A half century route to competitive collaboration: the Chemistry, Molecular and Materials Sciences & Technologies Virtual Community:

Antonio Laganà
Università di Perugia (UNIPG), IT

2.THANKS

- 1964 – 70 Laurea in Chemistry UNIPG – C Furlani, G Ciullo, A Sgamellotti – Research (Thesis) Quantum Chemistry (Electronic structure of coordination complexes) **JFK, GIOVANNI XXIII, RK, MLK**

- 1970 – 75 **Army service**, Laboratory demonstrator – G Volpi, G Liuti, V Aquilanti, F Vecchiocattivi – Research: collision dynamics (charge exchange) + (Orsay, C Moser)

- 1975 – 80 Temporary contract UNIPG, Research associate Manchester – JNL Connor (W Jakubetz, J Manz) – Research: Uniform semiclassical approximations, quasiclassical and 1D quantum reactive scattering

- 1980 - 85 Researcher and lecturer UNIPG, Visiting CALTECH, Cambridge. Parallel computing at CINECA and CNUCE – A Kupperman, DC Clary, E. Rossi, R. Baraglia, D Laforenza – Research: Hyperspherical collinear and Jacobi IOS reactive dynamics

- 1985 - 90 Associate professor UNIPG, Visiting scientist Los Alamos – RT Pack, GA Parker – Research: 3D Hyperspherical quantum reactive scattering

- 1990 – 95 Associate professor UNIPG, Visiting Scientist Bristol, Collaboration Bari – G Balint-Kurti, M Capitelli - Research: 3D time dependent reactive scattering and massively parallel trajectory calculations

