Information

Application of Grid technology in computational chemistry

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The key trends and prospects of development of computational chemistry that formed in the early 2010s are considered. The most advanced methods for solution of various types of challenges in the computational and quantum chemistry by calculations in the distributed environments (Grid) and on high-performance supercomputer installations and the application methods of parallel and distributed computations are demonstrated; the tailor-made technologies developed for these calculations are described.

Key words: computational chemistry, quantum chemistry, distributed calculations, Grid technology, supercomputers.

Introduction

Computational chemistry and quantum chemistry are branches of science that require large amounts of highly resource-intensive calculations. Currently, studies in the field of chemistry and related sciences are most often inefficient without such computations, which are performed to solve problems of various classes using either high-power supercomputer installations or distributed local and global computational grids. In addition, an integral part of these techniques is the use of superlarge databases (hundreds of terabytes), which can only be run on distributed computational environments.

The most demanded are large-scale calculations in the following fields of chemistry, chemical physics, and related sciences:

- study of the structure of matter,
- structure of molecules and solids,
- design of materials with specified properties,
- kinetics and mechanisms of complex chemical reactions,
- chemical physics of combustion and explosion phenomena,
- gas dynamics of extreme states,
- chemical physics of the polymer formation and modification processes,

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• predictive simulation of nanostructures and nanotechnologies,

• general problems of chemical physics.

Tackling of challenges in these fields requires a large volume of intense parallel and distributed calculations. For example, some molecular structure optimizations require up to 10^9 separate computations; this leads to the need of using either high-performance supercomputers or large distributed Grid polygons, which represent unions of geographically separated computer resources forming a common computational system.

Quantum-chemical calculations is a key line of work of the computational center of the Institute of Problems of Chemical Physics in Chernogolovka (IPCP RAS, http://www.icp.ac.ru).[1] The Institute has one of the most numerous libraries in Russia of parallel quantum chemical and molecular dynamics software (tailor-made, open source, and license programs). About 3000—4000 highly complicated computational problems are solved annually at the IPCP RAS and more than 400 publications appear based on the calculation results.

Key types of computational resources

These include supercomputer installations and distributed computational networks (Grid polygons). We will briefly describe both types of resources. Currently supercomputers are installations with productivity of more than 1 teraFlop (10^{12} operations per second), which are implemented in most cases as clusters of numerous homogeneous computation units combined into a computational network. The largest among them, in particular, Russian ones (Moscow State University, Lomonosov, April, 2011) have already exceeded the value of 1 petaFlop (10^{15} operations per second). Quantum chemical applications are often included in the software installed on these complexes. Note that leading countries (including Russia) aim to reach a 1 exaFlop performance of these installations (10^{18} operations per second) by 2018 and the development of software for the needs of computational chemistry is among the priority areas of development.

However, such installations are very expensive, difficult to manufacture, and costly to operate. In addition, for a number of reasons (inefficiency of problem paralleling, licensing restrictions of application program packages, *etc.*), they cannot fully implement their potential for the solution of many applied problems, in particular, in the field of chemistry. Therefore, in the 21st century, the concept of distributed computational networks (Grid polygons) is being developed. These are unions of geographically separated computer resources, within the framework of virtual organizations (VO), connected by high-speed data channels. The software developed for these polygons allows the users to automatically send their problems to the available free computational resources, retrieve the required data from the decentralized data banks, monitor the implementation of the problems, and collect the final results. Of course, the resources are allocated as free access and free resource exchange.

Thus, Grid polygons represent a computational environment (a sort of virtual supercomputer), which provides a flexible, safe, and coordinated splitting of computation and data storage resources and solution of problems adapted to its use. From the standpoint of the final user, the use of Grid environments resembles the use of Internet resources: a problem adapted to the Grid environment is sent to an arbitrary free available computational resource and is solved there, and the result returns to the user. The retrieval of the data stored in the Grid-polygon-connected data processing centers occurs in a similar way (it is transparent for the user). In the case of failures, the problem is automatically redireted to other resources.

