EGEE Generic Applications Advisory Panel
first meeting

Grid based Molecular Simulators

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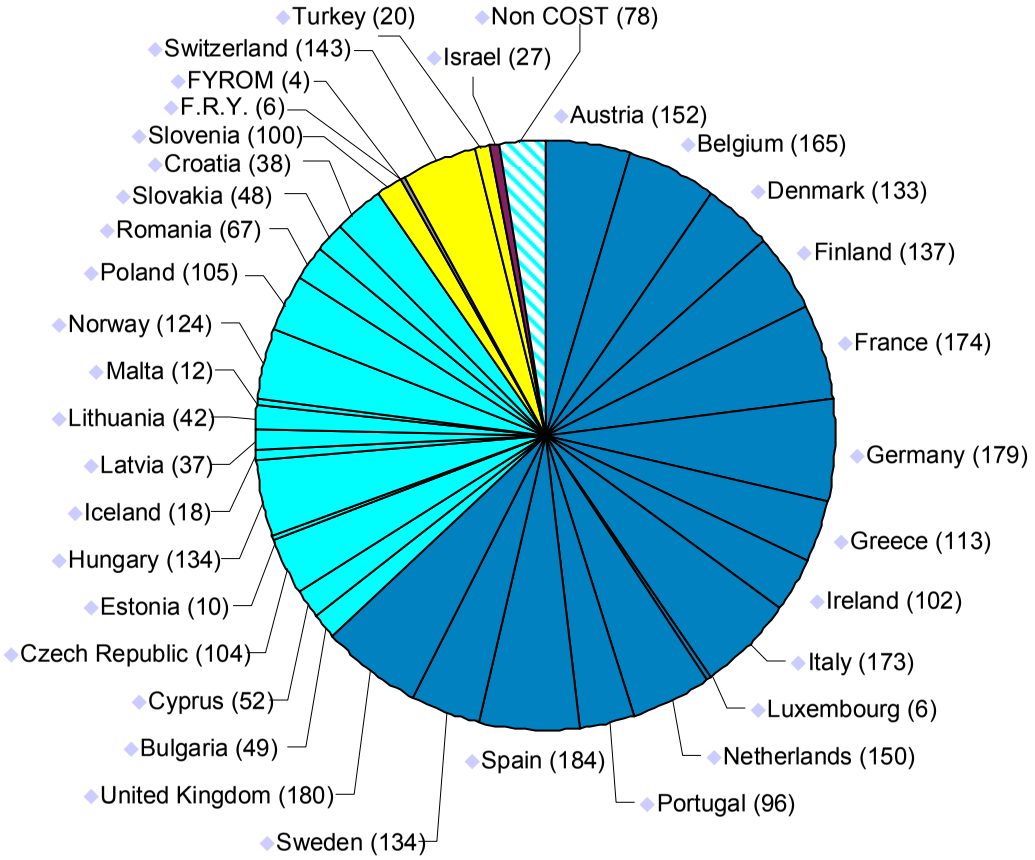
Osvaldo Gervasi
Dept. of Mathematics and
Computer Science
University of Perugia
ogervasi@computer.org

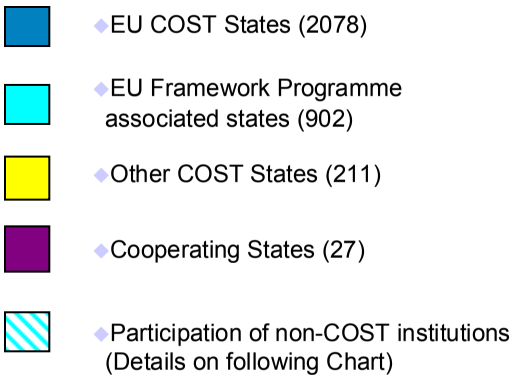
Antonio Laganà
Dept. of Chemistry
University of Perugia
lag@dyn.unipg.it

Summary

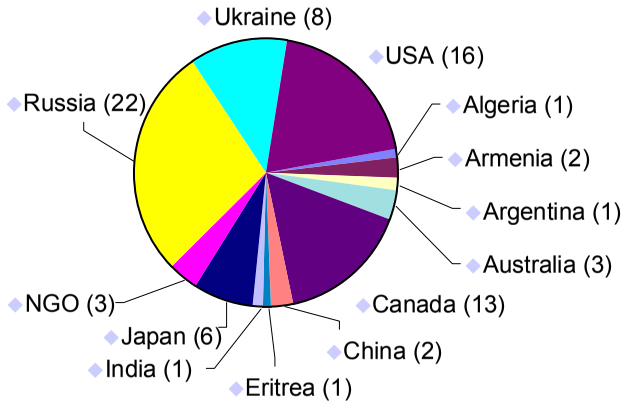
- COST Chemistry and METACHEM
- Ongoing metalaboratories in Chemistry
- Architecture of the Simulator
- Conclusions

