

# e-Science in a Virtual Laboratory

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# Outline

What is e-Science

Why is it important

How is it realized

Examples

Conclusions

# What is e-Science?

e-Science is enhanced science

# What is e-Science?

e-Science is enhanced science

# The what of e-Science

‘e-Science is about **global collaboration** in key areas of science, and the **next generation of infrastructure** that will enable it

John Taylor , 2001

# The what of e-Science

‘e-Science is about time and location independent global collaborative experimental science via sharing of facilities exploiting the next generation of (inter)national infrastructure that will enable it

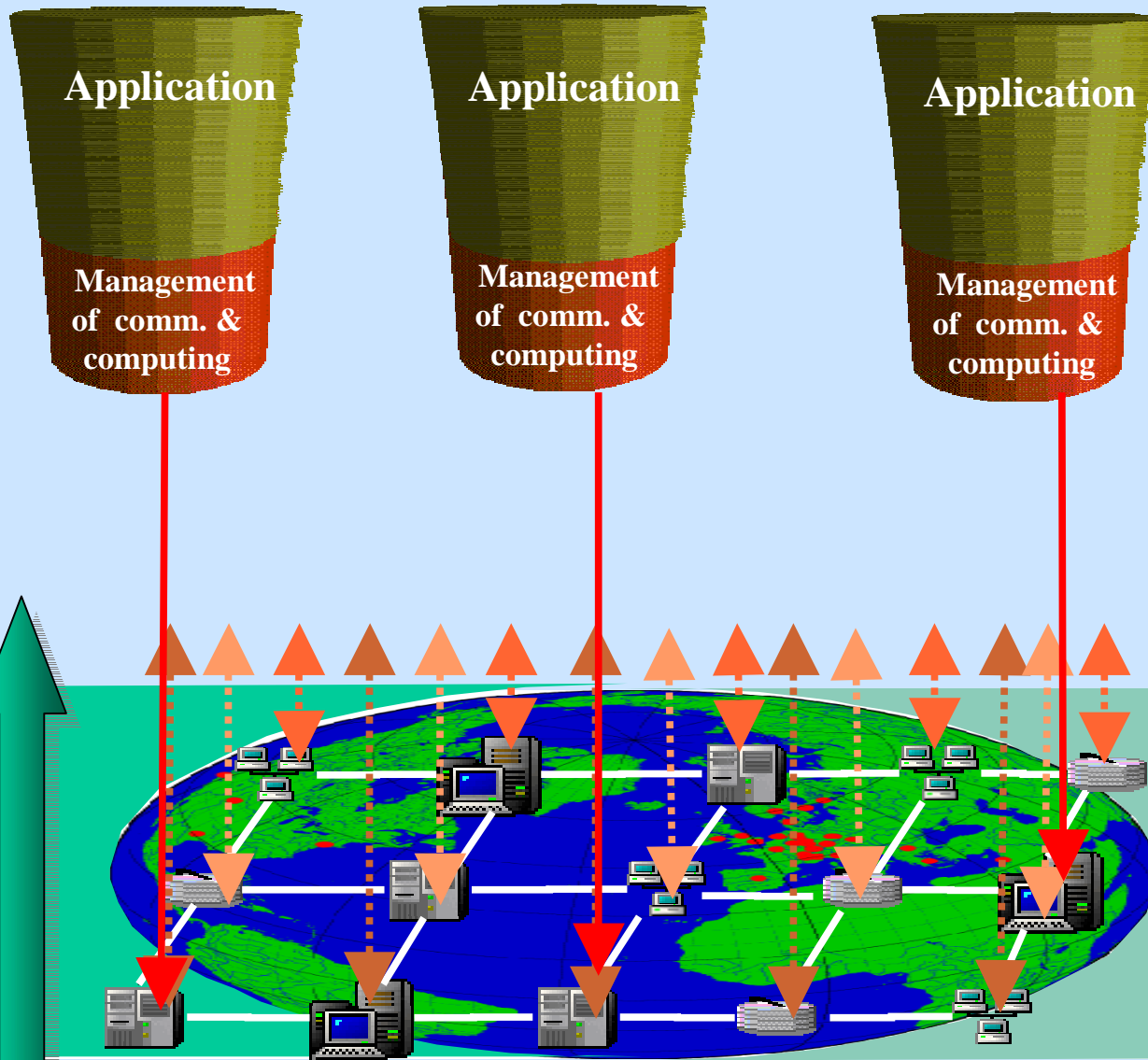
Bob Hertzberger (VL-E) , 2003

# The what of e-Science

- WEB was about **exchanging information**
- e-Science is about **sharing resources applying Grid:**
  - ✓ Experimental facilities
  - ✓ Data & Information repositories
  - ✓ Application services

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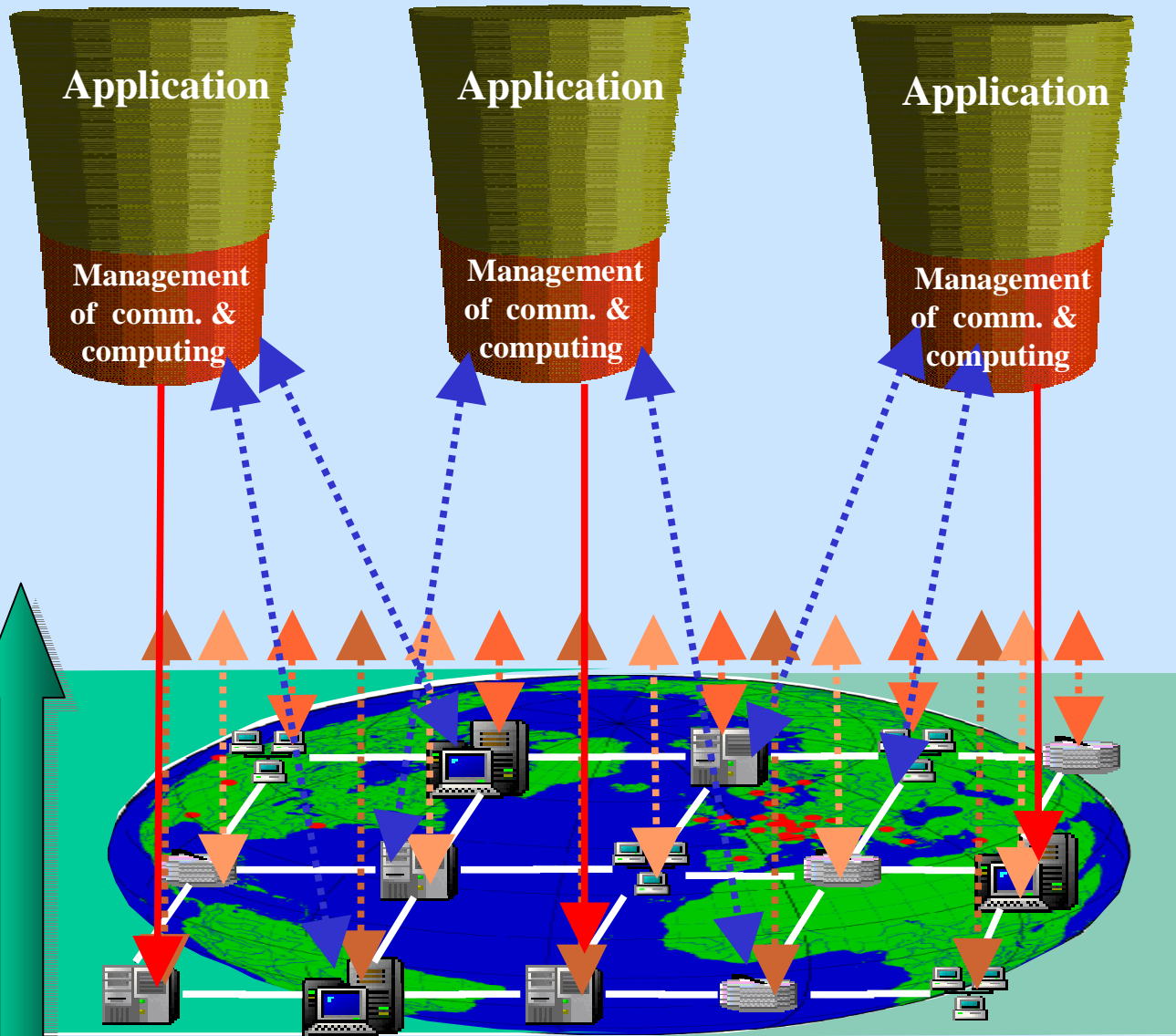
*Technology push*





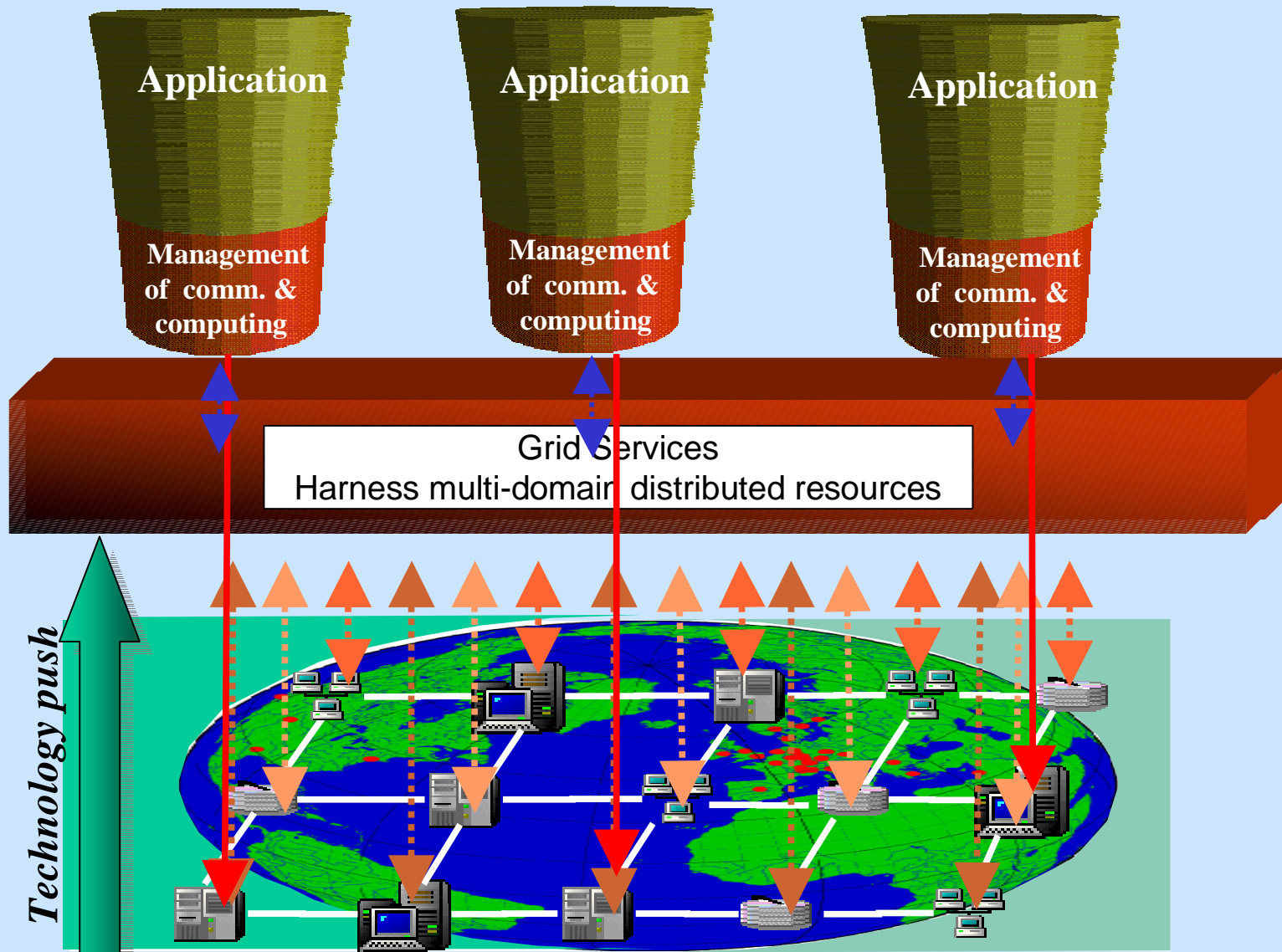
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*Technology push*



