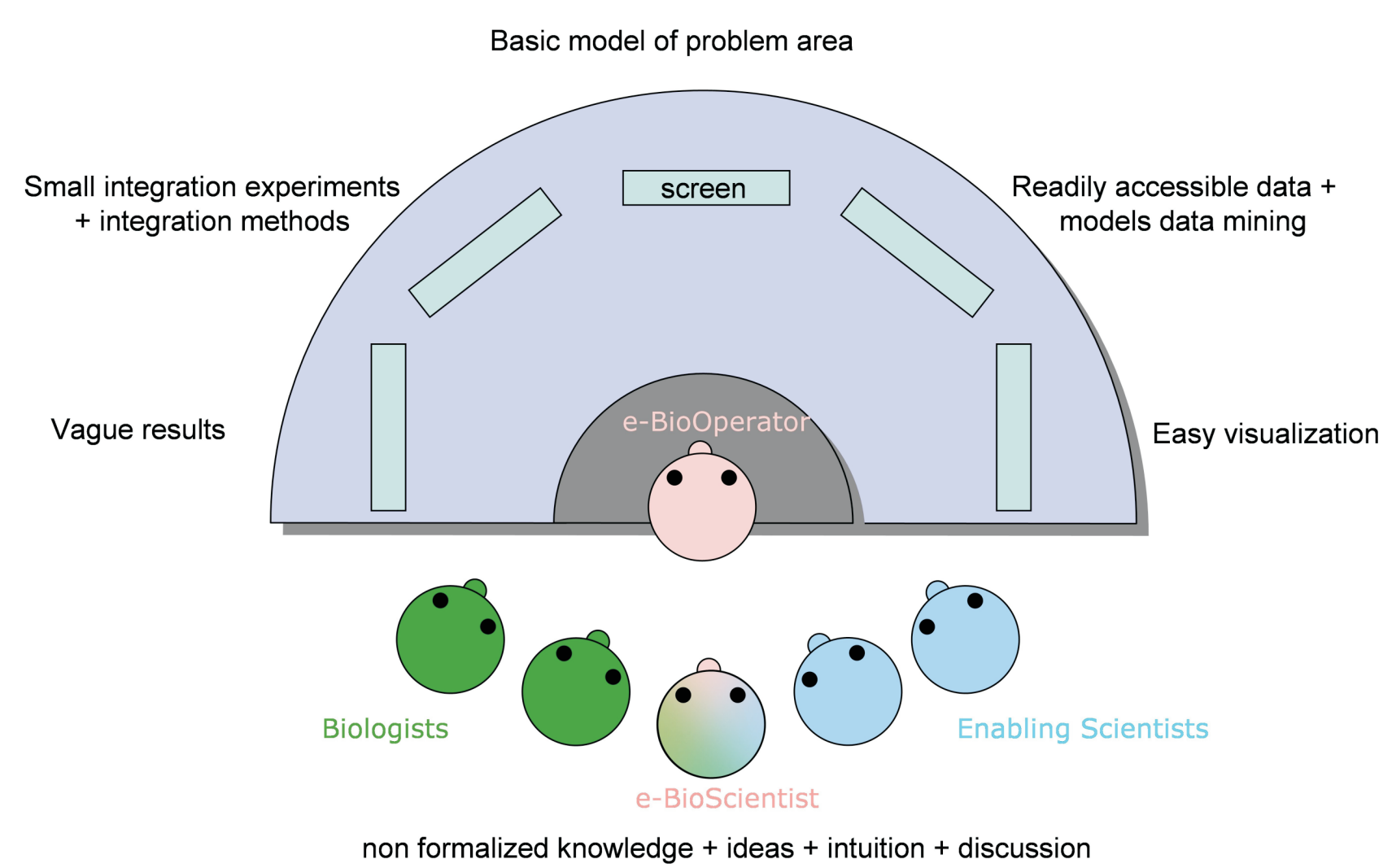# E-BioLabs: e-BioScience laboratories for enhancing 'omics' research

Han Rauwerda[1],Wim de Leeuw[1], Jorrit Adriaanse[2], Paul van der Vet[3],
Maurice Bouwhuis[2], Timo M. Breit[1]

[1]Integrative Bioinformatics Unit, Swammerdam Institute for Life Sciences, University of Amsterdam, 1098 SM, Amsterdam, SARA, Kruislaan 415, 1098 SJ, Amsterdam, [3]HMI Group, University of Twente, Enschede, The Netherlands.

