Demo and Poster Session

Erwin Laure
KTH

10 Demos

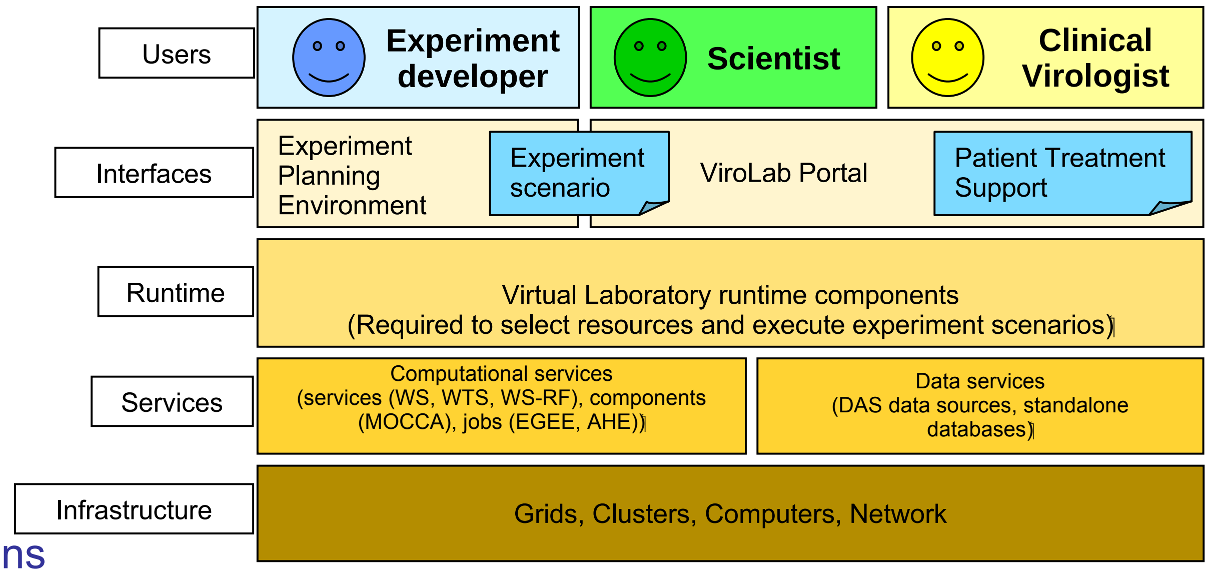
- Laboratory for Virtual Experimentation in Virology and Bioinformatics
  ACC CYFRONET AGH
- Grid Development Tools
  University of Marburg
- The Planck Process Coordinator workflow engine on the Grid
  Leibniz Supercomputer Centre
- Support for cooperative experiments in VL-e: from scientific workflows to knowledge sharing
  University of Amsterdam
- Interactive Simulations on the Grid
  Leibniz Supercomputer Centre
- UNICORE 6 - A European Grid Technology
  Juelich Supercomputing Centre
- Scientific Workflows in the UNICORE Rich Client
  Juelich Supercomputing Centre
- Jawari - A Grid Benchmarking and Monitoring Service for Grid Assessment
  Fraunhofer Institut ITWM
- DORII - Deployment of Remote Instrumentation Infrastructure
  Ludwig-Maximilians-Universität München
- The C3-Grid Project: Seamless Volume-optimized Access to Federated Climate Data
  Technische Universität Dortmund

KTH
VETENSKAP OCH KONST

VL vl introduction

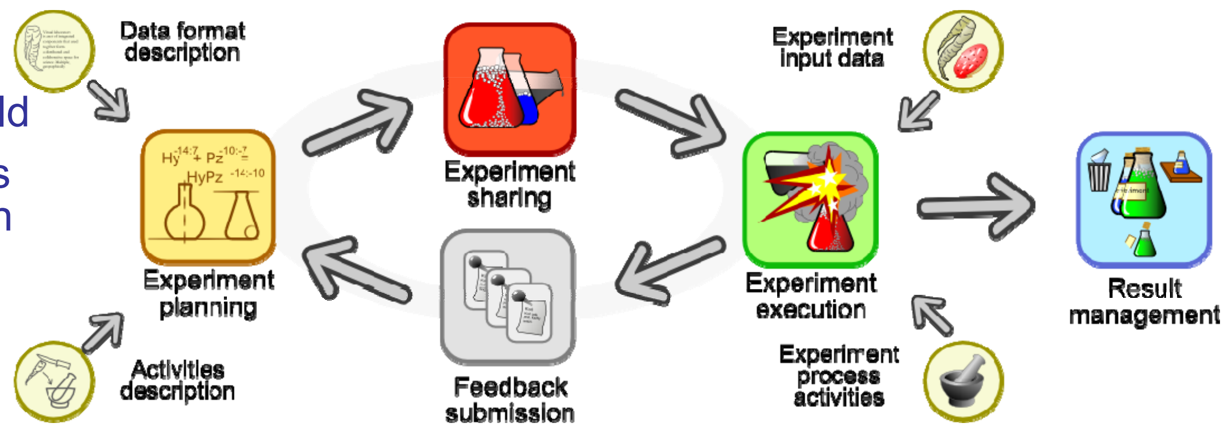
ViroLab virtual laboratory

- Distributed and collaborative e-research platform
- Integrates various data sources and computational resources
- Enables to build and execute experiments
- Facilitates knowledge sharing
- Dedicated to support virologists, epidemiologists and clinicians, but is also applicable in other domains



In silico experiment

- Mirrors an experiment in real world
- Defines input data and operations that need to be performed to obtain result
- Include experiment logic
- Expressed as a Ruby script



Scientific aspects and solution

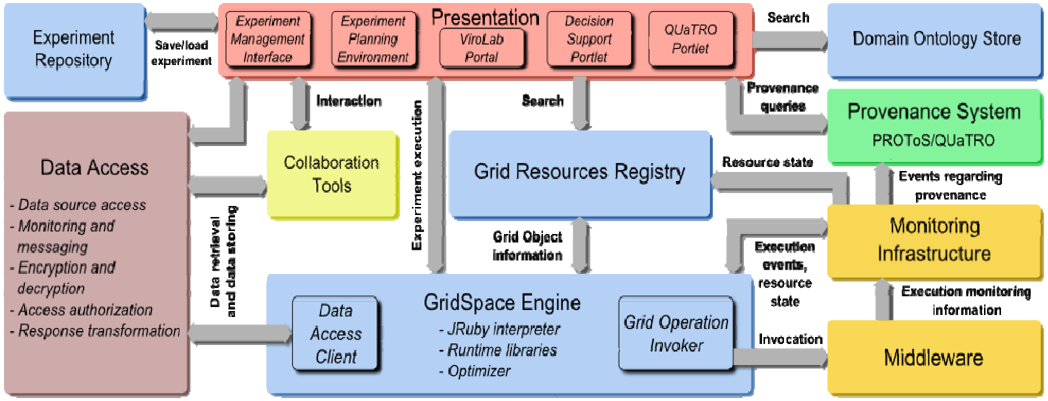
Scientific issues

– Heterogeneous computational and data resources

– Expressiveness vs simplicity

– Provenance of results and result reuse

– Collaboration (share data, knowledge and resources but preserve security)




```
require 'cyfronet/gridspace/goi/core/g_obj'
drs =
GObj.create('org.virolab.DrugRankingSystem2')
mut = 'P1M I2L S3T P4Q E6G V10N K11F'.split(' ')
ranking = drs.drs('ANRS', 'rt', mut)
puts ranking
```

Applications

– Virtual Patient Experiment Pilot ViroLab application

– Early Protein Folding

– Computational chemistry apps

–Data mining with WEKA

Links to remember

http://www.virolab.org/ http://virolab.cyfronet.pl/ http://gs.cyfronet.pl/

Grid Development Tools

http://mage.uni-marburg.de

- Grid Service Development
- Certificate Management
- Grid Browser
- Workflow Orchestration
- Workflow Execution
- Workflow Monitoring

Kay Dörnemann, Tim Dörnemann, Ernst Juhnke
and Prof. Dr. Bernd Freisleben

Demonstrators & Development Team

Kay Dörnemann
doernemk@mathematik.uni-marburg.de
Full-time research assistant
Research interests:
- Grid Computing in combination with P2P-Computing
- Grid Tools, responsible: Grid Service Development, Certificate Management, Grid Management