COST- Countries (2002)
Participating Institutions

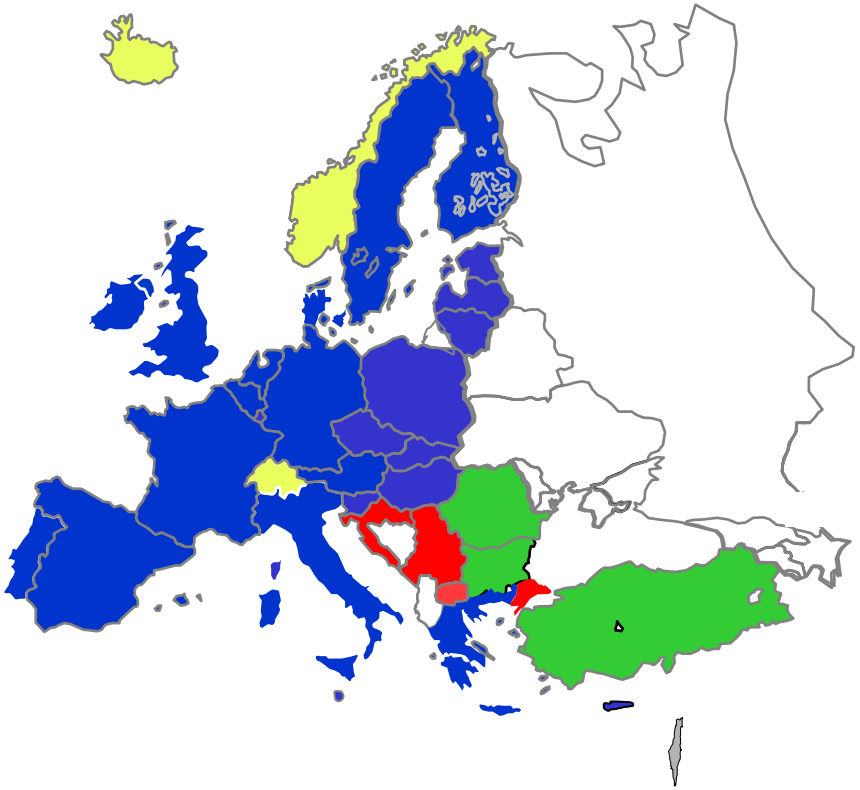




Participation of Non-COST Institutions (Total: 78)



COST Member States



- **The twentyfive EU Member States**
- **EFTA Member States**
  - Iceland
  - Norway
  - Switzerland*
- **Candidate Counties**
  - Bulgaria
  - Romania
  - Turkey *
- **Other Countries**
  - Federal Republic of Yugoslavia*
  - Former Yugoslav Republic of Macedonia*
  - Croatia *
- **Co-operating State**
  - Israel

* Not Associated to FP

The COST Chemistry domain

- Created in 1992
- 34 Actions launched since 1992 (12 completed with final evaluation)
- 22 running (10 had the mid term evaluation)
- Research Chemists from 31 COST Countries
- Associated Institutions from Australia, Japan, Russia, Ukraine and the USA

Second batch of Actions

- **Health and Therapy**
  - **D13** (New Molecules for Human Health),
  - **D18** (Lanthanide Chemistry for Diagnosis and Therapy),
  - **D20** (Metal Compounds in the Treatment of Cancer and Viral Diseases)

- **Biology and Prebiotic**
  - **D21** (Metalloenzymes and Chemical Biomimethics),
  - **D22** (Protein Lipid Interaction),
  - **D27** (Prebiotic Chemistry and Early Evolution),
  - **D28** (Natural Products as a Source for Discovery, Synthesis and Application of Pharmaceuticals)

Second batch of Actions

- **Nanostructures and new Functions and Materials**
  - **D14** (Functional Molecular Material),
  - **D17** (Oligomers, Polymers and Copolymers via Metal Catalysis),
  - **D31** (Organising Non-Covalent Chemical Systems with Selected Functions),
  - **D34** (Nanoscale Electrochemical and Bioprocesses at solid aqueous interfaces of industrial materials)
- **New Molecules and Clean Processes**
  - **D15** (Interfacial Chemistry and Catalysis),
  - **D24** (Sustainable Chemical Processes Stereoselective Transition Metal Catalysed Reactions),
  - **D25** (Applied Biocatalysis: Stereoselective and Environmentally Friendly Reactions catalysed by Enzymes)
  - **D29** (Sustainable Chemical Processes: Stereoselective Transition Metal-Catalysed Reactions)

Second batch of Actions

- **High Pressure and Energy**
  - **D30** (High Pressure Tuning of Chemical and Biochemical Processes),
  - **D32** (Chemistry in High Energy Microenvironments)
- **Theory and computing**
  - **D16** (Combinatorial Chemistry),
  - **D23 (**Metachem: Metalaboratories for Complex Computational Applications in Chemistry),
  - **D26** (Integrative Computational Chemistry)

Metachem: Matalaboratories for Complex Applications in Chemistry

- MURQM: Multireference Quantum Chemical Methods
- DIRAC: Four Component Relativistic Quantum Chemical Calculations
- SIMBEX: Simulation of Molecular Beam Experiments
- DYSTS: Dynamics and Spectroscopy of Systems : Relevant to Environment and Applied Chemistry
- ELCHEM: E-learning Technologies for Chemistry
- ICAB: Integration of Codes for Ab Initio Methods
- COMOVIT: Collaborative Molecular and Electronic Structure Visualization tools