Basic Concept

Basic model of problem area

Small integration experiments + integration methods — screen — Readily accessible data + models data mining

Vague results — e-BioOperator — Easy visualization

Biologists — e-BioScientist — Enabling Scientists

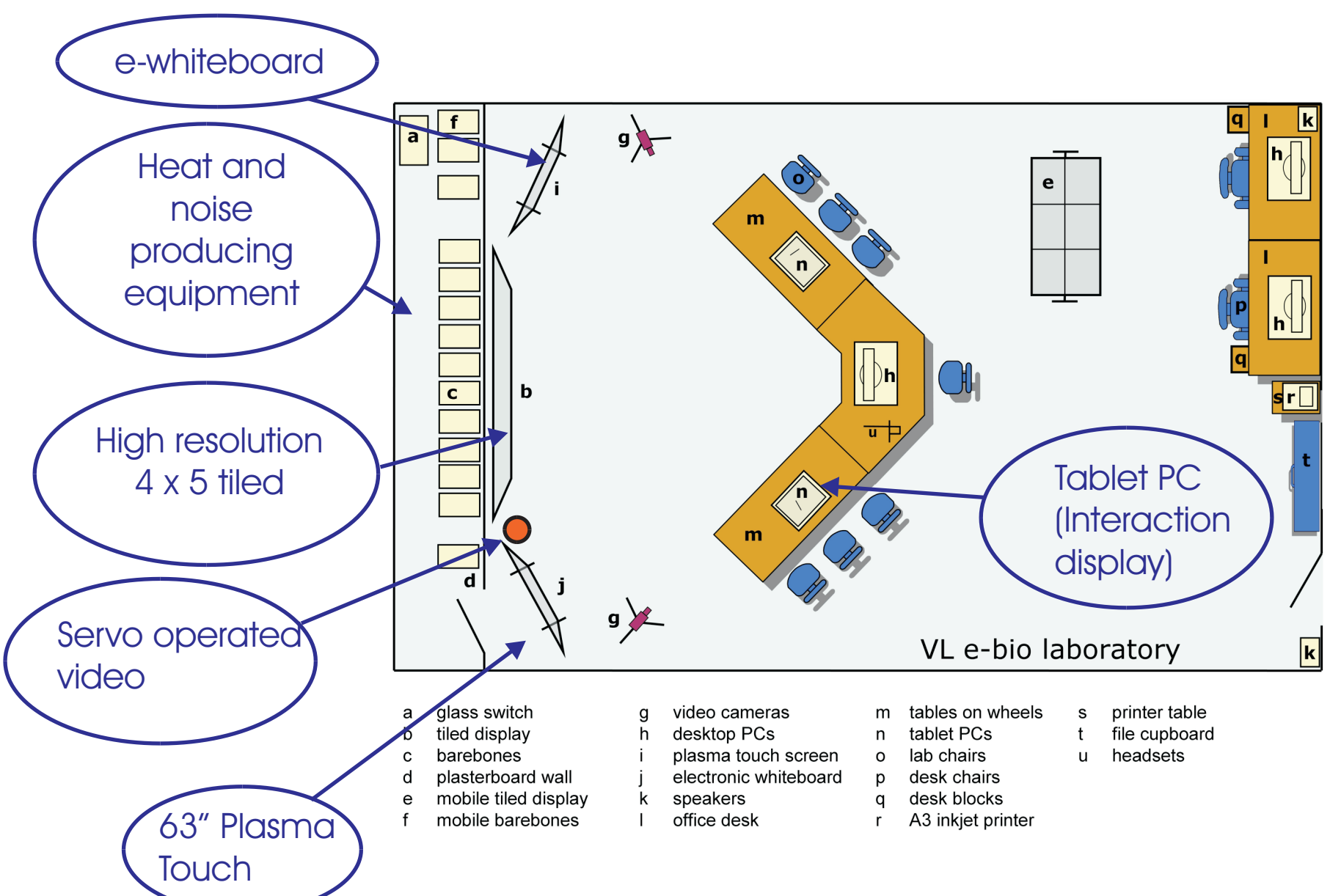non formalized knowledge + ideas + intuition + discussion

