GRID BASED A PRIORI REALISTIC ATOMIC AND MOLECULAR SIMULATORS

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Summary

- COST Chemistry and METACHEM
- Ongoing Metalaboratories in Chemistry
- Regional situations
- Proposed projects

WHAT IS A PRIORI MOLECULAR SIMULATION FOR

- Life and biological processes and structures
- Innovative Materials and nanodevices
- Environmental processes
- Food
- Astro and space processes
- ……

Metachem: Metalaboratories for Complex Computational Applications in Chemistry

- MURQM: Multireference Quantum Chemical Methods
- DIRAC: Four Component Relativistic Quantum Chemical Calculations
- SIMBEX: Simulation of Molecular Beam Experiments

Metachem: Metalaboratories for Complex Computational Applications in Chemistry

- 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

Il progetto GRID europeo: D23 COST action

Simbex

Murqm

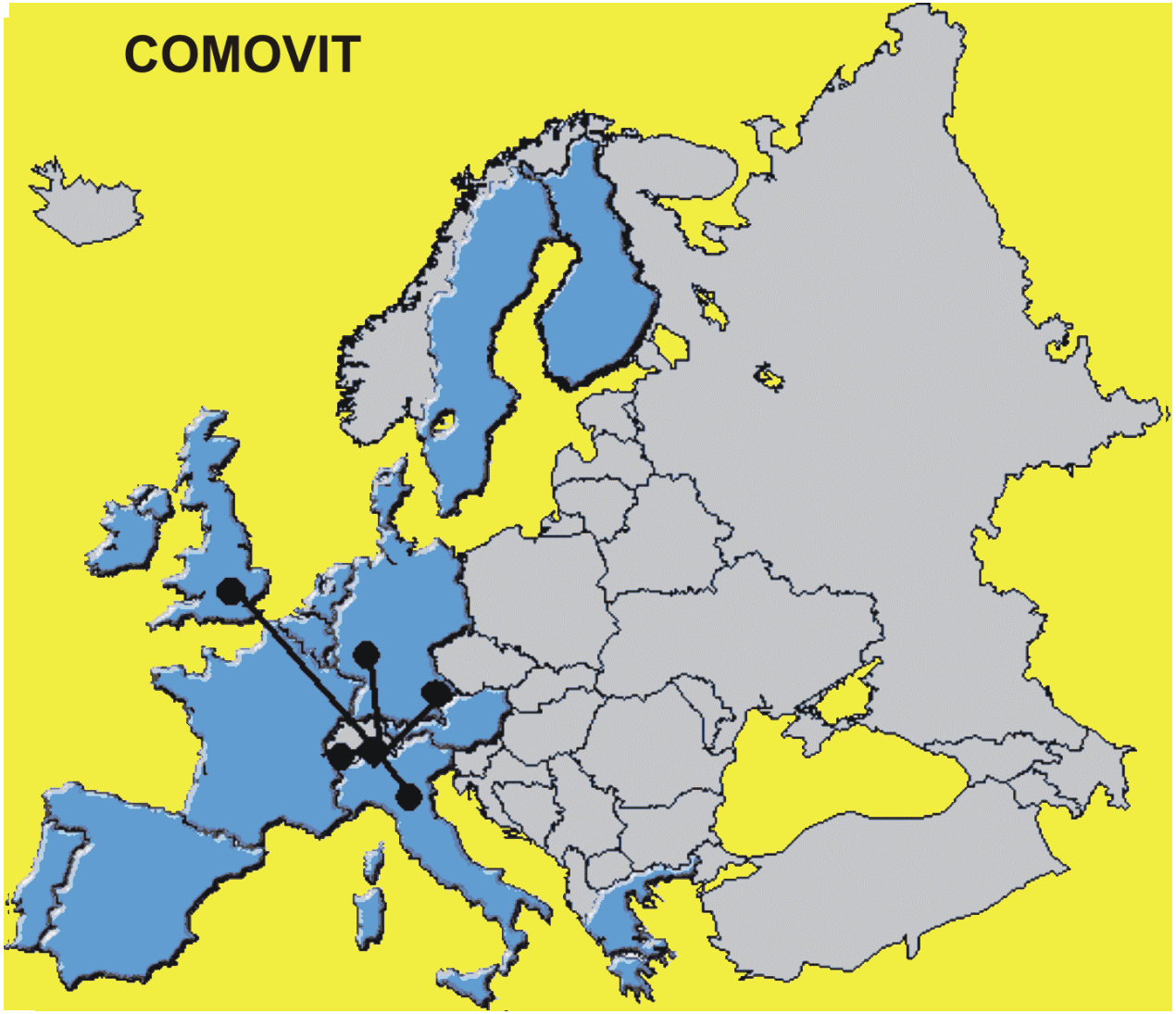
Dirac

Elchem

Icab

Dysts

Comovit



LABS per NATIONALITY (51)

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

DIRAC (K. FAEGRI, NO)

- Cooperative development of MC-SCF, gradient minimization, DFT capabilities, integral algorithms for relativistic accurate concurrent calculations
- 6 Laboratories

SIMBEX (O. GERVASI, I)

- Coordinated implementation of a problem solving environment to simulate molecular beam experiments and molecular processes. Ab initio, dynamics, kinetics and statistics codes will be assembled
- 10 Laboratories

DYSTS (A. AGUILAR, E)

- Environment and application driven dynamics and spectroscopy calculations distributed among the participating laboratories
- 4 Laboratories

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

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

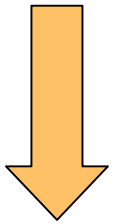
COMOVIT (H. LUETHI, CH)

- Design and development of multimedia distributed software to handle 3D molecular information of ab initio origin
- 6 Laboratories

QUANTUM DYNAMICS PROBLEM

$$i\hbar \frac{\partial}{\partial t} \Psi(\{W\},\{w\},t) = \hat{H}\Psi(\{W\},\{w\},t)$$

Born-Oppenheimer separation



Electronic Schrödinger equation:

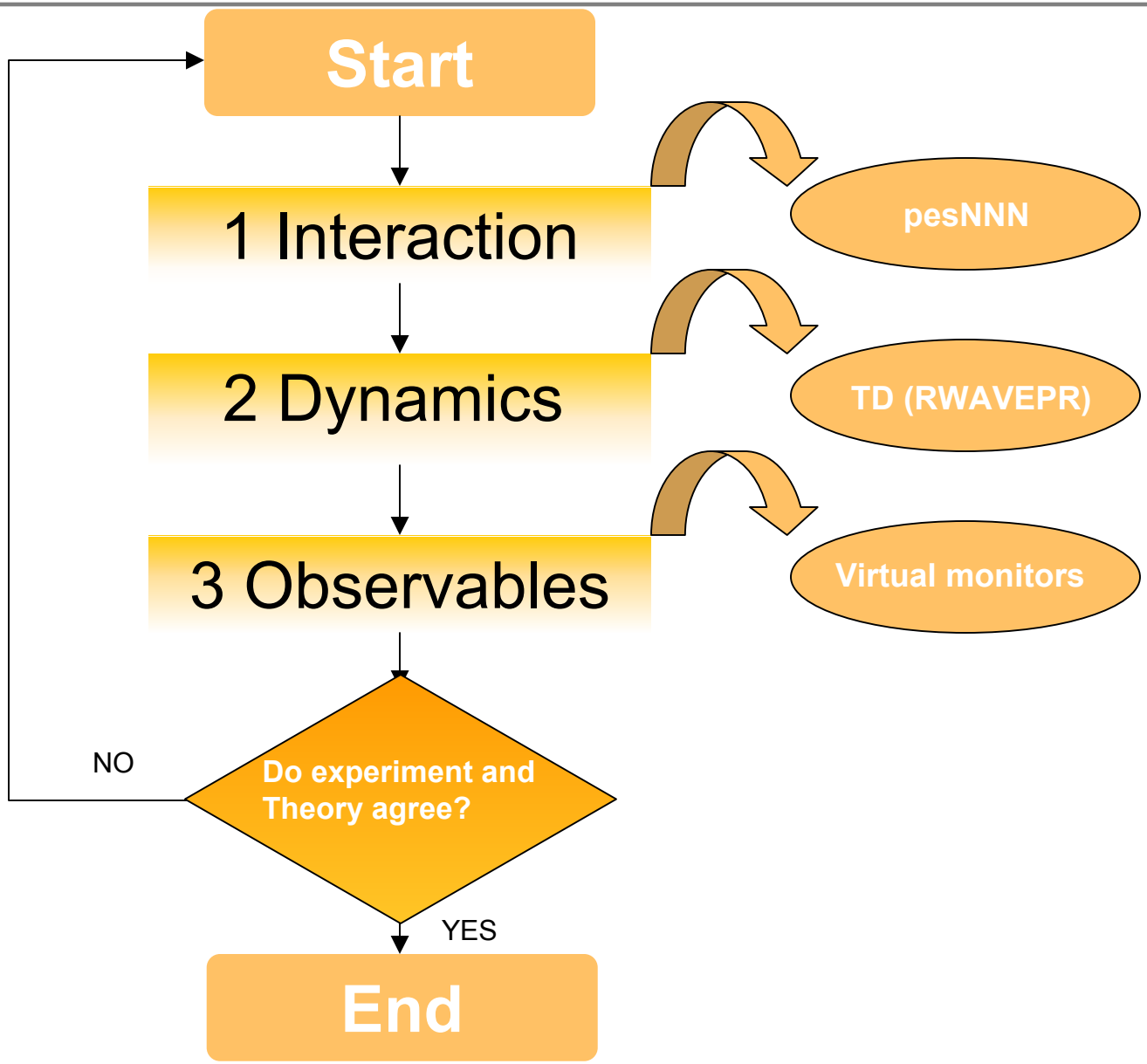
$$\hat{H}_{elec}\Psi_n(\{w\};\{W\}) = E_n(\{W\})\Psi_n(\{w\};\{W\})$$

Nuclear Schrödinger equation:

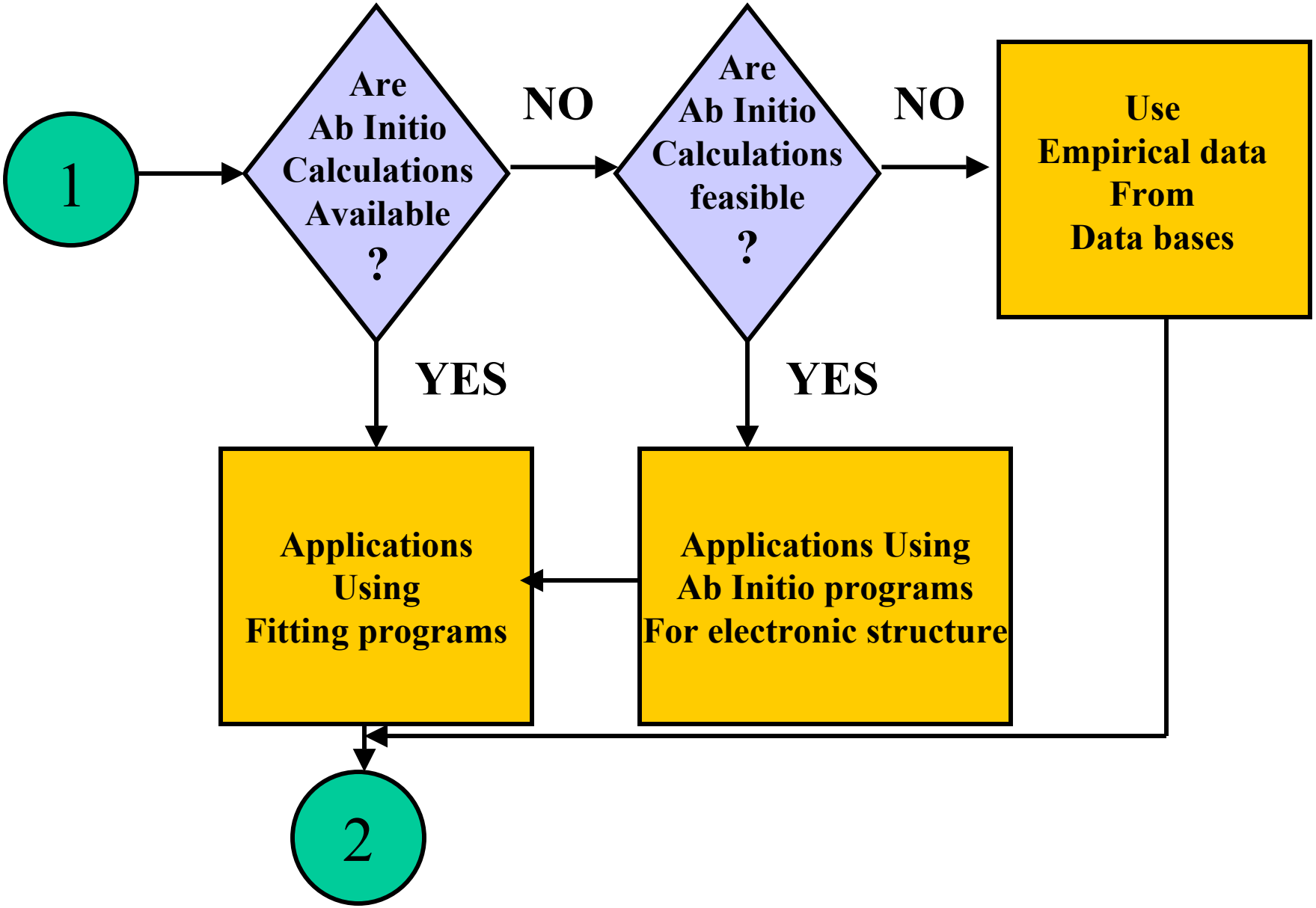
$$\hat{H}_n \chi_n(\{W\},t) = i\hbar \frac{\partial}{\partial t} \chi_n(\{W\},t)$$

$$\mathrm{d}/\mathrm{dt}\ [\mathrm{A}] = \mathrm{k}[\mathrm{A}][\mathrm{B}][\mathrm{C}]\ldots.$$