EU partners of D23 WGs

Simbex

Murqm

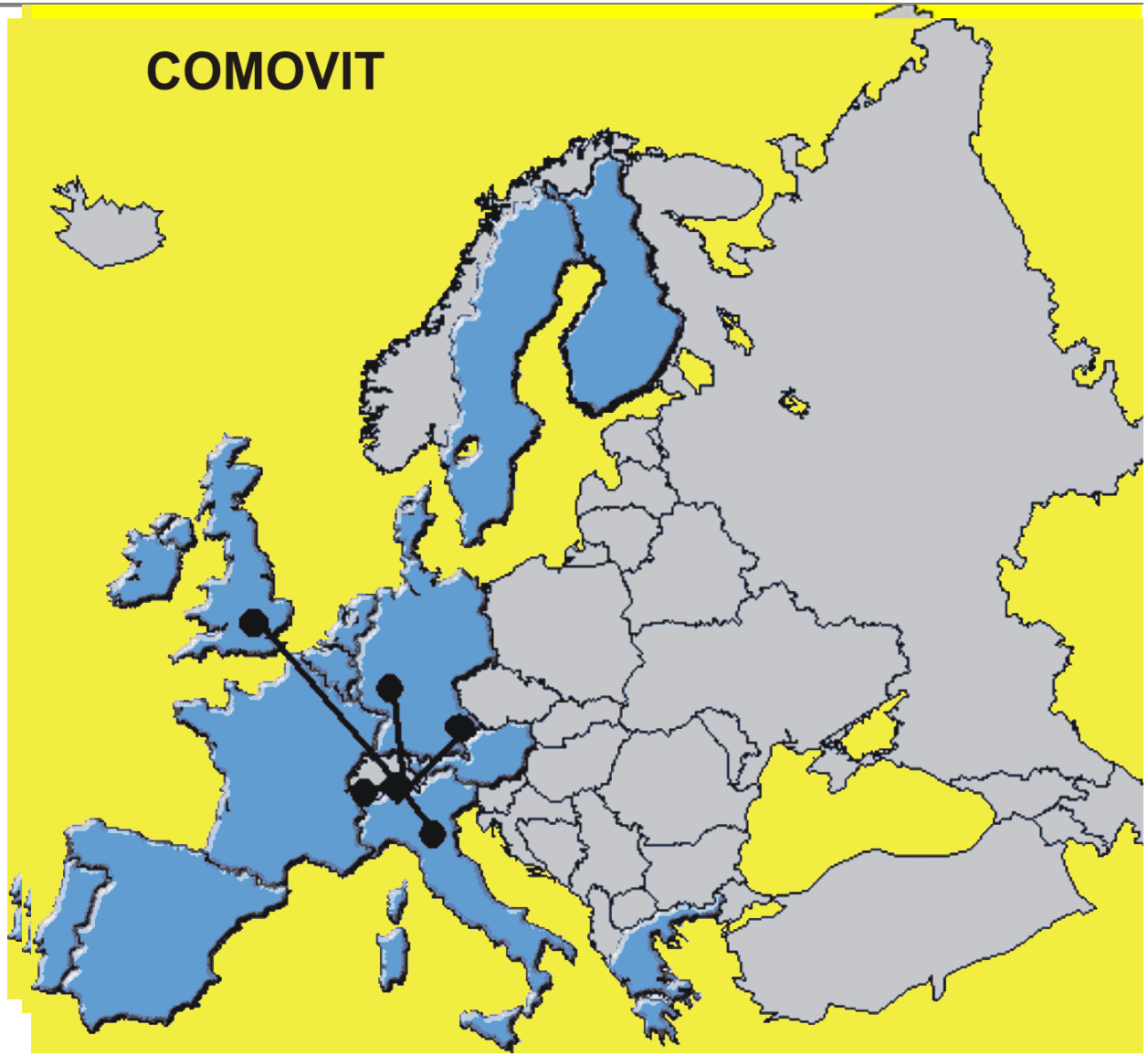
Dirac

Elchem

Icab

Dysts

Comovit



Labs per nationality

1 Isr,Pl,Sk,Nl

2 Cz,Ch, Fr, Dk, A, Sw, No

3 Hu

4 Gr

5 E

6 D, Uk,

9 I

MURQM (P. CARSKY, CZ)

- Ab initio codes are designed in a cooperative way. They deal with large matrices and linear algebra operations. Diagonalizations and minimizations. Construction of hypersurfaces of potential energy values bypoints
- 9 Laboratories (Petr Cársky - J. Heyrovsky Institute - Czech Republic, Jiri Pittner - J. Heyrovsky Institute - Czech Republic, Ivan Hubac - Comenius University – Slovakia, Stephen Wilson - Rutherford Appleton Laboratory –UK, Wolfgang Wenzel Universität Dortmund, Germany, Leszek Meissner - Nicholas Copernicus University – Poland, Volker Staemmler - Ruhr Universität – Germany, Constantinos Tsipis - Aristotle University of Thessaloniki – Greece, Aristides Mavridis - National and Kapodistrian Univ. of Athens - Greece)

DIRAC (K. FAEGRI, NO)

- Cooperative development of MC-SCF, gradient minimization, DFT capabilities, integral algorithms for relativistic accurate concurrent calculations
- 6 Laboratories (Knut Faegri - University of Oslo – Norway, Hans J. Aagaard Jensen University of Southern Denmark – Denmark, Uzi Kaldor -Tel Aviv University – Israel, Patrick Norman - Linköping University – Sweden, Trond Saue - Université Louis Pasteur – France, Lucas Visscher - Vrije Universiteit Amsterdam – Netherlands, Timo FleigHeinrich - Heine University - Germany)

SIMBEX (O. GERVASI, I)

- Coordinated implementation of a workflow management environment to simulate molecular beam experiments and molecular processes. Ab initio, dynamics, kinetics and statistics codes are assembled
- 10 Laboratories (Osvaldo Gervasi - Università di Perugia – Italy, Ernesto Garcia - Universidad del Pais Vasco – Spain, Gabriel Balint-Kurti - University of Bristol – UK, Gunnar Nyman - University of Goteborg – Sweden, Peter Kacsuk - MTA SZTAKI – Hungary, Jaroslaw Nabrzyski Inst. Bioorganic Chem., Poland, Francisco Tirado - Universidad Complutense – Spain, Ranieri Baraglia – CNR – Italy, Robert J. Allan – Daresbury Laboratory – UK, Gyorgy Lendvay – HAS -Hungary)

DYSTS (A. AGUILAR, E)

- Environment and application driven dynamics and spectroscopy calculations distributed among the participating laboratories
- 4 Laboratories (Antonio Aguilar-Navarro - Universidad de Barcelona – Spain, Vincenzo Aquilanti - Università di Perugia – Italy, Florent Xavier Gadea - Université Paul Sabatier – France, Paolo Palmieri - Universita di Bologna - Italy)

ELCHEM (A. LAGANA, I)

- Coordinated development of ubiquitous learning technologies and virtual laboratories. Design of distributed virtual reality tools at human and molecular level
- 10 Laboratories (Antonio Laganà - Università di Perugia – Italy, Ernst Bratz - TU Muenchen – Germany, Gustavo Avitabile - Università Federico II – Italy, Dimitra Kovala-Demertzi - University of Ioannina – Greece, Jens Josephsen - Roskilde University – Denmark, Paul Yates - Keele University – UK, Anna Croft - University of Wales – UK, Evangelia Varella - University of Thessaloniki – Greece)