Tim Dörnemann
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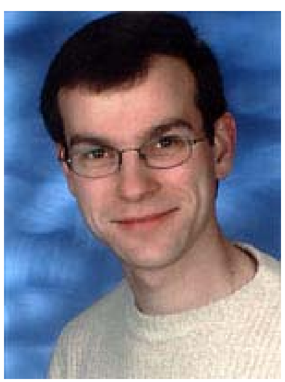
Full-time research and teaching assistant
Research interests:
- BPEL-based Workflow Modeling and Execution in Grid and Cloud Environments



Ernst Juhnke
ejuhnke@mathematik.uni-marburg.de
Full-time research assistant
Research interests:
- BPEL-based Workflow Modeling and Execution in Grid and Cloud Environments

Staff Developers:
- Kay Dörnemann
- Tim Dörnemann
- Ernst Juhnke
- Roland Schwarzkopf
- Thomas Friese
- Matthew Smith
- Steffen Heinzl
- Markus Mathes
- Dominik Seiler

Students
- Marian Harbach
- Fabian Schwarzer
- Stanimir Dimitrov
- Sebastian Kirch

Today´s Demonstration

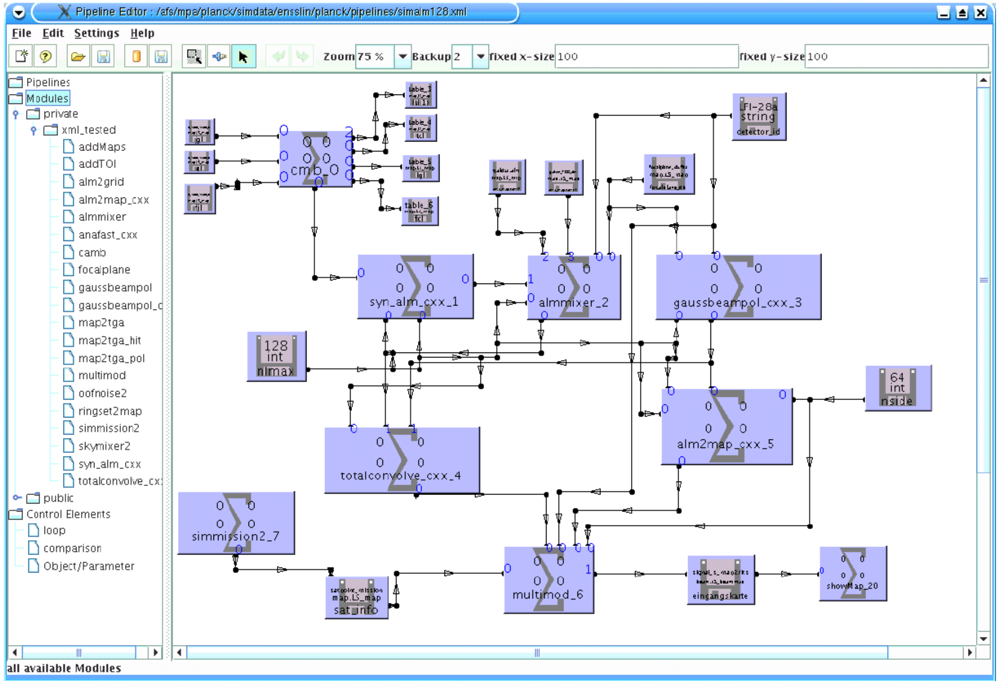
- Tool Support for the Entire Grid Software Development and Execution Lifecycle

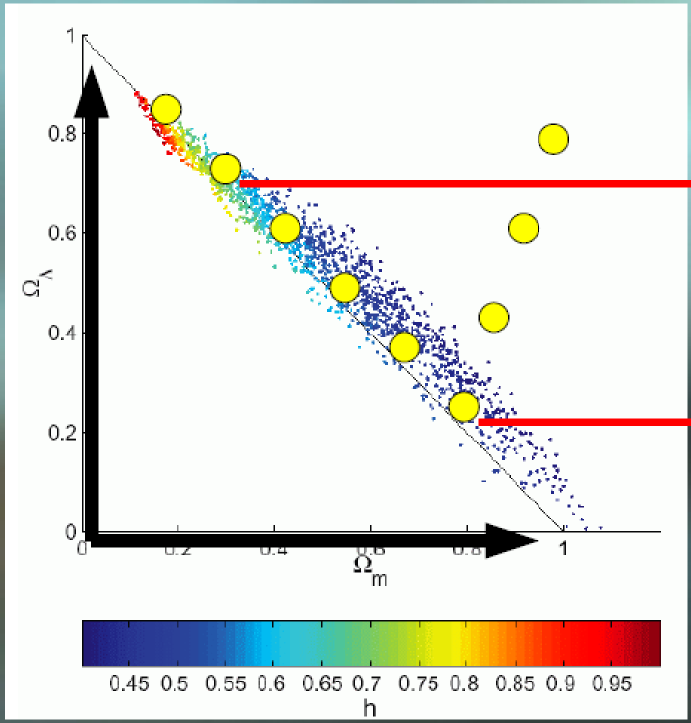
- Live demonstration of selected tools
  - Grid Service Development (Service Generator)
  - Workflow Orchestration
  - Workflow Execution
  - Workflow Monitoring
  - Certificate Management
  - Grid Browser

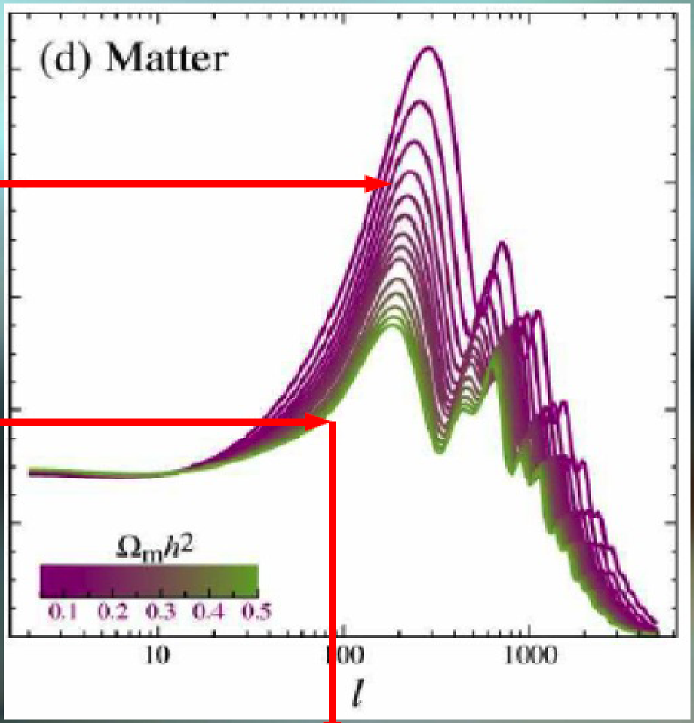
Visual Grid Service Orchestration (BPEL) and BPEL Workflow Engine

The Planck Process Coordinator workflow engine on the Grid

LRZ: Arthur Carlson, Ilya Saverchenko, Jarno Laitinen, …
MPA (ProC): Torsten Enßlin, Wolfgang Hovest, Thomas Riller, …
AEI (GAT): Alexander Beck-Ratzka, ...



