OPEN SCIENCE CLOUD (OSC)

INTRODUCTION to OPEN MOLECULAR SCIENCE CLOUD

Antonio Laganà

MASTER-UP srl and Department of Chemistry, Biology and Biotechnologies, UNIPG

Former Chair of the COMPUTATIONAL CHEMISTRY Division of EUCHEMS (2010-2016) and Member of the IGI Board (2010-2014)

"‥ The only way to gain the primacy of ideas is to become herald of a united Europe (of science) open to everyone"

Carlo Sforza, first Minister of Foreign Affairs of the Italian Republic (1948) and Rector of the University for foreigners, Perugia

OSC PARTNERS AND COMMUNITIES

JOINT OSC SCHOOL of the **ITN EJD TCCM Consortium, INFN, Department of Chemistry Biology and Biotechnologies** and **Department of Physics and Geology of the University of Perugia** with the operational support of **MASTER-UP srl.**

MAIN INVOLVED COMMUNITIES

PHYSICS: **MeV Big science and infrastructures (INFN paradigm)**

- Large Research Centers (CERN, Synchrotrons, ..)
- Backbone of EGI and IGI (Italian Grid Infrastructure)
- Extended Physics communities (Nuclear, Astro, ..)

CHEMISTRY: **meV Long tail of science (COMPCHEM paradigm)**

- Federated small Research Centers
- Departmental/group compute facilities
- Small theoretical, compute and experimental teams

1) COST D23 METACHEM (2000-2005)

- **OBJECTIVE**: build a European network of collaborative distributed computing groups (METALABORATORIES) to develop innovative solutions and paradigms for molecular science research

- **FUNDING**: only for meeting (not for building infrastructures)

- **METALABORATORIES IMPLEMENTED**:
  - Multireference quantum chemical methods
  - 4-component relativistic quantum chemical calculations
  - A priori simulation of crossed molecular beam experiments
  - Quantum mechanical studies of structure, dynamics and spectroscopy of systems relevant to environment
  - e-learning technologies for Chemistry
  - Code integration in ab-initio methods

2) FROM COST to an EGI VO and VRC

- **COST D37** (2006-2010): build within the grid infrastructure organizations and research environments suited to promote molecular science distributed computing activities in:
  - Photochemistry and photobiology
  - Dynamics engines for Grid molecular simulators
  - e-science and learning approches in molecular sciences
  - Codes interoperability in quantum chemistry
  - Computational chemistry workflows and data management

- **EGEE III –** establishing the **COMPCHEM** *Virtual Organization*

- **EGI-INSPIRE –** establishing the **EGI CMMST** Virtual Research Community (EGI-INSPIRE) with participation to **IGI**, **IBERGRID**, **PL-GRID** activities

3) OPEN MOLECULAR SCIENCE CURRICULA

ERASMUS+ MASTER TCCM (THEORETICAL CHEMISTRY & COMPUTATIONAL MODELING) 7 Universities

- GRONINGEN: *Magnetic Interactions in Molecules and Solids (2016)*
- LEUVEN: *Group Theory Applied to Chemistry (2013)*
- MADRID Autonoma: *Ab Initio Potentials and Wavefunctions*
- **PERUGIA**: *Chemical Reactions: Basic Theory and Computing (2017)*
- PORTO: *Ab Initio Biomolecules*
- TOULOUSE: *Ab Initio energies for Clusters*
- VALENCIA: *Nanostructured Materials*

- COFUNDING FOR WORLDWIDE APPLICANTS

4) OPEN MOLECULAR SCIENCE RESEARCH

ITN DOCTORATE TCCM CONSORTIUM 12 Universities

- PISA: *Modeling light harvesting by multi-chromophoric systems*
- GRONINGEN (2): *Modeling of photo-excitation processes in photovoltaics*
- **PERUGIA**: *Modeling chemical storage of renewable energies*
- TOULOUSE (2): *Electronic structure and dynamics of carbon nanotubes and Ruthenium complexes*
- VIENNA: *Modeling oxygen photosensitizers for photodynamics*
- MADRID (2): *Phototoxicity and stability of excipients and drugs, Dynamics of multiply charged biomolecules*
- PORTO: *Structural characterization of drug metabolites from collisional cross sections*
- PARIS: *Modeling nanoscale mixing of oxide materials*
- LEUVEN: *Predictive kinetics of organometallic catalysis*
- BARCELONA *Paramagnetic transitions in metal ions*
- PAIS VASCO *Aluminum-phosphate interactions*
- VALENCIA *Adsorption and separation of gases on graphene*.

5) SME TRAINING PARTNERS

THE 14 NON ACADEMIC ITN EJD TCCM TRAINERS

- ALYA TECH (ES)
- AΣ ATRIA SCIENCE SL (ES)
- BARCELONA SUPERCOMPUTING CENTER (ES)
- BIOLITEC RESEARCH GMBH (DE)
- CONSORZIO INTERUNIVERSITARIO CINECA (IT)
- GLAXO SMITKLINE RESEARCH & DEVELOPMENT LTD (UK)
- **MASTER-UP SRL (IT)**
- PARIS-SACLAY CAMPUS (FR)
- PLC SYSTEMS SRL (IT)
- SCIENTIFIC COMPUTING AND MODELING (NL)
- SIMUNE ATOMISTIC SL (ES)
- SMARTLIGS BIOINFORMATICA SL (ES)
- STOCKHOLM CAMPUS (SE)
- ZARAGOZA CAMPUS (ES)

6) VIRTUAL RESEARCH INFRASTRUCTURE

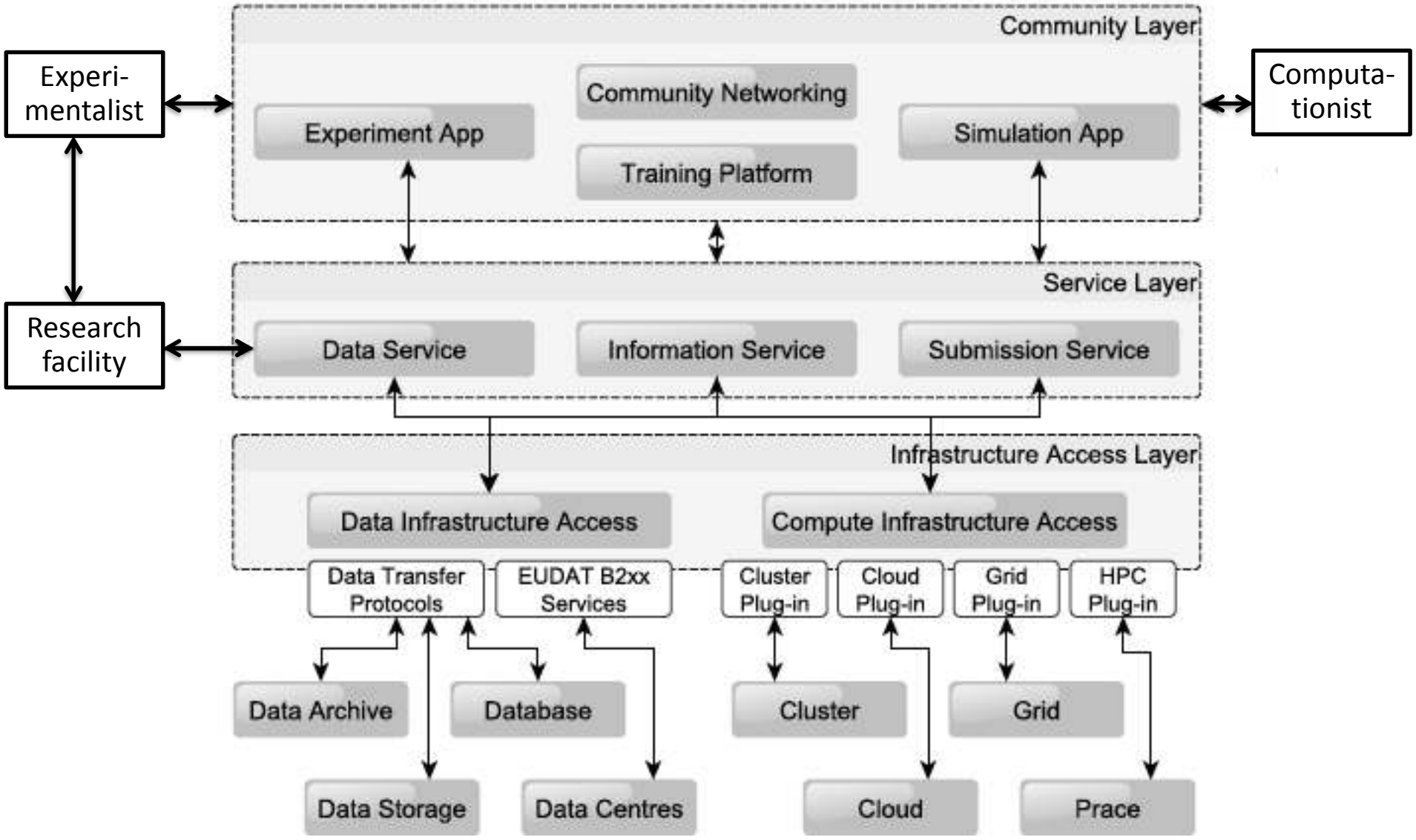
A H2020 PROPOSAL FOR A COLLABORATIVE MOLECULAR AND COMPUTER SCIENCE PLATFORM (not funded)