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Technology push



# The why of e-Science

‘e-Science will change the dynamic of  
the way science is undertaken’

John Taylor , 2001

# The Why of e-Science

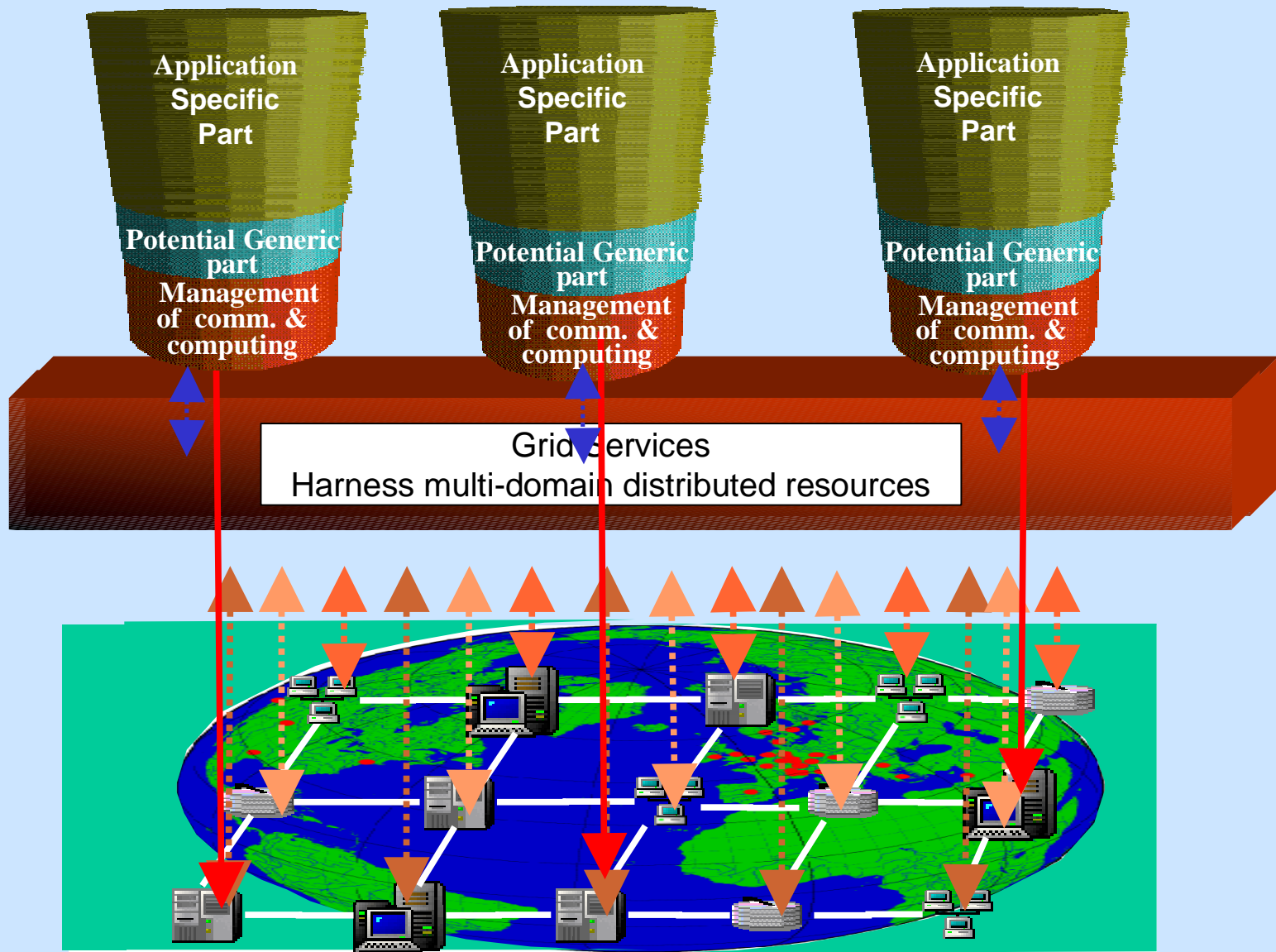
- Increased complexity of experiments results in:
  - ✓ More demands for multi-disciplinarity
  - ✓ Increased amounts & distribution of data and information
  - ✓ Increased complexity of:
    - ✓ analysis tools
    - ✓ variety of data & information

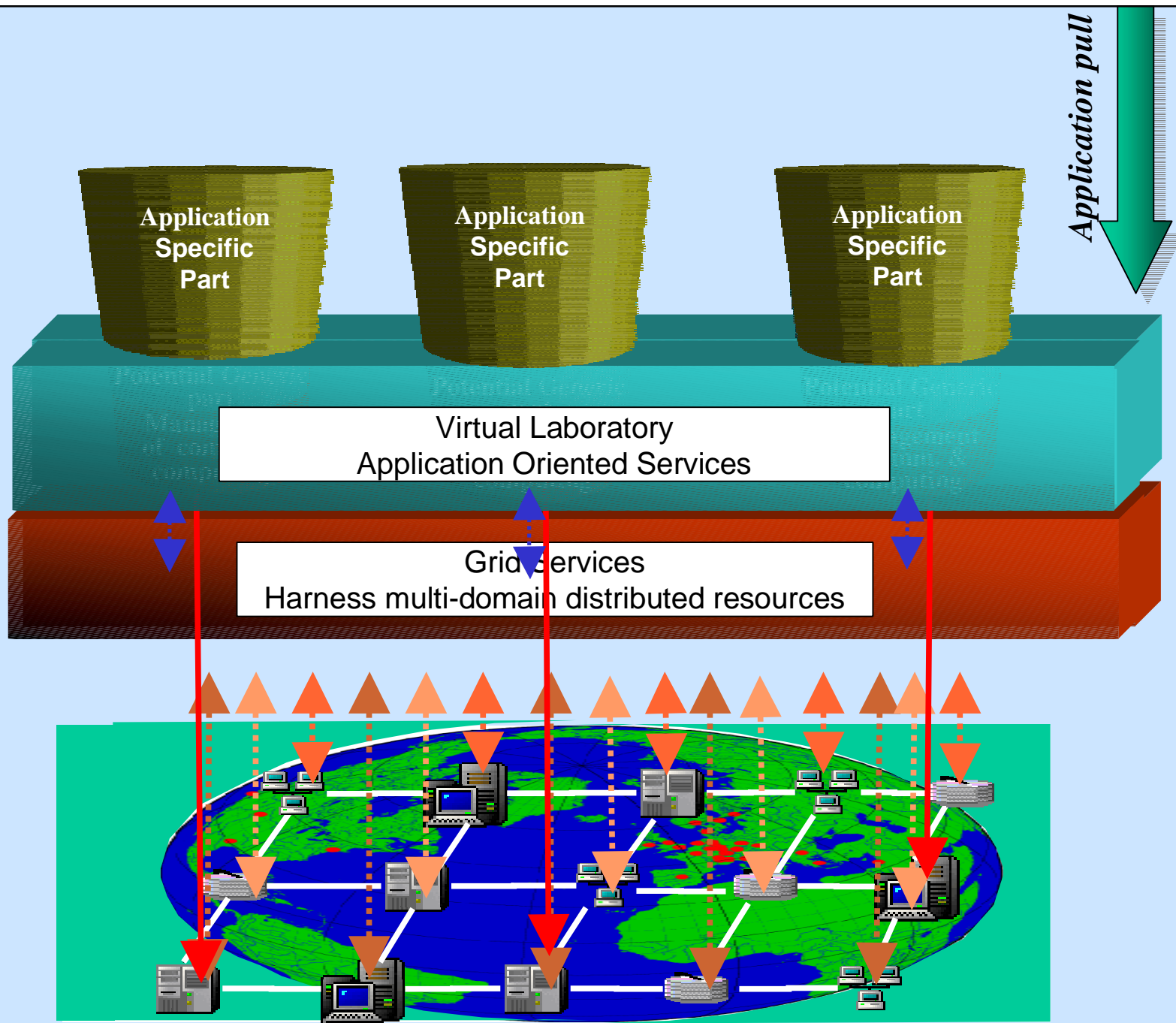
# Role e-Science in society

- Increased complexity of society
  - ✓ Science initiator of new solutions
  - ✓ Solutions become part of data driven society
    - Distribution of data & information sources
    - Access towards more & larger variety of data & information (multimedia)