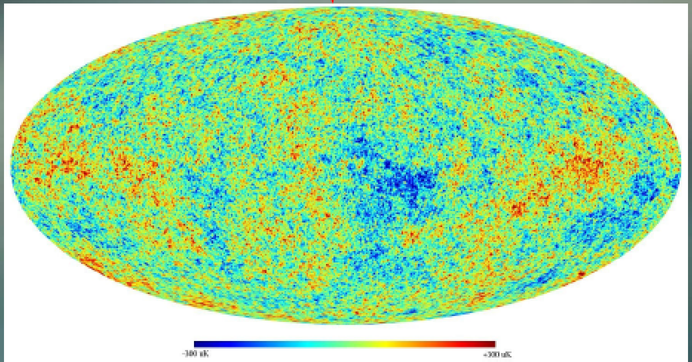




each point in parameter space configures a simulation workflow

each workflow is sent to a different computing host on the Grid

ProC & GAT hide Grid complexity from scientist



vl·e virtual laboratory for e·science

Cooperative experiments in VL-e: from scientific workflows to knowledge sharing

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Complex Scientific experiments model

Problem investigation:
- Look for relevant problems
- Browse available tools
- Define the goal
- Decompose into steps

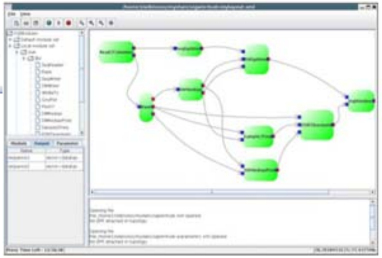
Experiment Prototyping
- Design experiment workflows
- Develop necessary components

Shared repositories

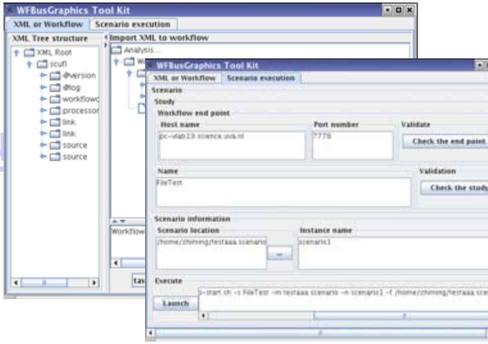
Results Publication
- Annotate data
- Publish data

Experiment execution
- Execute experiment processes
- Control the execution
- Collect and analysis data

Tools to support Cooperative experiments in VL-e



- **Virtual resource Browser**
  http://staff.science.uva.nl/~ptdeboer/vl
- **WSRF Grid-enabled workflow system**
  http://staff.science.uva.nl/~gvlam/wsvlam/



- **A WfBus for interoperability of scientific workflows.**
  http://staff.science.uva.nl/~zhiming/workflowbu /
- **Hybrid-bAsed Match-Maker for Resources**
  http://pc-vlab19.science.uva.nl:8081/ws-hammer

vl·e

virtual laboratory for e·science

From myexperiment to the Grid

SigWin-detector: is a grid-enabled *workflow 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.

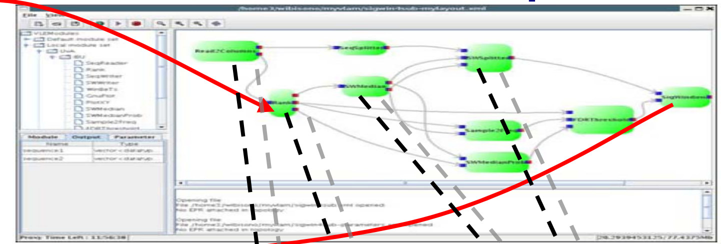
A significant window is a window in the input sequence for which the median value is significantly higher than expected, if assumed that the ordering of the numbers in the input sequence is random.

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 trancriptome map, the significant windows are called RIDGES and the output graph is called a RIDGEOGRAM.

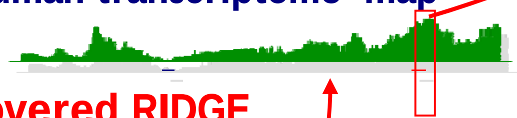
SigWin-detector runs under the WS-VLAM workflow management system.

myexperiment web site

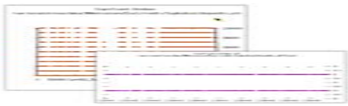
WS-VLAM composer



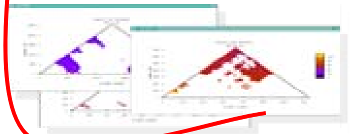
Human transcriptome map



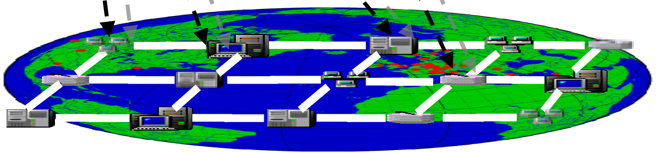
discovered RIDGE



Human transcriptome map



DNA curvature of the *Escherichia Coli* chromosome



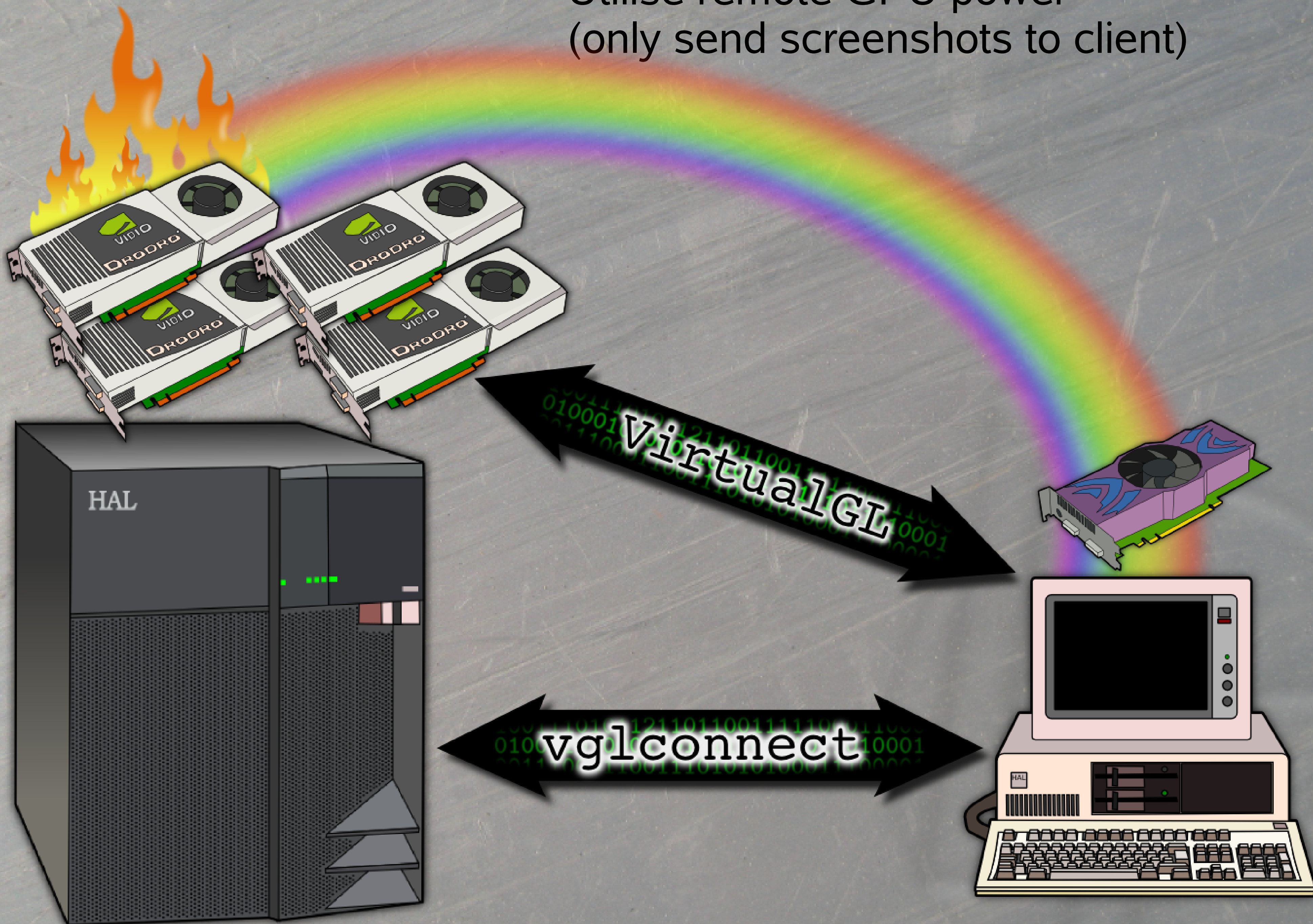
More details: http://staff.science.uva.nl/~inda/SigWin-detector.html

DEMO:
Interactive Simulations on the GRID

Dr. Helmut Satzger
Dr. Ferdinand Jamitzky

Remote Visualisation:

- Connect to remote server
- Utilise remote CPU power
- Utilise remote GPU power
  (only send screenshots to client)



Example: Interactive Simulations

HLRB II
Massive Parallel Simulation
NAMD

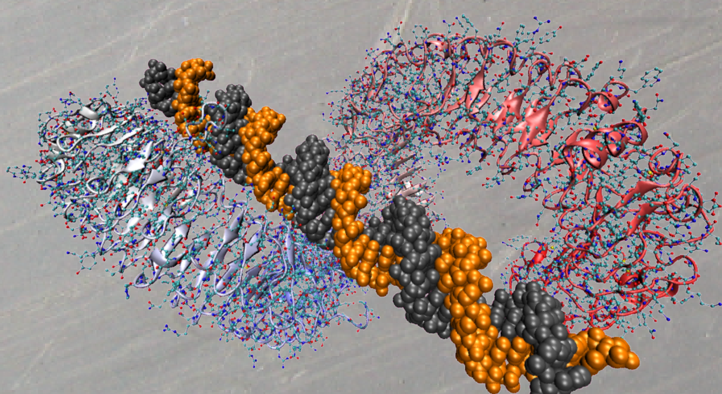
~1 GByte/s

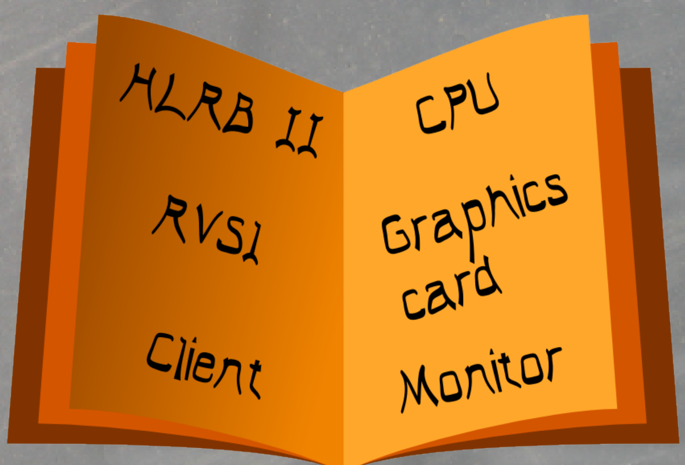
RVS1
Visualisation
VMD

~800 KByte/s

Client
Display
vglrun

1,000,000 atoms
2000 cores compute
20 iterations/second





UNICORE 6

A European Grid Technology

http://www.unicore.eu

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Jülich Supercomputing Centre (JSC)