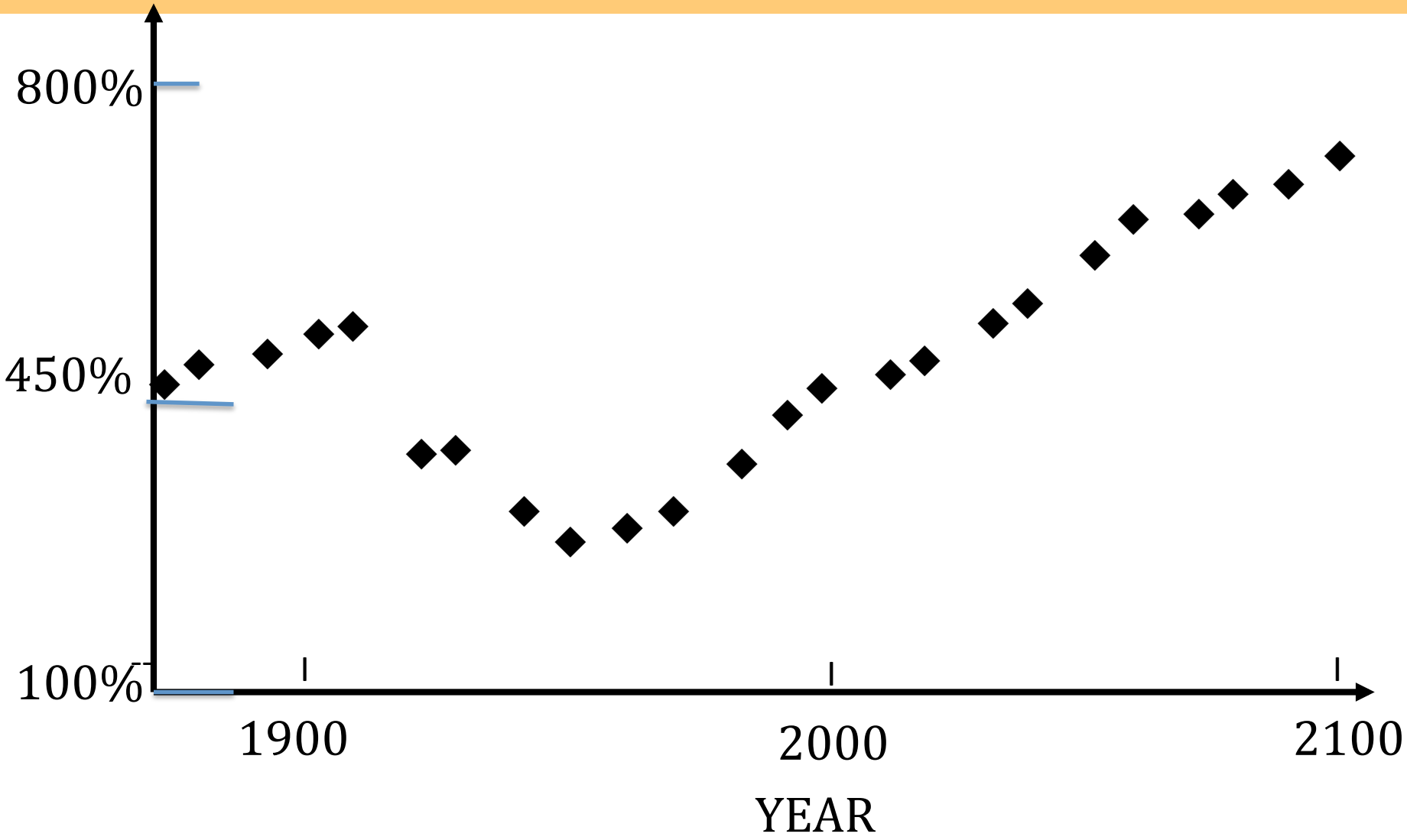
3.THANKS

- 1994 - Full Professor - COST, ECTN ECHEMTEST and EUROLABELS (AK Smith, E Varella, R. Whewell, T. Mitchell), Director of the UNIPG Computer center
- 2000 - Director of the UNIPG Department of Chemistry
- Further UNIPG collaborations (F Pirani, P Casavecchia, G Grossi, R Candori, S. Cavalli, N Balucani, A Lombardi,)
- Other collaborations (UNIPG Dept of Math and Inf., Barcelona, Salamanca, Vitoria, Vancouver, Budapest, ECSEC Rome, EPCC Edinburgh, Crete, …)
- G. Cruciani allowing the Department to carry out research to social targets
- STUDENTS: O. Gervasi, S. Crocchianti, E Garcia, A Riganelli, N Faginas Lago, L Pacifici, V Piermarini, S Rampino, A. Costantini, C. Manuali, … .

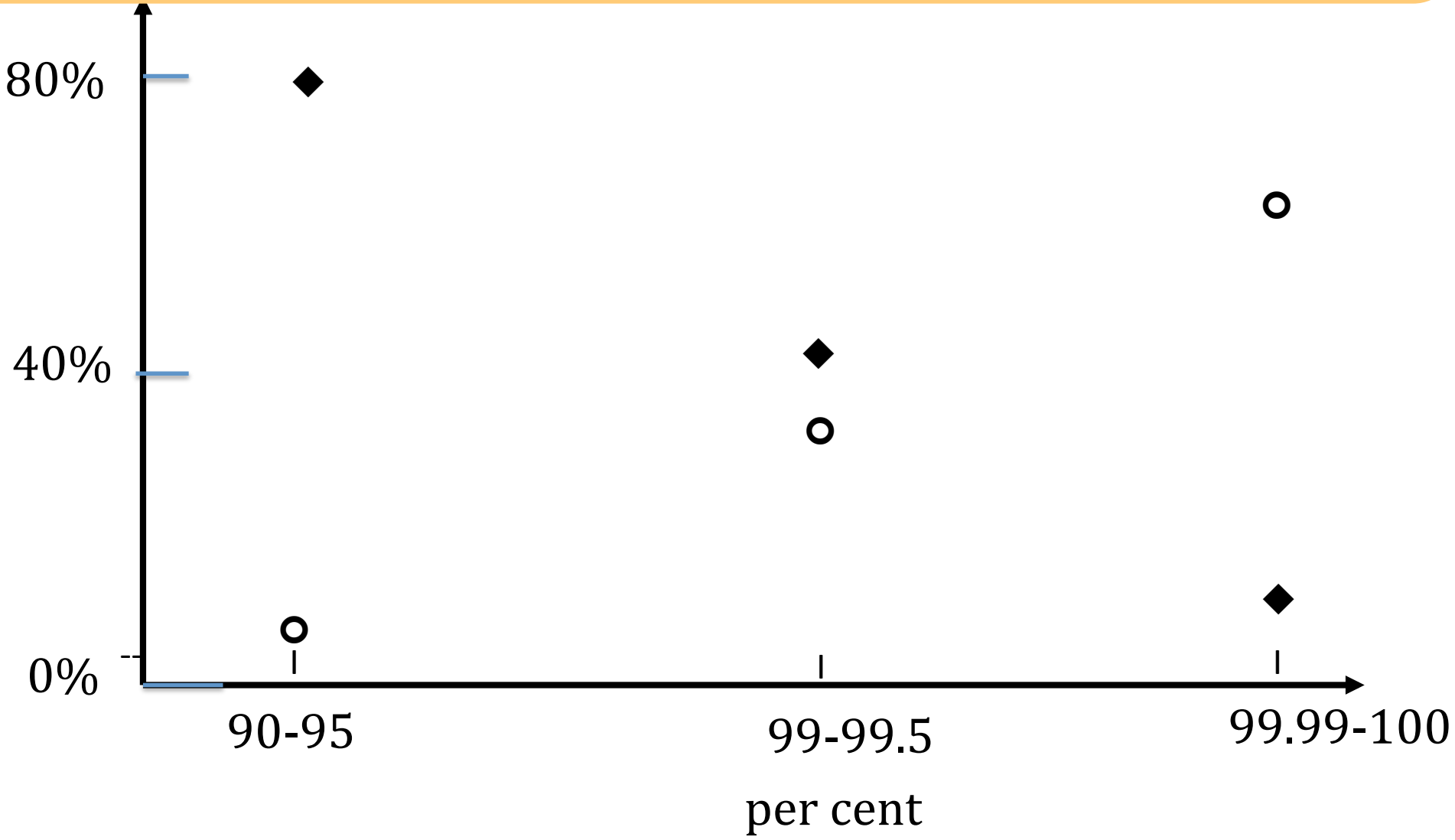
- **THIS IS THE ACADEMIC ENVIRONMENT I ENJOIED WORKING IN. RESEARCH AND EDUCATION CONSIDERED AS "PER SE" VALUES**