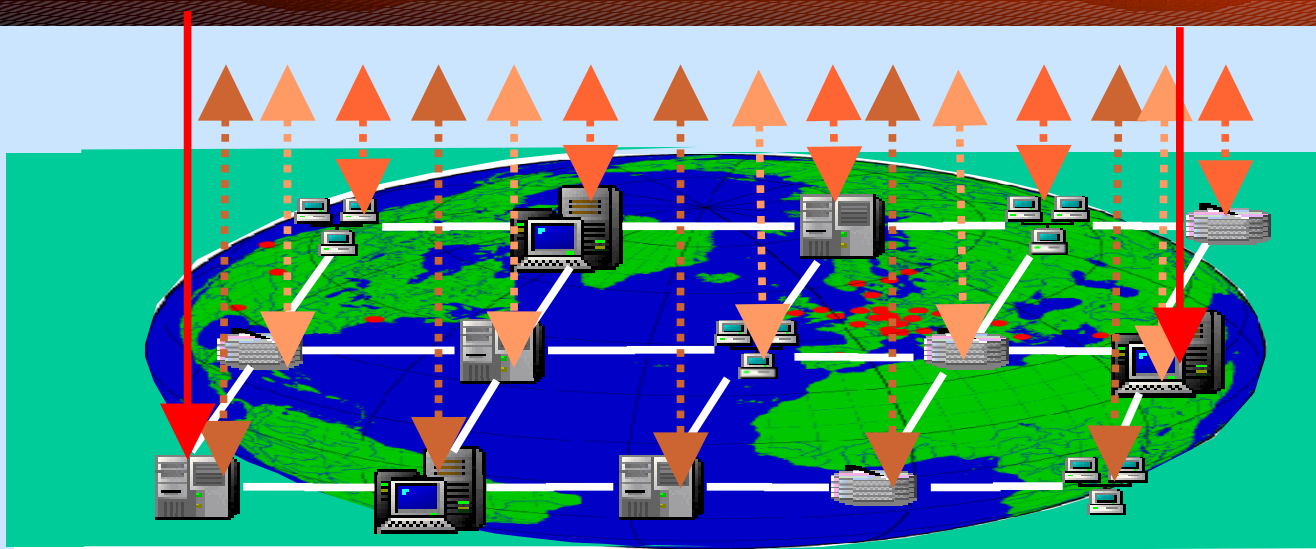
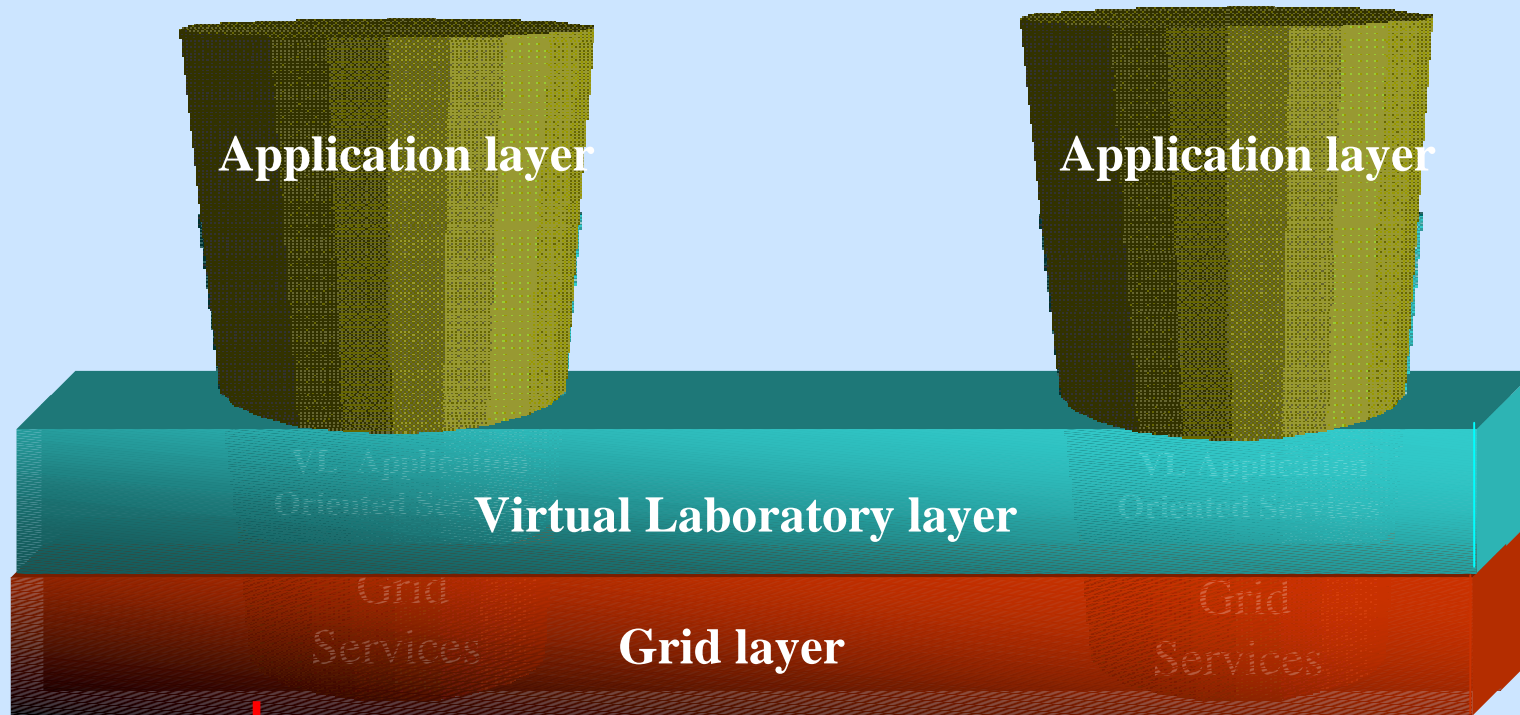
# The How of e-Science

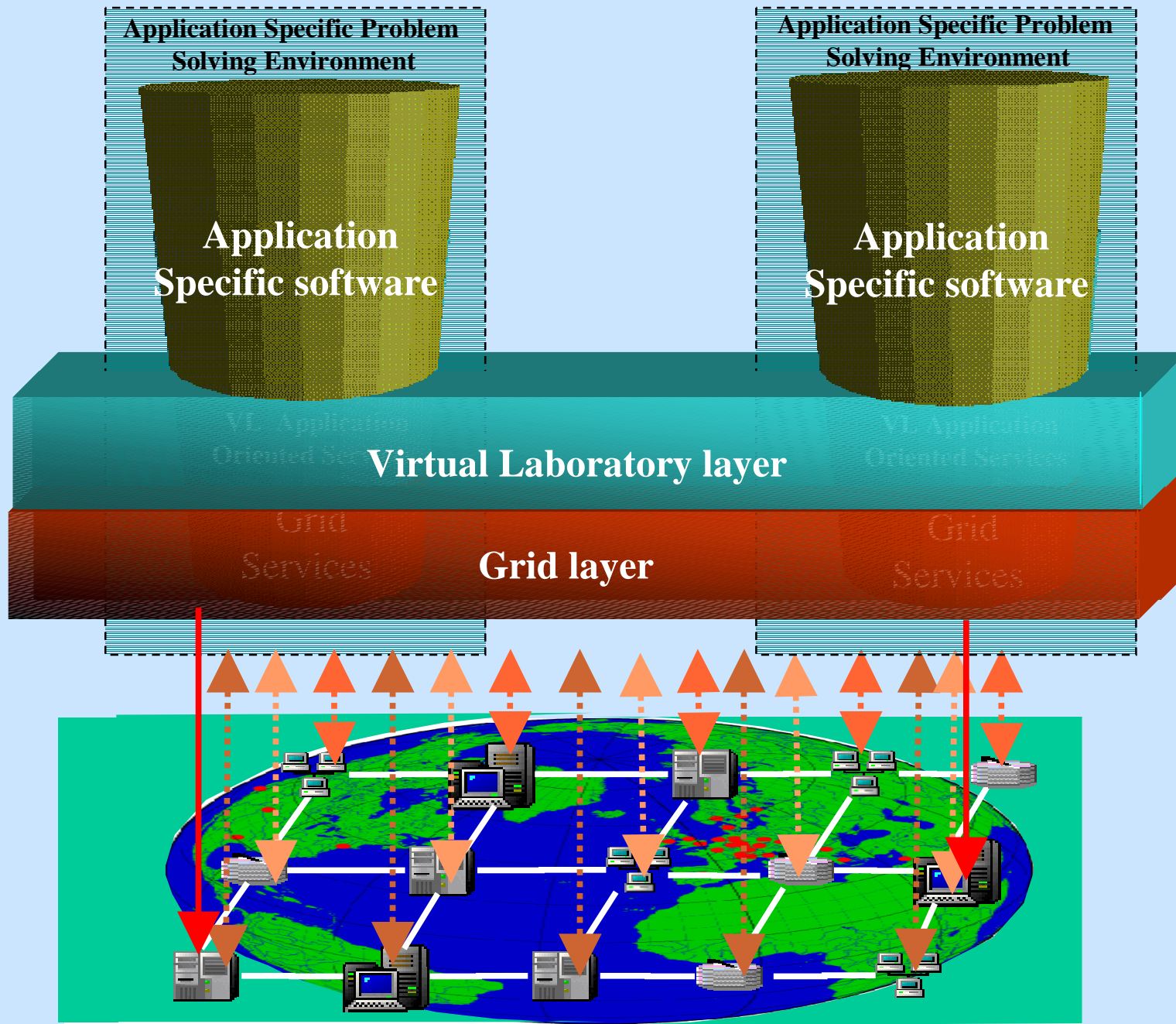
- Multi-disciplinary activity between:
  - ✓ Domain scientist
  - ✓ ICT scientist
- Combining human expertise & knowledge
- Next generation infrastructure is differentiator
- For us via VL methodology