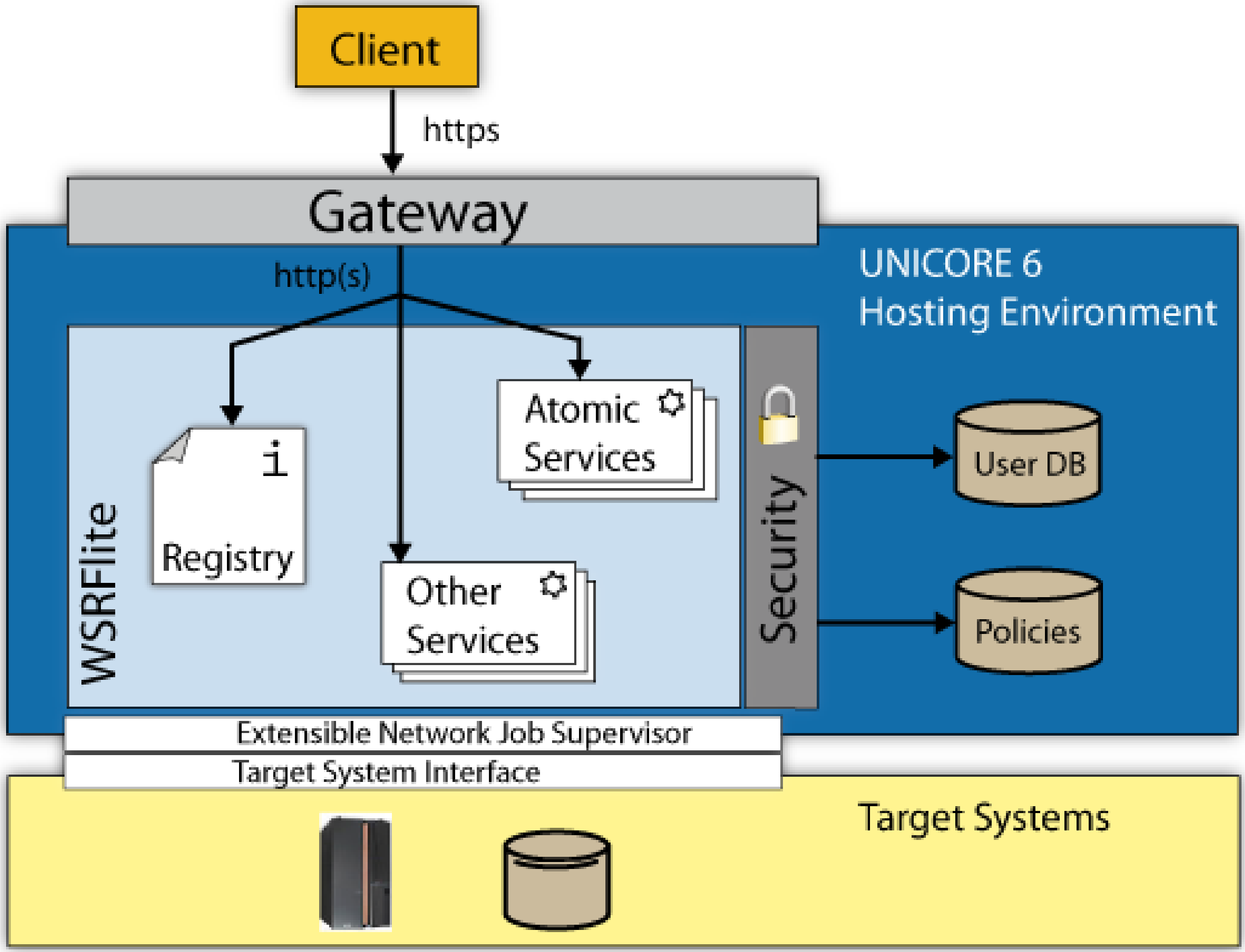
JÜLICH
FORSCHUNGSZENTRUM

A few facts

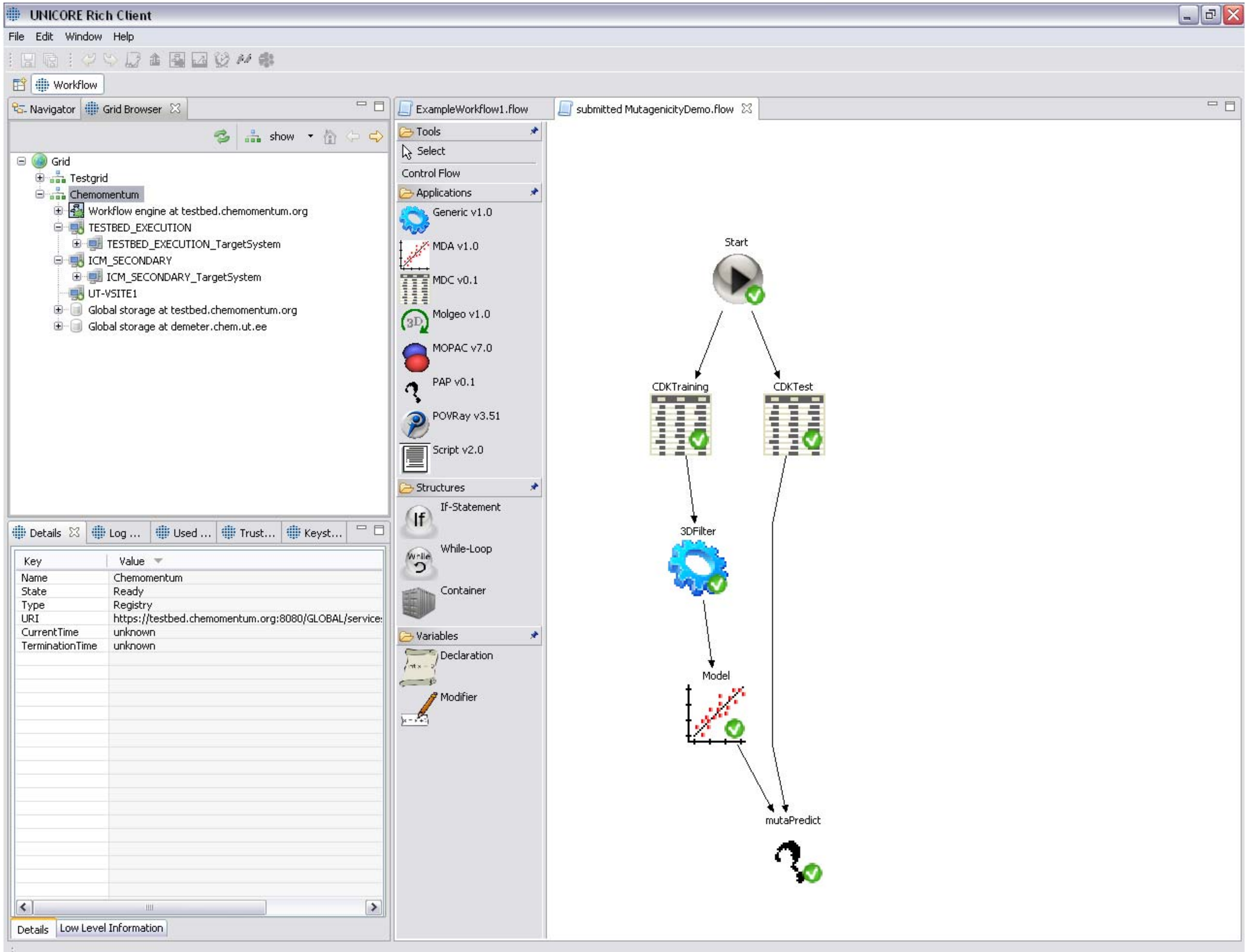
- **UN**iform **I**nterface to **CO**mputing **Re**sources
  - seamless, secure, and intuitive Grid middleware
- In continuous development since 2002 in several EU projects
- Open Source community development since Summer 2004
  - BSD license
  - hosted on SourceForge

Guiding Principles, Implementation Strategies

- **Standards-based**: OGSA-conform, WS-RF 1.2 compliant
- Open, extensible **Service-Oriented Architecture** (SOA)
- Mature **Security**: X.509, proxy and VO support
- Tightly integrated **workflow** support, highly extensible by different workflow languages and engines
- **Application integration** mechanisms on the client, services and resource level
- Variety of **clients**: graphical, command-line, API, portal, etc.
- Quick and **simple installation** and configuration
- Support for many operating and batch systems
- Implemented in **Java** to achieve platform-independence


Client
https
Gateway
http(s)
UNICORE 6
Hosting Environment
Atomic
Services
Registry
Other
Services
WSRFlite
Security
User DB
Policies
Extensible Network Job Supervisor
Target System Interface
Target Systems

UNICORE Rich Client (URC)



UCC – Commandline Client

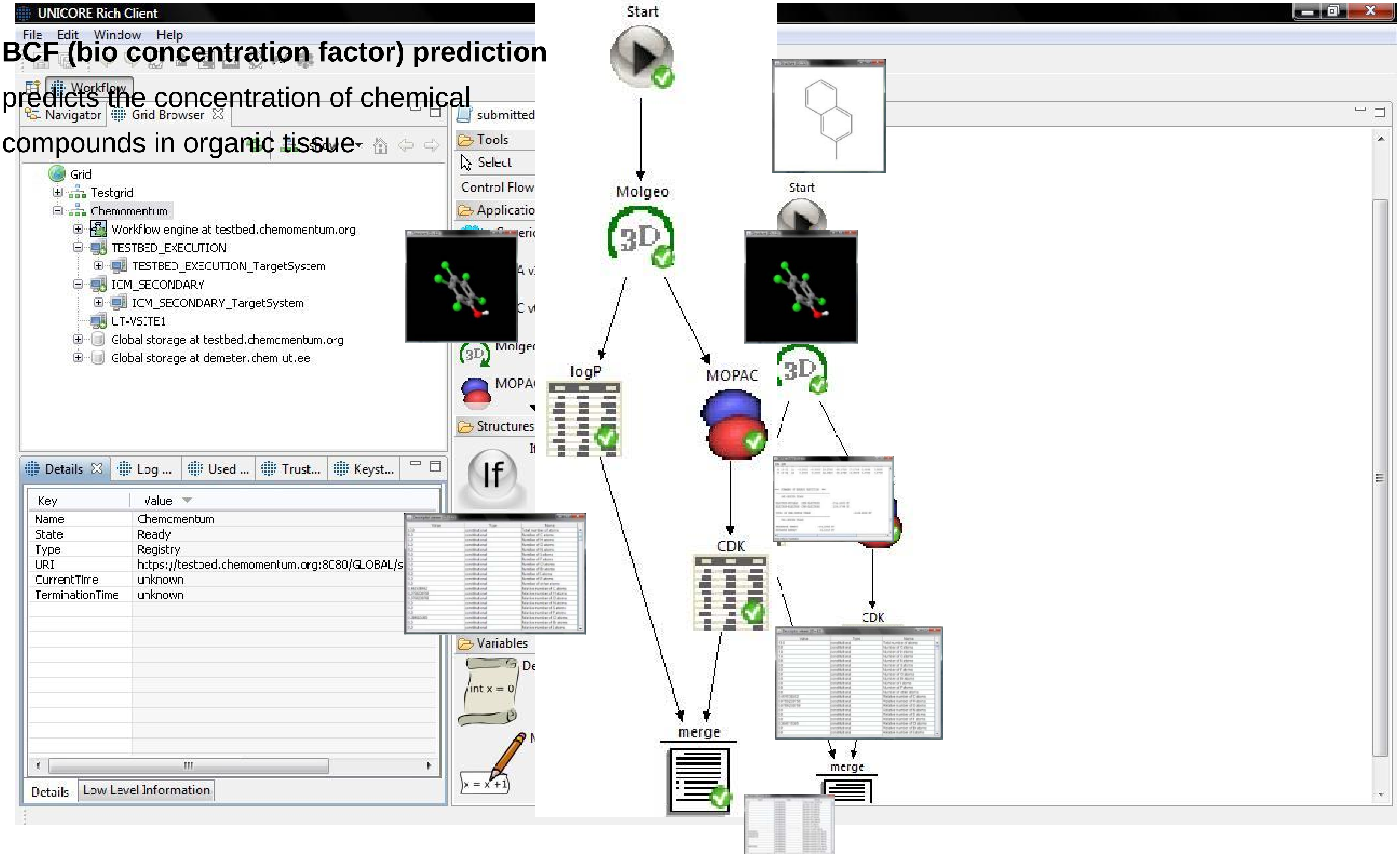
```
>ucc -h
UCC version 1.2-SNAPSHOT
Usage: ucc <command> [OPTIONS] <args>
The following commands are available:
Data management:
 ls                    - list a storage
 copy-file-status      - check status of a copy-file
 get-file              - get remote files
 find                  - find files on storages
 resolve               - resolve remote location
 copy-file             - copy remote files
 c9m-get-file          - get remote files
 put-file              - puts a local file to a remote server
General:
 connect               - connect to UNICORE
 list-applications     - lists applications on target systems
 list-jobs             - list your jobs
 list-sites            - list remote sites
 c9m-system-info       - Checks the availability of services.
Job execution:
 run                   - run a job through UNICORE 6
 get-status            - get job status
 abort-job             - abort a job
 batch                 - run ucc on a set of files
 get-output            - get output files
Other:
 shell                 - Starts an interactive UCC session
 loadtest              - load tests services
 issue-delegation      - Allows to issue a trust delegation assertion
 wsrf                  - perform a WSRF operation
 run-groovy            - run a Groovy script
Workflow:
 c9m-submit            - submit a workflow to Chemomentum
 c9m-trace             - trace info on a workflow in Chemomentum
 c9m-control           - control a workflow in Chemomentum
 c9m-workflow-info     - lists info on workflows in Chemomentum
Enter 'ucc <command> -h' for help on a particular command.
>
```