- IN THE REAL WORLD, INSTEAD, THE THEORY OF MARGINAL PRODUCTIVITY (THE SALARY SHOULD CORRESPOND TO THE ADDITIONAL PRODUCTION THAT ONE GENERATES) IS DOMINANT

4. T Piketty, The capital in the XXI century, Bompiani, 2014
The ratio capital/incomes in the world 1870-2100 (continuous after world wars increase)



5 .T Piketty, The capital in the XXI century, Bompiani, 2014
Percentage Incomes from work ◆ incomes from capital O
Richest minorities have larger shares of capital



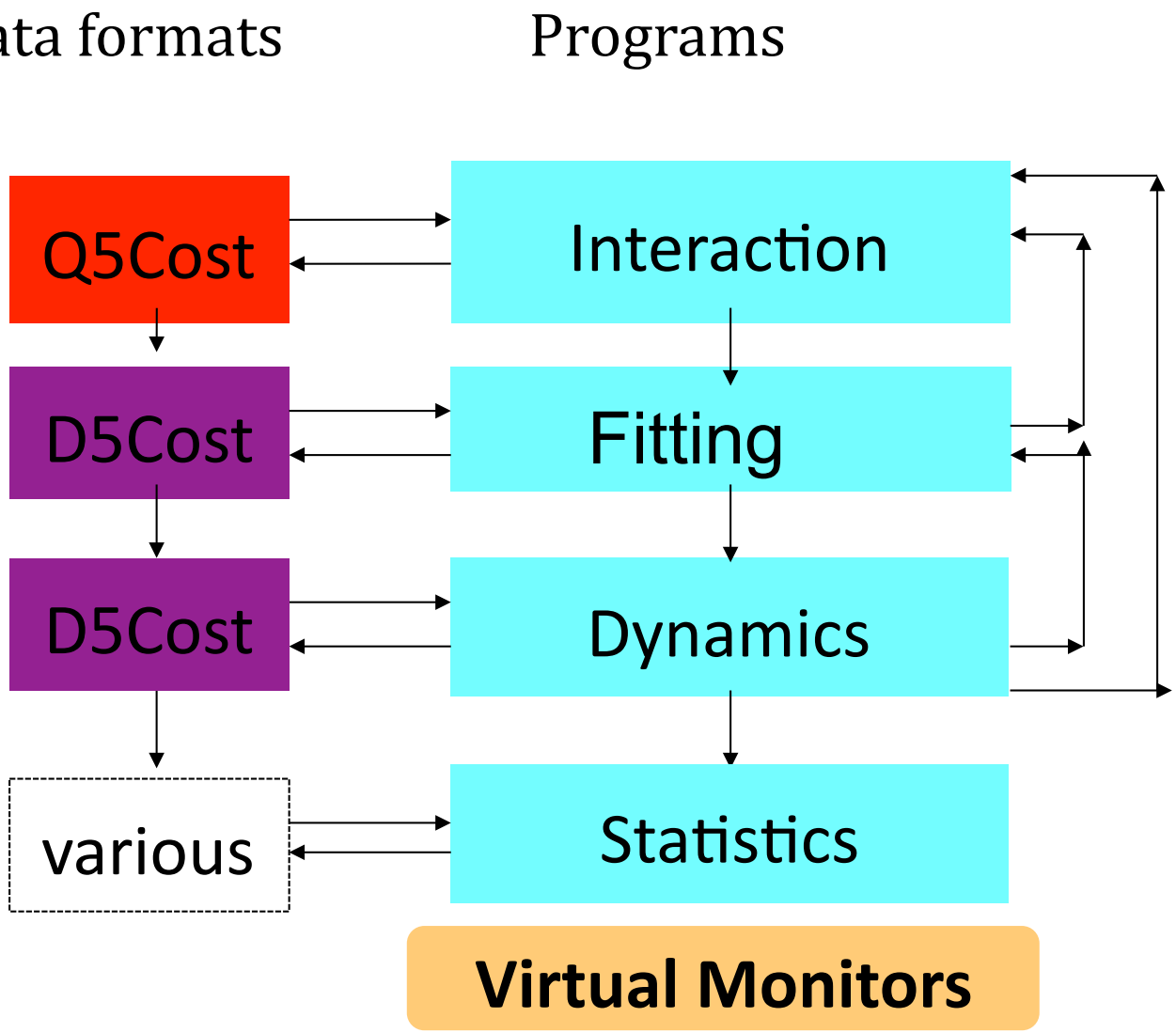
6. MARGINAL PRODUCTIVITY neglects HUMAN CAPITAL (solution: COMPETITIVE COLLABORATION)