This concept allows one to involve in the calculations large numbers of computational resources with simultaneous use of tens and hundreds of clusters (*i.e.*, thousands of processors) and hundreds of terabytes of data from distributed storages, perform simultaneously tens of thousands independent tasks. Note that the supercomputer installations can serve as such resource units of Grid polygons, which markedly facilitates the user´s work.

Key types and classes of computational chemistry problems. Computational chemistry as a promising tool of modeling of material objects

Why quantum chemical computations are so important and how big may be the demanded computational resources? They are important for studies of the structure of matter and nanomaterials, solid state physics, biophysics, and other fields of science related to investigation of the electronic structures of compounds.

Consider an application of computational chemistry requiring high-performance and fairly resource-intensive calculations. The design of materials with pre-specified functional properties including the manufacture of new materials and extension of the scope of functions of existing materials is currently one of the most promising and demanded areas in computational chemistry and related sciences. The physicochemical and functional properties of these materials are defined in micro- and nanometer spatial ranges. From the physicochemical standpoint, these materials and structures refer to molecularly structured and nanostructured systems.

Therefore, methods of computer modeling of molecular systems and nanosystems become especially important. These methods have to be sufficiently fast and accurate to ensure detailed prediction of the properties and structures of materials being manufactured or designed, including their behavior under external treatment under variety of physicochemical conditions. The purely experi-

mental approach to solving these problems has been almost exhausted due to the very large number of compounds and physical states to be evaluated and also due to time and cost restrictions. Direct experiments in molecular and nano-technologies are replaced more and more often by computer modeling of the structure of substances based on the use of high-performance computing systems: supercomputers and distributed computing networks.

Numerous applied program packages and tailor-made programs on quantum chemical and molecular dynamic modeling of atomic and molecular systems have been developed. Using various paralleling techniques, it is possible to perform calculations for systems containing up to several thousands of atoms and calculate system dynamics for more than millions of atoms in the range of lifetimes down to several nanoseconds. This allows for hierarchical multiscale approach to the modeling of any material objects ranging from quantum to macroscopic ones. In this case, at every lower level, parameters needed to construct the next, higher-level models are calculated. The goals attained at the upper level of the hierarchical modeling determine the lower-level modeling tasks. The *ab initio* quantum chemical modeling is performed for small clusters comprising 10—100 atoms to determine the existence of phases possible in the material and describe the electronic energy spectrum, the eigenfunctions, and the density of states for an isolated cluster at a constant position of the nuclei, and the potential energy of the system with electron-nuclear subsystem contributions.

The next quantum statistical level makes use of models that take into account also the environment of the clusters. Then the evolution of non-equilibrium systems comprising hundreds of clusters under various external conditions is studied at the kinetic level. Molecular dynamics methods (with solution of mechanics equations) considering atoms as classical particles can also be applied at this level. It becomes possible to consider systems comprising from 1 thousand to 1 million atoms and to describe objects with sizes of 100—1000 nm^3 and also to simulate the operation of molecular-size devices. The kinetic coefficients, equations of states, equilibrium structures, phase transitions, and non-equilibrium processes are determined at this level. Then it is possible to switch to the meso level and to the level of continuous media for which one can calculate the viscosity, the heat capacity, friction coefficients, and other macroscopic properties of materials and also wave processes in the elements.

The results of this model are applied to determine the parameters of the finite element method and related methods, which implement the models of continuous medium or structural models (theory of mechanisms and machines, complex systems). The successive hierarchical modeling of material objects is suitable for predicting their properties at any level, which is exceptionally important for the construction of process chains for the manufacture of new materials or materials with altered properties. One can plainly see that the computational chemistry supports the first levels of the described model construction chain: modeling of molecular systems and nanosystems, as well as biological objects at the quantum chemical, quantum statistical, and kinetic levels by means of molecular dynamics methods based on both known and newly developed applied program packages that allow for parallel computations. Thus, the most advanced computational chemistry using high-performance calculations defines the basis of the subsequent modeling of material objects and undoubtedly becomes the leading tool in chemistry and related fields of science.