UCC

Life Science Workflow

BCF (bio concentration factor) prediction

predicts the concentration of chemical compounds in organic tissue



UNICORE in use – some examples

- Supercomputing
  - DEISA (EU)
  - Clinical Supercomputing (USA)
  - SKIF-GRID (Russia, Belarus)
- National Grids (Germany)
  - D-Grid
  - AeroGrid
  - BIS-Grid
- Commercial
  - T-Systems SfR
  - 52° North

UNICORE

software, source code, documentation, tutorials, mailing lists, community links, and more:

http://www.unicore.eu

Goal

Support for Quality of Service Assessment and Assurance in Grids

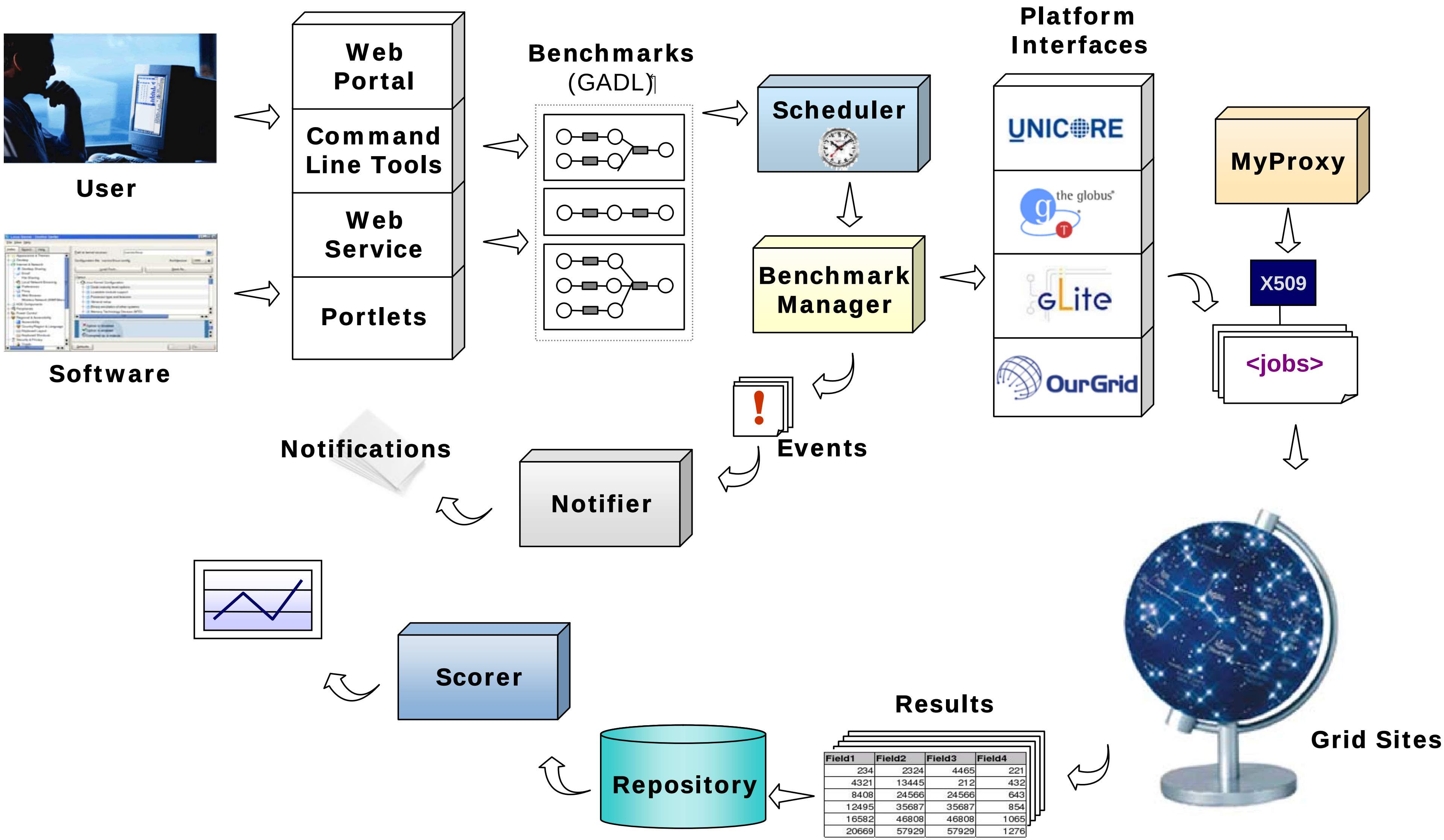
Components

- Benchmarking and Monitoring Service
- Performance Prediction Tools

Characteristics

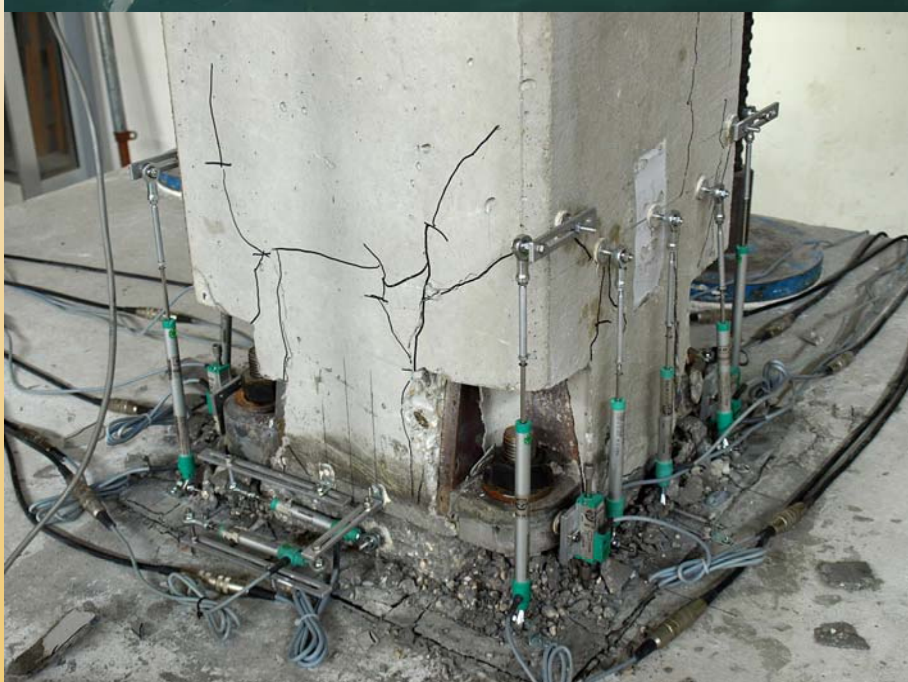
- Open Source
- Free of Charge
- Extensible
- Multiplatform
- Focused on Grid Services
- In production for 3 years
- Simple to use
- Mimics an End-user