Dont get trapped into popular tenets. Brave by following your heart and your intuition.
Steve Jobs, June 2005

Tor Norretranders
The generous man: how helping others is the Sexiest thing you can do
Better world Books 2009

If you have not to worry about your future, donate to the future of your and next generations … by sharing and participating.
Harvard Sara Lawrence-Lightfoot, School of life, London

7. COLLABORATIVE SIMULATION WORKFLOWS and DATA FORMATS HELP SCIENCE PROGRESS



A. Laganà, A. Costantini, O. Gervasi, N. Faginas Lago, C. Manuali, S. Rampino: *COMPCHEM: progress towards GEMS a Grid Empowered Molecular Simulator and beyond,* **Journal of Grid Computing, 8(4), 571-586 (2010)**

E.Rossi, S. Evangelisti, A. Laganà, A. Monari, S. Rampino, M. Verdicchio, C. Angeli, K. Baldridge, G.L. Bendazzoli, S. Borini, R. Cimiraglia, P. Kallay, H.P. Luethi, K. Ruud, J. Sanchez-Marin, A. Scemama, P. Szalay, A. Tajti, *Code interoperability and standard Data Format in Quantum Chemistry and Dynamics: the Q5/D5cost Data Model*, **Journal of Computational Chemistry 35(8): Code Interoperability 611-621 (2014);**

8. THE H + H_2 REACTION SIMULATOR

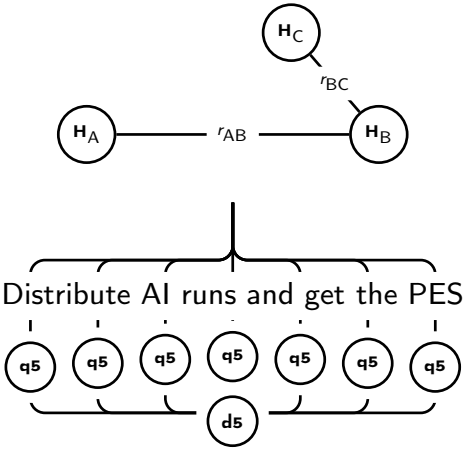
THE ATOM-DIATOM PROTOTYPE

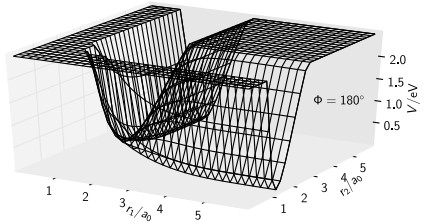
Interaction module (high level ab initio)

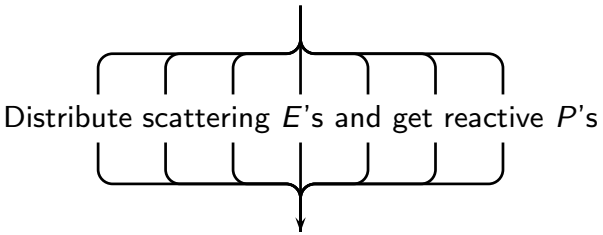
Fitting module (bond bond formulation)