A. Laganà (Perugia, IT), G. Terstyanszky (Westminster, UK), J. Kruger (Tubingen, DE)

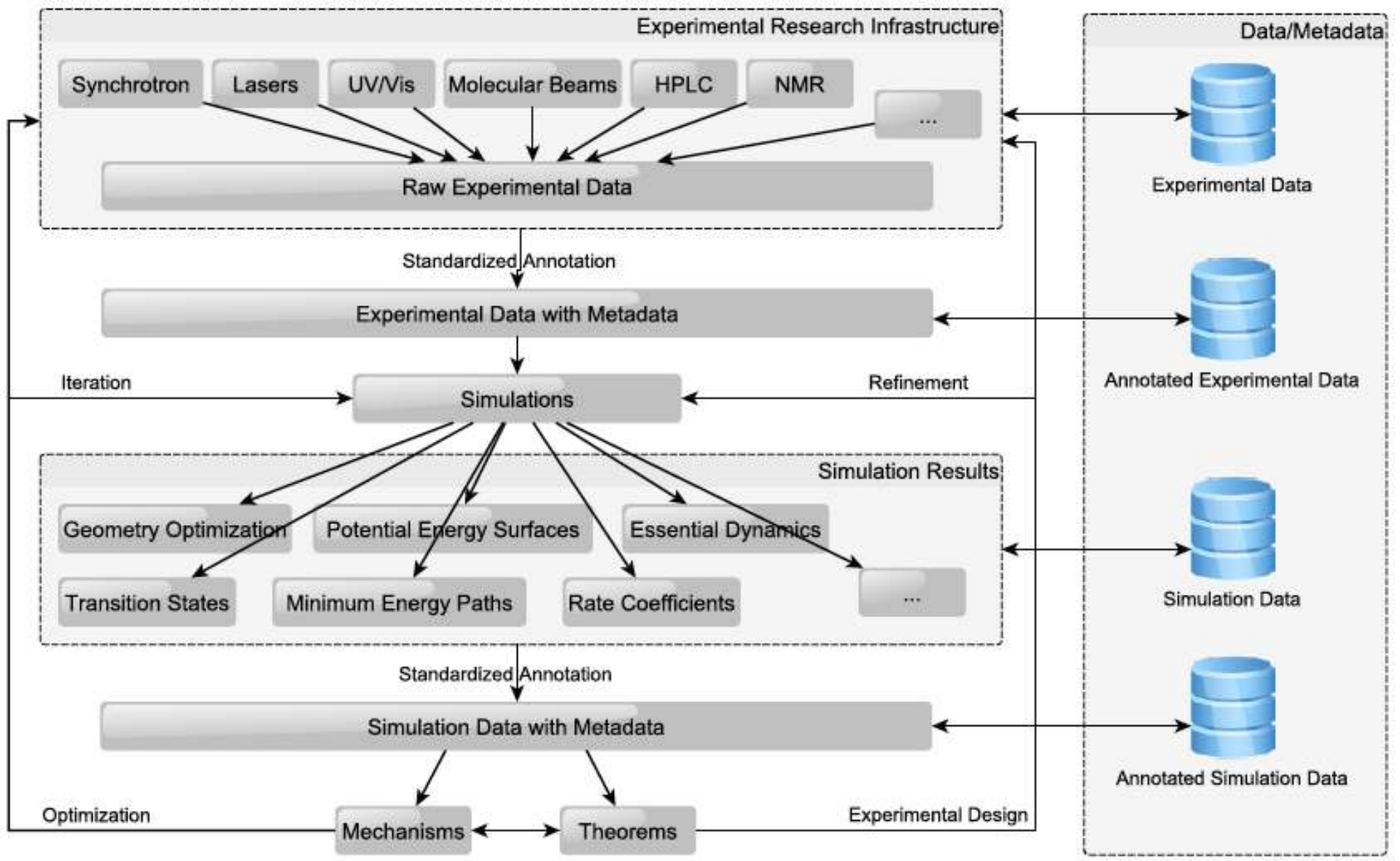
In collaboration with 12 Universities and Research Centres

- Provide an environment for the development of Open Molecular Science applications by federating computers and data
- Create an infrastructure and procedures suited for the utilization of Open Molecular Science services
- Drive interdisciplinary data to knowledge and innovation for societal needs

Access to data and computers



Data flows


Experimental Research Infrastructure
Synchrotron
Lasers
UV/Vis
Molecular Beams
HPLC
NMR
...
Raw Experimental Data
Standardized Annotation
Experimental Data with Metadata
Iteration
Simulations
Refinement
Simulation Results
Geometry Optimization
Potential Energy Surfaces
Essential Dynamics
Transition States
Minimum Energy Paths
Rate Coefficients
...
Standardized Annotation
Simulation Data with Metadata
Optimization
Mechanisms
Theorems
Experimental Design
Data/Metadata
Experimental Data
Annotated Experimental Data
Simulation Data
Annotated Simulation Data

EXPERIMENTAL INFRASTRUCTURE

research facility and infrastructures	Provider	EU	NA	RE	TRL	use cases
ELETTRA synchrotron facility	Elettra Sincrotrone Trieste	X			9	1, 3,4
FERMI free electron laser facility	Elettra Sincrotrone Trieste	X			9	All
non-linear spectroscopy	LENS, Firenze	X			9	1,2,4
FLASH free electron laser	DESY, Hamburg	X			8	1,2,4
PETRA III accelerator	DESY, Hamburg	X			9	4
crossed beams and beam gas facility	Beamlab, Perugia		X		8	2, 3, 5,6
plasma facility	Beyond Nano RI, Bari		X		9	3,5
ultrafast lasers + spectroscopy	CLUR/UCM, Madrid		X		8	2,3,4, 5
shock wave combustion experiments	CNRS, France		X		9	6-7
laboratory burners	CNRS, France		X		9	6-7
Jet-stirred and plug flow reactor	ENSIC, France			X	8	6-7
shock wave spectroscopy	ENSIC, Nancy			X	9	6-7
cyclonic and engine burner	CNR-IRC, Napoli			X	9	6-7
sodium-cooled fast and plug flow reactor	CNR-IRC, Napoli			X	8	5,6-7
experimental kinetics laboratory	Ljubljana			X	8	8
UV/Vis, Raman facilities	Aachen			X	8	4