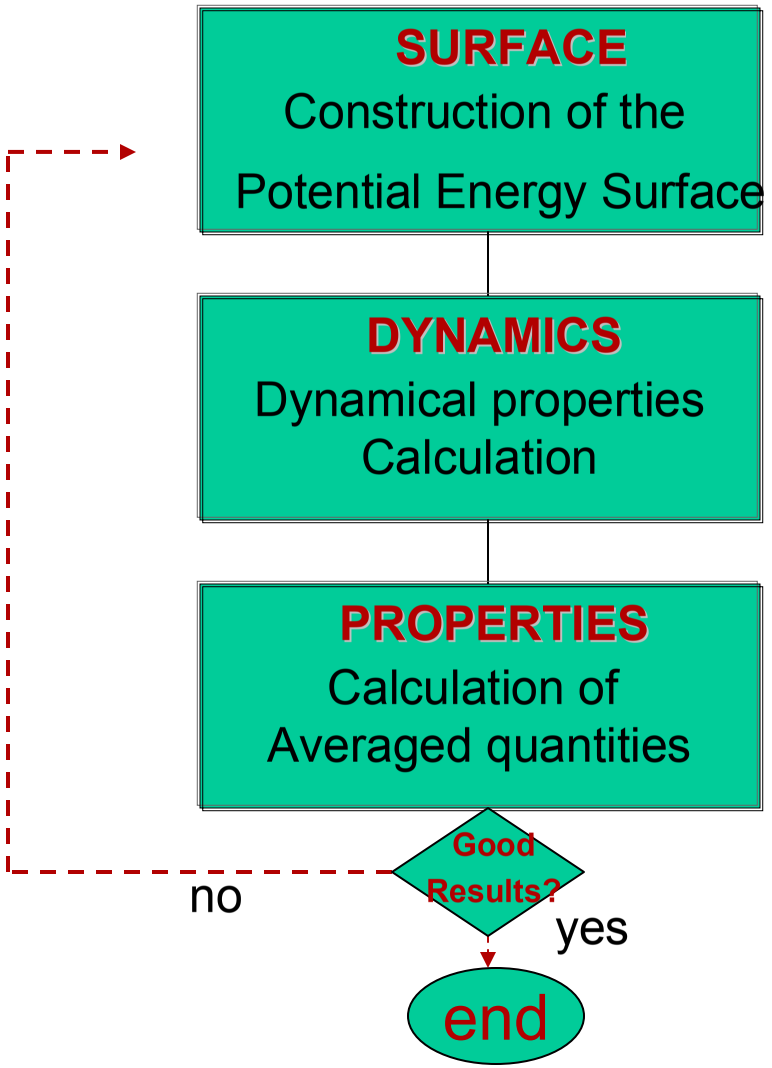
ICAB (E. ROSSI, I)

- Coordinated development of linear scaling methods for ab initio calculations with particular emphasis on chemical data transfer and handling
- 6 Laboratories (Elda Rossi – CINECA –Italy, Renzo Cimiraglia - Università di Ferrara – Italy, Daniel Maynau – IRSAMC – France, José Sanchez-Marin - Universitat de Valencia – Spain, Peter Szalay - Eötvös Loránd University – Hungary, Rosa Caballol - Universitat Rovira i Virgili Spain)

COMOVIT (H. LUETHI, CH)

- Design and development of multimedia distributed software to handle 3D molecular information of ab initio origin
- 6 Laboratories (Hans Peter Luethi, ETH - Zurich - CH)

The architecture of the Simulator



Electronic Structure calculation and representation

- Isolated (gas phase) small molecules
- Isolated (gas phase) large molecules
- Condensed phase and solid state calculations
- Topological studies
- Modeling and functional representations of the potential energy surfaces

Molecular Dynamics calculations

- Exact quantum dynamics for small systems
- Semiclassical and mixed classical-quantum for intermediate systems
- QM/MM and Car Parrinello
- Classical dynamics

Observable Properties

- Structure and stability calculations for aggregates of various sizes
- Kinetics and fluid dynamics calculations
- Thermodynamics properties
- Direct Monte Carlo calculations
- Condensed phase and liquid crystals
- Cross sections and rate coefficients

Electronic Structure Programs

- Small molecules (GAMESS-UK, GAMESS US, MOLPRO)
- Large molecules (GAUSSIAN03)
- Topological analysis of the interactions (AIMPAC, TOPOND)
- Modelling and fitting of the potential energy surfaces (FITTING)

Molecular Dynamics Programs

- Car-Parrinello (CPMD)
- Classical dynamics (ABCtraj, VENUS96; DL_POLY)
- Quantum dynamics (TD)
- Semiclassical dynamics (ABCsem)

Observable Properties Programs

- Direct Monte Carlo (DSMC)
- Energy and angular distributions

Critical Features of the Individual Programs

- AB INITIO METHODS (molpro, gamess, adc, gaussian,) resource requests are proportional to N^3 (N is the number of electrons) and to M^D (M is the number of grid points per dimension D) for CPU and disc demand.
- EMPIRICAL FORCE FIELDS (Venus, dl_poly, …) resource requests are proportional to P! (P is the number of atoms)

Critical Features of the Individual Programs (ii)

