
WISDOM open day

Bonn-Aachen International Centre for Information Technology (B-IT)

December 16, 2005



Fraunhofer Institute
Algorithms and
Scientific Computing



Where are we here ...



Bonn – Aachen International Centre for Information Technology (B-IT)

- established in 2002
- international master curricula in media informatics, autonomous systems and life science informatics
- based on a cooperation between the University of Bonn, the University of Applied Sciences in Sankt Augustin, the Technical University of Aachen, and the Fraunhofer Institutes in Sankt Augustin

Why are we here ...



- First meeting at *PharmaGrid* retreat 2003 in Welwyn (UK)
- Vincent Breton suggests to start an initiative to use grid computing to fight *neglected diseases*
- On the *Healthgrid conference* in January 2004 we decide to do a first pilot experiment. Lots of discussions with interested partners.
- In 2005, IN2P3 in Clermont-Ferrand and Fraunhofer SCAI in Sankt Augustin deploy a first biomedical application on one of the largest grids in the world: the EGEE grid

Today, we are here to critically review what has been done so far and to develop a roadmap towards sustained cooperation and coordination of healthgrid activities to battle neglected diseases.

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In particular ...

.....we would like to discuss the following aspects

Grid aspects

- How do we make the grid-approach taken in WISDOM more robust?
- How do we make the virtual screening approach smarter?

Biology aspects

- How do we integrate our in silico activities with experimental molecular biology laboratories?

Political aspects

- How do we coordinate our activity with other initiatives in this field and how do we align with the strategies of stakeholders such as EU, WHO, national research organisations?

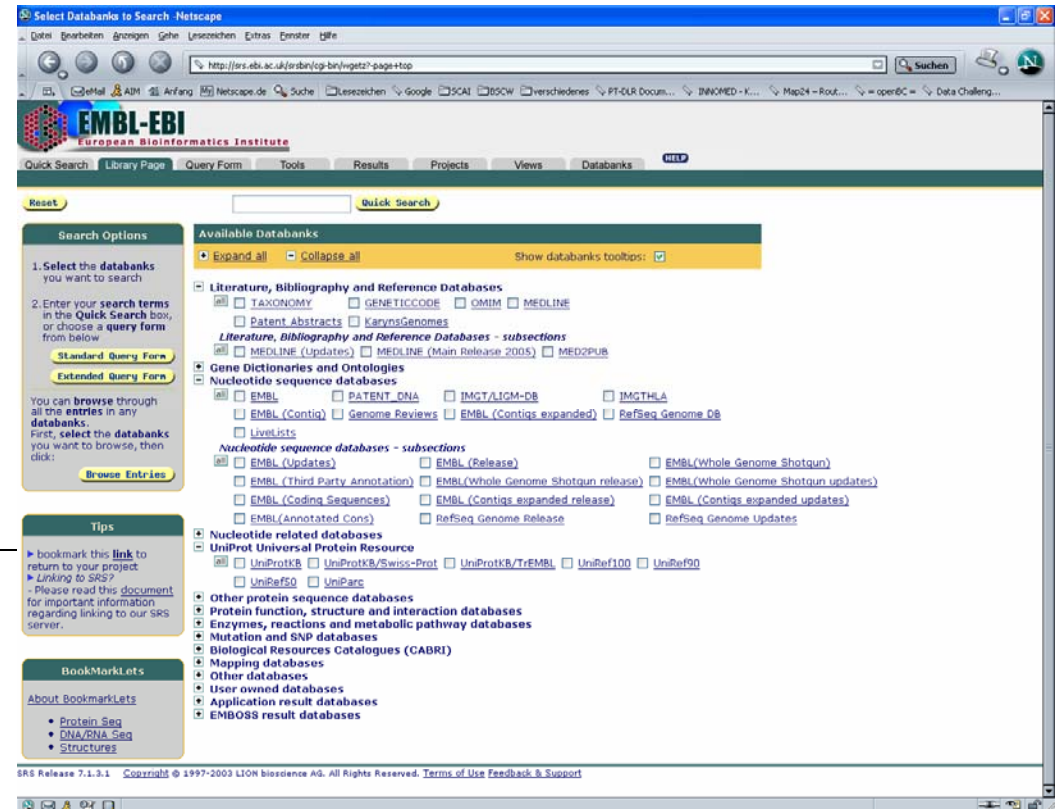
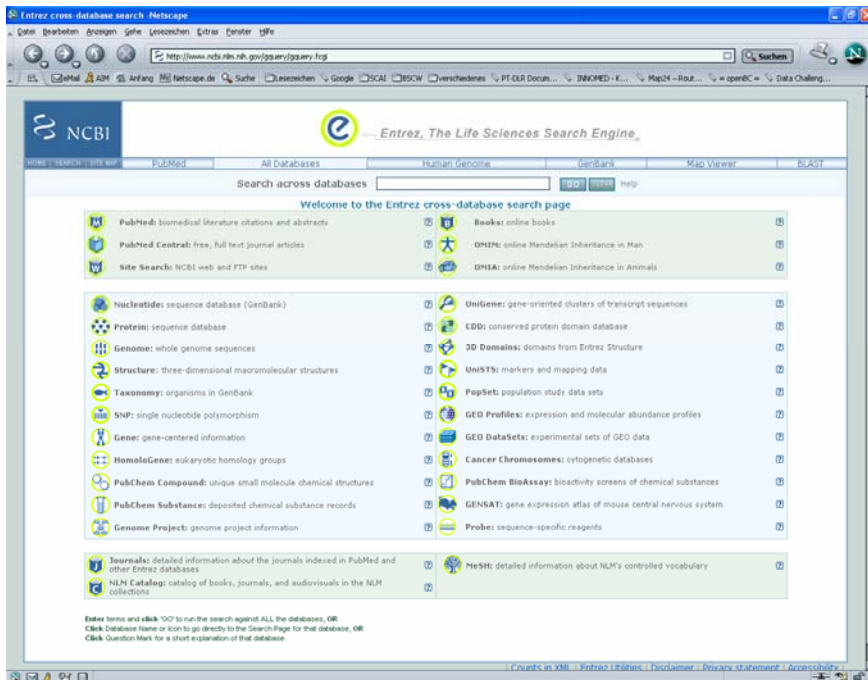
Why GRID COMPUTING ? ...

If you are old enough, you may have experienced molecular biology or experimental pharmaceutical research in the times before the internet was available for everybody



Why GRID COMPUTING ? ...

From the mid of the 1990s on we had access to online biomedical information through the well established “knowledge” portals. These portals are useful to retrieve relevant information, but do not support collaborative experimentation ...



Why GRID COMPUTING ? ...

Since the idea of eScience has been brought up with the beginning of the new millenium, a new paradigm has been established to share compute resources, data sources and services on the grid. Of course, grid computing as a new discipline is still in its infancy, but the first promising results have already been achieved (see e.g. the myGrid project in the UK or the BIRN project in the US). In the pharmaceutical industry, grid computing has gained momentum as a tool to increase the efficiency of hardware investments for compute-intensive applications such as molecular docking (e.g. at NOVARTIS).

Acknowledgement

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- B-IT for providing the infrastructure
- The speakers for coming here and investing their time (and money) for this workshop
- Special thanks to BioSolveIT GmbH for their generous support (use of FlexX & license management)
- The PRISM forum (Rene Ziegler / Manuel Peitsch (Novartis)) for continuous feedback on our discussions to use grid computing for virtual screening
- The EGEE compute nodes for their contribution of CPU power
- The teams at Fraunhofer and IN2P3 for their hard work (and the catering ...)