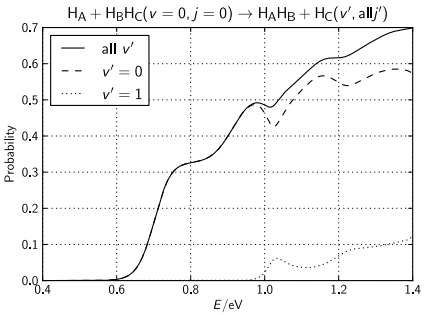
Dynamics module (quantum, semi, quasi)

Observables module (P, σ, k, I)









S. Rampino, A. Monari, S. Evangelisti, E. Rossi, A. Lagana', *A priori modeling of chemical reactions on computational grid plat-forms: workflows and data* **Chemical Physics 398,192-198 (2012)**

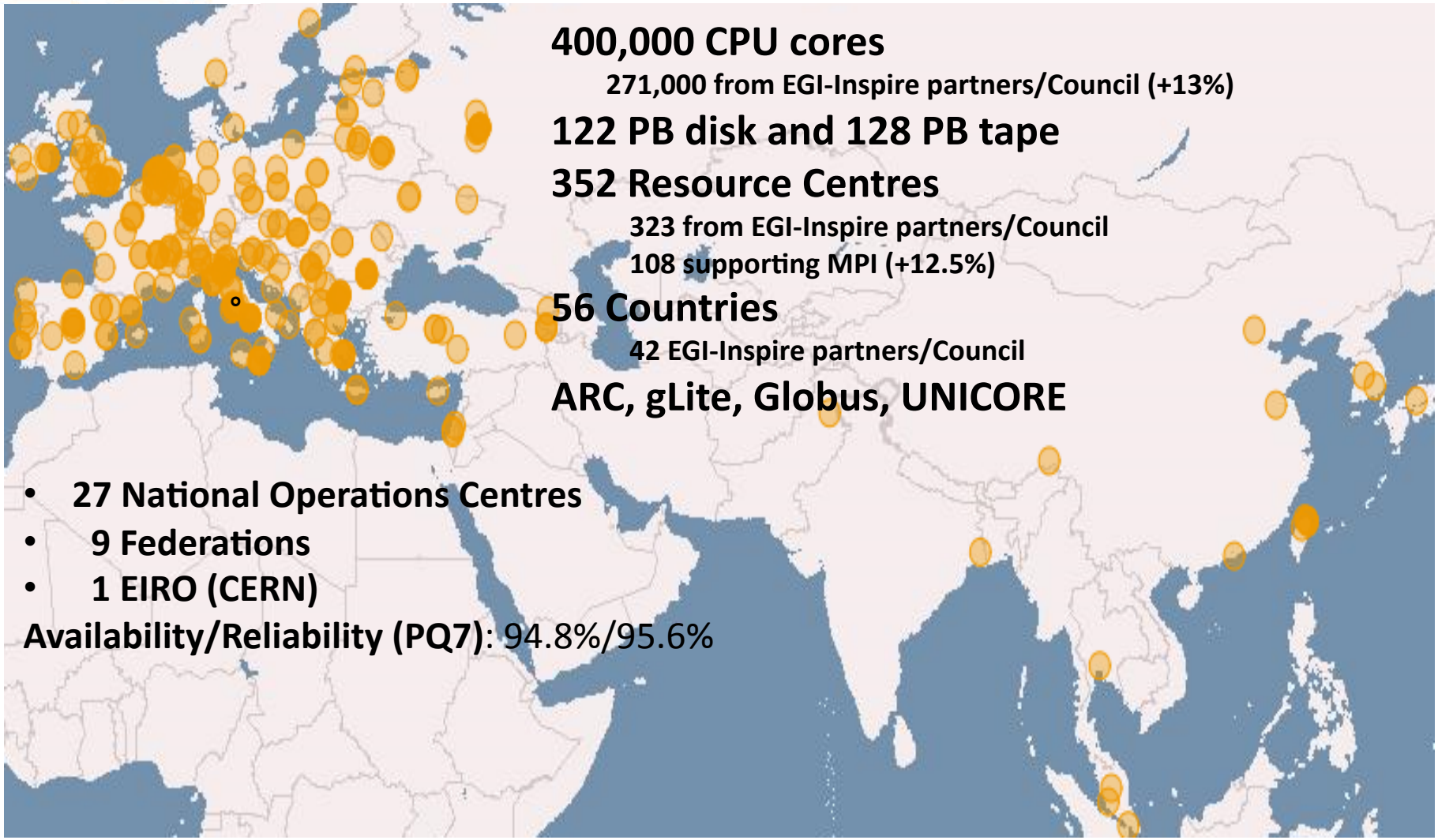
9. GRID COMMUNITIES

- **Virtual Organizations: a set of individuals and/or institutions that share resources under agreed rules**
  - *Sharing is highly controlled,* resource providers and consumers define clearly and carefully what is shared, who is allowed to share, and the conditions under which sharing occurs

