



e-Infrastructures:

A view from
Bioimage Informatics

Christoph Best

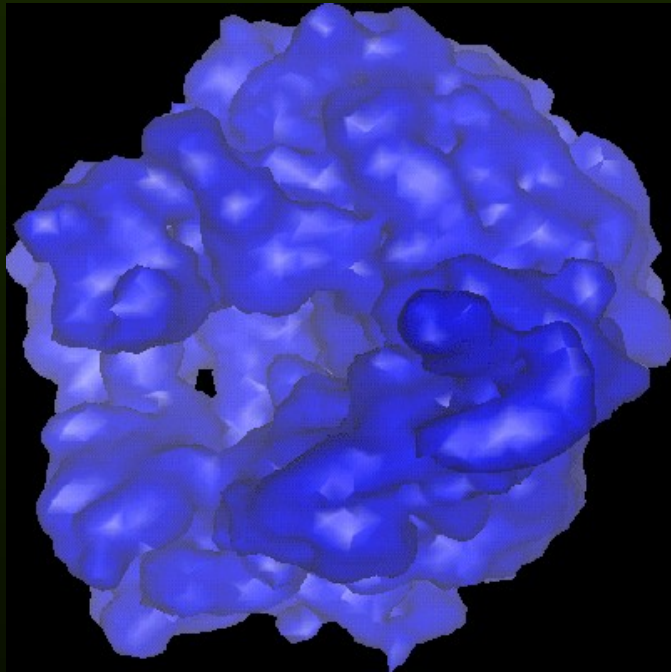
Electron Microscopy Data Bank
PDB Europe
European Bioinformatics Institute,
Cambridge, UK

EMBL-EBI



Electron Microscopy Data Bank

EMDB-1003

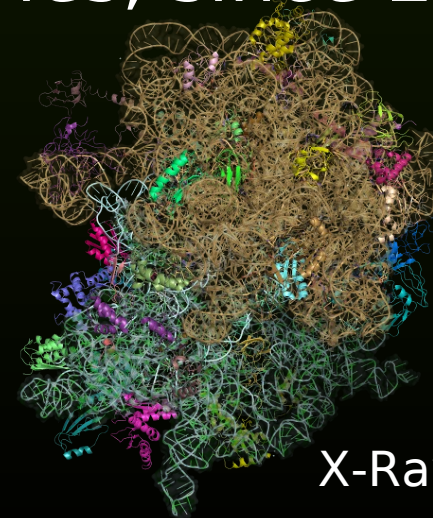


Gabashvili IS, Agrawal RK, Spahn CM, Grassucci RA, Svergun DI, Frank J, Penczek P

Solution structure of the E. coli 70S ribosome at 11.5 Å resolution.