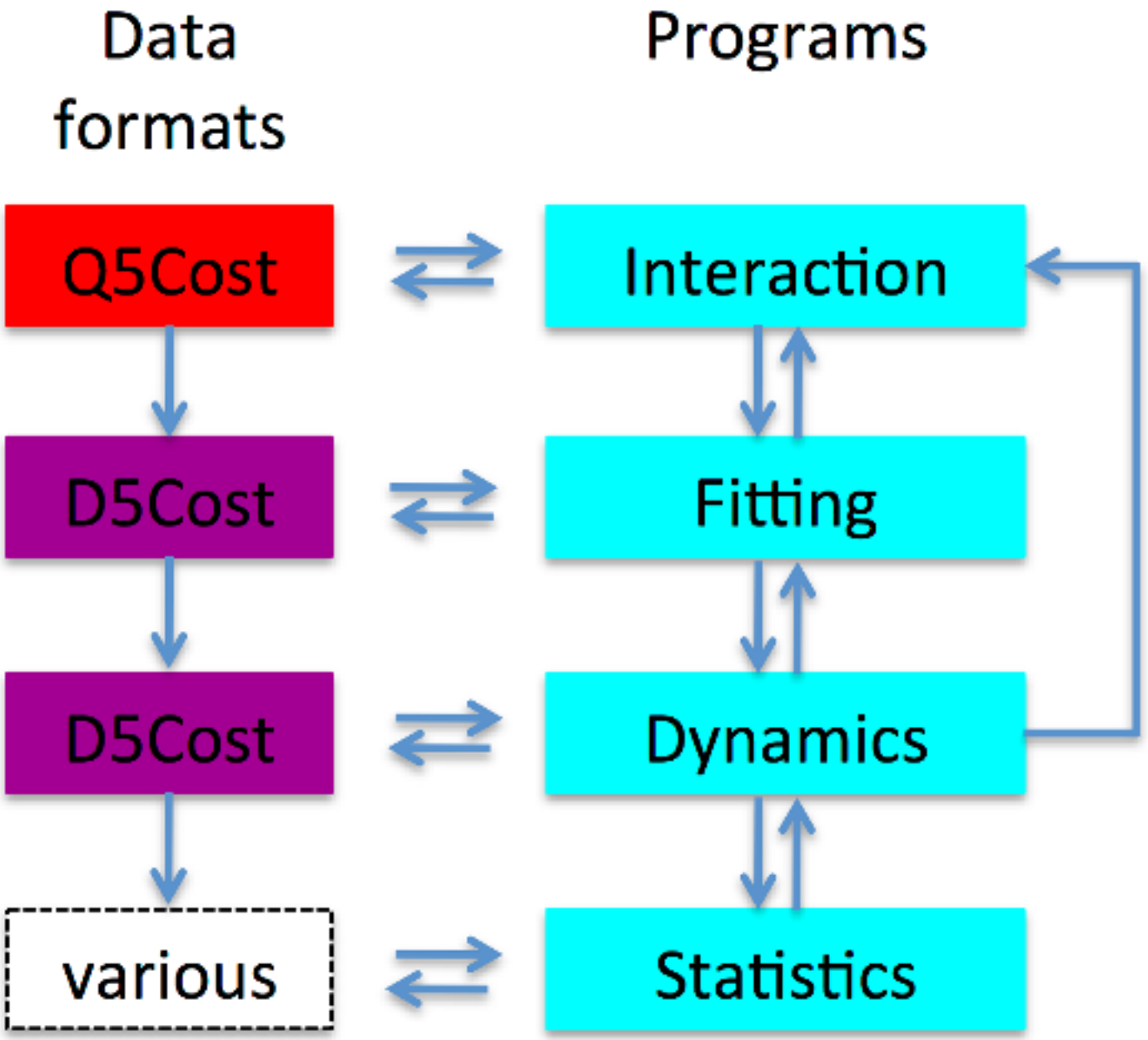
COMPUTATIONAL INFRASTRUCTURE

computing resources	Provider	EU	NA	RE	TRL	use cases
EGI Federated Cloud + Grid	EGI	X			9	All
CINECA	PRACE	X			9	All
CMAST	Roma	X			9	2,3,5
CRESCO	Roma	X			8	2,3,5
RECAS	Bari		X		9	2,3,5
ZIH	Germany		X		9	1,2,4
MoSGrid	Germany		X		9	3,4,5
UCM Computer cluster	Madrid			X	9	2,3,4
Computer Center. Nat. Inst. Chem	Ljubljana			X	8	8
Openstack cloud	Perugia			X	7	2,3,5
Linux cluster	Perugia			X	8	2,3,5
FLAVUS cluster	Tübingen			X	8	4

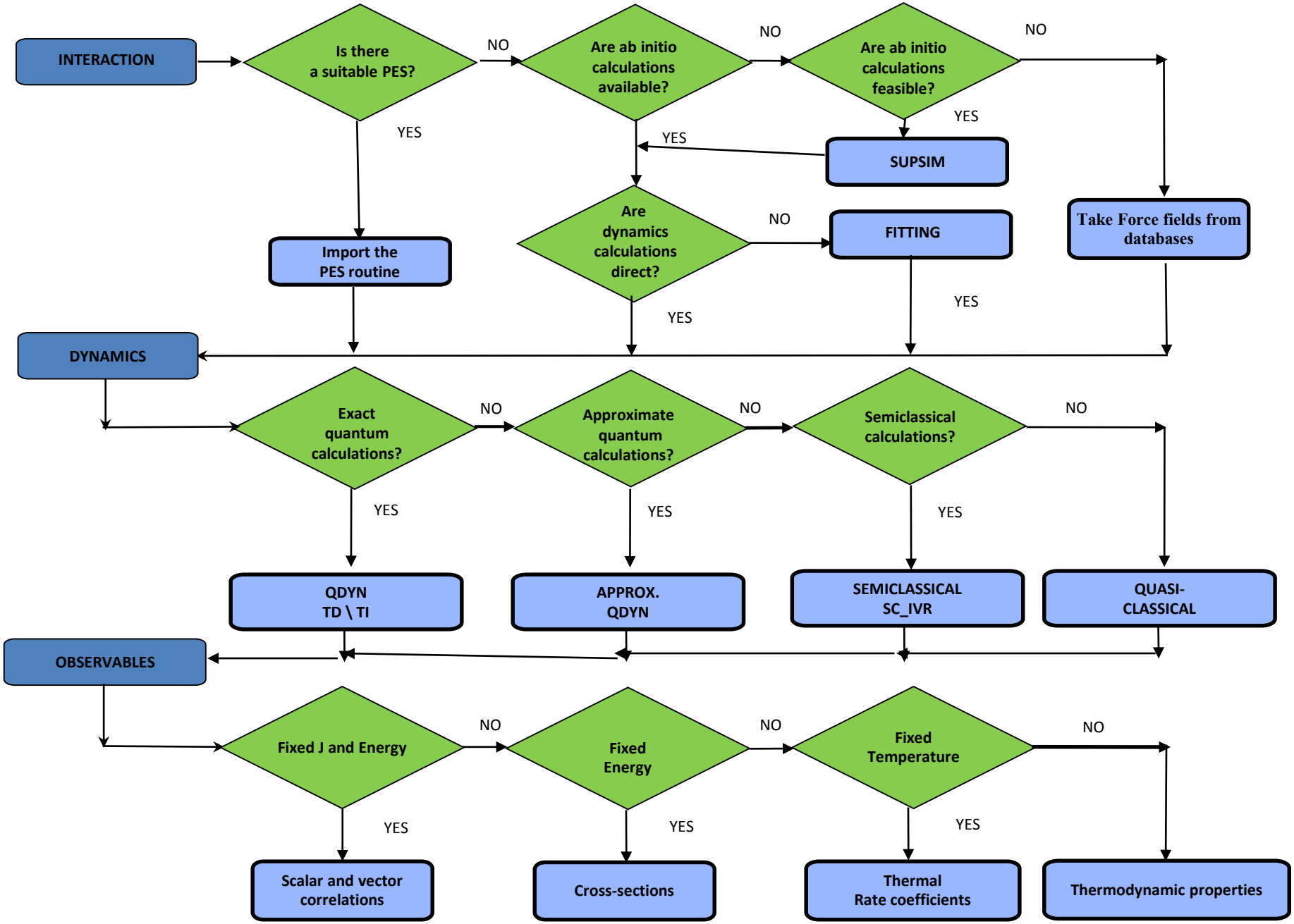
7) GEMS: the grid Molecular Simulator

- **TOPICS**: Highly accurate chemical dynamics and energetics for systems made of reasonably small molecules.
- **Experiments**: Beams, femto- and nano-second pulsed lasers, pump-probe and laser spectroscopy, time-of-flight mass spectrometry, ion and photoelectron imaging techniques, non equilibrium plasmas, catalysed gas phase processes.
- **Computing**: High level ab initio electronic structure packages together with quantum, quantum-classical and quasi-classical molecular dynamics codes plus statistics implemented on different machines.
- **Innovative chemical processes**: renewable energies storage, carbon neutral fuels, new materials, etc.