E-BioLab ~ a Collaborative Working Environment

- A *physical space* in which scientists enjoy working
- A room to discuss analysis results in the context of a biological question by *visualization*
  - equipped with *Problem Solving Environments* for a number of scientific domains
    - analysis tools and methods made available
    - visualizations can be produced (semi)-instantenously
    - integration of tools and methods (workflows)
- Allows to separate data manipulation and discussion by:
  - production of visualizations by e-BioLab operator
  - advanced automation (workflows)
- Keep track of discussions by e-BioLab Journal
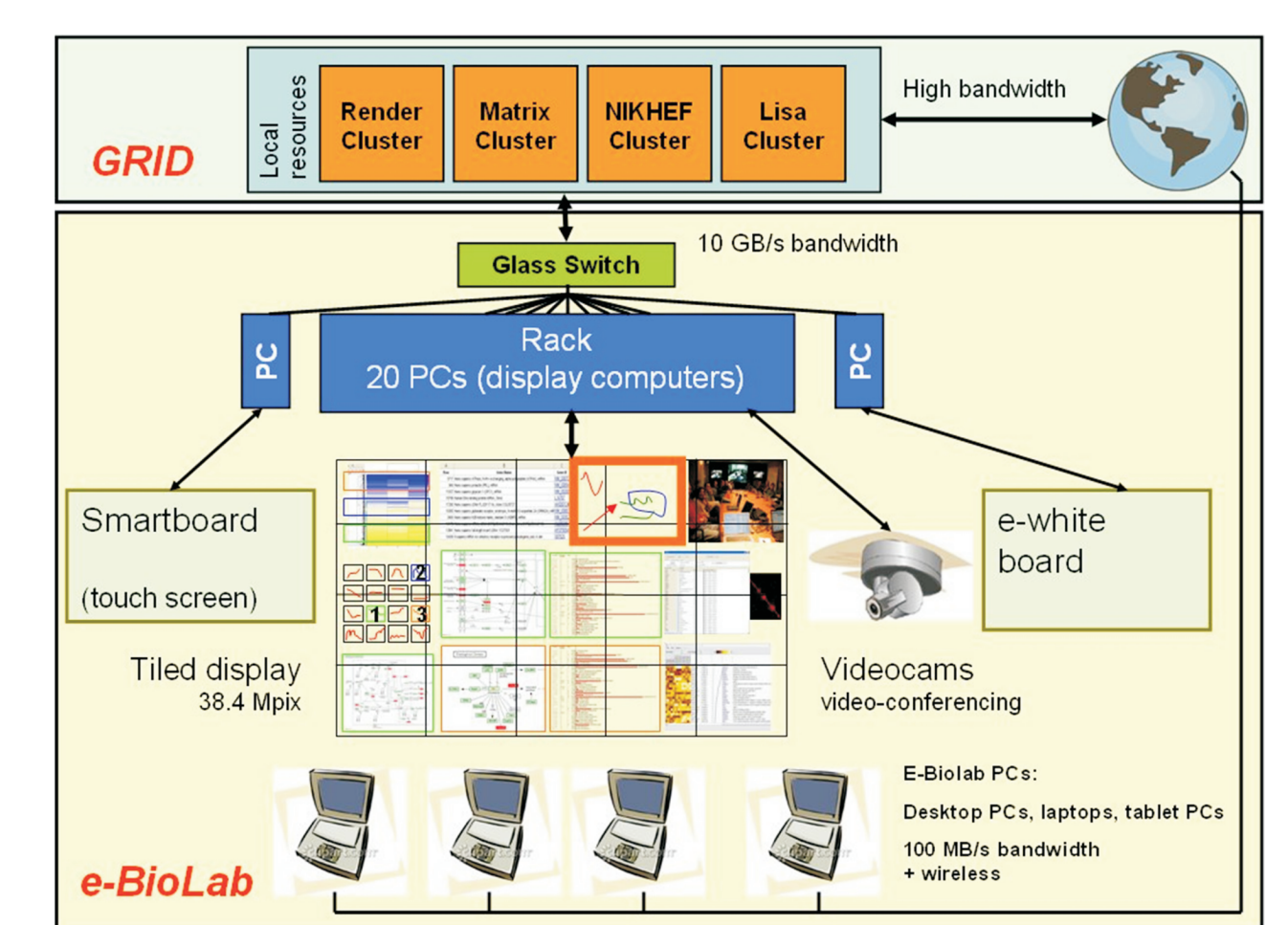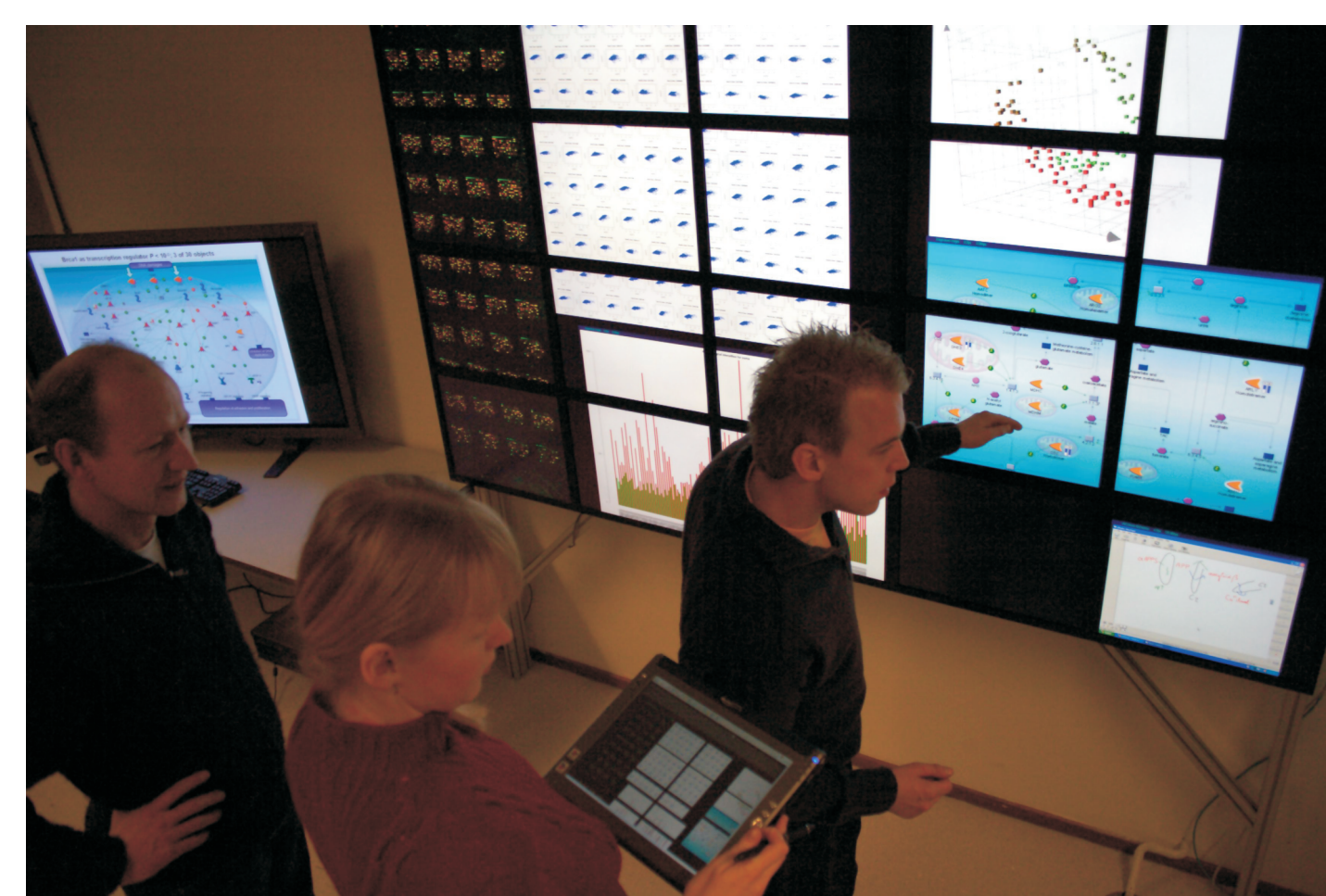- Facilities for remote collaboration