10. MEMBERSHIP of the COMPCHEM VO

Membership Level	Short Description
1. User	*Passive*: Runs programs implemented by other VO members.
	Active: Implements at least one program for personal usage.
2. Software Provider	*Passive*: Implements at least one program for use by other members.
	Active: Manages at least one implemented program for collaborative usage.
3. Infrastructure Provider	*Passive*: Confers to the infrastructure at least a small cluster of processors.
	Active: Contributes to deploy and manage the infrastructure.
4. Manager (Stakeholder)	Takes part to the development and the management of the VO.

11. THE EUROPEAN GRID



400,000 CPU cores

271,000 from EGI-Inspire partners/Council (+13%)

122 PB disk and 128 PB tape

352 Resource Centres

323 from EGI-Inspire partners/Council

108 supporting MPI (+12.5%)

56 Countries

42 EGI-Inspire partners/Council

ARC, gLite, Globus, UNICORE

- **27 National Operations Centres**
- **9 Federations**
- **1 EIRO (CERN)**

Availability/Reliability (PQ7): 94.8%/95.6%

12. GriF: a QoS tool for grid empowering computational applications

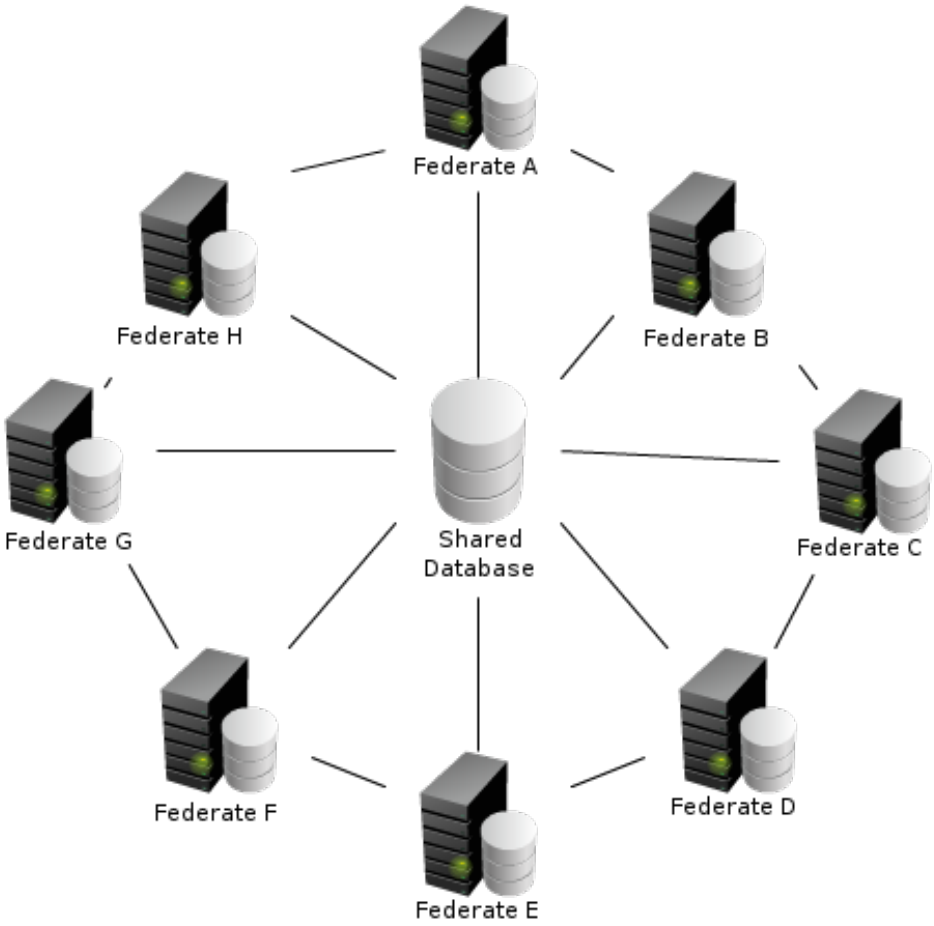
- Make grid applications **black box like** and **an optimized distribution of tasks over the grid** automatic.
- Adopt **a collaborative JAVA Service Oriented Architecture (SOA) framework** articulated as a set of **grid services**
- Provide **users with standard operational modalities** based on **friendly user driven services** allowing the **composition of one or more services** transparently to their implementation details.
- Conveniently **direct the jobs to the appropriate** machine