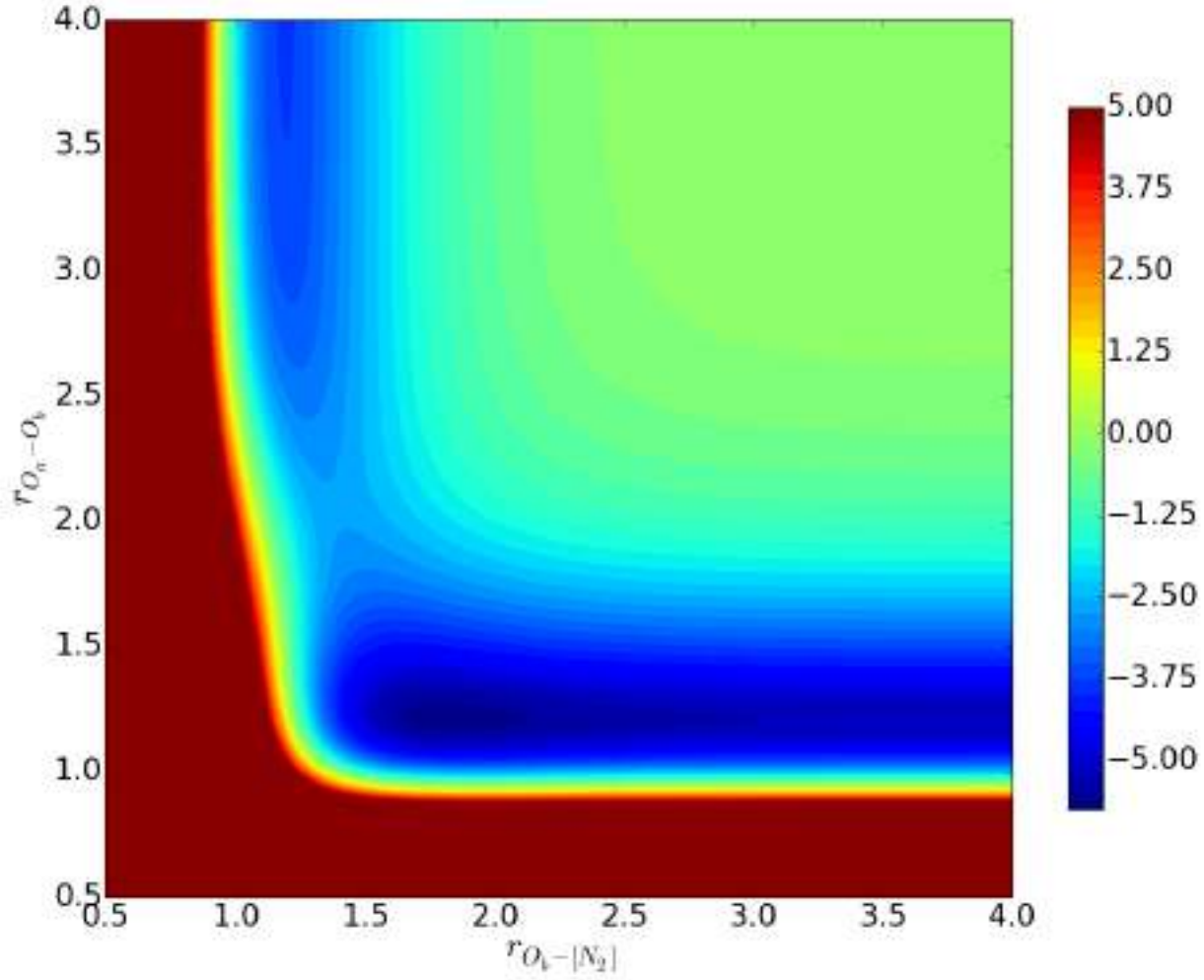
7a.1) WORKFLOW BASICS (Rampino)



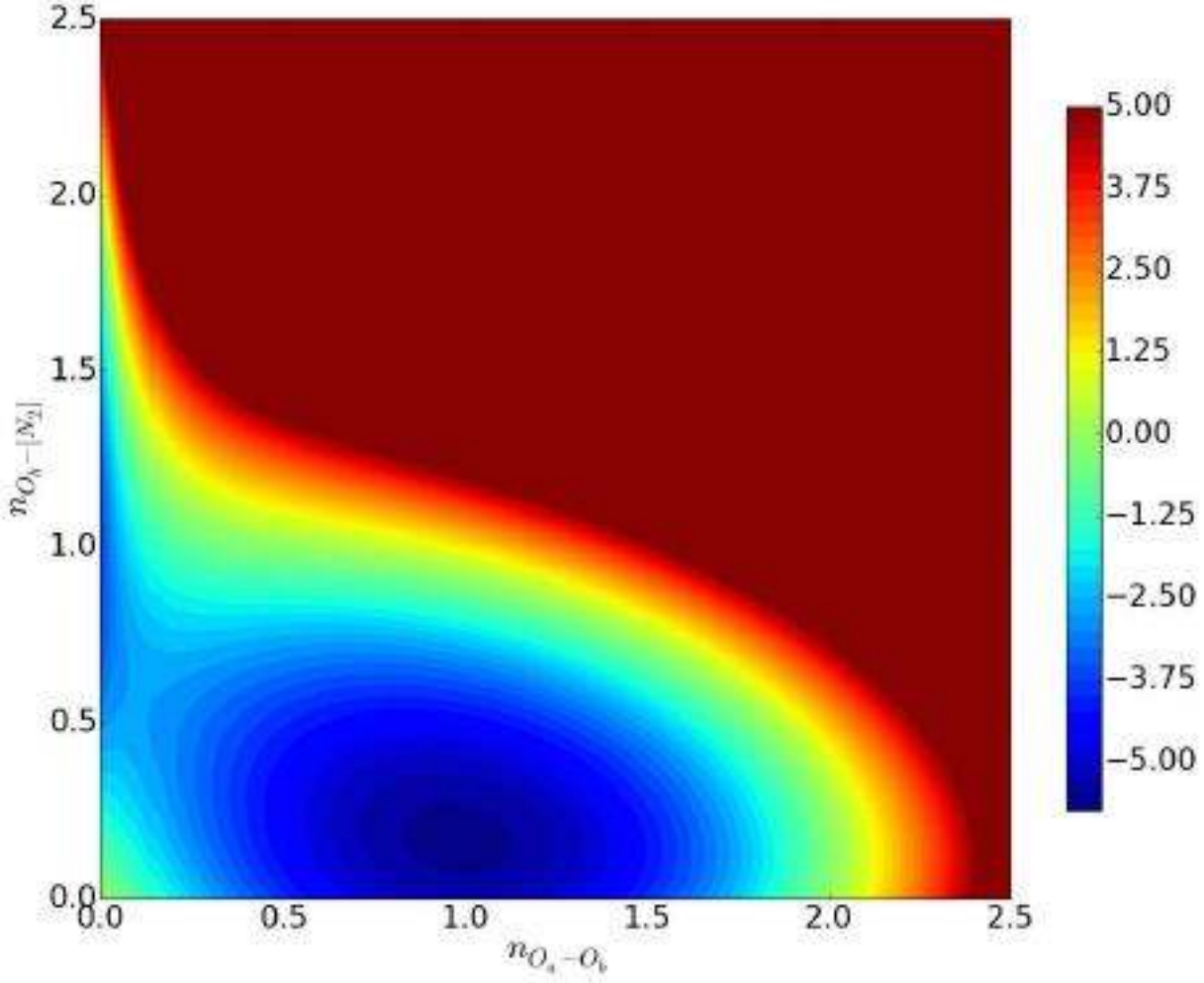
7a.2) WORKFLOW DETAILS (Rampino)