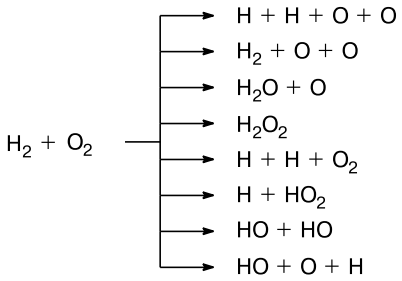
In view of our experience in performing this type of calculations,[1—4] the resource-intensive quantum-chemical problems can be classified into two types:

1) problems that split into a set of almost independent tasks, their number depending on the number of problem parameters and/or the degree of detailing of the splitting network of the desired data domain;

2) problems that represent a single computation process requiring, most often, one-time allocation of a lot of resources (the number of processors, RAM, disc space, *etc.*).

Typical examples of the problems of the first and second types are shown in Scheme 1 and Fig. 1, respectively.

Scheme 1



Scheme 1 shows an example of investigation of the path cross-sections of the potential energy surfaces of chemical reactions (the calculation time for one path varies from fractions of a minute to several hours, the total calculation time is up to several years of operation of a single processor; the initial conditions include four mutual orientation angles; impact parameter; two vibrational quantum numbers; two rotational quantum numbers; collision energies; and altogether 1—10 million independent paths).

Problems of the first type are most demanded in operation in the distributed environments, because by directing independent task to a multitude of small clusters (every cluster comprises 10—20 processors, and the task can be paralleled), it is possible to attach high efficiency of using computation resources. It is possible to use large polygons (up to 10^3—10^4 processors) both local ones (in hetero-

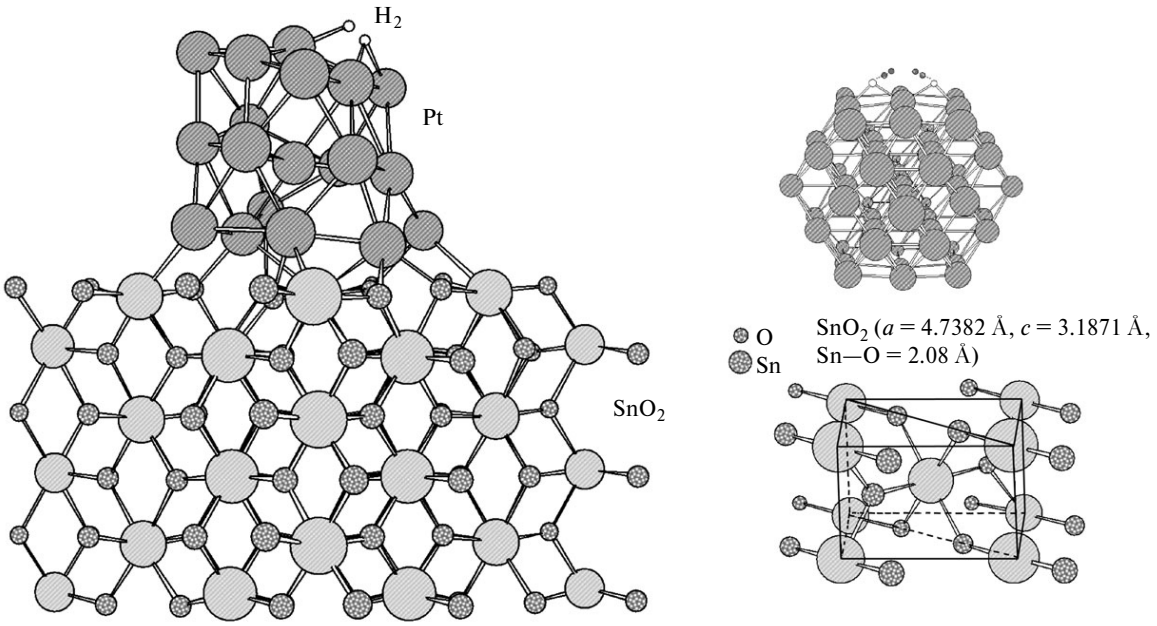


Fig. 1. Adsorption of H_2 on an octahedral cluster Pt_{19} located on the SnO_2 surface. The calculations on the Chebyshev SKIF-MGU complex (VASP program) used up to 200 CPU, the run time was 15 h, 10 optimization steps out of the needed 100—200 steps were performed.

geneous environments such as Condor) and geographically distributed Grid environments (set of computation clusters, resource sites).