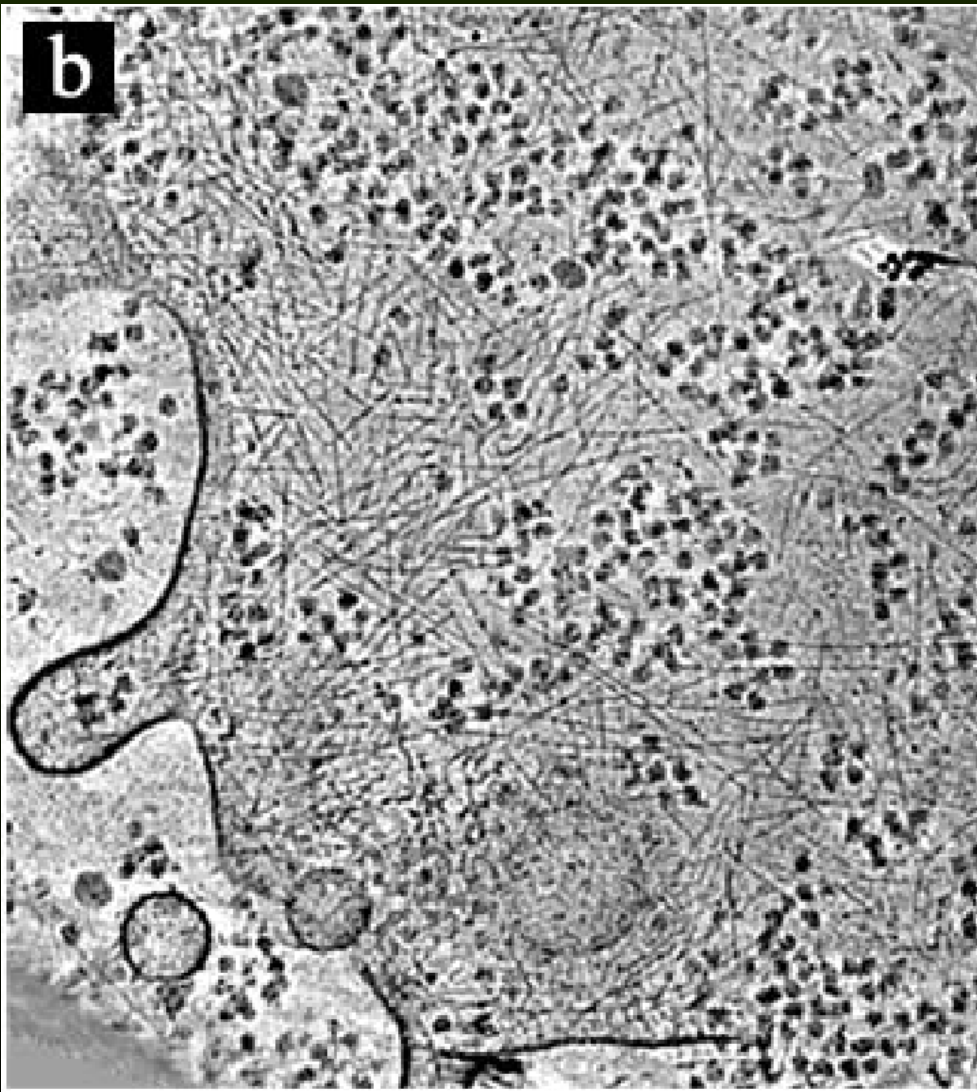
Cell 100, 537 (2000)

- Repository of 3D density maps
 - Macromolecular Complexes
 - Subcellular Structures
- Integrated into [wwPDB](#) (X-ray crystallography)
- 700 entries, since 2002



X-Ray structures

Cryo-Electron Tomography



- Bridging Structural and Cellular Biology

“Structural Systems Biology”

Future technologies:

- X-ray microscopy
- Superresolution light microscopy
- Free electron laser

O. Medalia, 2002

Bioimage Informatics

Informatics Support for Bioimaging

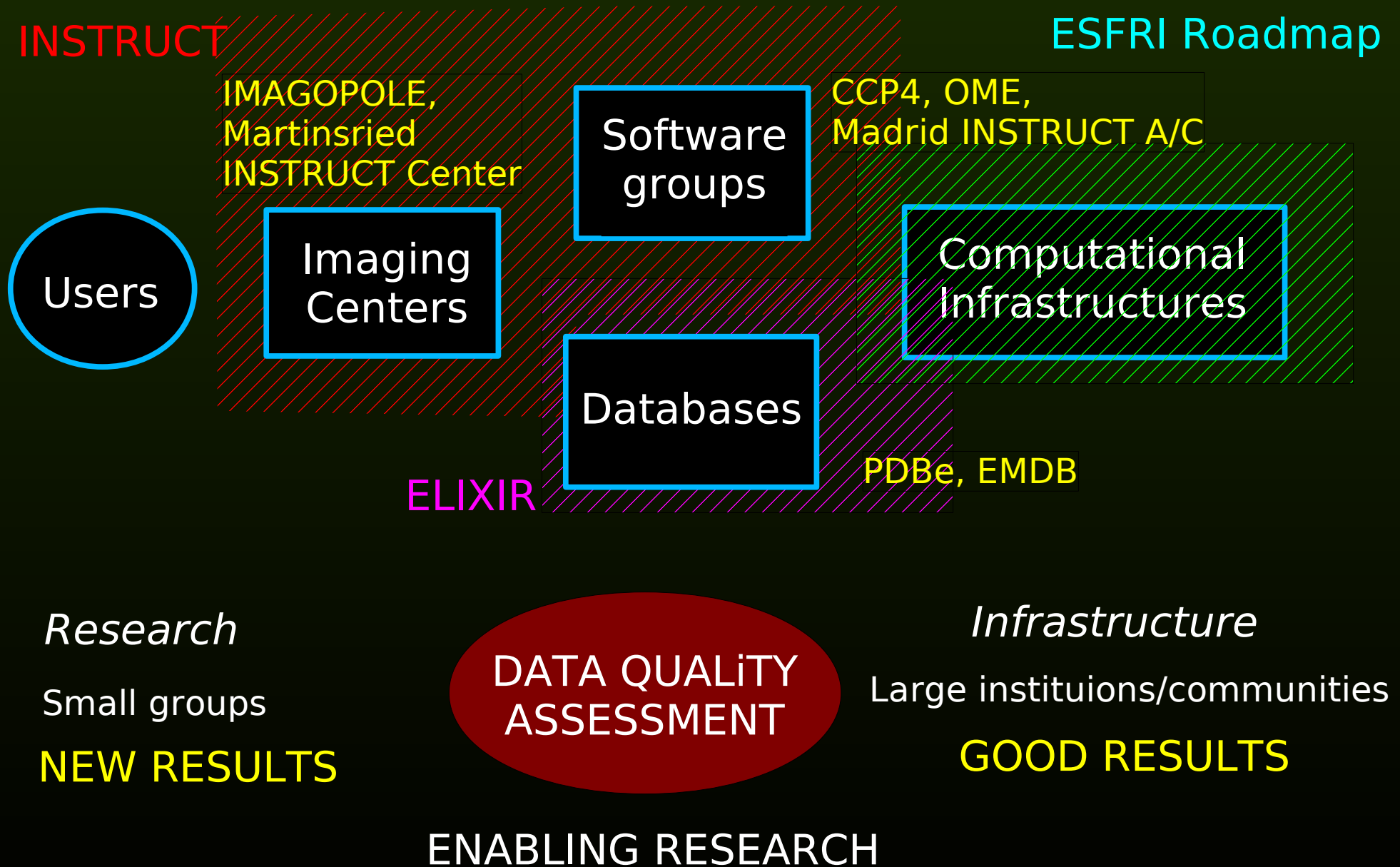
More and more results come from computers!

The **intermediate scale**:

- Computing: 100s of hours or 100s of cores
- Data: 100s of Gigabytes
- People:
 - O(100) labs worldwide, O(500) active scientists
 - **close integration of wet-lab and computing**

VERY WELL SUITED FOR UTILITY COMPUTING

A bioimaging research community



What we need

- Grid/cloud replaces the local cluster
- Virtualization:
 - Simplicity: Flexible software environment
 - Security
- Cloud storage “Time Machine”
- Software appliances, Software-as-a-service
 - Virtual machines with EM software pre-installed
 - User configurable and extensible Linux “distributions”
 - Deployment on request “like my own cluster”
 - Web-based interface + command line
Google AppEngine

Institutional support for resources

- Resources need **long-term** strategy
 - Cannot be run by Ph.D. students or postdocs
 - Need **competitive** salaries, transparent contracts
 - Research scientist **career track** parallel to teaching track
 - Examples: **NIH National Resource Centers**, National labs, CERN, EMBL
- Above all: resources are science
 - Emphasis on **technical excellence**
 - Possibility to **participate in research**
 - ... and not just to get the next postdoc contract!

Conclusions

- Bioimage Informatics exemplifies increasing relevance of computers -> “e-science”
- Virtual Research Communities naturally form around software and data services
- Focus on data quality and validation complements “new results” focus
- Cloud computing, virtualization, software-as-a-service
- Institutional framework for research resources