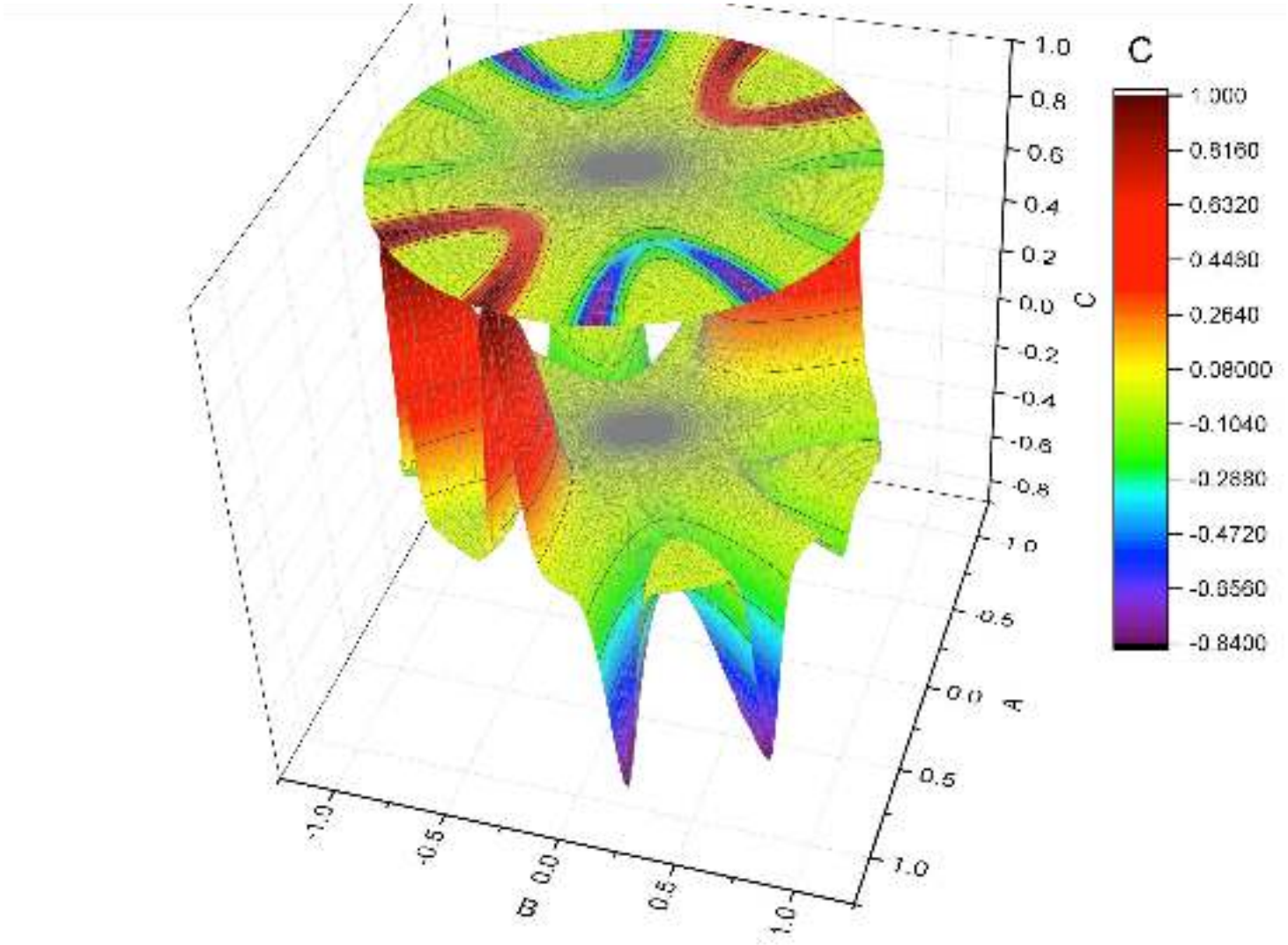
7b.1) HIGH LEVEL AB INITIO POTENTIALS INTERNUCLEAR DISTANCE FORMULATION



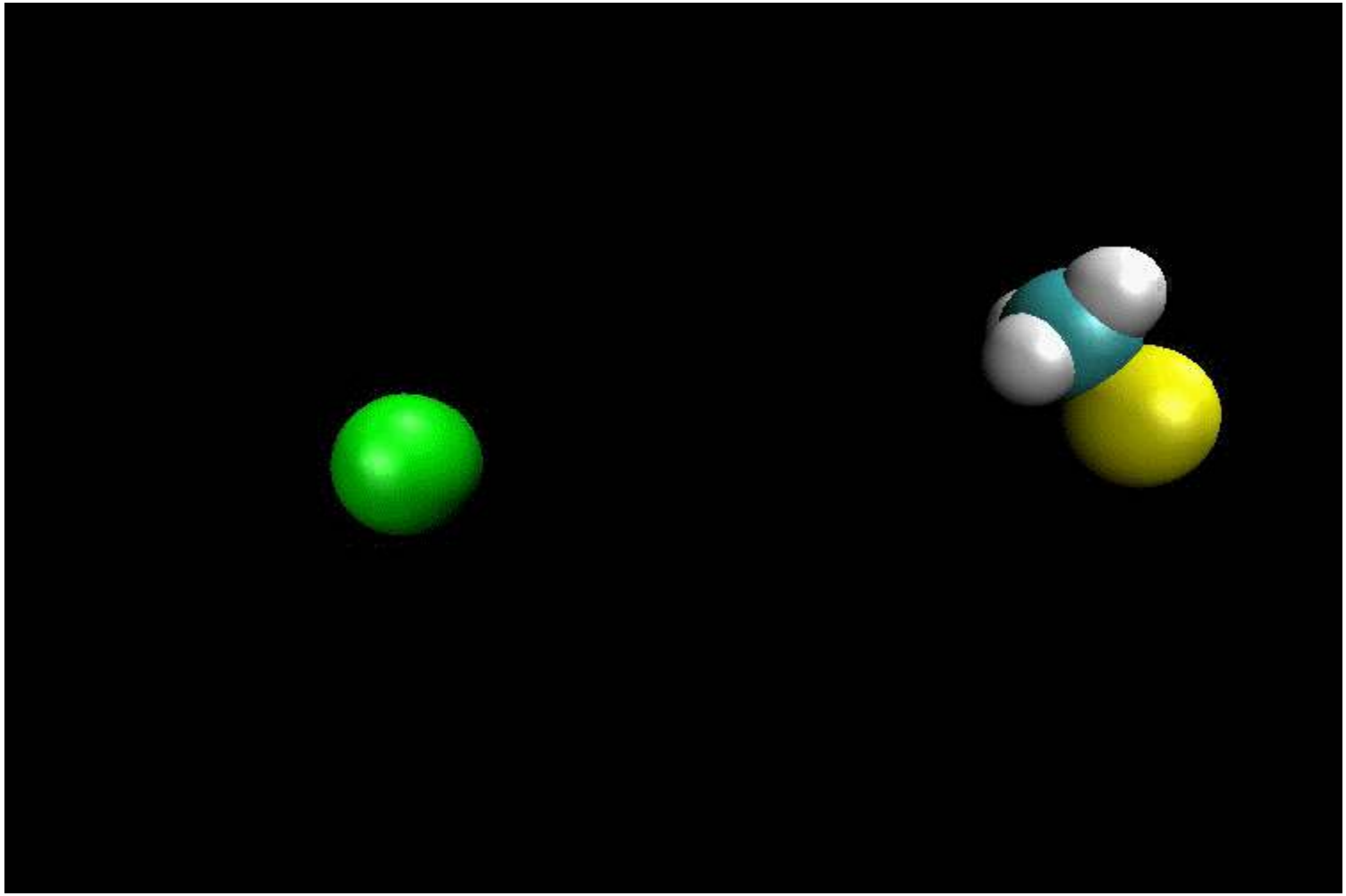
7b.2) BOND ORDER FORMULATION (Rampino)