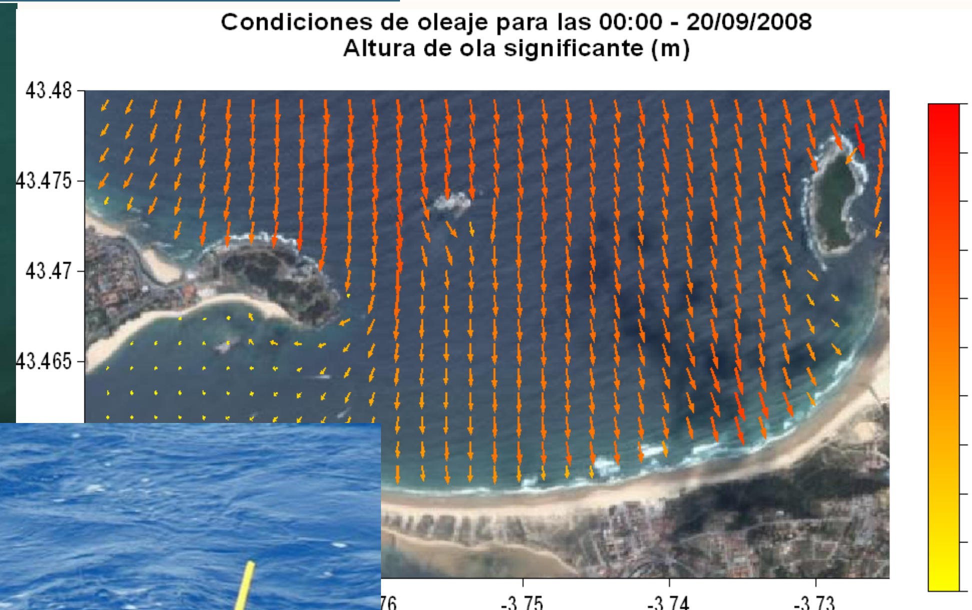
How it works

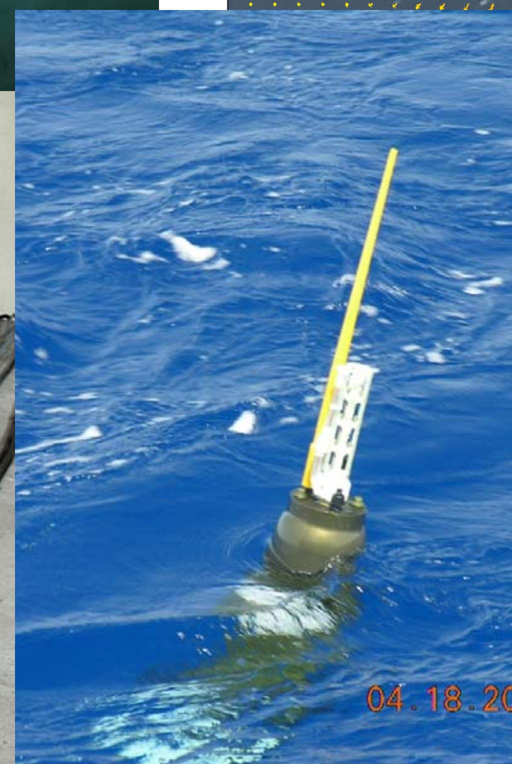


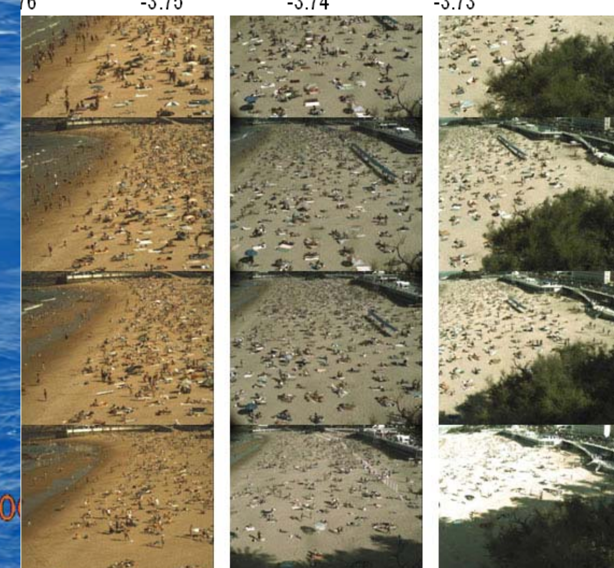
jawari.net

Deployment of Remote Instrumentation Infrastructure

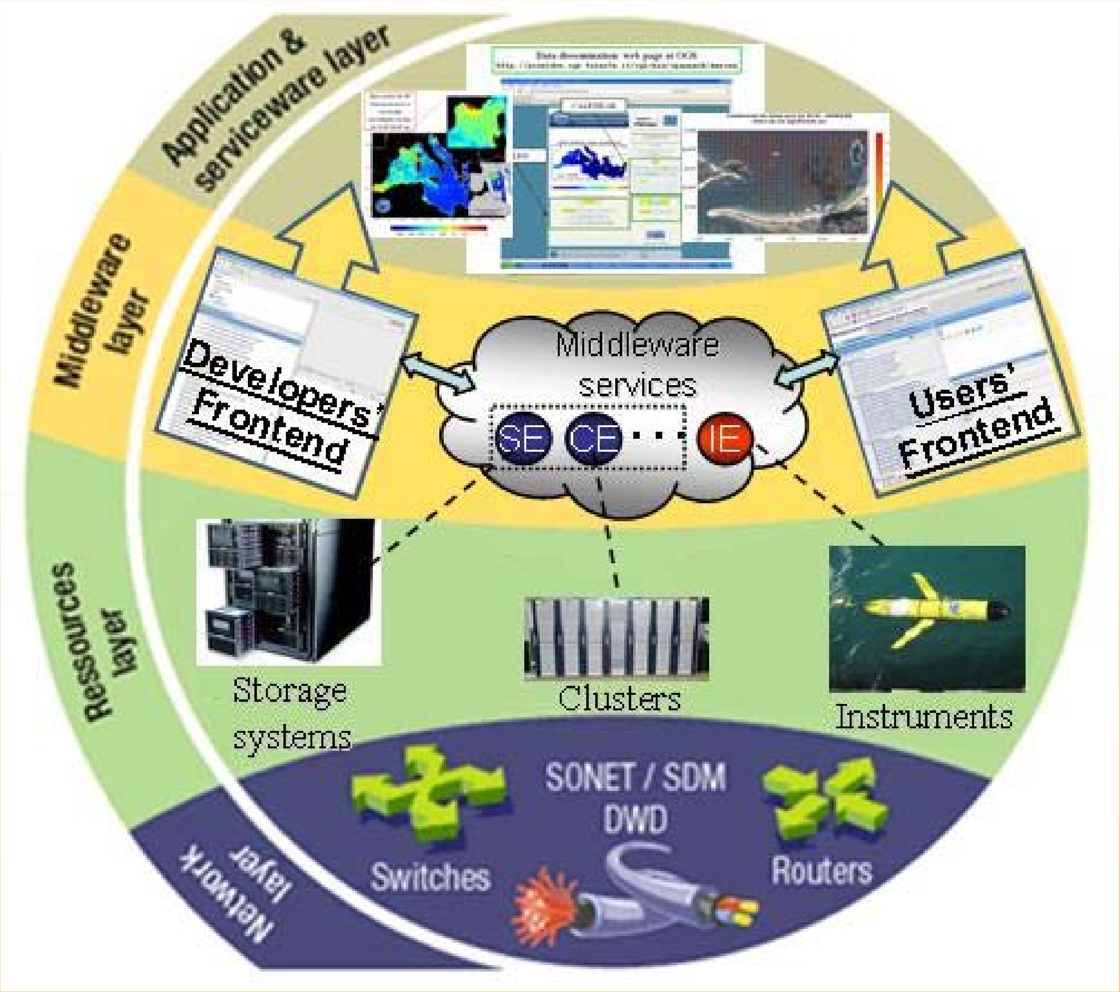








Remote Instrumentation Infrastructure



Applications: Oceanographic-, Earthquake-, Experimental-Science, Coastal-Observation

Middleware: adding Instrument Element support, basing on gLite, User/Developer support: VCR and g-Eclipse

Resources: Gilders, Floaters, Earthquake-Sensors, Cameras, Synchrotron, CEs, SEs, ...

Network: GEANT, Internet, Iridium, ...