(center column)

Omics research projects share the characteristic of producing large amounts of data, applying a multitude of methods from different scientific fields, and using many resources, such as data and computational resources. Many e-science solutions, such as Virtual Lab e-Science (VL-e) are currently being developed worldwide to support these multidisciplinary omics endeavors. From our experience, particularly face-to-face meetings speed up scientific progress in multi-disciplinary projects. [1] We therefore have set up a laboratory to accommodate meetings of multidisciplinary project teams. In this e-bioscience laboratory (e-BioLab) project teams have the methodological and computational resources from the different enabling disciplines at their disposal. Results of analyses can be displayed with state of the art visualization capabilities and facilities to annotate and capture analysis results are available.

E-BioLab Layout

e-whiteboard

Heat and noise producing equipment

High resolution 4 x 5 tiled

Servo operated video

63" Plasma Touch

Tablet PC (Interaction display)

VL e-bio laboratory

a glass switch
b tiled display
c barebones
d plasterboard wall
e mobile tiled display
f mobile barebones
g video cameras
h desktop PCs
i plasma touch screen
j electronic whiteboard
k speakers
l office desk
m tables on wheels
n tablet PCs
o lab chairs
p desk chairs
q desk blocks
r A3 inkjet printer
s printer table
t file cupboard
u headsets

Technical Infrastructure

- Part of the infrastructure provided by the *Virtual Laboratory for e-Science (VL-e)*
- high bandwidth connectivity (10Gbit/s) through switch
- VL-e framework
  - grid oriented, flexible, secure resource sharing
    - Globus
    - Storage Resource Broker (SRB)
    - Vbrowser (management of visualizations)
  - web-services oriented workflow management
- *Tiled display* operated by
- 20 commodity PCs
- SAGE window management software (EVL, Chicago)[3]
  - OpenGL, VNC clients
- TOPS software (SARA)[2]
- Access Grid for *Video Conferencing*

GRID — Render Cluster, Matrix Cluster, NIKHEF Cluster, Lisa Cluster — High bandwidth
Glass Switch — 10 GB/s bandwidth
Rack 20 PCs (display computers)
Smartboard (touch screen)
e-white board
Tiled display 39.4 Mpix
Videocams video-conferencing
e-BioLab PCs: Desktop PCs, laptops, tablet PCs 100 MB/s bandwidth + wireless
e-BioLab

