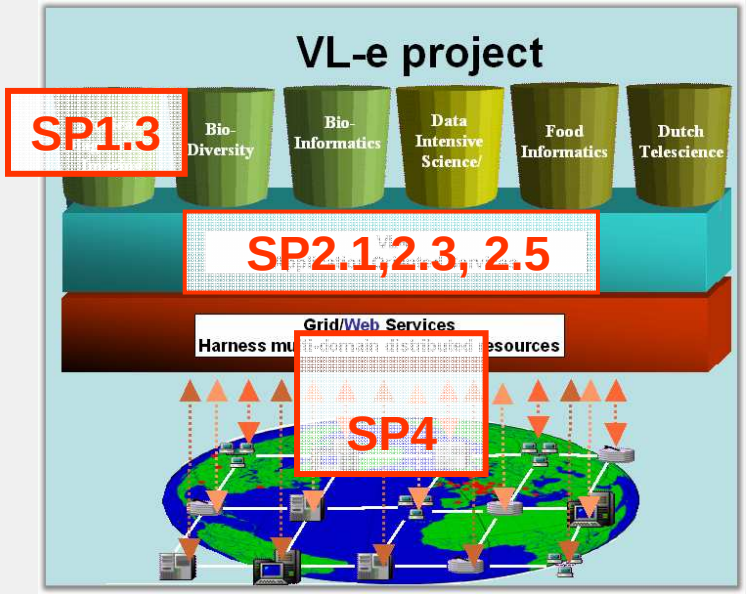
- What we are trying to do is no "rocket science", but we get no "free lunch" …
  - Evolving technology and requirements
  - Evolving/unstable/poorly documented infrastructure
  - Tools with low usability for "end users"
  - Insufficient experts for application development
  - Difficult communication 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) Team

- IvI
  - Ketan Maheshwari, Silvia Olabarriaga (SP1.3)
  - Piter de Boer, Adam Belloum (SP2.5)
  - Breanndán Ó Nualláin (SP2.1)
  - Abdullah Ozsoy, Robert Belleman (SP2.3)
- AMC (SP1.3)
  - Jeroen Snel, Johan Alkemade
  - Aart Nederveen, Matthan Caan
- SARA (SP4)
  - Maurice Bouwhuis
- NIKHEF (SP4)
  - Jan Just Keijser
  - Dennis van Dok
- VUMC (SP1.3)
  - Keith Cover
  - Jasper Sluijmer



Additional Thanks to…

- Dr. Paul van Hooft (IvI, UvA)
- grid-support @{ sara | nikhef }.nl
- Bart Heupers (SARA)
- Prof. Dr. Kees Grimbergen,
  Prof. Dr. Ard den Heeten (AMC)
- Prof. Dr. Bob Hertzberger

The VL-e project is supported by a BSIK grant from the
Dutch Ministry of Education, Culture and Science
and is part of the ICT innovation program of the Ministry of Economic Affairs.

Thanks for your attention!

Questions?

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vl·e

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