The C3-Grid Project

Seamless Volume-optimized Access to Federated Climate Data

B. Fritzsch, S. Kindermann, A. Papaspyrou,
and the C3-Team

AWI Alfred-Wegener-Institut für Polar- und Meeresforschung

Deutsches Klimarechenzentrum

technische universität dortmund

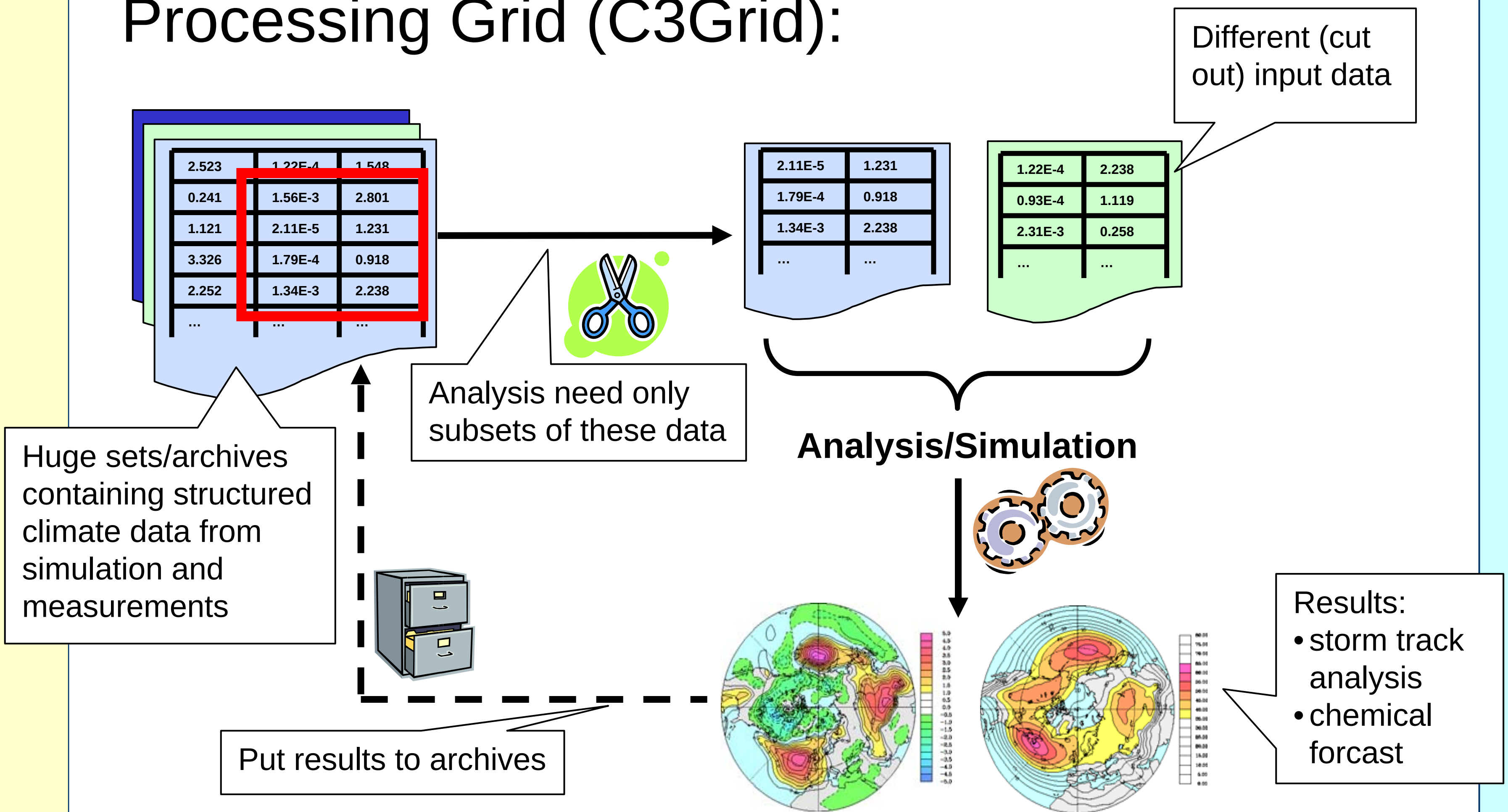
GEFÖRDERT VOM Bundesministerium für Bildung und Forschung

Grid Computing in Climate Research

- Earth System Science Applications
  - short term weather forecast
  - subsystem modelling
  - stormtrack analysis
- Current Situation
  - no coherent working environment
  - manual staging and transportation of relevant data
  - problem of heterogeneous resources, distributed data and different access policies
- Identfied requirements for C3Grid
  - fairly typical Grid Use Cases
  - but: some special characteristics
    - comprehensive metadata support
    - special structure of data

Scientific Workflow

Collaborative Climate Community Data and Processing Grid (C3Grid):



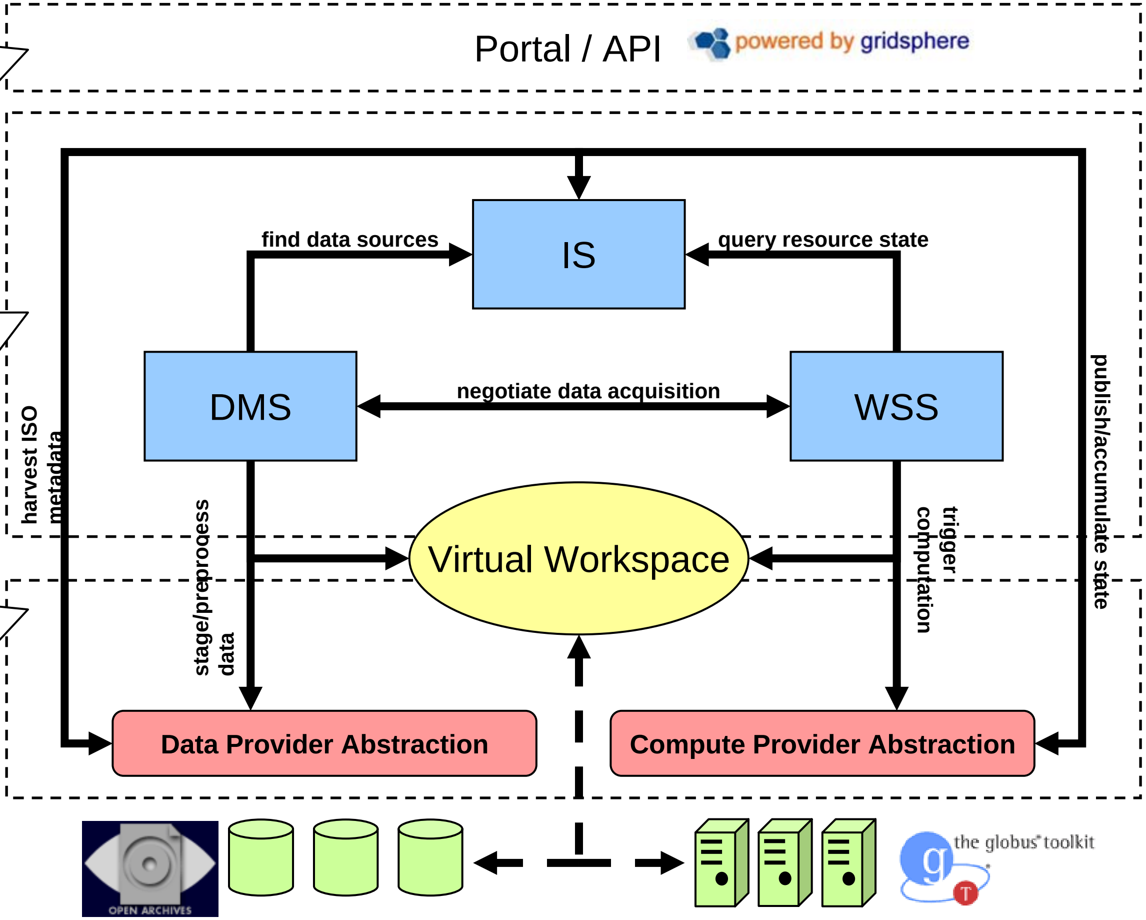
C3-Grid Architecture

General: Service Oriented Architechture (SOA)

Portal Layer:
- **interface for Grid user**
- **programming interface**

Middleware Layer:
- **distributed Grid infrastructure**
- **information and data related services**

Abstraction Layer:
- **data provider abstraction**
- **compute provider abstraction**



5 Posters

- Maintaining Reference Graphs of Globally Accessible Objects in Fully Decentralized Distributed Systems
  Bjoern Saballus, Thomas Fuhrmann

- Adaptive Run-time Prediction in Heterogeneous Environments
  Christian Glasner, Jens Volkert

- Performance Prediction Based on Hierarchy Parallel Features Captured in Multi-Processing System
  Jiaxin Li, Feng Shi, Ning Deng

- CLOUDLET: Towards MapReduce Implementation on Virtual Machines
  Shadi Ibrahim, Hai Jin, Bin Cheng, Song Wu, Haijun Cao, Li Qi

- Investigating Software Transactional Memory on big SMP machines
  Ruibo Wang