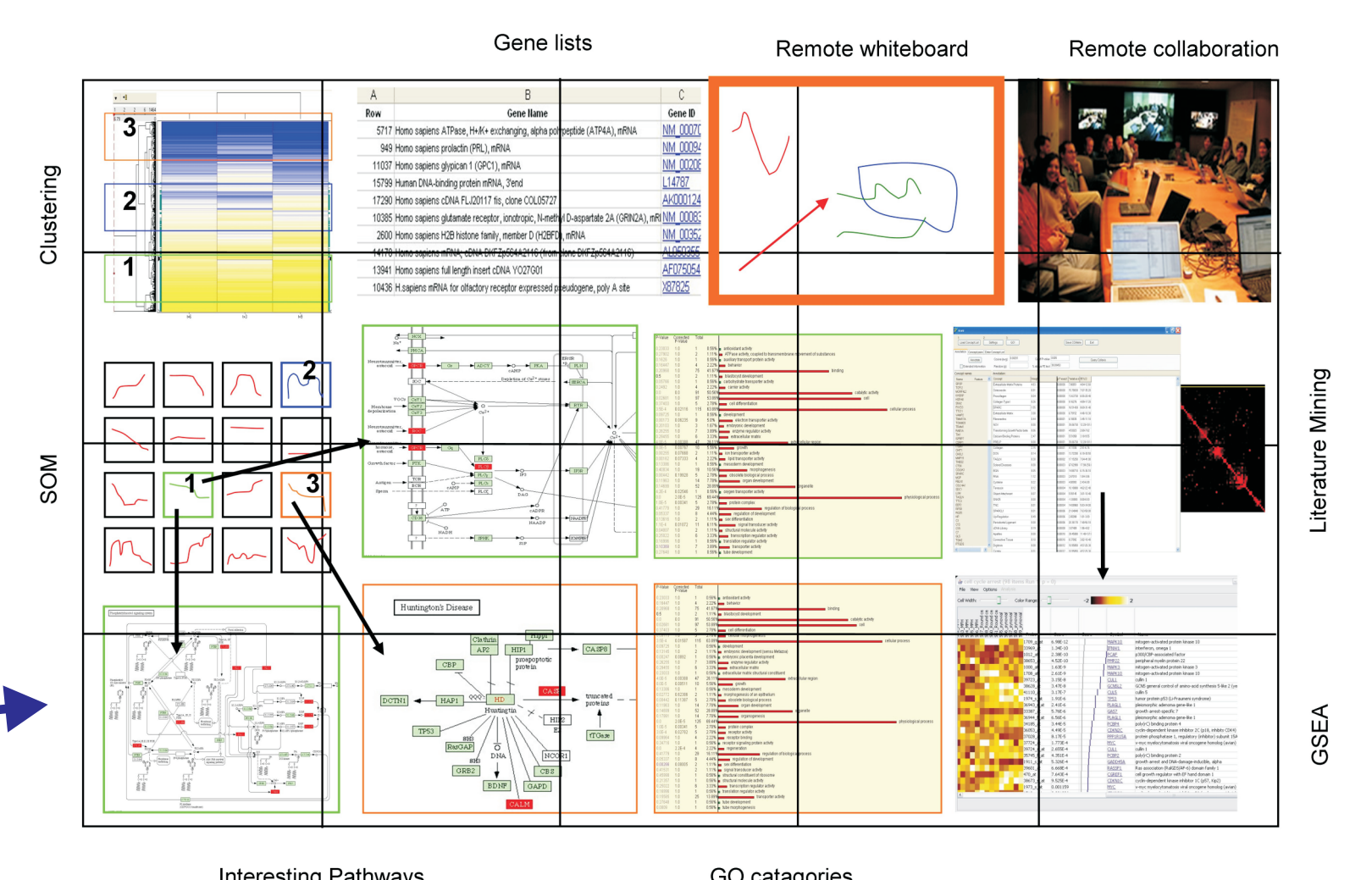## Example: Micro-array Problem Solving Environment

The e-BioLab provides configurations of the VL-e framework dedicated to a specific problem area, e.g. a microarray analysis problem solving environment (MA-PSE).

Available elements:
- Oligo reannotation (Oligorap)
- HybridizationQuality Control (HybQC)
- Argos image analysis for microarrays
- Model Optimization
- Grid Submission of mixed effect linear models