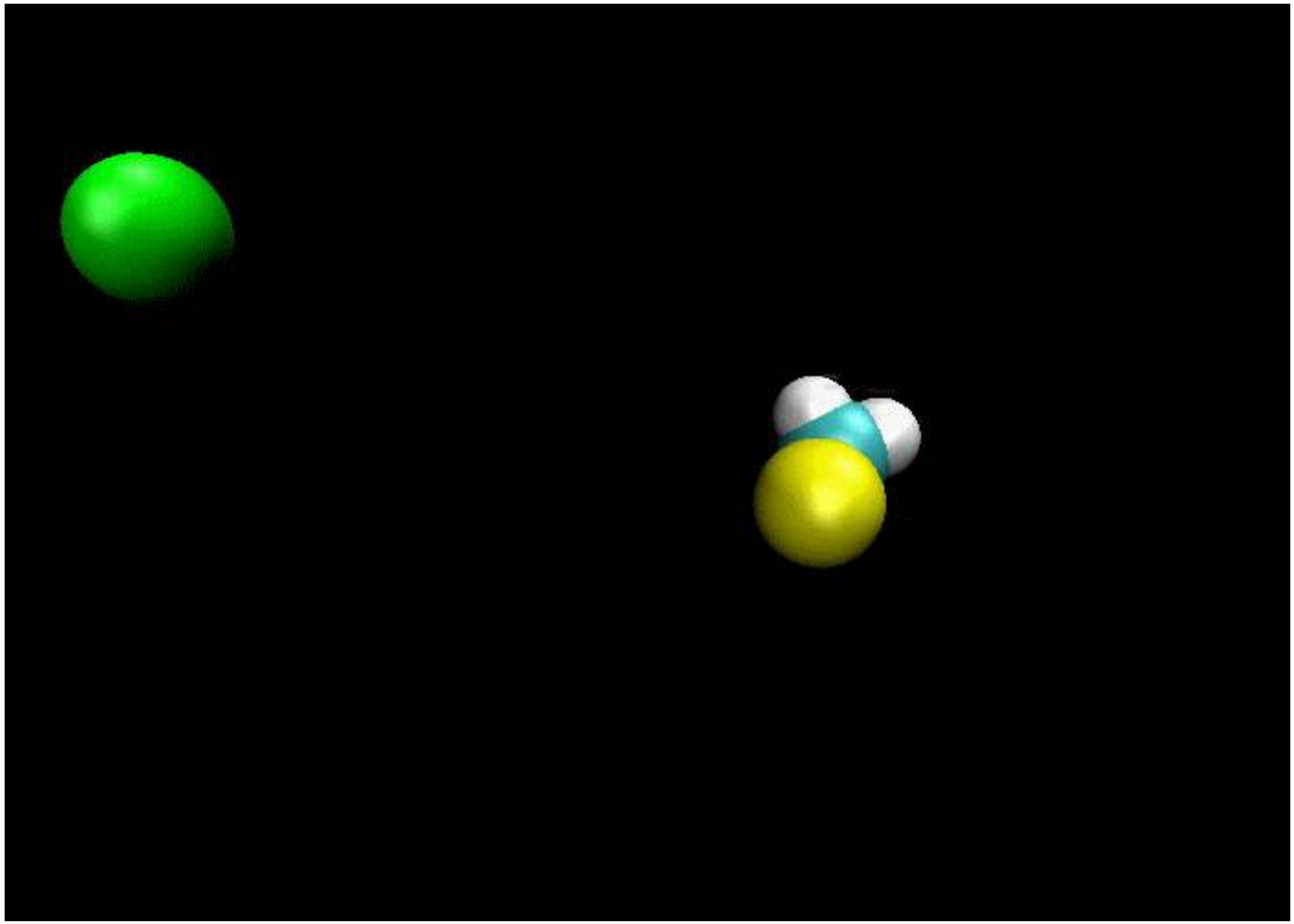
7b.3) HYPERSPHERICAL QUANTUM DYNAMICS: THE H_3 SYSTEM (Rampino)



7c.1) MOLECULAR DYNAMICS: DIRECT MECHANISMS (Faginas)

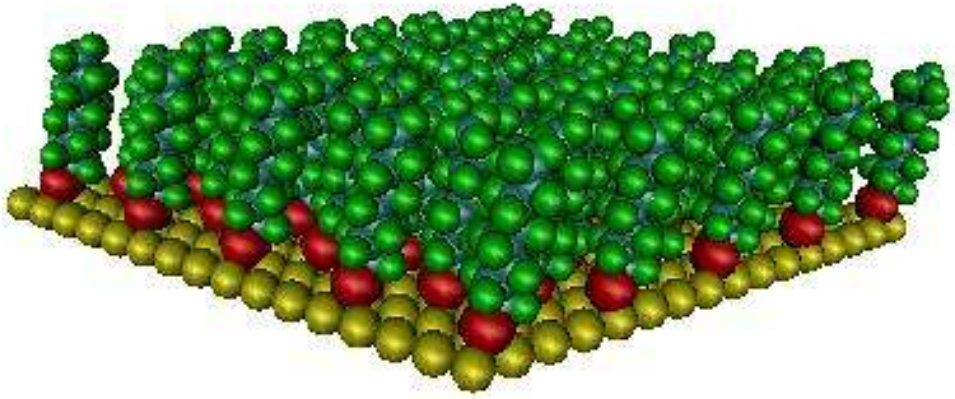


7c.2) MOLECULAR DYNAMICS: COOPERATIVE MECHANISMS (Faginas)

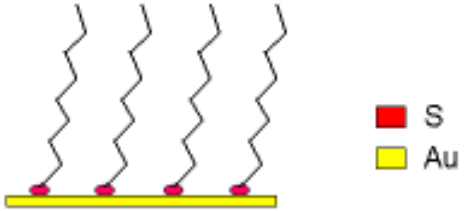


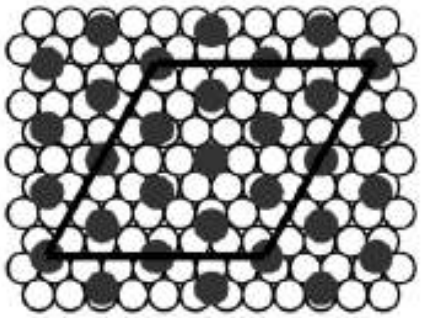
7c.3) MOLECULAR DYNAMICS: CATHALYSIS (Faginas)

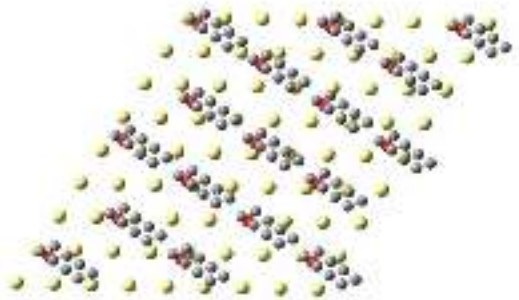
Protonated peptide



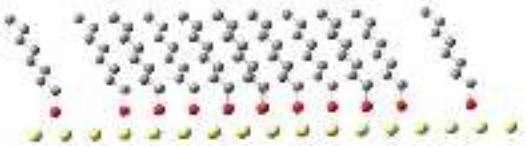
Surface: $CF_3(CF_2)_7S$-Au





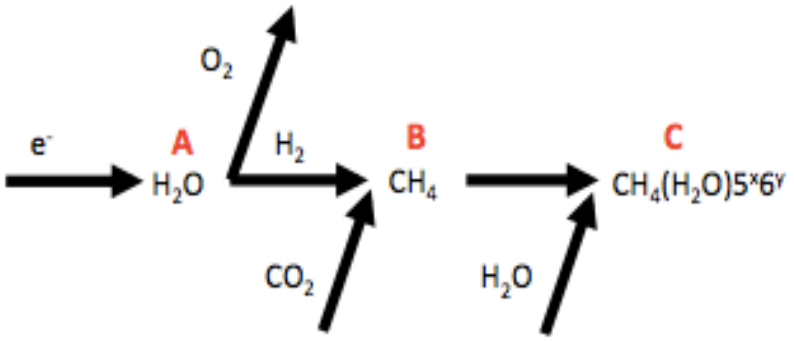


TOP VIEW



SIDE VIEW

7d.1) INNOVATION: from RENEWABLE ENERGIES to METHANE (Master-UP)



7d.2) The PLAYERS

DCBB & DICA
University of PG



R.P.C srl
(Roma)


ENEA (Frascati)