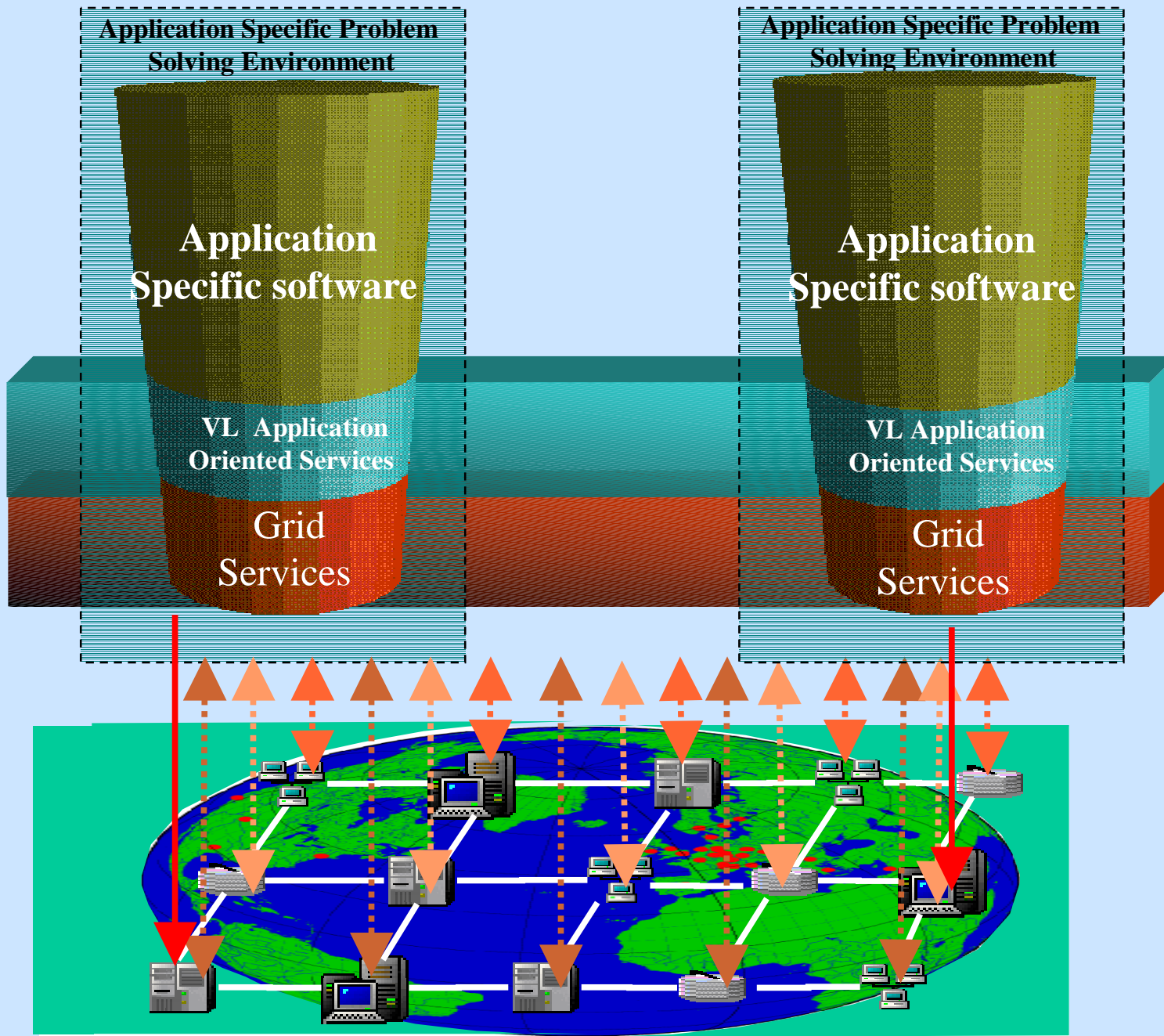


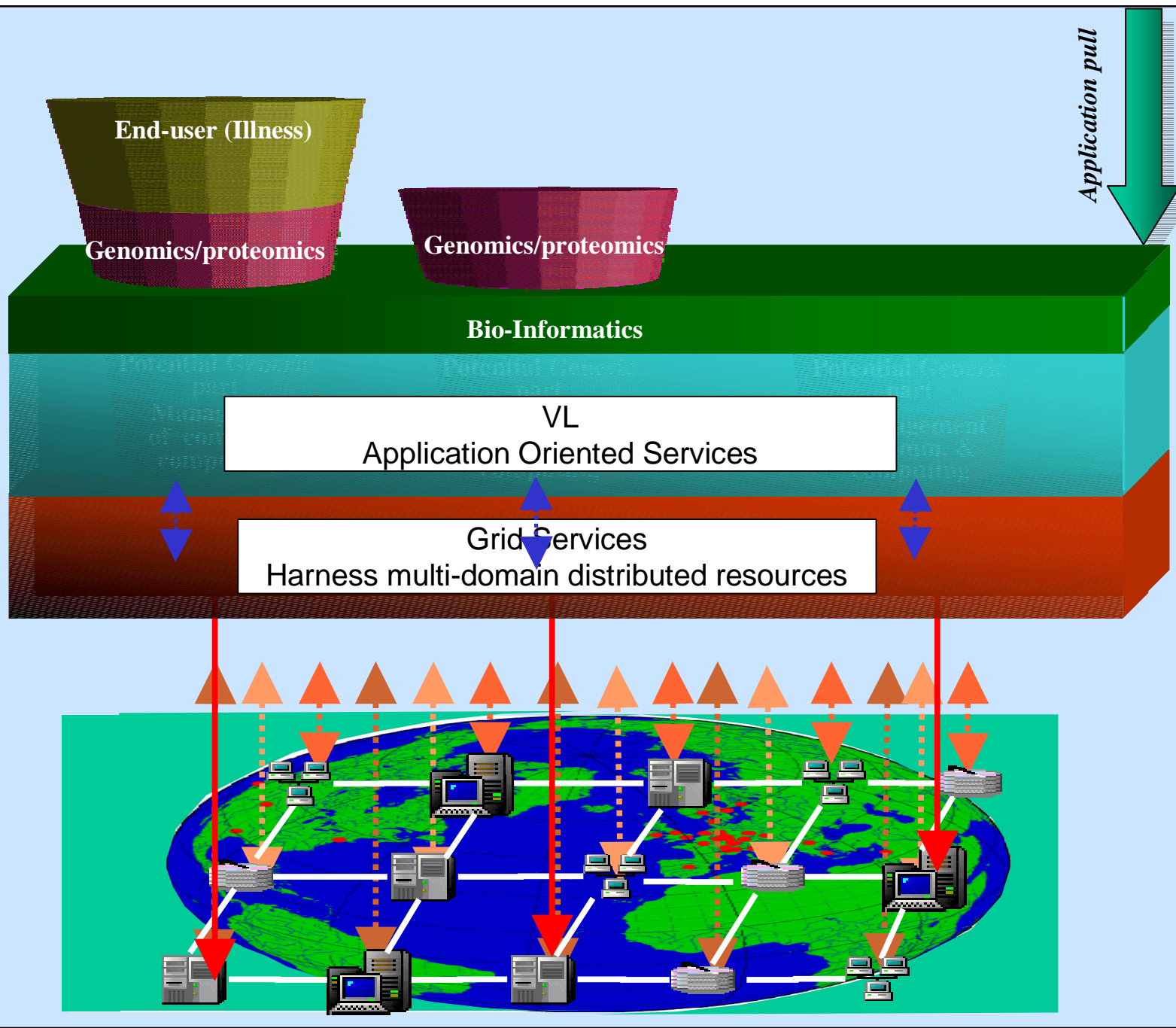


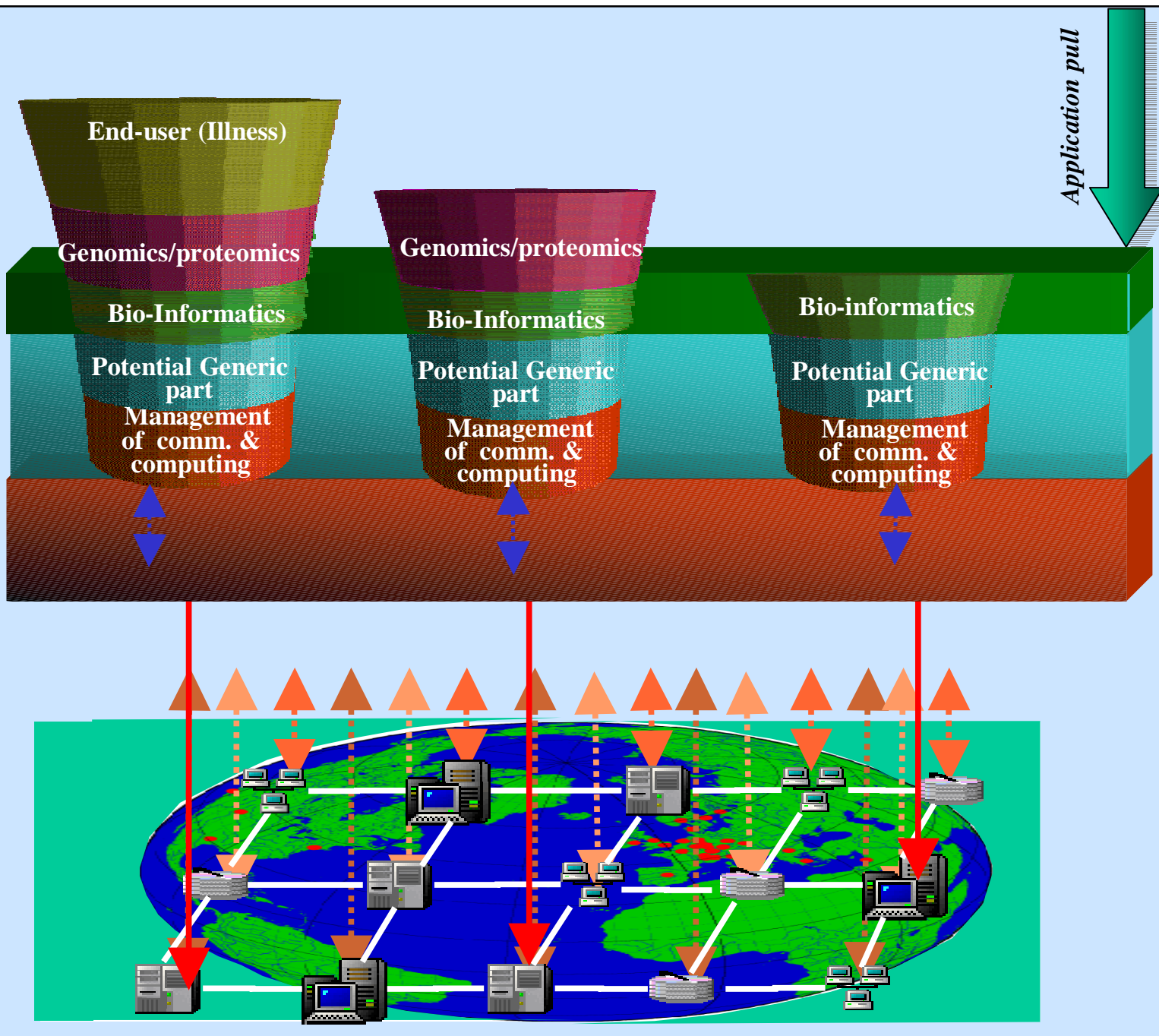




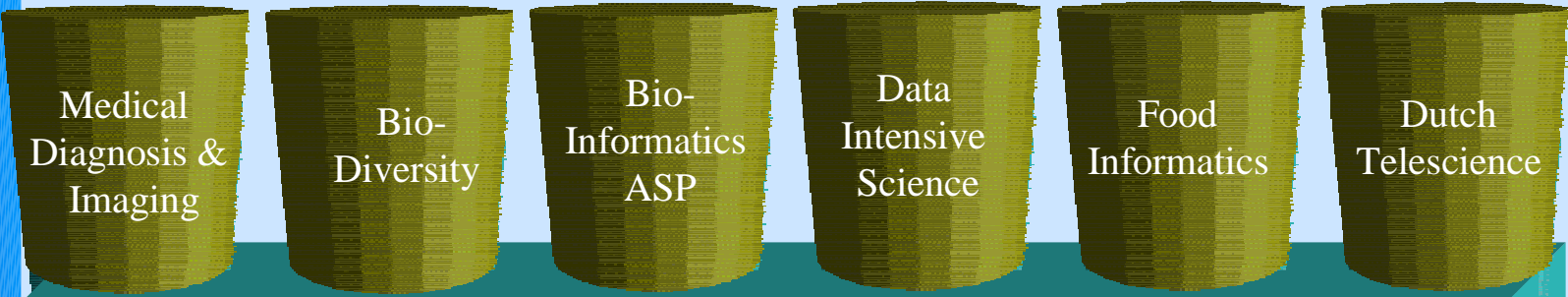






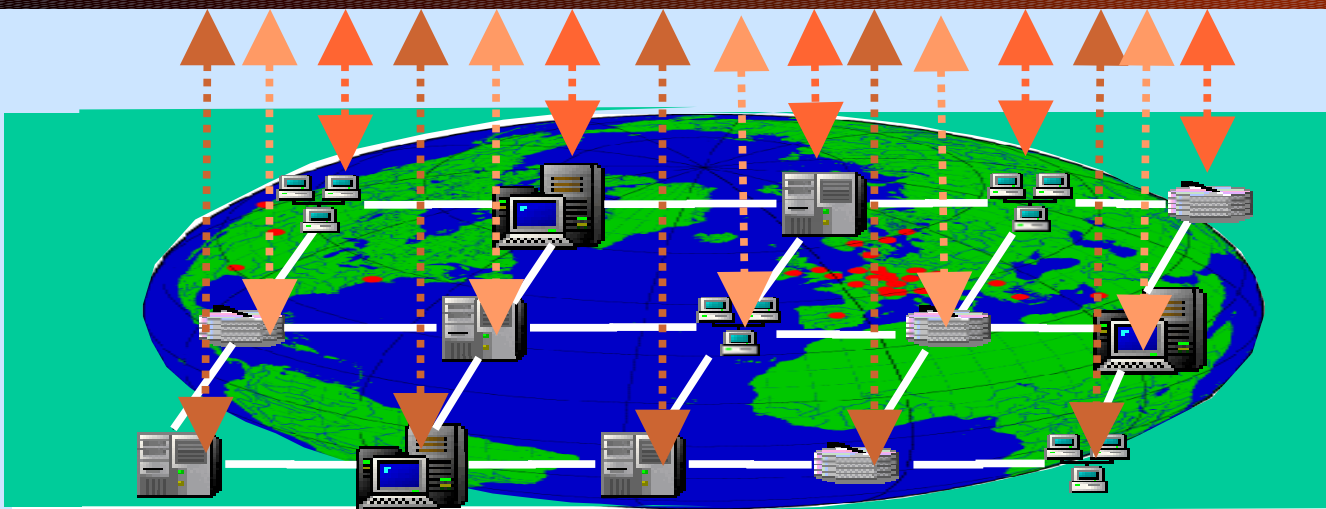


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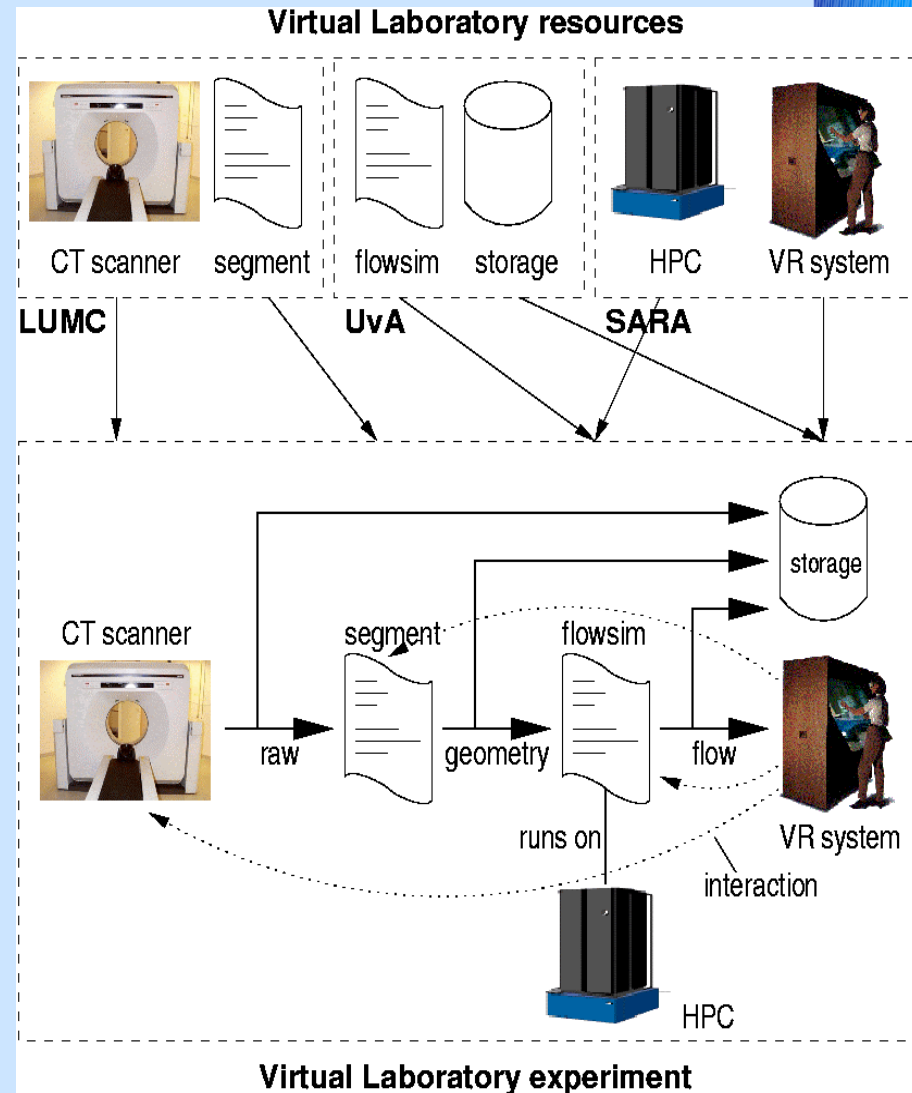