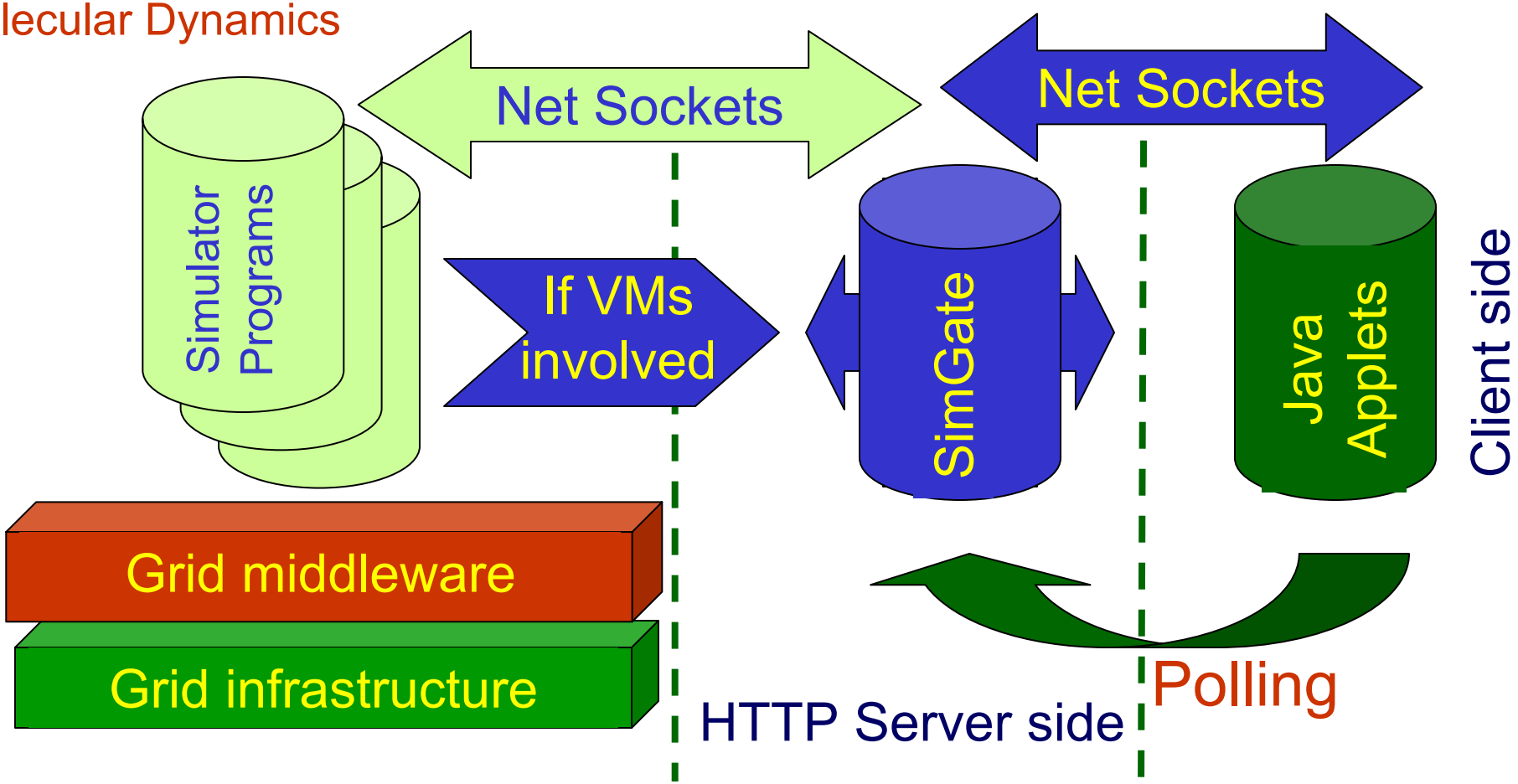
- DYNAMICS (APH3D, TIMEDEP, …) these programs use as input the output of the previous module most critical dependence is on the total angular momentum **J** value that can increase up to several hundred units and the size of the matrices depend on 2J+1
- KINETICS PROGRAMS use dynamics results for integrating relevant time dependent applications

The model architecture of a Simulator

Ab-initio techniques,

PES fitting,

Molecular Dynamics



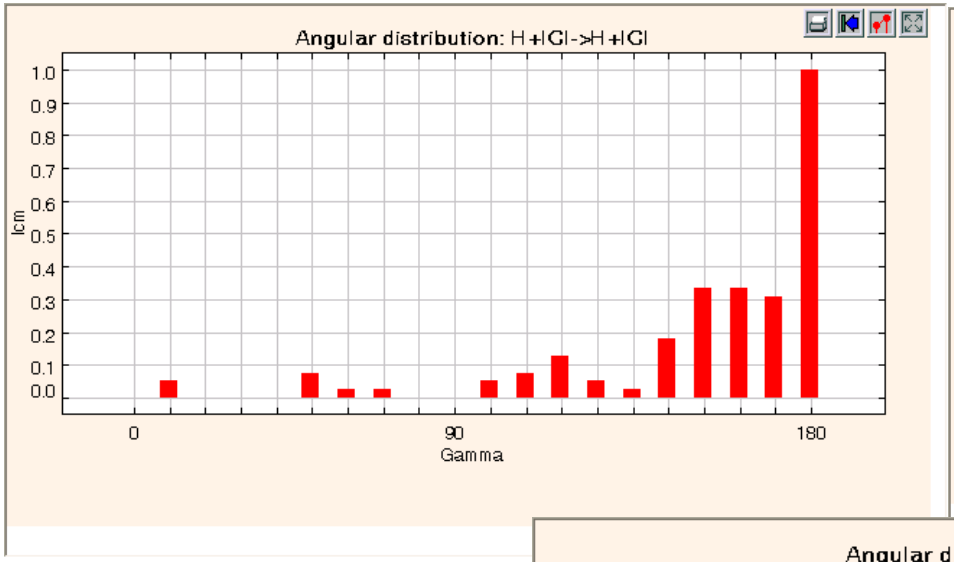
Local Platforms

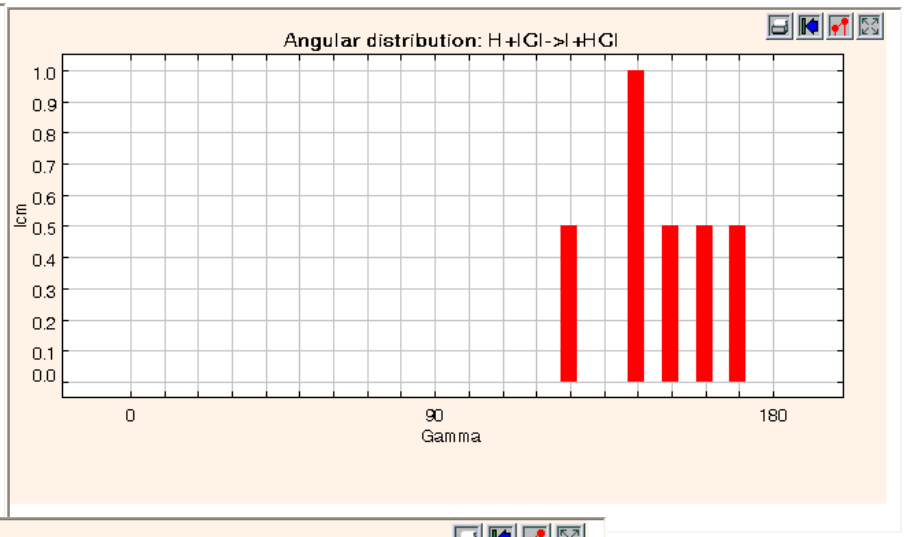
- Several workstations (IBM, Sun, SG, HP, ..)
- Clusters of PC
- Parallel machines (IBM SP, Origin, Sun multiprocessor, …)
- Supercomputer centers (CINECA, EPCC, CESCA, ..)