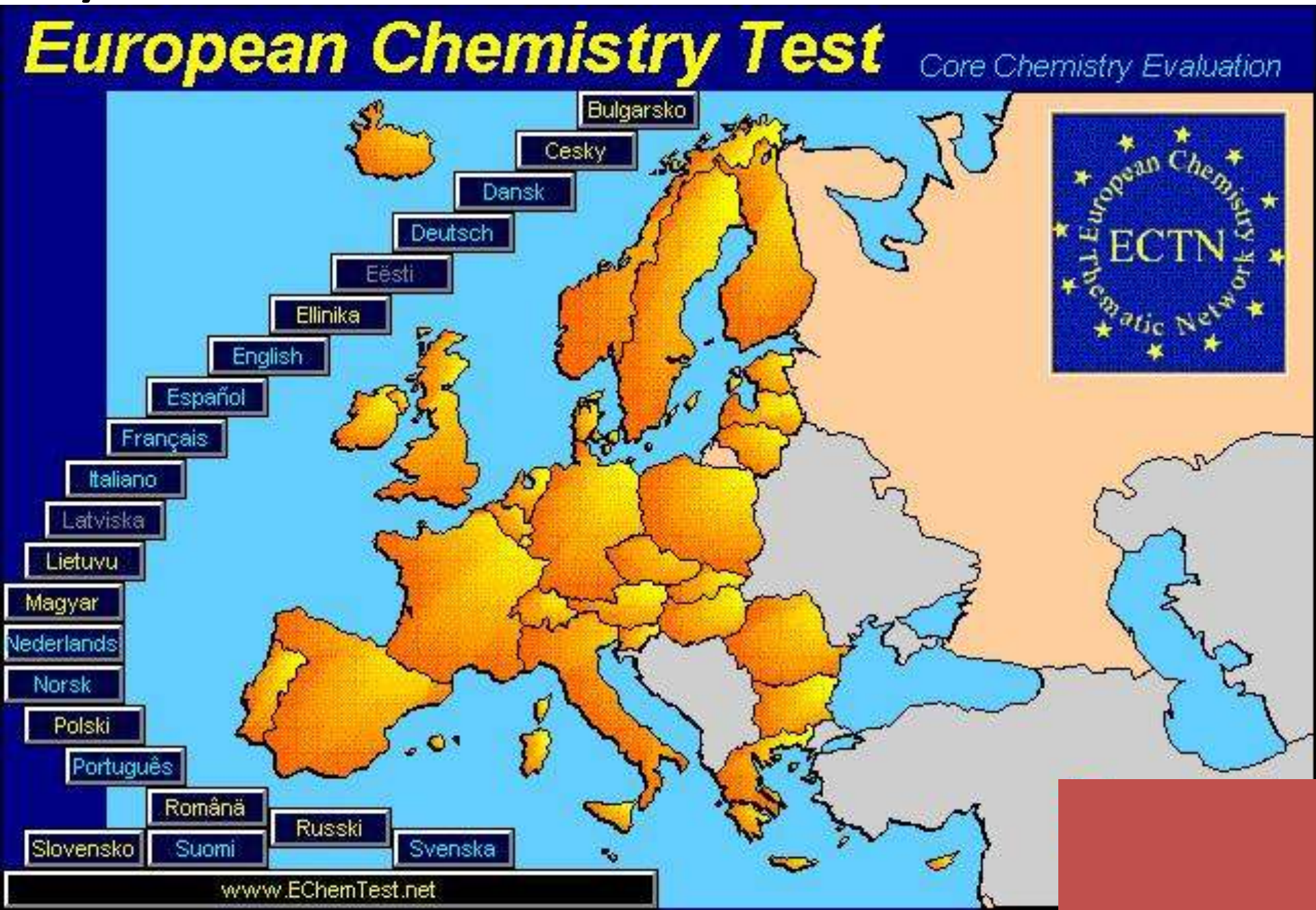
RDPower
srl (Terni)


MASTER-UP
srl (Perugia)

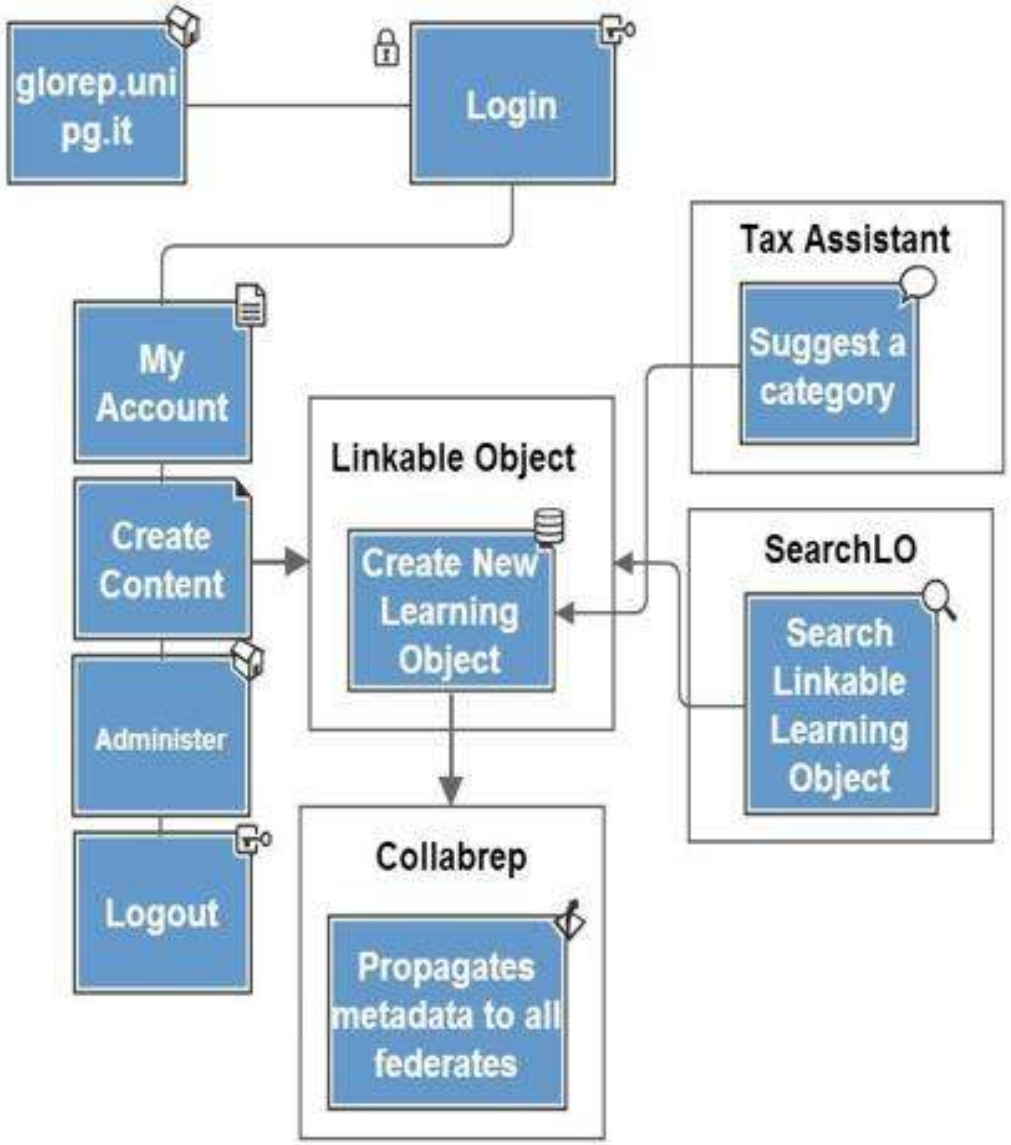

8) A MOLECULAR SCIENCE PILOT
Thematic Platform Partnership Model

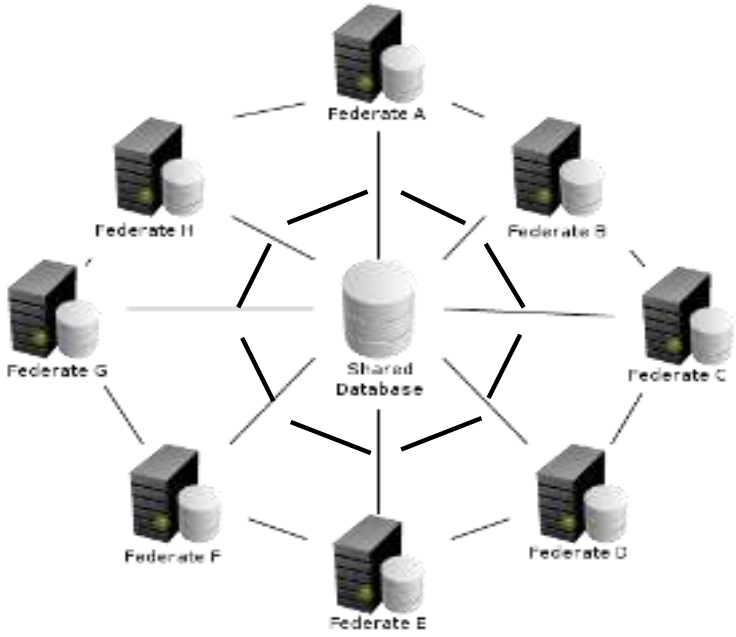
- (Service) From You (operated) By You
  - ✓ Thematic platform partner operates services
  - ✓ Thematic platform partner owns Intellectual Properties (IPs)
  - ✓ EGI supports the thematic platform with e-Infrastructure services
- Thematic platform partner is responsible for:
  - ✓ Provision of the thematic service (incl. e.g., cost for operation, support)
  - ✓ Maintenance and further development of the service (new features)
  - ✓ Meeting the terms & conditions of entering the EGI marketplace
  - ✓ End-user customer relations
- EGI responsible for:
  - ✓ Provision of underlying services (e.g. cloud, grid) – based on SLA
  - ✓ Marketing of service in marketplace
- Shared responsibilities
  - ✓ Agreed access rules and policies
  - ✓ Interoperable services