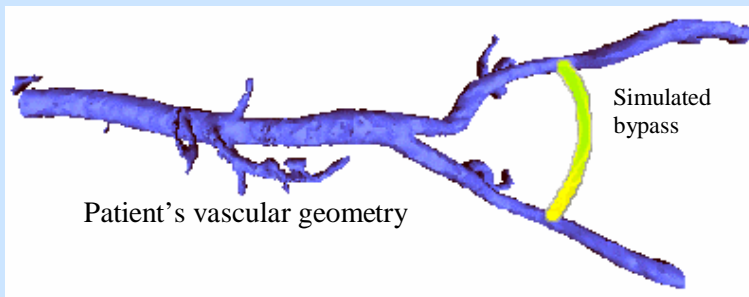
VL  
Application Oriented Services

Grid Services  
Harness multi-domain distributed resources



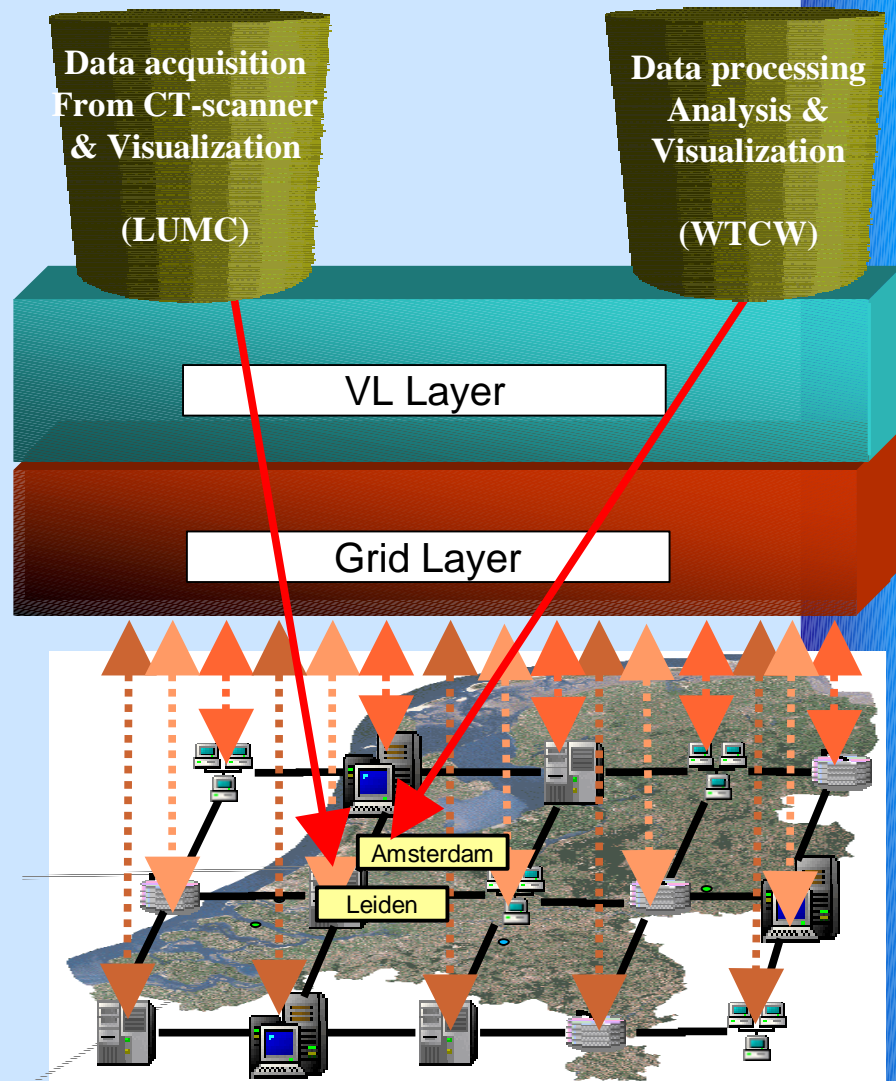
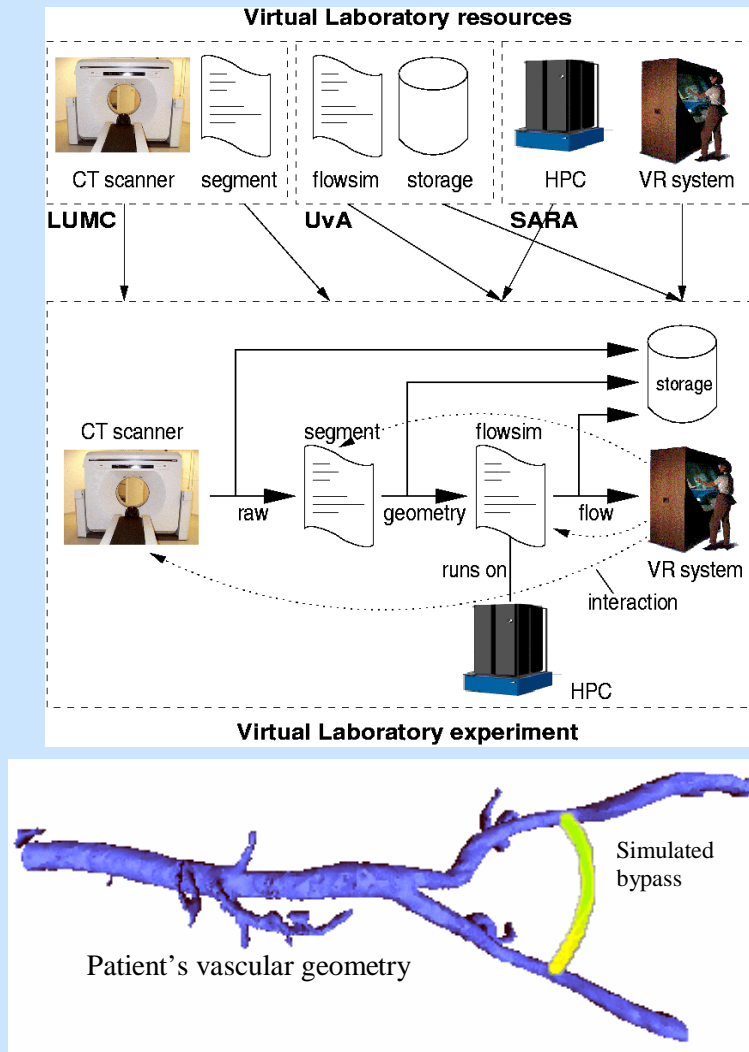
# Simulated Vascular Reconstruction (Example)