13. THE CREDIT ECONMY

- GENERALIZE the "service oriented" APPROACH
- Introduce a METRICs for the VO work
- Develop algorithms for the calculation of QoS and QoU
- Implement a system of credits for work and cost for services

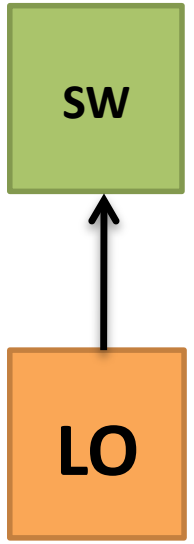
C. Manuali, A. Lagana'
GRIF: A New Collaborative Framework for a Web Service Approach to Grid Empowered Calculations
Future Generation of Computer Systems, 27(3), 315-318 (2011) DOI 10.1016/j.future.2010.08.006

14. E-LEARNING DISTRIBUTED REPOSITORIES

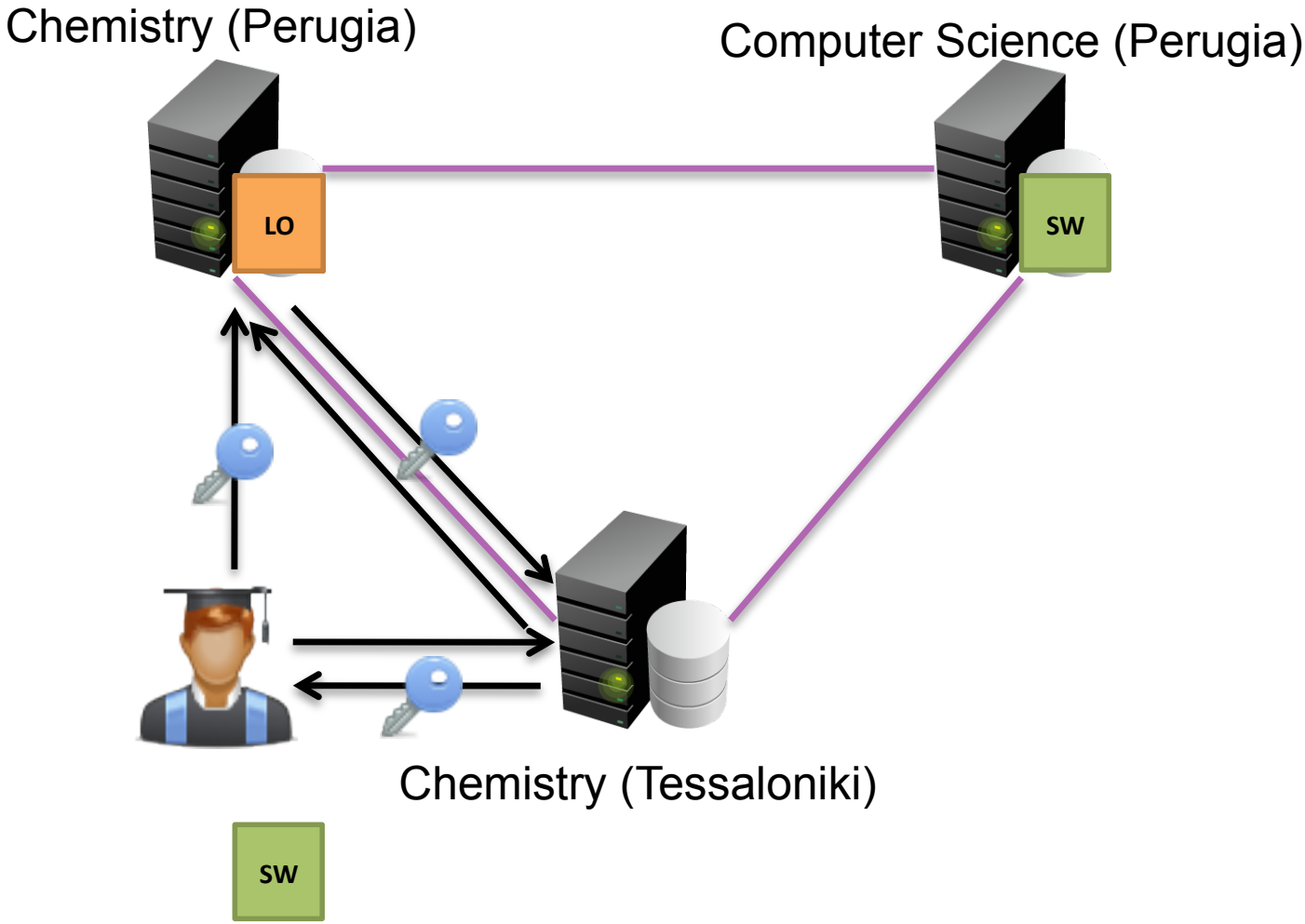


Our results

- Federation of autonomous repositories
- Automatic content sharing
- Downloadable content (for registered users)
- Simplified content import from Moodle
- LO Dependency management