9a) EU SHARED Molecular Science e-Tests



9b) GLOREP: MOLECULAR SCIENCE LEARNING OBJECTS DISTRIBUTED REPOSITORY

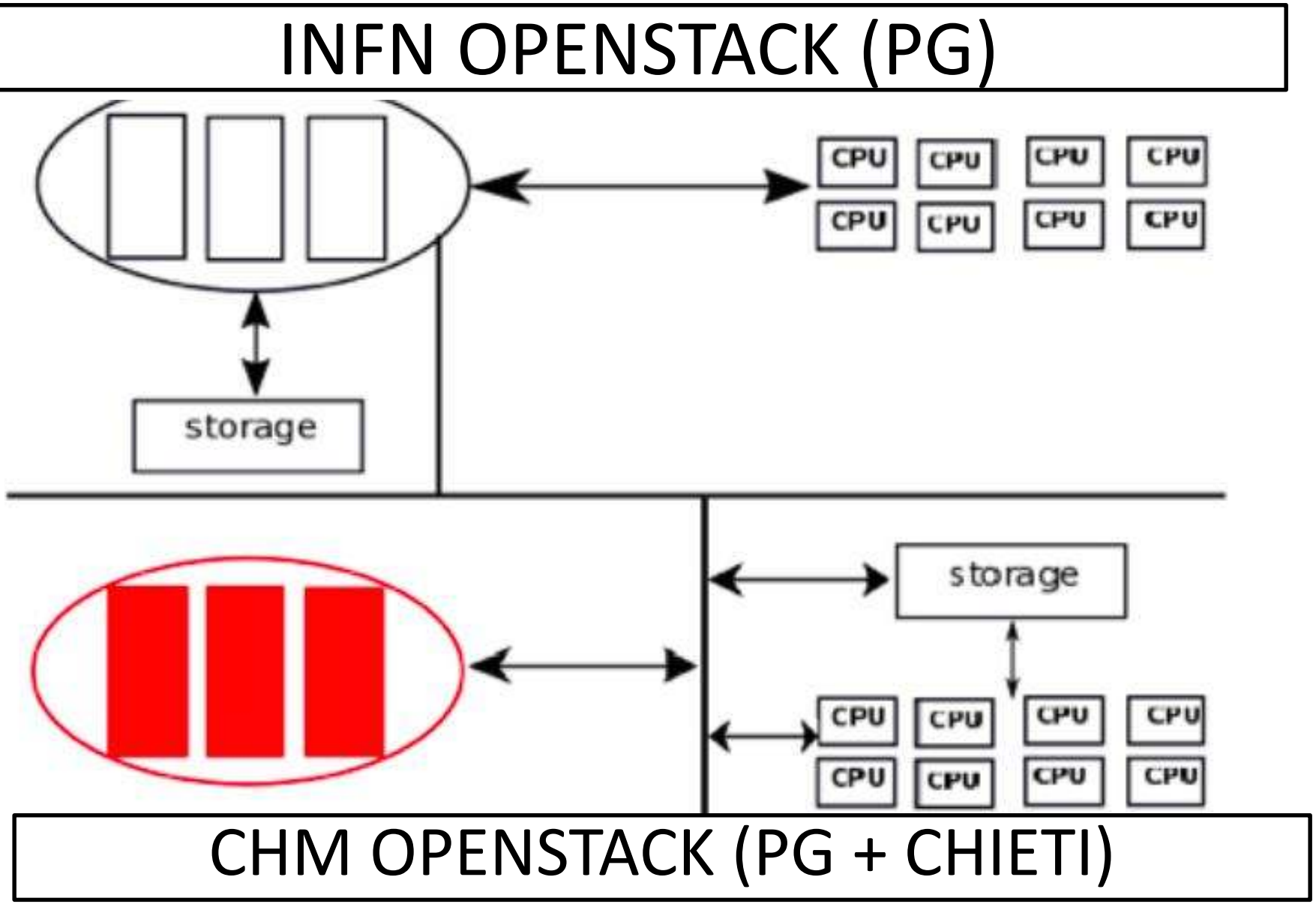




THE PG MOLECULAR SCIENCE CLUSTER

- **RESEARCH PARTNERS:**
  - **UNIPG** GROUND AND EXCITED ELECTRONIC STRUCTURE
  - **UNIPG** QUANTUM AND CLASSICAL MOLECULAR DYNAMICS
  - **UNIPG** DRUG DESIGN AND CHEMOMETRICS
  - **UNIPG** E-TESTS AND LEARNING OBJECTS
  - **ISTM-CNR** SOLID STATE
- **COMPANIES**:
  - **MASTER-UP** srl (Computer services and renewable energies storage).
  - **MOLECULAR HORIZON** srl (Drug design and chemometrics)
- **COLLABORATION**:
  - PERUGIA **INFN, PHYSICS** & **GEOLOGY, MATHEMATICS** & **INFORMATICS** DEPARTMENTS UNIVERSITY of PERUGIA
  - **UNIVERSITY** of CHIETI

LOCAL CLOUD PLATFORM



THANKS

SOSC BASICS (Mon-Tue)

- M. Mazzucato: *Scientific computing an historical and inspired view*
- A. Zoccoli: *Perspectives, funding, European model*
- C. Grandi: *Big experiments: Computing Challenges*
- F. Giacomini: *Scientific Programming (Hands on)*
- D. Salomoni: *Cloud computing; Science in Openstack*
- P. Vicini: *Parallel Computing*
- G. Terstyanszky: *Workflows in Molecular sciences*
- D. Spiga et al.: *Cloud/Parallel/HPC (Hands on)*

SOSC APPLICATIONS (Wed-Thu)

- M.N Faginas Lago: *Molecular Dynamics*
- S. Rampino: *Quantum dynamics*
- M.N. Faginas Lago: *Molecular Dynamics (Hands on)*
- S. Rampino: *Quantum dynamics (Hands on)*
- T. Dorigo: *Statistical Methods in Data Analysis*
- T. Dorigo: *Statistical Methods in Data Analysis (Hands on)*
- E. Ricci: *Deep Learning*
- E. Ricci: *Deep Learning (Hands on)*

SOSC EDUCATION (Fri)

- S. Tasso: *OMS GLOREP*
- S. Tasso, M. Rui: *OMS GLOREP (Hands on)*
- O. Gervasi: *EChemTest on LibreEOL*
- O. Gervasi, M. Rui: *EChemTest on LibreEOL (Hands on)*

THANKS

- ITN EJD TCCM CONSORTIUM

- INFN, UNIVERSITY PG (Dept. Chem. Biol. Biotech, Dept. Phys. Geo, Dept. Math. Inf)

- MASTER-UP

- **ALL PARTICIPANTS**

PRACTICAL HINTS

- LECTURES: *PHYS-GEO Department*
- LUNCHES: *UNIVERSITY REFECTORY sign with Noelia during the morning*
- ACCOMMODATION: *HOTELS and Students' houses*
- MATERIALS: *submit to lagana05@gmail.com to publish on the **VIRT&L-COMM** e-magazine*
- ANY PROBLEM: *refer to the SOSC front desk*

Partnership Model 2:
Thematic Platform Supplier

- (Service) From You (Operated) By EGI
  - ✓ Thematic platform supplier passes service ownership (IPs) to EGI
  - ✓ EGI operates and maintains the thematic platform
  - ✓ EGI supports the thematic platform with e-Infrastructure services
- Thematic platform supplier is responsible for:
  - ✓ Service component(s) support based on OLA if EGI members
  - ✓ Service component(s) support based on UA if non-EGI members
  - ✓ Maintenance and further development of the service (new features)
- EGI is responsible for:
  - ✓ Provision of the thematic platform (and operations)
  - ✓ End-user customer relations
  - ✓ Provision of underlying services (e.g. cloud, grid) – based on SLA
  - ✓ Marketing of service in marketplace
- Shared responsibilities (subject to negotiation)
  - ✓ Maintenance and further development of the service (new features)
  - ✓ Training, documentation, and technical supports
  - ✓ Costs