- *Simulated Vascular Reconstruction in a Virtual Operating Theatre*
  - patient specific vascular geometry
  - blood flow simulation
  - pre-operative planning
- In cooperation with Leiden University Medical Center (LUMC, prof. Reiber)



# Simulated Vascular Reconstruction (Example)

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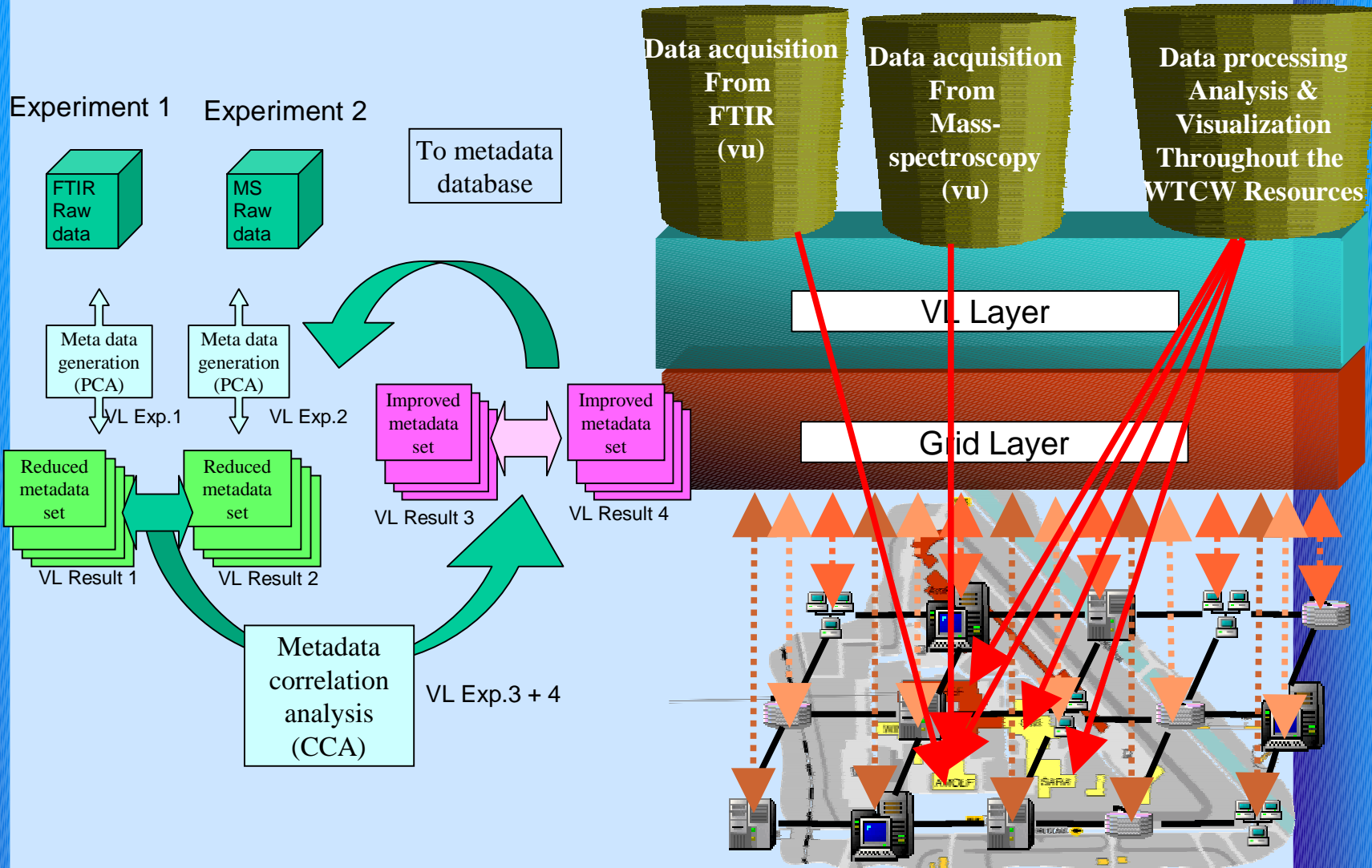
The anatomy of a painting:  
*Scrutinizing Rembrandt in multiple dimensions*



*The anatomy lesson of dr. Tulp, Rembrandt (1632), Mauritshuis, Inv nr. 146*

# MACS: Material Analysis of Complex Surface

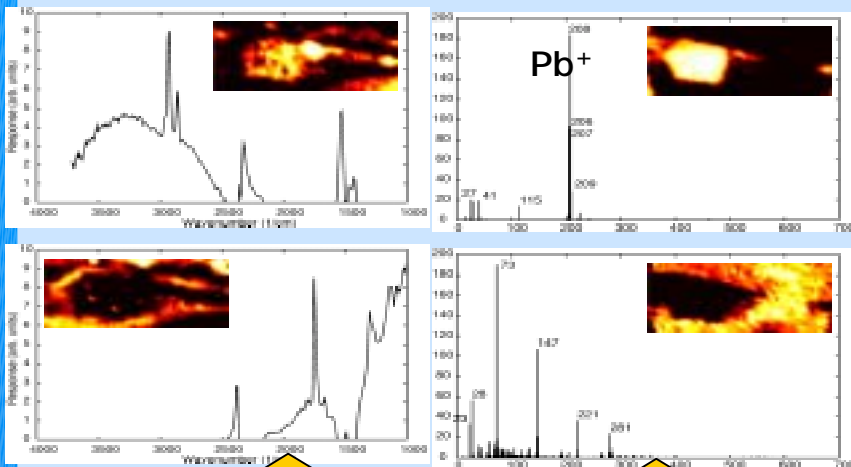
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### Principal Component Analysis

FTIR PC1 43.0% var

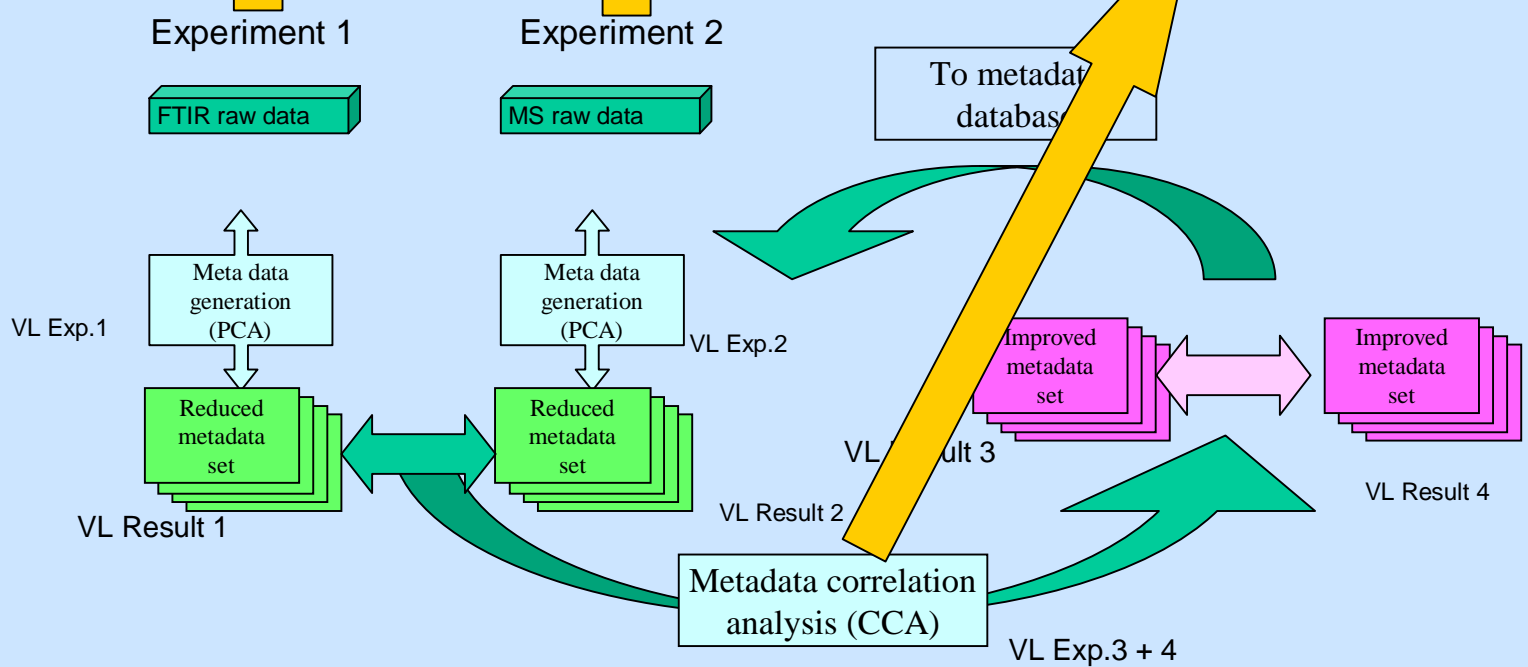
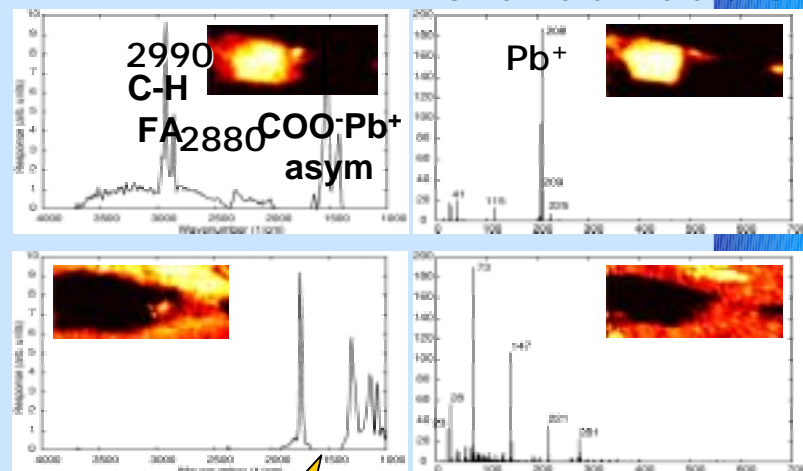
TOF-SIMS PC1 6.1% var



### Canonical Correlation Analysis

FTIR CV1 15.9% var

TOF-SIMS CV1 5.6% var



# VLAM-G

## Virtual Laboratory AMsterdam

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A collaborative analysis environment  
for applied experimental science