An example is provided by the path calculations of chemical reactions. A typical reaction is $H_2 + O_2$. The elementary collision event is modeled by classical paths. The calculation of the full reaction cross-section requires variation of two mutual orientation angles for each molecule, the vibrational and rotational quantum numbers, the collision parameter, and the relative collision energy. As a rule, the calculation of one path takes from several seconds to several minutes. The successive addressing of these parameters results in calculation of tens of million paths, which is unrealistic when local resources are used, *i.e.*, it is necessary to switch to distributed polygons.

A similar approach is suitable for solving multiparametric problems of chemistry characterized by relatively independent addressing of multidimensional networks of input parameters. A major part of these problems are solved not for a single set of input data but for a detailed input data network. The number of tasks into which the problem can be split increases exponentially as a function of the number of variable parameters and the degree of detailing of the input data splitting. A number of tasks of 10^8—10^{10} ensures an accuracy of the computational experiment unattainable by other methods.

Unfortunately, researchers are still compelled to either considerably decrease the number of variable parameters of the problem, which results in inadequate consideration of some physicochemical effects, or "coarsen" the input data networks, which leads to the loss of some non-monotonic results (edge effects, local extrema, "potential wells", *etc.*). An increase in the accuracy of calculations for such problems often reveals results that have not been predicted beforehand by the theory.

The problems of the second type are usually meant for supercomputers, as the efficiency of solving them is directly related to the high requirements to the resources of both the supercomputer (a large number of processors is involved) and the computing units (considerable amounts of RAM and disc space) and also parallel computing. For typical problems related to nanostructures and molecular crystals, it is possible to use up to several thousand processors with processor time consumption of about a month, *i.e.*, teraFlop-level clusters.

Unfortunately, the problem of effective paralleling of programs remains topical, and the developed algorithms for quantum chemical software considerably lag behind the capacity of the existing computation systems. For example, for the GAUSSIAN program, there is an empirical rule: the scalability is proportional to the cube root of the number of processors. In the case of GAMESS, the scalability is much better but it remains practically linear only when at most several hundreds processors are used. VASP type programs were scaled in a similar way. The increase in the efficiency of solving problems on supercomputers is one of the key problems the developers face en route to the use of petaFlop- or higher-level computers.

This was also implemented in Grid polygons where free resources with the most suitable parameters are se-

lected automatically. The problems are sent to these resources, after which the Grid environment itself monitors their solution on supercomputers.

The resource Grid center of the IPCP RAS, structure and potential

The work with distributed compuring systems were started at the IPCP RAS in 2004—2005 within the framework of various Russian and international programs. The key areas of authors´ research as follows:

1) adaptation of the most demanding applied packages in the computational (quantum) chemistry to the distributed environments and providing for the broad access of chemists to them;

2) development of the resource Grid center (as the aggregation of resource sites for several Russian Grid polygons), which acts as both a polygon for the computation experiments and the means for solving important fundamental and research-and-practice tasks;

3) development of new methods for the calculation and arrangement of computing services in distributed environments.

These areas were chosen considering the main strategies of the development of Grid polygons in Russia and in the world; this brings the final user (chemical scientist) closer to the wide-scale utilization of distributed computing resources and ensures the possibility of solving problems that are currently difficult to solve on single computing complexes.