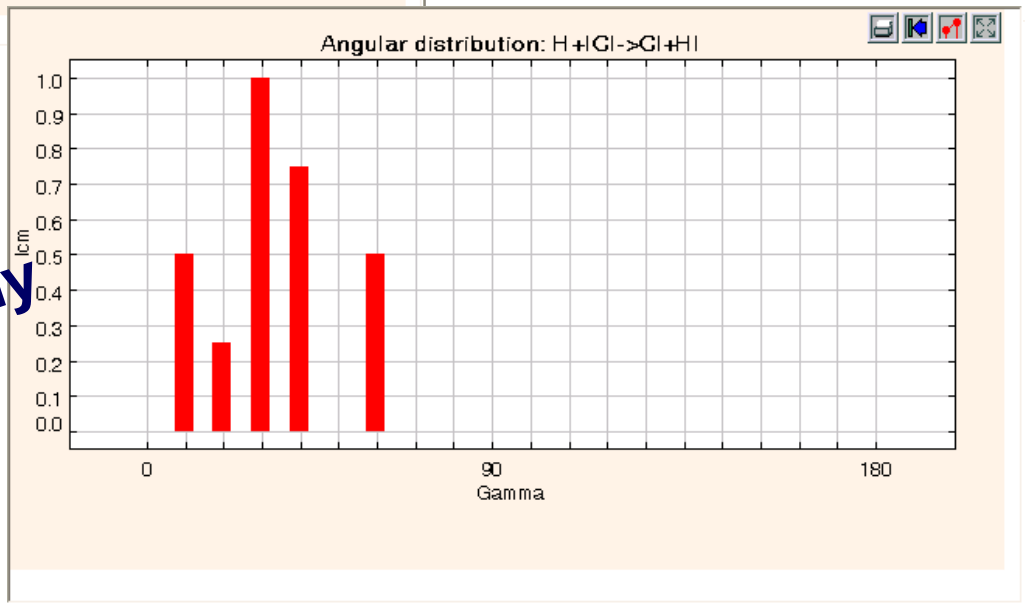
Metalaboratories components

- Molecular expertise centers
- Specialized software fabric (programs, interfaces, ..)
- Grid middleware
- Grid infrastructure
- Users

Virtual Monitors of the Angular Distribution of $H + ICl$



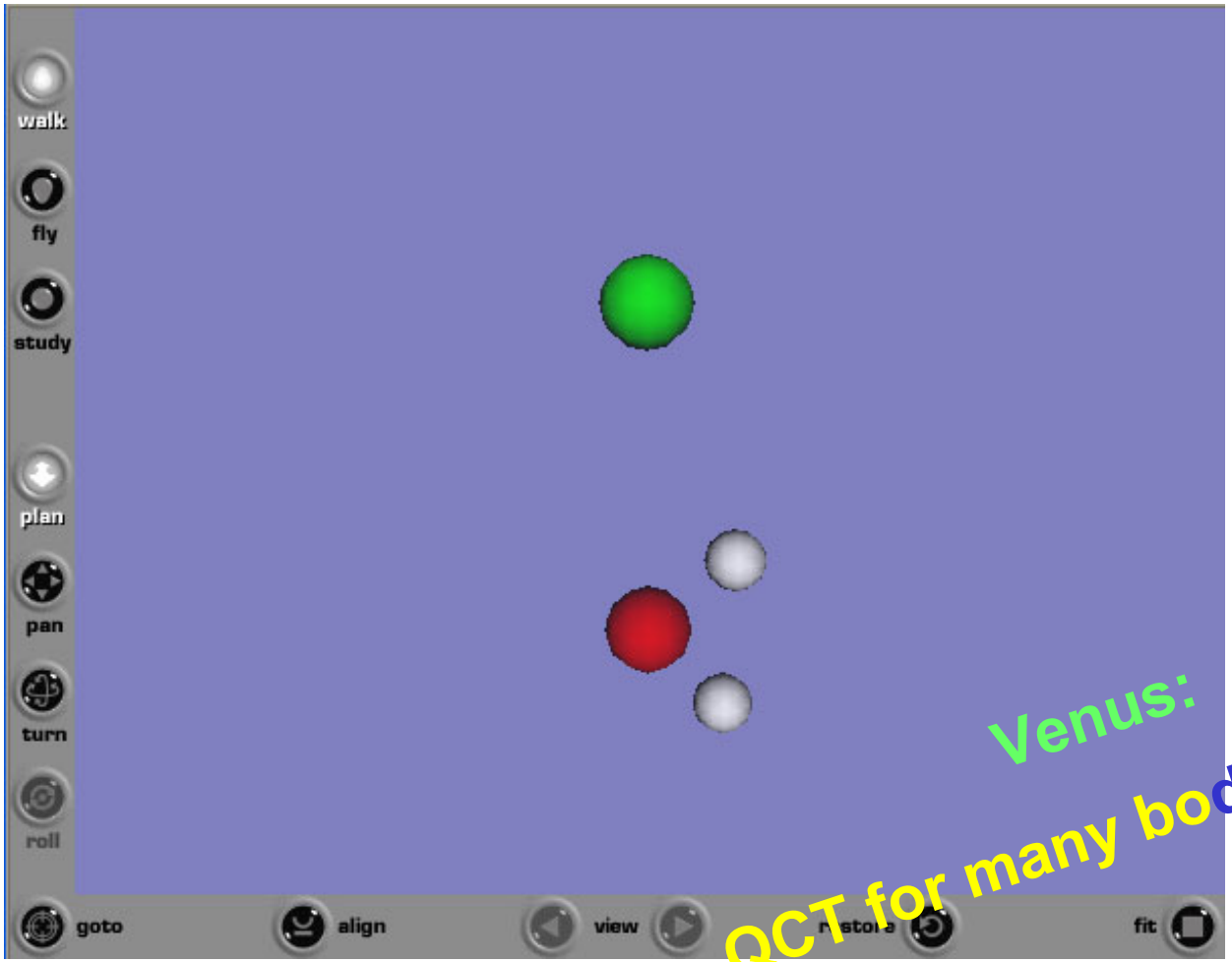




ABCtraj:

