

# Estimation of the physico-chemical parameters of materials based on rare earth elements with the application of computational model

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**Abstract.** Computational model, technique and the basic principles of operation program complex for quantum-chemical calculations of material's physico-chemical parameters with rare earth elements are discussed. The calculating system is scalable and includes CPU and GPU computational resources. Control and operation of computational jobs and also Globus Toolkit 5 software provides the possibility to join computer users in a unified system of data processing with peer-to-peer architecture. CUDA software is used to integrate graphic processors into calculation system.

## 1. Introduction

Universal and specialized program packages of simulation are applied while carrying out the research of new functional material creation. Significant computational resources are needed to model atomic structures properties of sold materials. The requirements to the volume of computational resources are being raised multifold with the development of mathematical apparatus techniques and the increase of model description precision.

Characteristics and properties of atomic structures are studied in the program complexes GIMM\_FPEIP, MATLAB and also in program complexes GAMESS, Firefly, Gaussian, HyperChem, MOPAC, ORCA, ADF, PRIRODA, SPARTAN and others. All of them have individual peculiarities. In some cases, the broad functionality of these program packages or narrow specification on the contrary does not allow you to apply these programs to model characteristics of alloys with rare-earth metals additions in case of variable external actions in a wide range of values.

The automation of research process is especially attended while modeling the properties of atomic structures. A large volume of data is accumulated in the course of modeling and the data should be stored in the full amount. Specialized supercomputers and clusters are used to carry out quantum-chemical calculations what makes it possible to carry out calculations in acceptable time. In this connection, the way of data processing, storage, aggregation and analysis have to be automated as much as possible in order to solve problems of researching new material successfully [1-5].

The aim of the work was to create a program complex for modeling atomic structure characteristics of alloys with rare-earth metals additions. The program complex would provide users with relatively cheap computational and informational resources for automated data processing and for storage and analysis of modeling results.

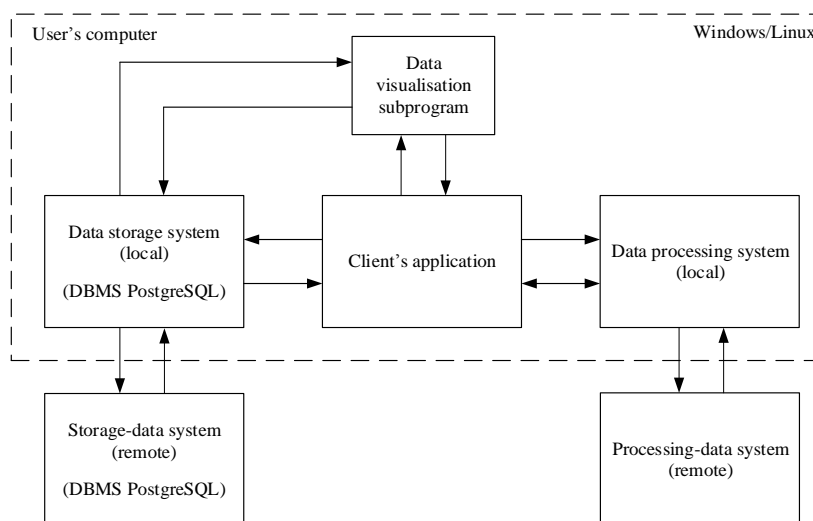


## 2. The data processing system structure

A lot of attention was paid to the unification of data format for interaction of Antares components in the course of its development. In turn, this made it possible to provide needed functionality and relatively easiness of its implementation.

The program complex has functions which allow carrying out model calculations on the basis of heterogeneous computing resources of GRID network [6]. Calculations can be carried out on GPU graphics accelerators which surpass streaming CPU joined as clusters in speed of carrying out mathematical operations.

In program complex Antares CUDA hardware-software architecture is used to parallel computational jobs [7]. Antares general structure is presented in Figure 1.



**Figure 1.** General structure of program complex Antares

The set of experimental data formed in the course of material research is stored in local and remote systems.

Local and remote data storage systems comprises DBMS server PostgreSQL and FTP file server.

The database structures in a user's computer and in remote DBMS server have an identical structure and set of tables.

Remote processing system is a remote Data Processing Center (DPC) which provides a user without sufficient computational resources with a possibility to operate data on GPU basis.

Internal data processing system in its structure and functions similar to the external one and allows data processing by means of a user's computer with the help of CPU or GPU, if available.

