

ECRI 2007[★]


★ *european conference on research infrastructures*

Global Virtual Communities

Wolfgang von Rueden, CERN, Geneva

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The Communities

- Users of large scientific instruments
 - High Energy Physics (example LHC)
 - Large telescopes, Fusion
 - Future: ESFRI supported Research Infrastructures
- Global science
 - Bio-medical community (example Wisdom)
 - Digital Libraries
 - Multi-disciplinary teams
- Numerous small communities
 - infrastructure allows virtual communities to be created dynamically with little overhead

Example LHC Computing Grid

- Based on two major e-infrastructures: EGEE and OSG
- World-wide collaboration supporting 7000 scientists
- Operational now with real data taking in early 2008
- All hardware resources and most of the personnel contributed by the project partners, plus significant contributions from EC and DOE/NSF funded projects
- Preparation started back in 2000, project will run for 10-15 years => sustainability!!

Millions of potential drugs to test against interesting proteins!



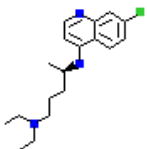
~~High Throughput Screening
1-10\$/compound, several hours~~

Too costly for a neglected disease!

Compounds:

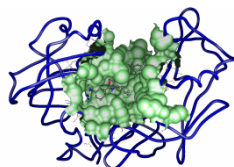
ZINC: 4.3M

Chembridge: 500 000



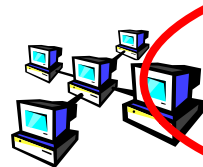
Targets:

PDB: 3D structures



Molecular docking (FlexX, Autodock)

~1 to 15 minutes

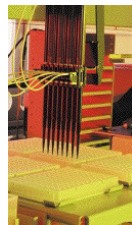


Data challenge on **EGEE**

~ 2 to 30 days on ~5000 computers

Cheap and fast!

Selection of the best hits



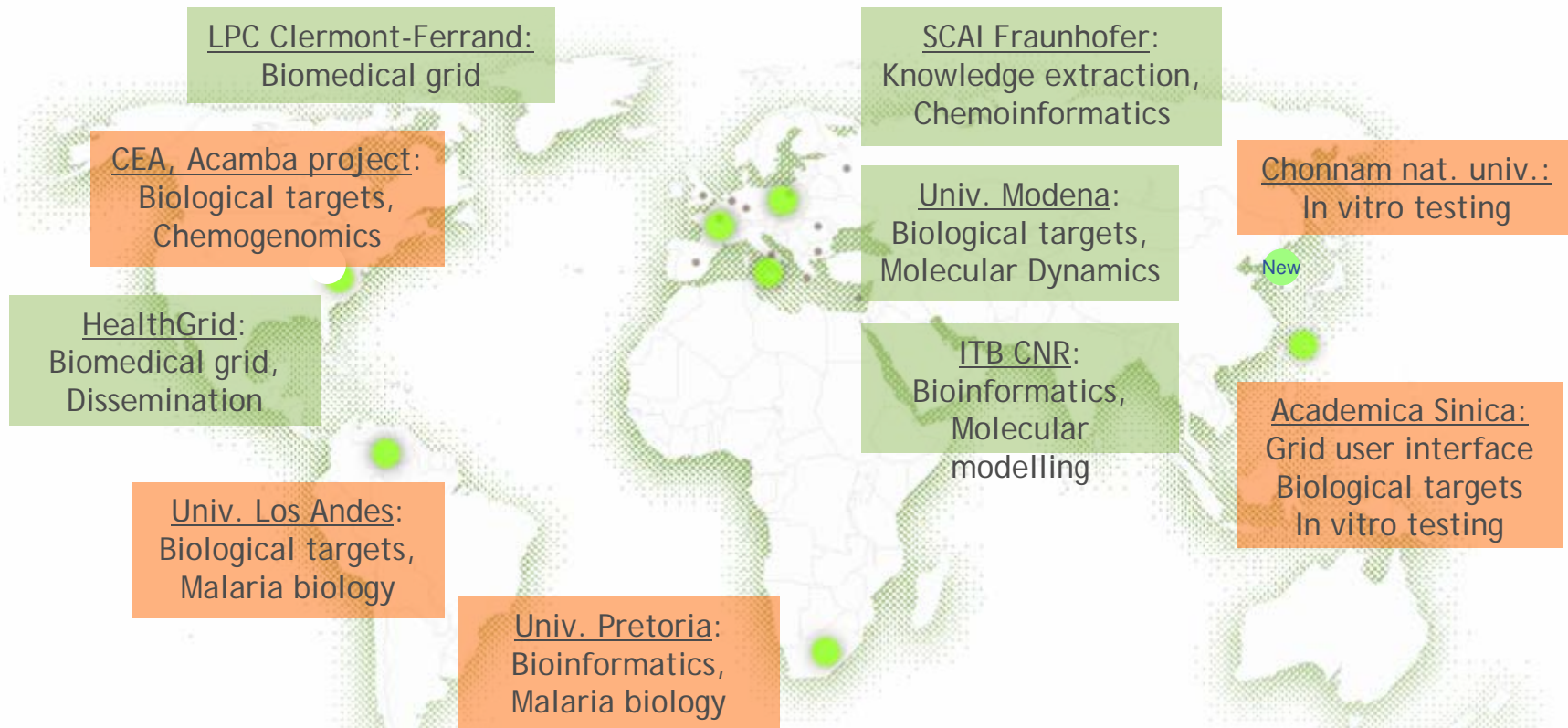
Hits screening using assays performed on living cells