QCT for 3 body systems

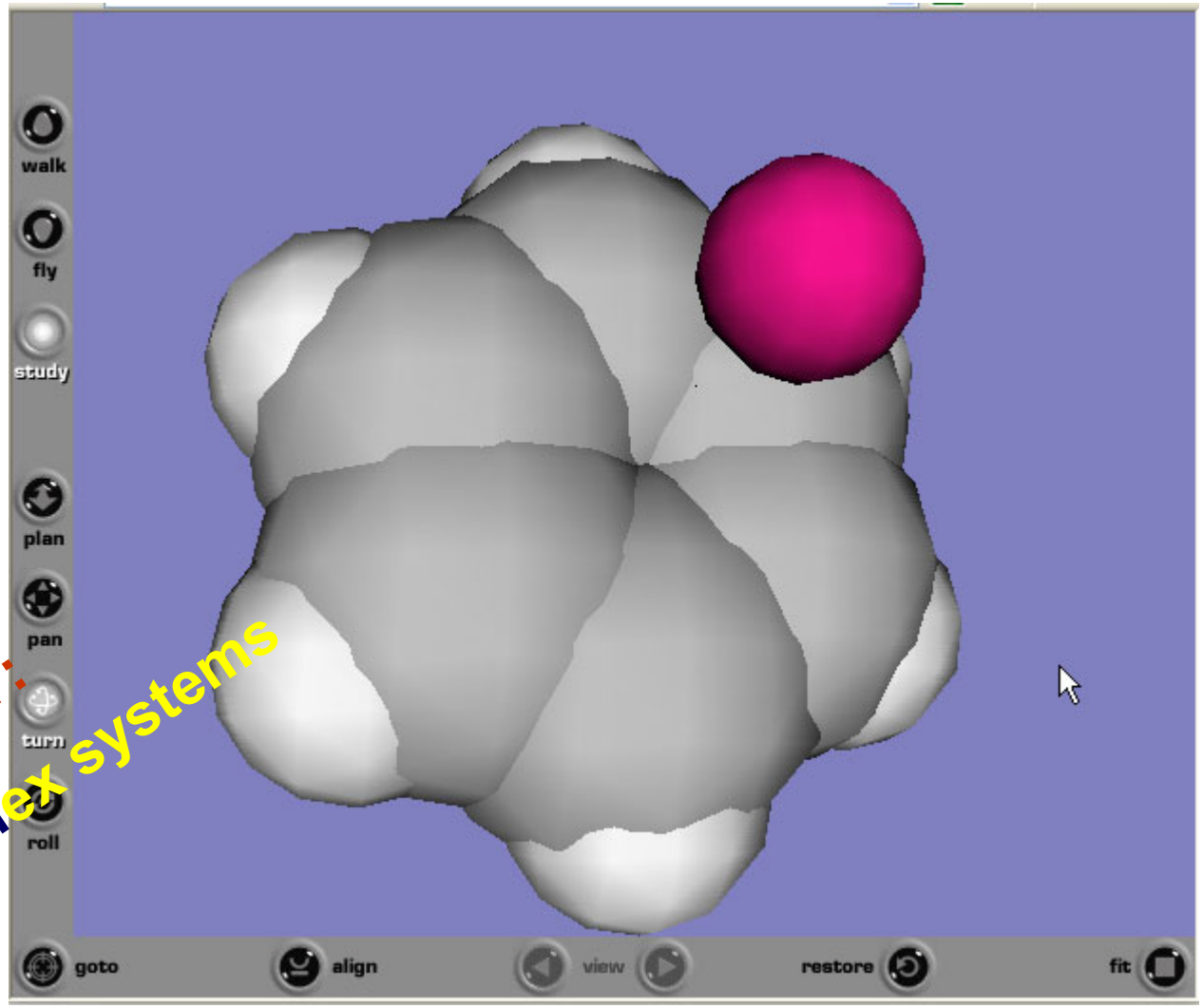
OH-HCl trajectory



Venus:

QCT for many body systems

Virtual Monitor of $Ar+C_6H_6$



DL-POLY:

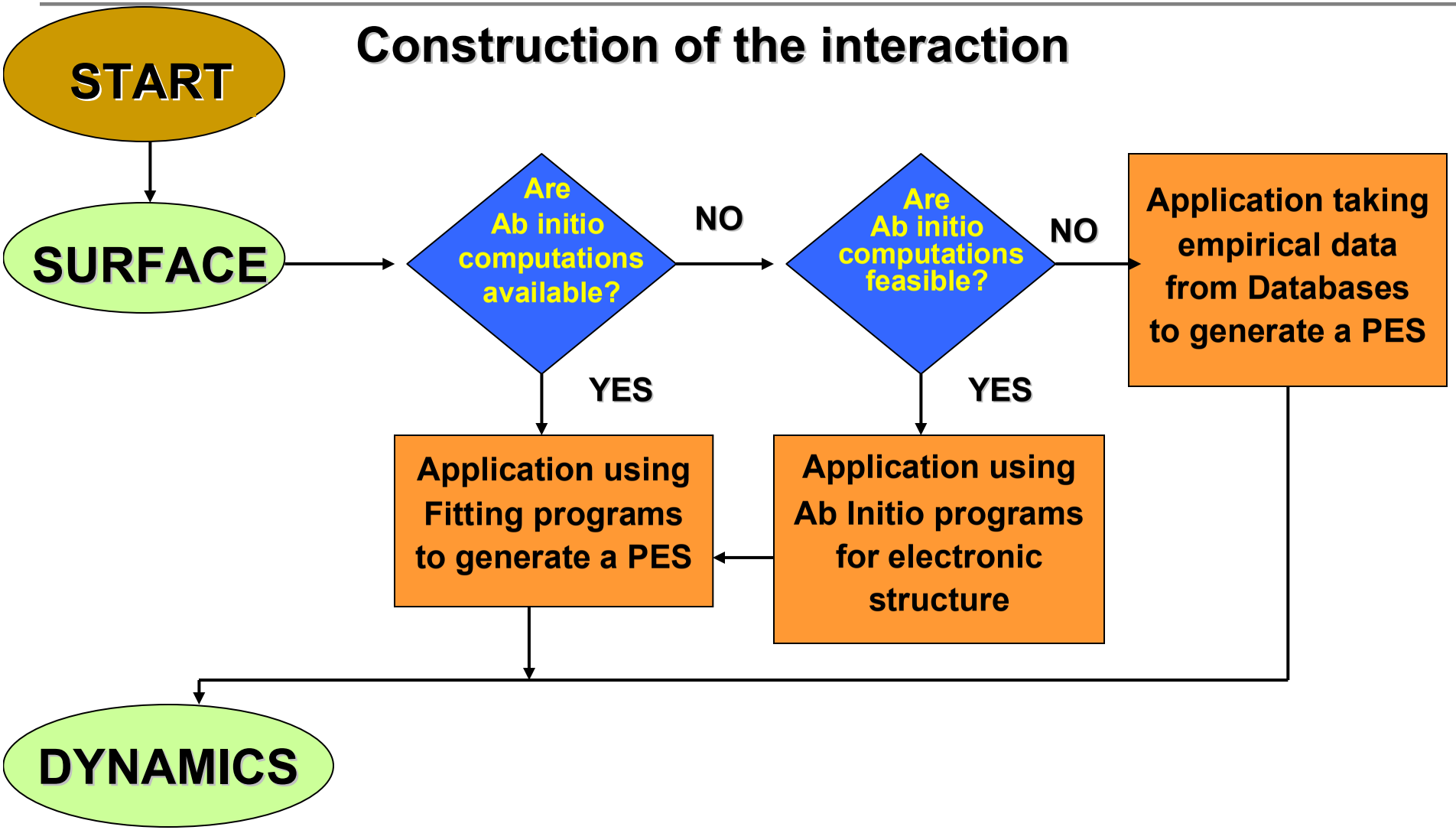
QCT for complex systems

Conclusions

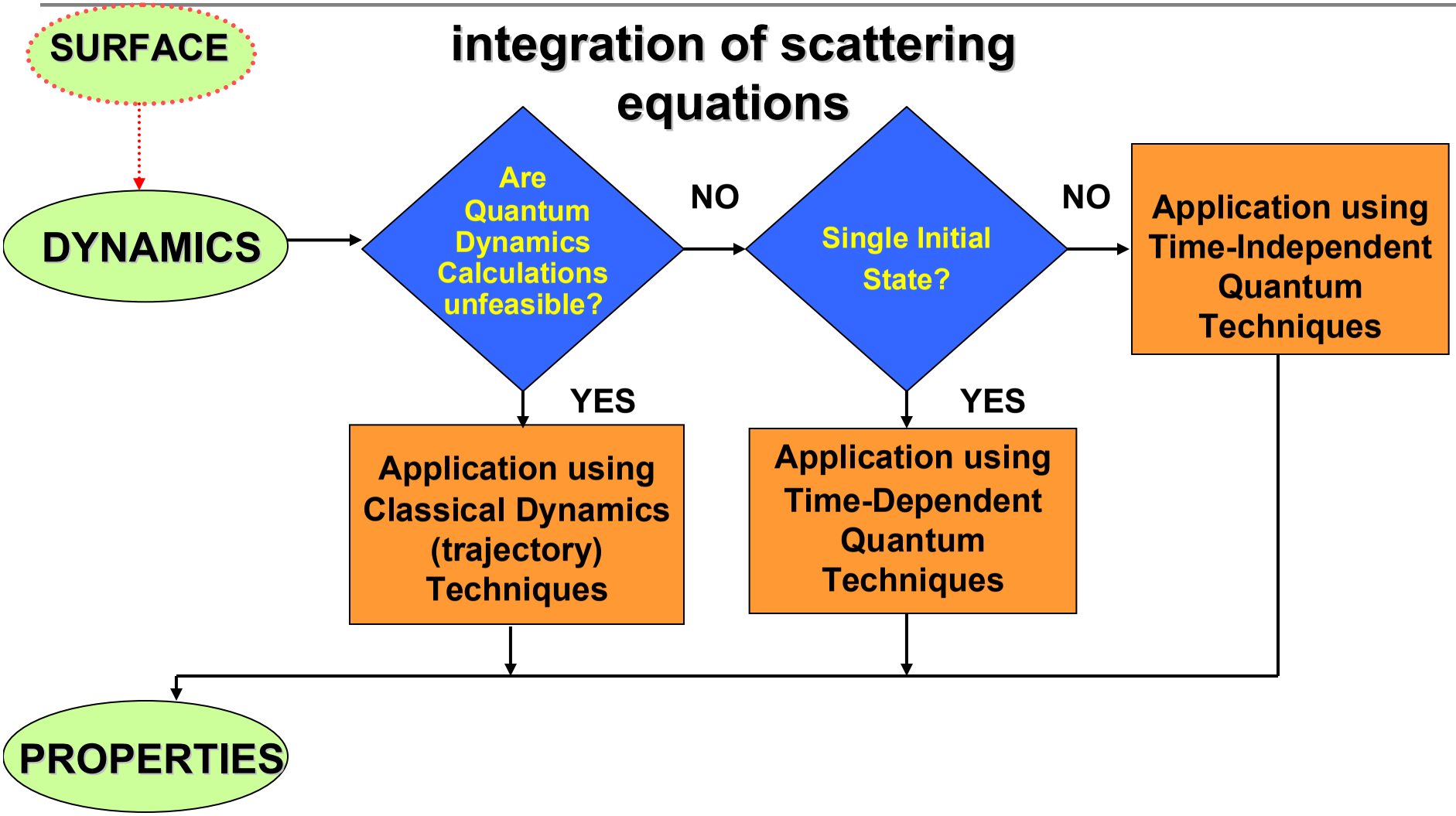
- A proposal to deploy a Chemistry Grid Application aimed at building molecular simulators is presented
- It is based on the activities of some already established Metalaboratories in D23 COST Action, some of them already involved in EGEE activities.
- It will impact all research activities in which complex simulations need to be carried out to govern advanced experiments and a priori rationalizations of real systems.

SURFACE

Construction of the interaction



DYNAMICS


SURFACE
integration of scattering equations
DYNAMICS
Are Quantum Dynamics Calculations unfeasible?
NO
Single Initial State?
NO
Application using Time-Independent Quantum Techniques
YES
YES
Application using Classical Dynamics (trajectory) Techniques
Application using Time-Dependent Quantum Techniques
PROPERTIES

PROPERTIES

Reconstruction of reaction properties