# Objectives

- Enable VLAM-G users to **define, execute, and monitor** their experiments
- Provide to VLAM-G users:
  - ✓ location independent experimentation,
  - ✓ familiar experimentation environment
  - ✓ assistance during their experiments
  - ✓ Easy way to bring/port new/existing applications to the Grid
- Developing application prototypes to check ideas and to learn

# Experiment Steps



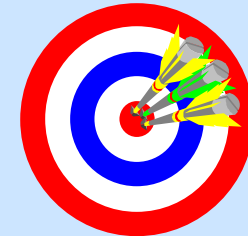
*designing the  
experiment*



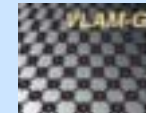
*performing the  
experiment*



*analyzing the  
experiment results*



*Success*



# Realization Methods

- Application layer
  - ✓ Case studies
- Virtual Laboratory layer
  - ✓ Provides VLAM-G modules
  - ✓ Offers an information management system
- Grid Layer

# VIMCO: **V**irtual **L**aboratory **I**nformation **M**anagement for **CO**-operation

## *Assisting Information Federation*

- VIMCO objectives for **scientists**:
  - ✓ *Assistant*
  - ✓ *Enabler / Facilitator*
- VIMCO objectives for **VLAM-G**:
  - ✓ *Service & Session Information Manager*

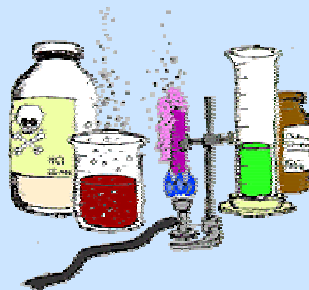
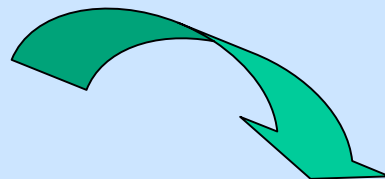


# Experiment Steps & Difficulties



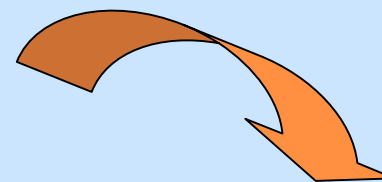
*designing the  
experiment*

*Knowledge and Expertise!  
Experiment Archiving!*



*performing the  
experiment*

*Information Organization!  
Logging Information/Data!*

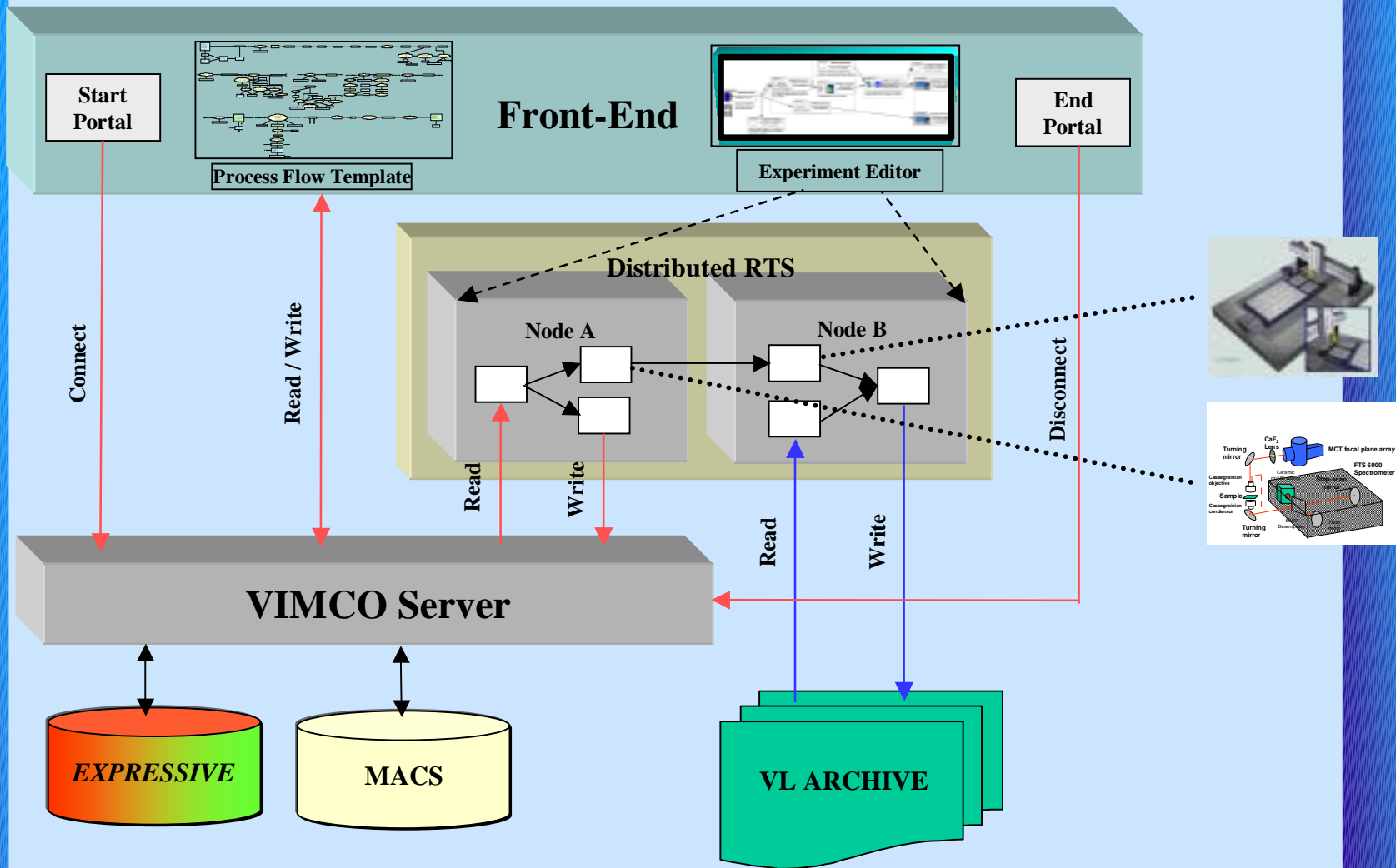


*analyzing the  
experiment results*

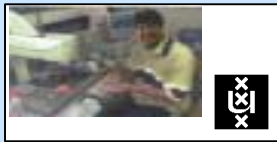
*Approach to Data  
Analysis and Tools!*

# Experimentation in VLAM-G

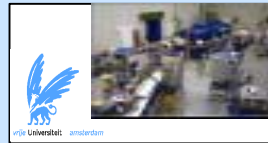
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# VLAM-G Experimentation Environment Data Model



DNA micro-array  
experiment

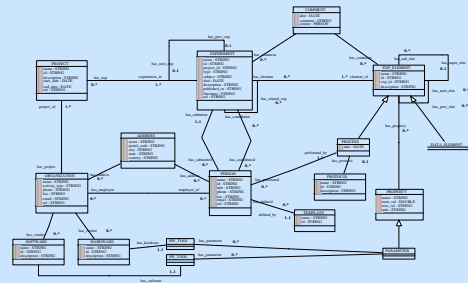
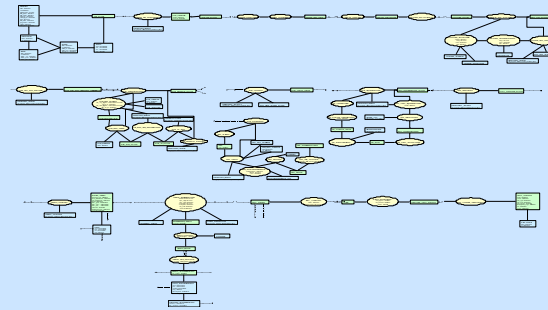


Micro-beam  
experiment

*Common aspects of  
an experiment*



*Process and data flow  
in an experiment*



Experimentation Environment  
Data Model

**Process Flow Template**

*Annotations on an  
experiment*



Application databases

# Assistant for Scientists Information Presentation

## Process-Flow Template

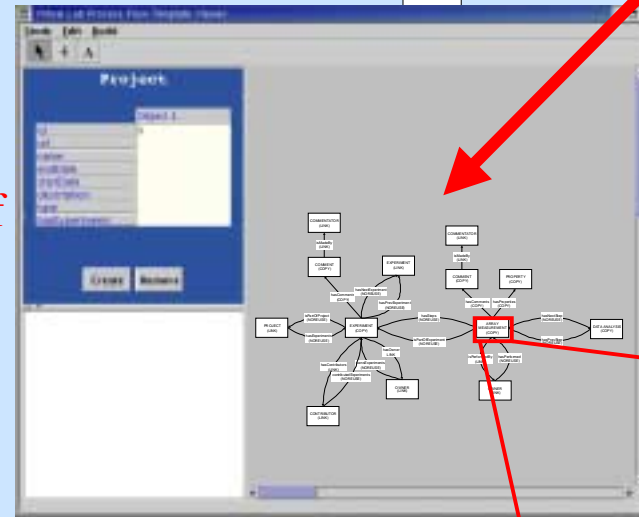
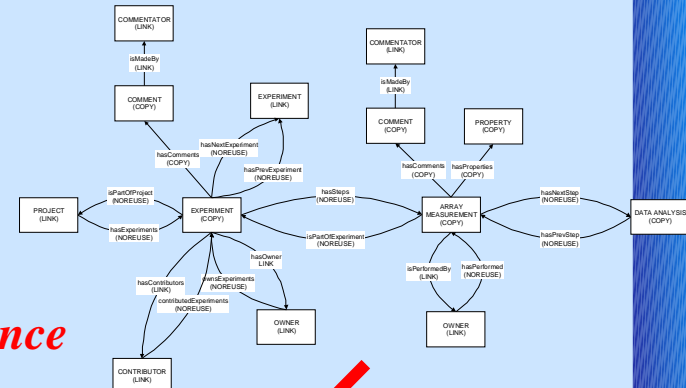
- Graphical representation of **data elements** and **processing steps** in an **experimental procedure**
- Information to support **context-sensitive assistance**