Leads
Clinical testing
Drug

The grid added value

- The grid provides the centuries of CPU cycles required on demand
- The grid provides the reliable and secure data management services to store and replicate the biochemical inputs and outputs
- The grid offers a collaborative environment for the sharing of data in the research community on avian flu and malaria



Role of e-infrastructures

- Provide general services similar to scientific networks
 - NRENs plus GÉANT are excellent examples
 - Aim for “out-of-the-box” solutions in the long-term
 - Requires standardization
 - Needs to be inclusive
- Requires sustainability
 - Short-term funded projects encouraged rapid development
 - Understanding is now mature enough to take next step
- Shared infrastructure helps multi-disciplinary teams to work together

Status of e-infrastructures in Europe

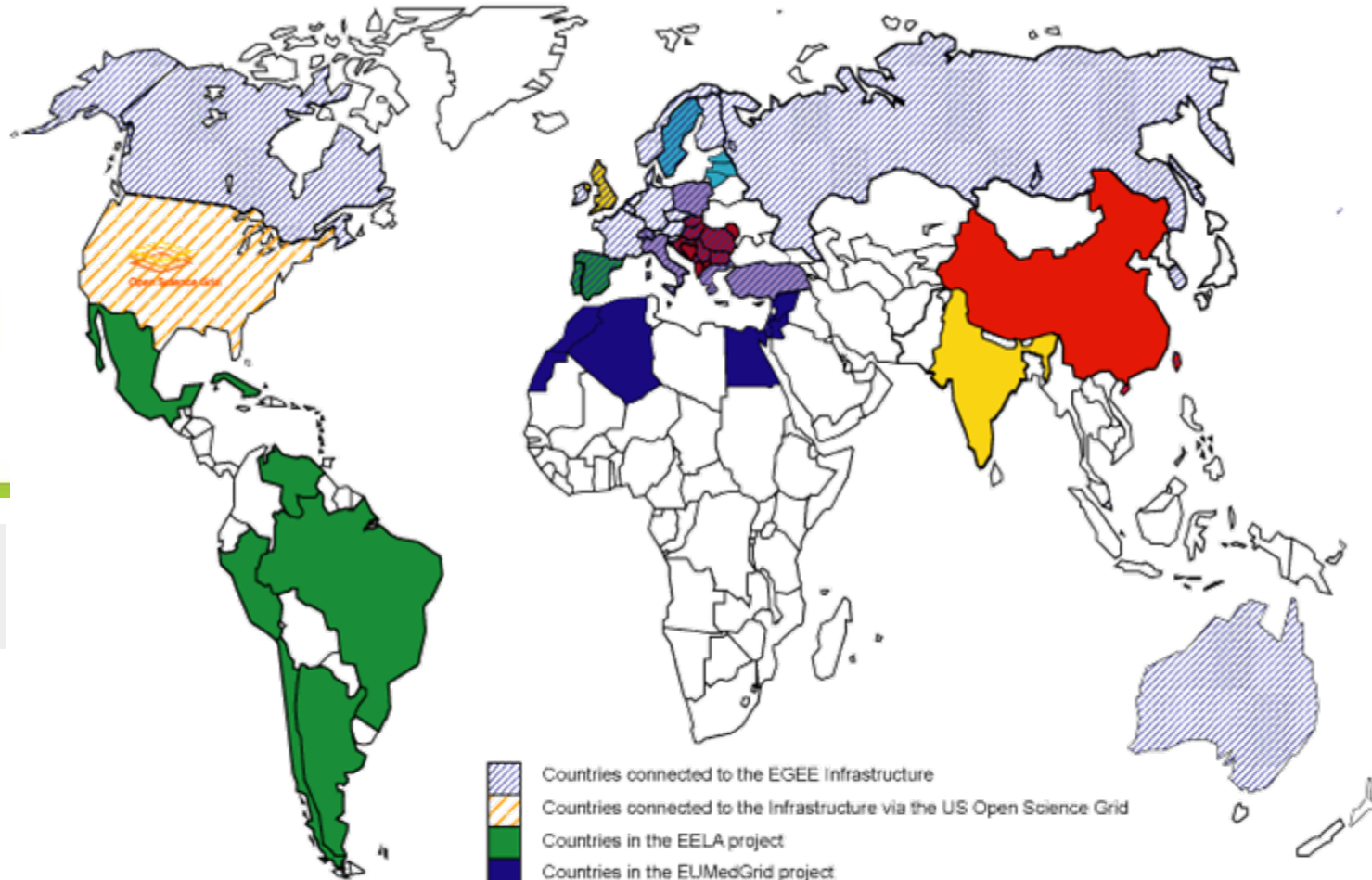
- Europe has made very respectable investments
 - EC: spent 400 M€ on e-infrastructures for FP5+FP6 and will spend 575 M€ in FP7
 - Significant national programmes in EU member states
- Large variations between countries
 - From very small to very large, big diversity
 - Leading: UK and Italy
- Largest European examples: DEISA, EGEE and GÉANT
- Active collaboration and successful interoperability outside Europe
- Effort required to bring HPC and Grids together for the benefit of the communities requiring both



omii europe
open middleware infrastructure institute



TeraGrid



- Countries connected to the EGEE infrastructure
- Countries connected to the Infrastructure via the US Open Science Grid
- Countries in the EELA project
- Countries in the EUMedGrid project
- Countries in the BalticGrid project