The works with distributed environments are based on the resource Grid center established at the IPCP RAS,[1—3,5] which combines the resource sites of the following Russian Grid polygons:

• the consortium unit EGEE-RDIG (Enable Grid for E-sciencE and Russian Data Intensive Grid, http://www.egee-rdig.ru, from May, 2010, EGI, European Grid Infrastructure) based on the gLite environment (http://glite.web.cern.ch), access to computer powers of up to 700—1000 processors and disc space of about 15—30 terabyte in several geographic areas (Moscow, Dubna, Khar´kov, Chernogolovka, *etc.*);

• A-category site of the SKIF polygon (http://skif-grid.botik.ru) based on the intermediate Unicore software (http://www.unicore.eu), the access to SKIF-MGU, Syberia (Tomsk), SKIF-Avrora (Chelyabinsk), IPS RAS, North Caucasian State University, and other resources (up to 1500 processors);

• National Nanotechnology Network site (GridNNN, http://www.ngrid.ru, the virtual NanoChem organization), a Globus Toolkit 4 environment, http://www.globus.org); total number of processors of more than 8000, a large number of VO including those suitable for quantum chemical calculations. Within the framework of GridNNN, the IPCP RAS has established and headed the VO Nanochem for performing quantum chemical calculations.

These resource sites allow one to solve the incoming problems both using applied quantum chemical packages adapted to distributed environments and general ones. The resource sites comprise also a set of user interfaces for the interaction of adapted quantum chemical applied software with the Grid environments. They allow launching the outgoing problems of computational chemistry on the distributed resources of these polygons, thus ensuring the formation of tasks, running the resources on remote sites through brokers, monitoring of task progress, collection of the results, and statistics.

An important part of the IPCP RAS resource center is the Grid portal (http://grid.icp.ac.ru, Grid Enabled Chemical Physics, see below), which joins high-level www interfaces into a system of Grid services and markedly facilitates the Grid calculations for a chemical researcher.

Main Grid services for solving problems of computational chemistry

Work in the distributed environments with applied computational chemistry packages and tailor-made programs. We verified and tested the use of Grid resources for real calculations using standard applied program packages (including parallel) that are used in the computational chemistry and various programs tailor-made at the IPCP RAS and Chernogolovka Scientific Center of the RAS. Of particular interest is adapting these programs for the distributed computations at the maximum of available resources of the Russian and international Grid infrastructures. The adaptation in all of the above-mentioned distributed computing environments (see above) was done for the applied program packages most demanded by the IPCP RAS users:

GAMESS-US (http://www.msg.ameslab.gov/GAMESS), a highly popular program for the theoretical studies of the properties of chemical systems, the second best known after GAUSSIAN, suitable for calculating the molecular energies, structures, vibration frequencies, various properties of molecules in the gas phase and in solutions in the ground and excited states. The key trend is the development of calculation methods for superlarge molecular systems.

VASP (Vienna University, http://cms.mpi.univie.ac.at/vasp) and **PWscf** (http://www.pwscf.org, Plane-Wave Self-Consistent Field), programs that are designed for the simulation of the volume and the surface of a solid within the framework of *ab initio* approaches based on the density functional theory (DFT) using periodic boundary conditions and plane wave basis sets. The program package is suitable for structure optimization and molecular dynamics modeling of the processes on the surface and in the bulk of a solid (first of all, catalysis and ionic conductivity). Modeling at the quantum chemical level is performed

for small clusters comprising 10—100 atoms, which determine the existence of possible phases in the material. The modeling object is described by the system wave functions and Hamiltonian. The target values include the electronic energy spectrum, the eigenfunctions, the density of states of an isolated cluster at a constant position of the nuclei, and the potential energy of the system with electron-nuclear subsystem contributions.

GAUSSIAN-03 (http://www.gaussian.com), a quantum chemical program package most popular among chemists. The main reasons are the broad scope of implemented quantum chemical procedures, high performance, and convenient user interface. The modern versions of the GAUSSIAN package extend the scope of quantum chemical methods and their modifications. The GAUSSIAN package is suitable for calculating the molecular energies, structures, vibration frequencies, various properties of molecules in the gas phase and in solutions in the ground and excited states. The key trend of new versions is the development of calculation methods for superlarge molecular systems. The use of the package in distributed environments is held up by license agreements.

DALTON-2 (http://www.kjemi.uio.no/software/dalton/dalton.htm), a program suitable for calculating the singlet—singlet excitations, electronic structures, rotational and vibrational spectra of molecules and for considering the relativistic and solvation effects.