Micro-array experimentation Pipeline
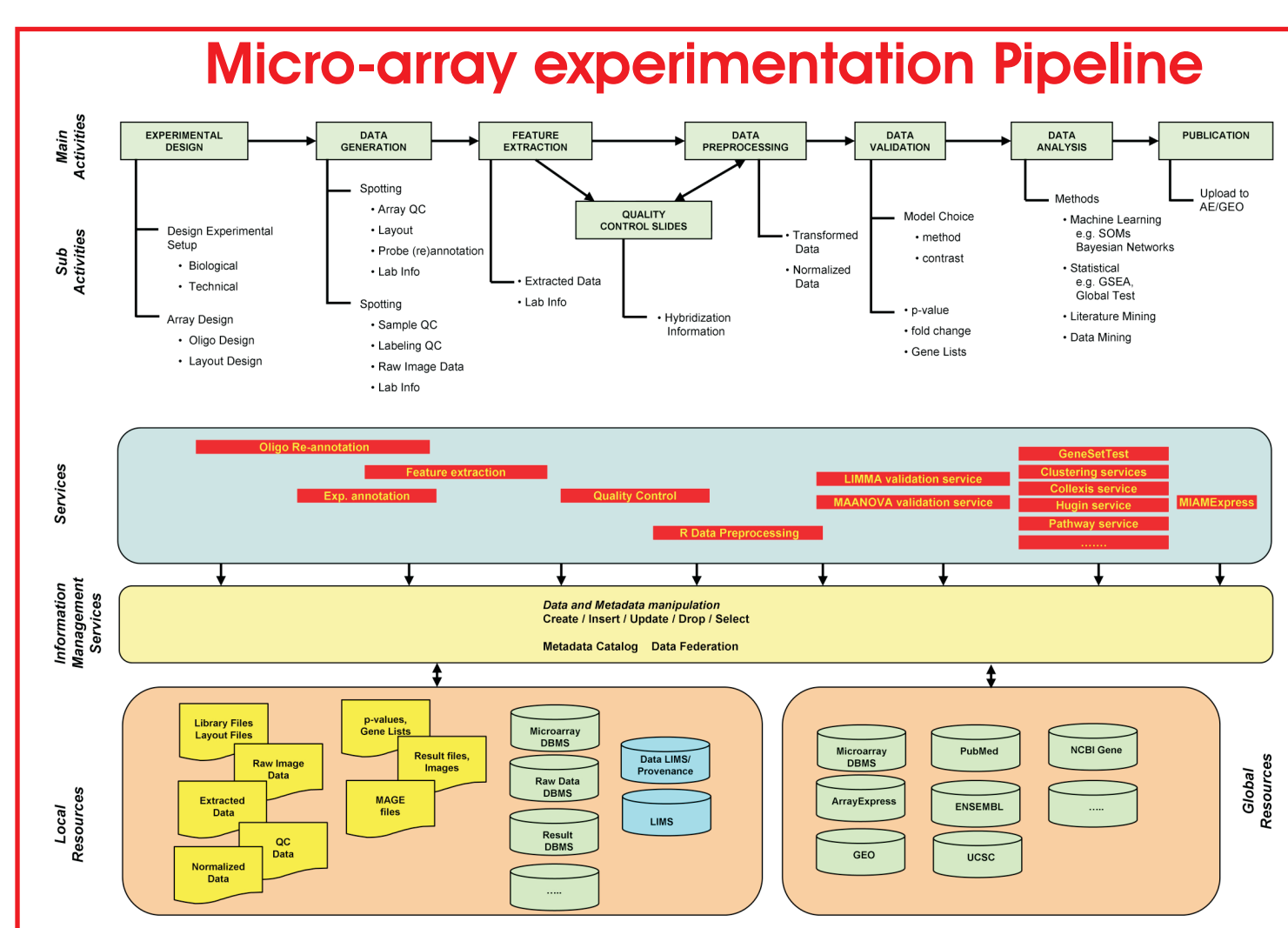
E-BioLab Challenges and Opportunities

- Building *Problem Solving Environments* for scientific disciplines
- Development of *e-lab journaling software*
  - identification of requirements
  - software engineering
- Development of *interactive operation of the tiled display*
  - development of positioning functionality in SAGE
  - research into usage of e-BioLab by groups
  - development of interactive mode in SAGE
- *Application integration and brushing*
  - data integration at application level
  - propagation functionality of selection on tiled display

Gene lists — Remote whiteboard — Remote collaboration
Clustering — SOM — Literature Mining — GSEA
Interesting Pathways — GO catagories

Remote collaboration by e-BioLabs
Currently Leiden University, Wageningen UR and Nijmegen Radboud University intend to set up e-BioLabs:
- Connect e-BioLabs by switchless   -connections
- Sychronize tiled displays
- Set up remote video conferencing through Access Grid