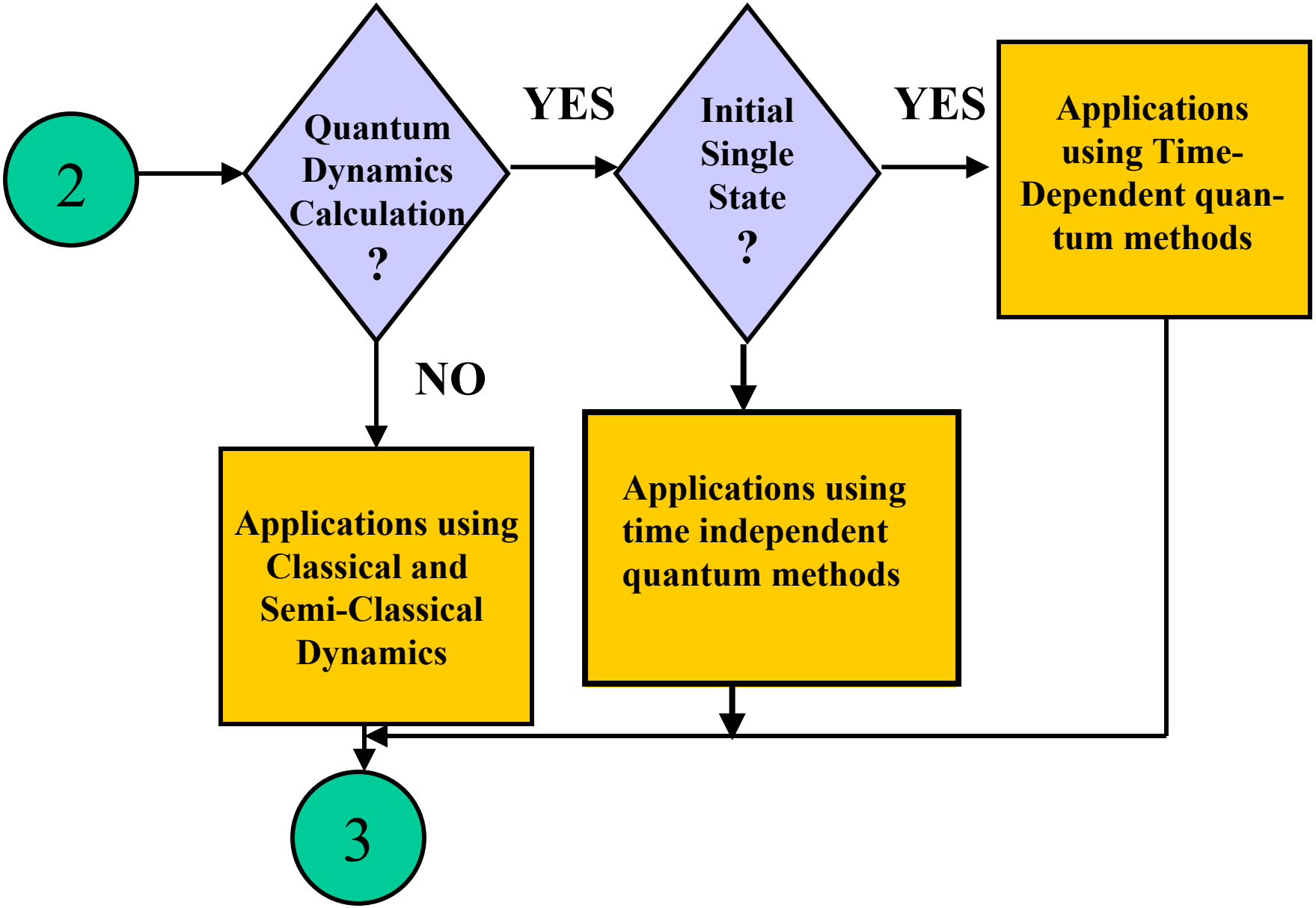
The molecular simulator SIMBEX



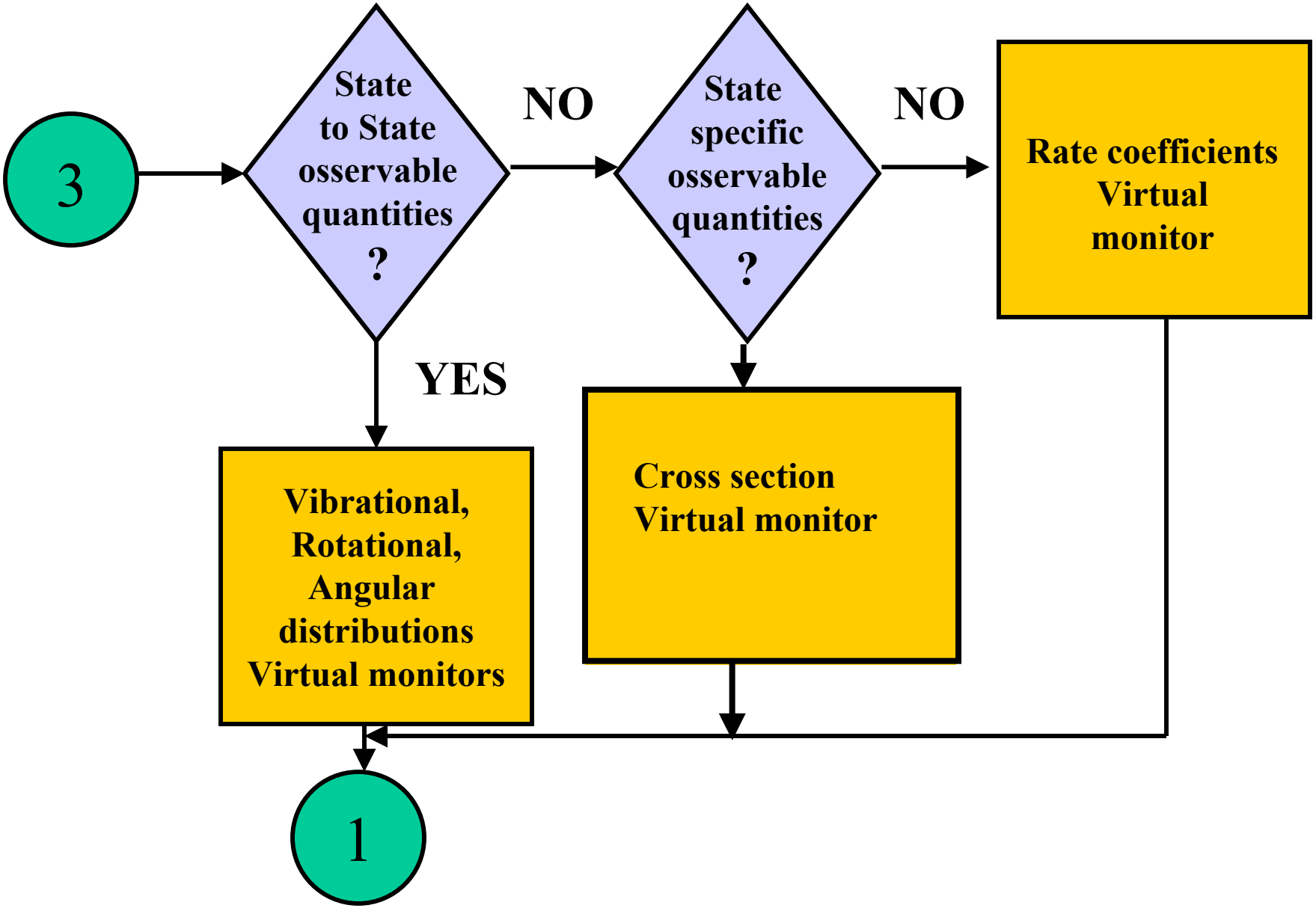
MODULE 1


1
Are
Ab Initio
Calculations
Available
?
NO
Are
Ab Initio
Calculations
feasible
?
NO
Use
Empirical data
From
Data bases
YES
YES
Applications
Using
Fitting programs
Applications Using
Ab Initio programs
For electronic structure
2

MODULE 2


2
Quantum Dynamics Calculation ?
YES
Initial Single State ?
YES
Applications using Time-Dependent quan-tum methods
NO
Applications using Classical and Semi-Classical Dynamics
Applications using time independent quantum methods
3

MODULE 3


3
State to State osservable quantities ?
NO
State specific osservable quantities ?
NO
Rate coefficients Virtual monitor
YES
Vibrational, Rotational, Angular distributions Virtual monitors
Cross section Virtual monitor
1

ELECTRONIC STRUCTURE CALCULATIONS AND REPRESENTATIONS

- 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 (CP)
- 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 (the number of electrons) and to M^D (M is the number of grid points per dimension D) for cpu and disc.
- EMPIRICAL FORCE FIELDS (Venus, dl_poly, …) resource requests are proportional to P! (P is the number of atoms)

- 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 te matrices depend on 2J+1
- KINETICS PROGRAMS use dynamics results for integrating relevant time dependent applications