CPMD (http://www.cpmd.org), a program for molecular dynamics calculations.

NAMD (University of Illinois at Urbana-Champaign, Computational Biophysics Group, http://www.ks.uiuc.edu/Research/namd), well scalable molecular dynamics program, one of the fastest programs for parallel calculations on a large number of processors. The program is actively used at the IPCP RAS to calculate micelles.

Tailor-made programs (designed by the IPCP RAS) for solving multiparametric problems in quantum chemistry and molecular dynamics.

For the sets of software, features of various implementations of single-processor and paralleled versions were studied, the adaptation strategies of the chosen types of quantum chemical calculations to various distributed environments. For most applied program packages, low-level interfaces for running in distributed computation environments were designed and tested. These interfaces include numbers of scripts for the formation of the outgoing tasks, launching the resources at remote units, monitoring of the problem solutions, retrieval of the obtained results from remote resources, and the assembly of the final results to the user interface. The interfaces for single-processor and paralleled software versions were implemented. The applied software was run through the infrastructure of the above-described Grid polygons on the resource Grid unit of the IPCP RAS, which was used as the remote distributed resource. Currently, the resource sites of the IPCP RAS can be used to solve the computational chemistry problems as the incoming problems using all of the quantum chemical packages mentioned above.

The implementation of Grid services as high-level web interfaces. A constituent part of the resource center of the IPCP RAS is the Grid portal combining Grid and web services. High-level web interfaces that enable more efficient utilization of all advantages of Grid calculations were formed in this portal. This environment allows the users to obtain more easily the access to the Grid resources and services, activate and configure them by means of the web browser. The Grid portal architecture is based on the idea that the portal system is a container for low-level user interfaces providing the work with Grid services. The advantage of this architecture is that it allows rather easy building-in of interfaces of Grid services and alteration of the existing ones. The portal services control and visualize the user interface.

At the IPCP RAS, a Grid portal (http://grid.icp.ac.ru, Grid Enabled Chemical Physics, GECP) with www interfaces was formed for the following applied packages:

1. The quantum chemical GAMESS-US program package suitable for parallel *ab initio* calculations.

2. A data parallel set of procedures for the calculation of multiparametric functions for solving chemical physics problems.

These web interfaces are designed for determination of the input parameters and conditions (including the data loading, creation and edition of the configuration files, end-user license operation), formation of complex primary start-up files, running (after user authorization) of the required software in distributed environments, monitoring of the task implementation, and collection of the results. The operation, through web interface, of bunches of independent tasks for the data domains being obtained by splitting and the operation by the formation of virtual containers were integrated for the GAMESS-US package (see below). Note that the major part of the program code of web interfaces is not directly related to the chosen distributed environment; therefore, the web interfaces are connected to all three mentioned Grid polygons (EGI-RDIG, SKIF polygon, GridNNN) and, hence, supports three distributed environments (gLite, Unicore, Globus GT4). The designed web interfaces decrease substantially the user effort both for the formation of tasks and for the primary data and markedly facilitate the subsequent running the package in the distributed environments.

Solution of Grid problems using the "virtual container" method. Note that most of the applied packages of computational chemistry (and also of other fields of science and technology) is distinguished by the complexity of configurations and enhanced requirements to the execution environment, especially for parallel calculations. Usually this problem is solved by creating virtual organizations, *i.e.*, communication through the distributed environments

of largely similar (as regards the installed software and preferences) computing resources. In this case, the chosen applied packages (together with the configuring and setting-up means) are distributed from a common repository (for example, as CERN applied packages: Atlas, CMC, Alice and the like).

In most cases, an unprepared resource site does not have the required pre-installed applied software or is not properly configured. For these resources, running of complex applied packages for quantum chemistry that have not be pre-installed usually fails. Therefore, the resource units of distributed media are adjusted manually or semiatomatically, in particular, the packages are installed, the central and computing units are configured (including setting of environment variables, common NFS resources, PBS queues), additional system libraries and executable files are installed (including parallel environments such as Mpich-2). After this, the packages can be run on distributed resources (as this is done for the resource sites of the IPCP RAS for solving the incoming problems).