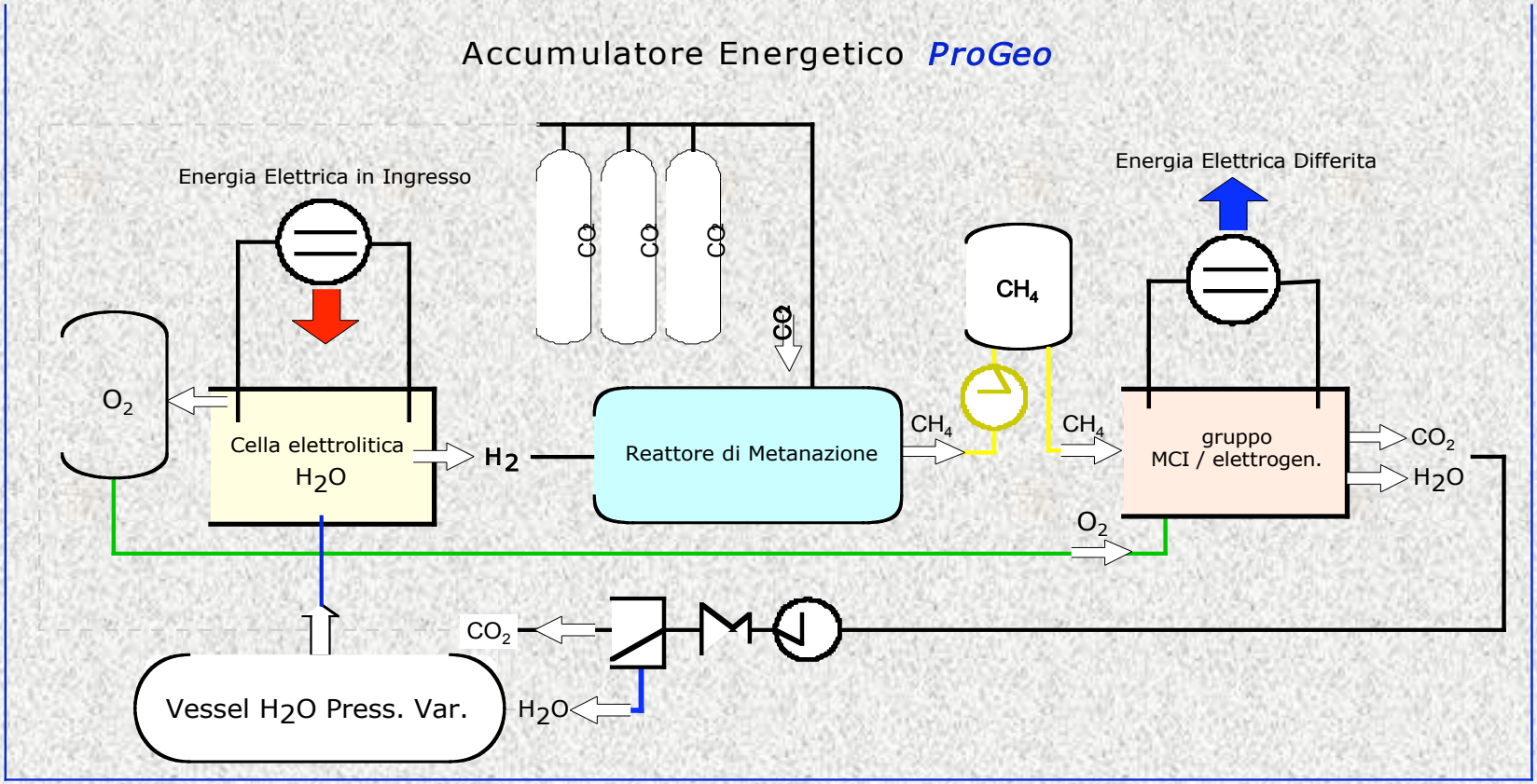
15. A use case


Chemistry (Perugia)
Computer Science (Perugia)
LO
SW
Chemistry (Tessaloniki)
SW

16. GREEN METHANE TO STORE RENEWABLE ENERGY

THE PROGEO INDUSTRIAL PROTOTYPE

Enea, DCBB, RPC, PLC, Master-up



THANKS

to all of you for attending and to Gabriele for hosting us