## Study

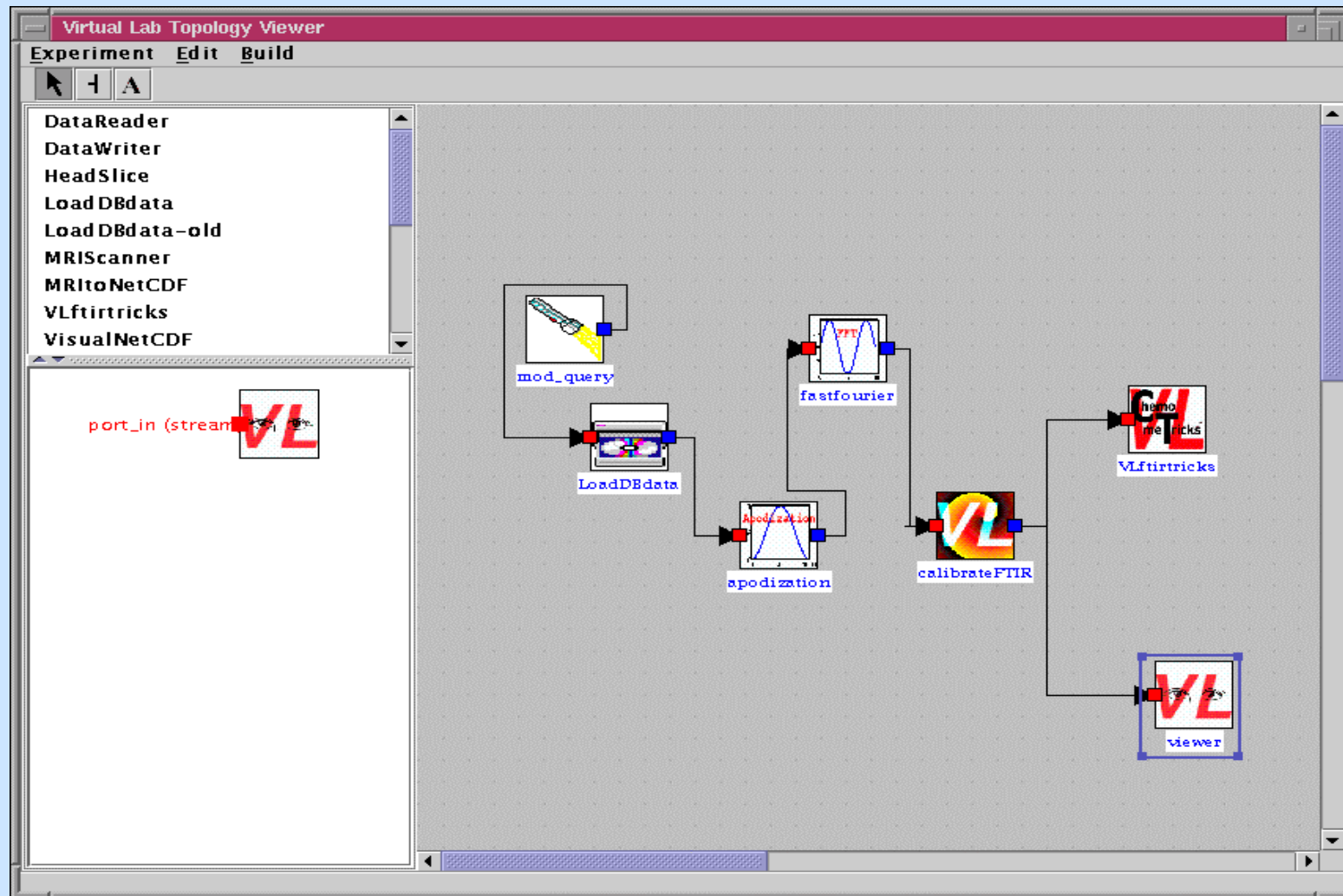
- Descriptions of experimental steps represented as an **instance of a PFT** with references to experiment topologies

## Experiment Topology

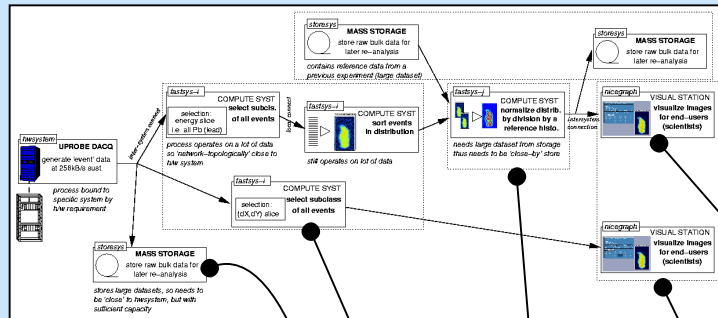
- Graphical representation of **self-contained data processing modules** attached to each other in a **workflow**



# Snapshot of the VLAM-G experiment editor/viewer



# Porting the Experiments to the Grid



*Experiment Editor* allows the user to attach a set of software modules to define the execution workflow.

*RTS* executes the modules in the workflow on the Grid in a distributed manner using the Globus toolkit

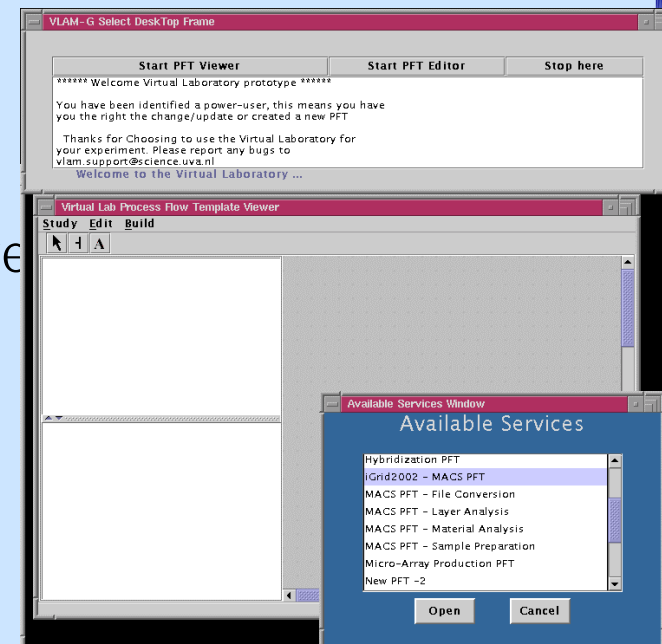
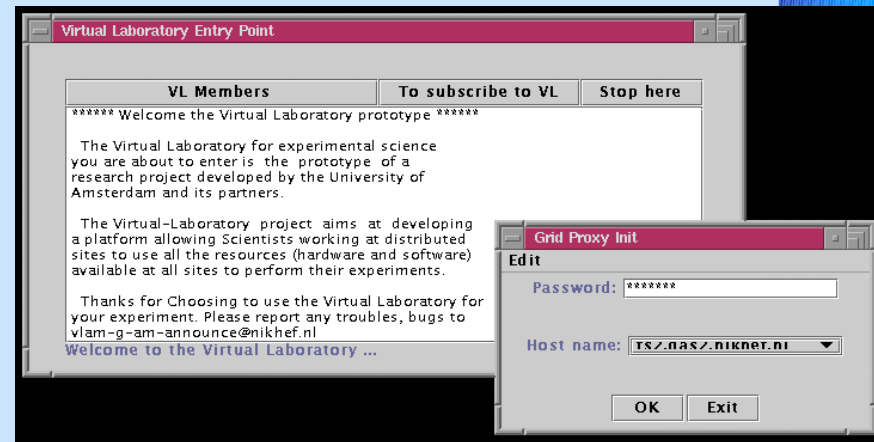
VLAM-G Run Time System

Grid / Globus Services

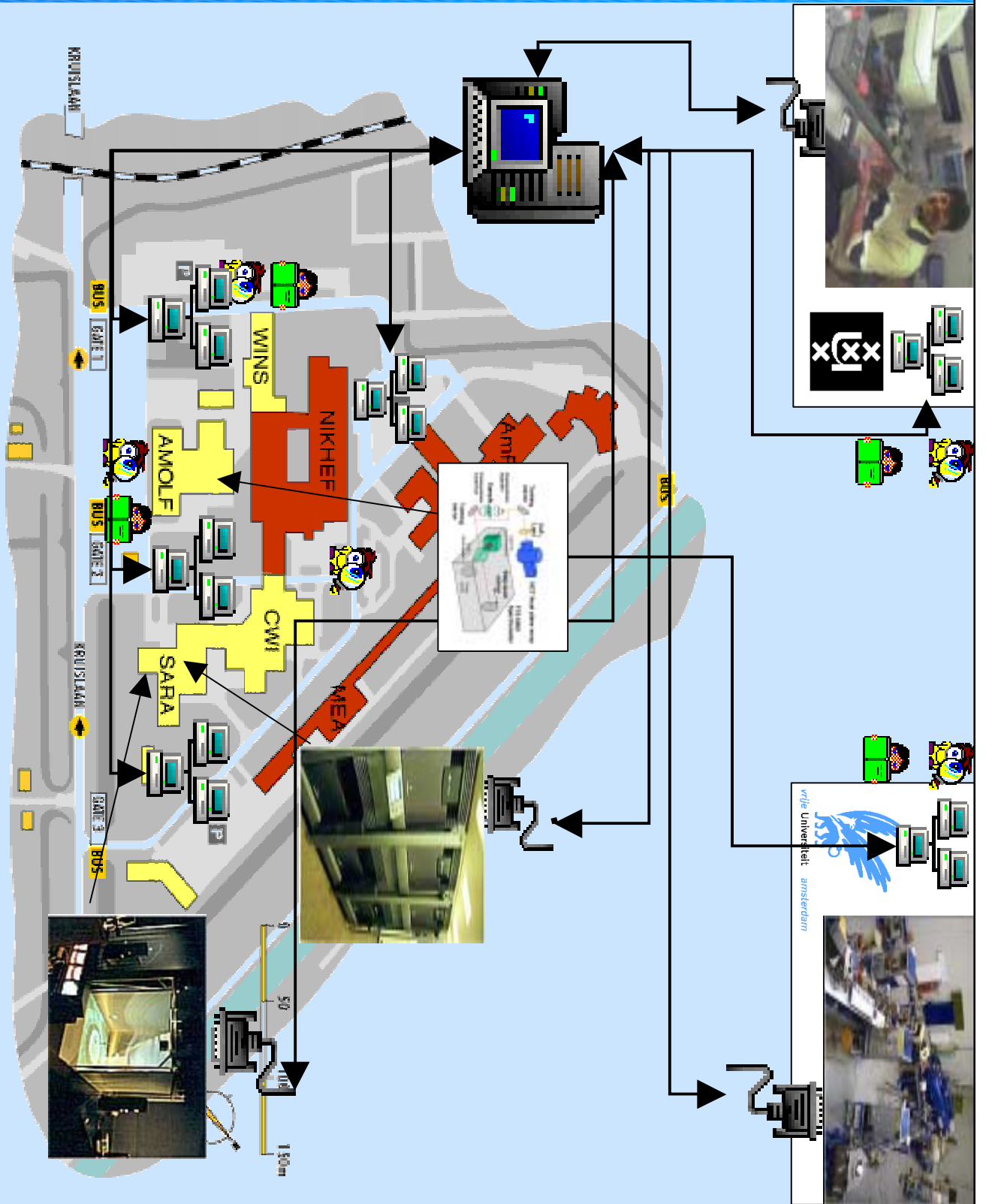


# Using VLAM-G toolkit

1. User **logs-on** to VLAM
  - ✓ VLAM Middleware
  - ✓ User Interface
  - ✓ Authentication
2. Select a service
  - ✓ Web-based interface to access the VLAM resources
    - Physical devices,
    - specialized-analysis software
    - etc.



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# Conclusion

- e-Science model & work has to include whole technology chain
  - ✓ Application
  - ✓ Virtual Laboratory
  - ✓ Grid
- Application cases provide feedback to generic layer
- Workflow analysis very useful to capture knowledge
- Content Management: VLAM-G middleware

# Thanks to

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# Participants