For partial solution of this problem, the method of movable virtual software containers was developed. A container comprising the proper applied program, the set of required system files and libraries, the scripts for deployment and configuring of the execution environments, data files, and configuration files are delivered to a remote unit of the Grid environment by standard means of the *middleware* distributed programs.

The use of these containers is suitable for delivering a pre-set environment as a single task that requires no additional configuring or complex installation and setting procedure, which are to be performed, most often manually, by the cluster administrator. Having arrived to the resource unit, the container deploys the package and the required system libraries, adjusts the execution environments (including the parallel environment), runs the task, and after that dispatches the results to the user interface and cleans the execution environment, *i.e.*, brings the resource to the initial state. This may solve the installation, setting, and OS and other software incompatibility problems and resolve the conflict of identical applications.

Operation of bunches of formally independent tasks. Running of bunches of independent tasks with the access to all resources of the distributed environment is a method developed to solve a wide range of multiparametric problems of computational chemistry using Grid technology.[6] As noted above, a class of chemical physics problems requires successive addressing of a large number of parameters. The complete problem is split into a multitude (up to 10^9) of independent subproblems (each is defined by the set of parameters).

Automation of the splitting procedure of the complete problem into fragments provides convenient use of the system. A typical example is a fundamental problem of the theory of elementary chemical processes: tunneling reactions induced by electromagnetic radiation. Parameters include the radiation frequency and amplitude. The computational complexity of the problem is high; however, the calculations at each network point are independent of one another. Therefore, it is possible to split the computing area into numerous non-overlapping sub-areas and to solve the problem for each point on different processors.

The procedure of running a bunch of tasks was developed for all of the available resources of the chosen distributed environment. A program package for running the task bunches and obtaining results by means of the user interfaces (UI) of the gLite, Unicore, Globus, and GT4 environments was written in Perl. For the solution of multiparametric quantum chemistry problems, methods of formation of the bunches of independent tasks with variable parameters were developed (up to 10^4 (in prospect, up to 10^7) of this tasks per problem).

The chosen data domains are cut by tailor-made scripts, then the independent tasks are formed, and queues are formed and launched followed by dispatching to the resources. After that, the scripts are periodically run (by operation system tools) to monitor the task execution, check the execution time, restart the failed tasks, and collect the results of the executed tasks (using the database and tables therein to check the current state of the task, *i.e.*, "waiting", "launching", "execution", *etc.*). After completion of the calculations, the "atomic" results are collected to a single output file.

The key drawback of task bunch operation is the limited possibility for the users to monitor their own tasks in the Unicore and Globus GT4 environments. However, in general, the new, fully asynchronous mechanism for launching a task bunch requires of the user only to select the desired resource, which can be done using the web portal.

Conclusion

Using the described Grid computation techniques, a fairly complete range of Grid services for large-scale high-level calculations in chemistry was established at the IPCP RAS.

A set of applied program packages for computational chemistry adapted to various Grid environments (gLite, Unicore, Globus GT4) with different-level interfaces (from low-level interface up to the web portal) was designed.

New calculation procedures (formation of bunches of independent tasks, virtual containers, *etc.*) in distributed and parallel environments using computational chemistry software were developed.

A resource center (comprising the resource units of the EGI-RDIG polygon, SKIF polygon, and GridNNN, and web portal) was established combining both the resources for execution of incoming tasks in the gLite, Unicore,

Globus and GT4 environments and user interfaces to these distributed environments for solving the outgoing problems at the external resources.

As a result, a computational center was founded suitable for performing calculations in different fields of chemistry in the distributed environments on large-scale polygons (in prospect, up to 10^4 CPU on multiteraFlop-scale units). The applicability of the created resources to the solution of practically important chemical problems on high-performance computational polygons was demonstrated. This allows one to set and solve both fundamental and applied computational problems, which was earlier unavailable in the chemical science due to the limited capacity of computing resources. The main scientific areas of application of Grid technology include chemical physics, quantum chemistry, investigation of nanostructures, molecular dynamics, pharmaceutics, development of fuel cells, *etc*.

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