- Countries in the SEE-GRID project
- Countries in the EUIndiaGrid project
- Countries in the EUChinaGrid project
- Countries in several regional projects

What next?

- Achieve sustainability at National and European level
 - Create a National Grid Infrastructure (NGI) in each country
 - Create one European Grid Infrastructure

- Steps towards this goal
 - EGEE-III forms Joint Research Units in all participating countries in view of creating NGIs
 - EGI Design Study prepares proposal for European coordination

Issues

- Large diversity of solutions and visions in Europe (≥5 middleware stacks) – when will we converge?
- See Ian Foster's blog in May (<http://ianfoster.typepad.com/>)
- NGIs: More effort needed to arrive at a minimal set of common function while taking into account national needs
- EGI
 - Needs to add value to the NGIs
 - Focus on providing reliable services and support
 - Seamless continuation from present projects
 - Although “supported” by all countries in principle, more efforts are needed to obtain a real commitment

Conclusion

- e-infrastructures support global virtual communities
- New communities are being formed therefore
- Communities rely on stable long-term support
- Europe has achieved a lot, but much more needs to be done
- Progress is hampered by a lack of global thinking
- Lack of political support in many countries
 - a consequence of mixed messages to politicians?
- We should not waste our investments – we can do better

References

- CERN: www.cern.ch
- DEISA: www.deisa.org/
- EGEE: www.eu-egee.org
- EGI: www.eu-egi.org
- ESFRI: cordis.europa.eu/esfri/
- GÉANT: www.geant.net/
- LCG: www.cern.ch/lcg
- OSG: www.opensciencegrid.org
- Wisdom: wisdom.eu-egee.fr/