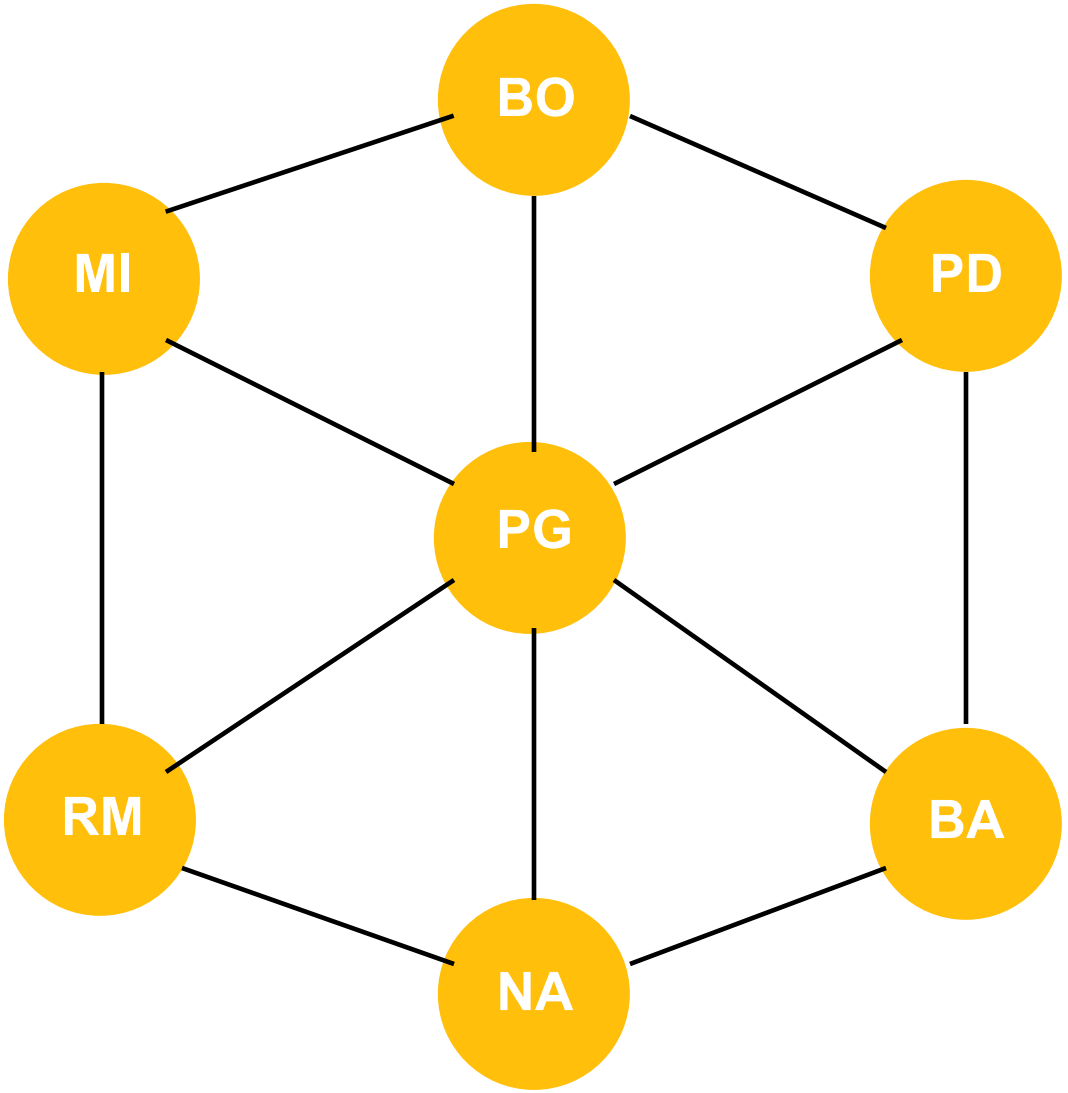
LOCAL PLATFORMS

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

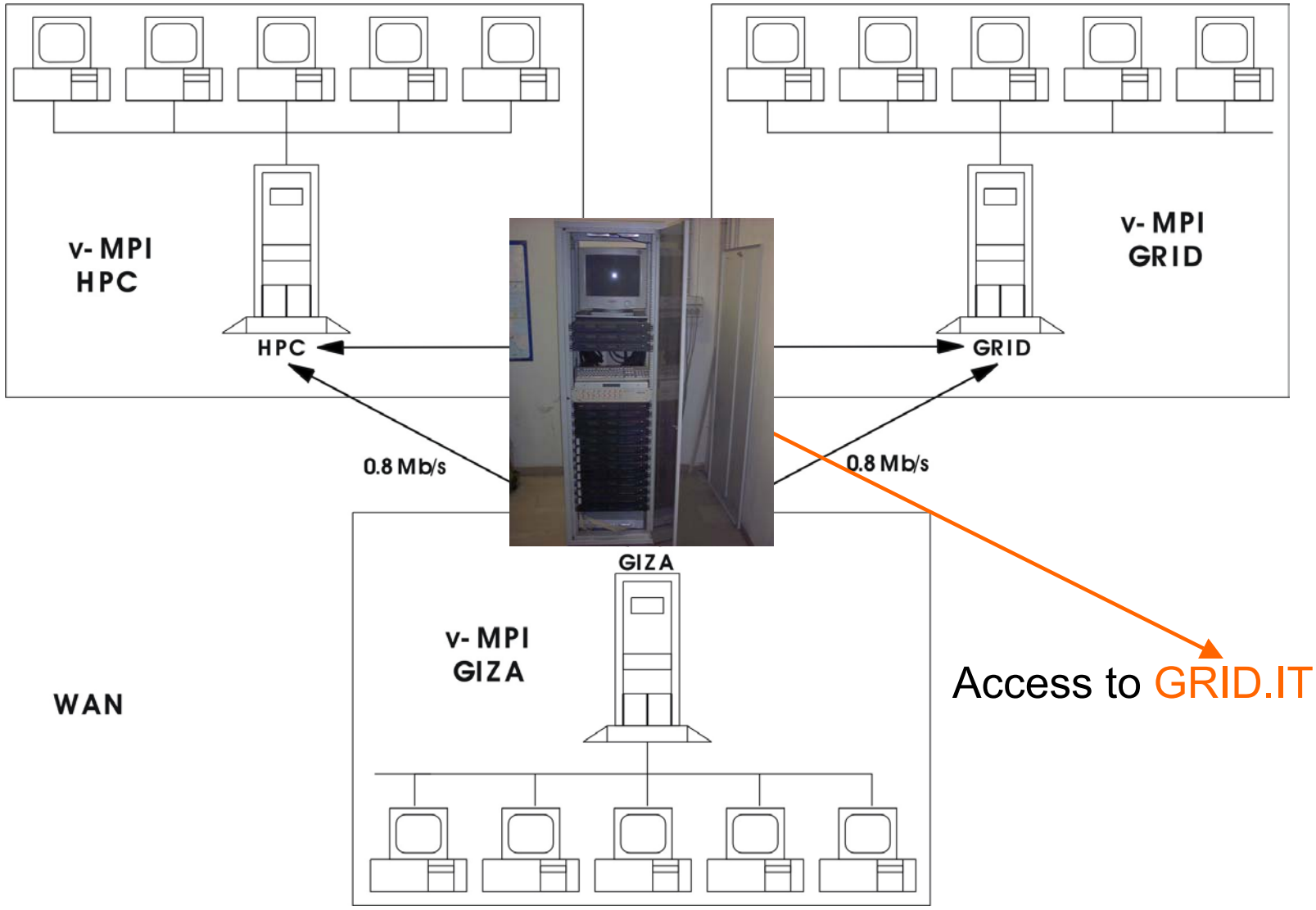
LOCAL CLUSTERING (geographical

- Nordic grid
- Hungary
- Italy

ChemGrid.it: the Italian Grid for Chemistry



ChemGrid: the Perugia node



Metalaboratories components

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

CONCURRENCY LEVELS

INDEPENDENT CALCULATIONS

LOOSELY COUPLED CALCULATIONS

STRONGLY COUPLED CALCULATIONS

TWO POSSIBLE PROJECTS

- Materials by molecular simulation design on grid
- Chemical knowledge on the grid

MATERIALS BY MOLECULAR SIMULATION DESIGN

- Develop a general purpose molecular simulator on grid
- Develop user friendly interfaces for external (experimentalists, engineers, designers, environmentalists …)

CHEMICAL KNOWLEDGE

- Mark up languages for handling chemical knowledge
- Virtual laboratories for handling chemical procedures