Nijmegen — Wageningen — Amsterdam — Rotterdam
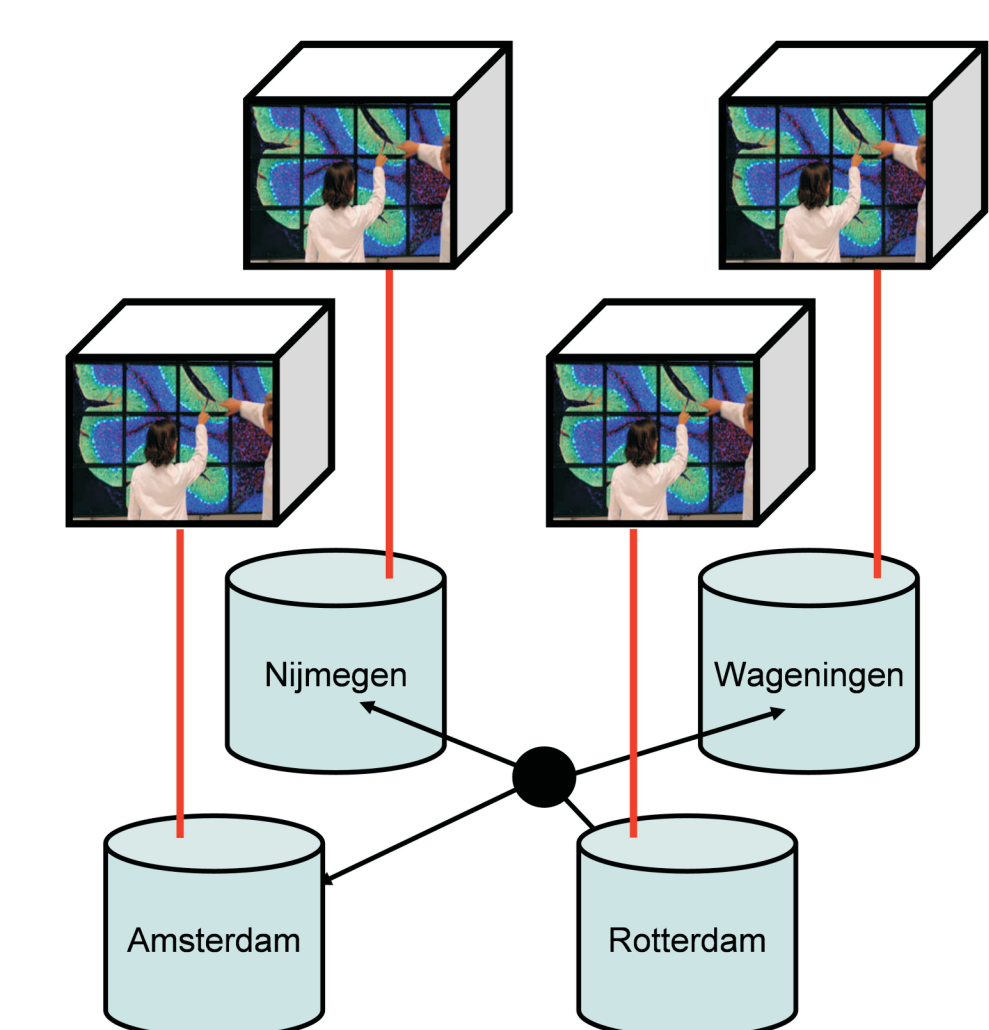
[1] H. Rauwerda, M. Roos, B. O. Hertzberger, and T. M. Breit, "The promise of a virtual lab in drug discovery," Drug Discov Today, vol. 11, pp. 228-36, 2006.
[2] B. Stolk and P. Wielinga, "Building a 100 Mpixel graphics device for the OptiPuter," Future Generation Computer Systems, vol. 22, pp. 972-975, 2006.
[3] J. Byungil, R. Jagodic, L. Renambot, R. Singh, A. Johnson, and J. Leigh, "Scalable Graphics Architecture for High-Resolution Displays," Proceedings of IEEE Information Visualization Workshop 2005, Minneapolis, MN, 2005.