A user's computer is both a client and a server, which can give its informational and computational resources or it can use distributed network resources to solve the problems of modeling. In order to store experimental data, a user can engage own computer memory resources or the user can engage resources of dedicated remote data storage server that is included in DSS. The client application allows initiating data communication between the local and remote DSS servers, and also to initiate the visualization of experimental data in order to carry out analysis and it allows you to run computing jobs.

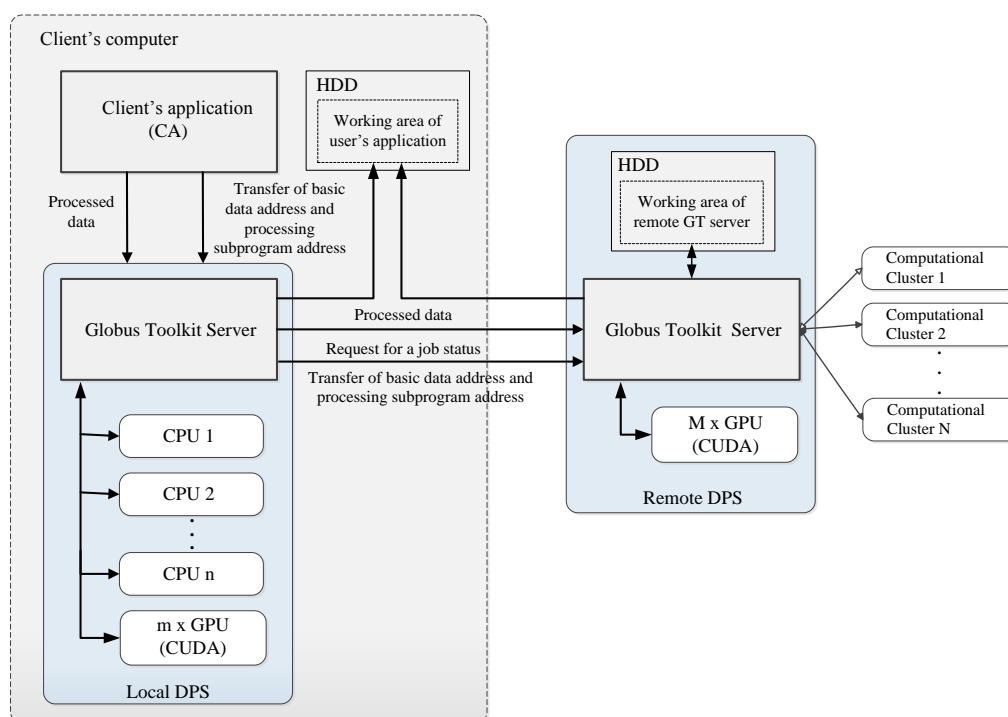
The results of the conducted experiment are stored as a set of files in the working directory of the client's application. Files contain the calculated functional of a model, calculation results, executable code of parallel calculations, and other metadata. There is the header XML-file in each directory of a certain experiment, this file contains the experiment identification number, the basic characteristics of the modeled material and pointers (links) to all files relating to a certain experiments.

The header XML-file is used to identify files in a separate experiment. Data from the header XML-file is copied into database while preserving the experimental results and that fact allows the user to search for required materials according to a set of supplied parameters. The possibility of synchronizing data between local and remote servers is introduced into DSS functionality of Antares program complex. The exchange of data between servers is carried out by means of PostgreSQL DBMS.

Data synchronization allows backing up user's data to ensure its safety and it gives the possibility to analyze the data by other users.

Synchronization request is sent to the DBMS of a remote server at the moment when user's computer connects to DSS network. The remote DBMS connects to the DBMS of a local DSS server and searches for new records in a user's database. In the case of finding new records, the remote DBMS copies from the local file server header XML-files which contain key information about the location of new data in the memory of a local file server. A stored procedure (subprogram) executes the process of copying files with the results of new experiments; this subprogram is run by the DBMS on a remote server. At this time new records are created in the database of a remote DSS server. These records have information about main material parameters and links to experiment files.

The formation and the start of computational jobs in a local or remote data processing system (DPS) is done by means of a client application. The functions of user's interaction with the ODS include the following: the volume assessment of free computational resources, the sending of a job into DPS and the controlling of an assignment in current status. The interaction scheme of a client's application of program package Antares with DPS is presented in Figure 2.



**Figure 2.** The scheme of interaction between a client's application and DPS

Globus Toolkit software is the basis of the local and remote DPS server. The local DPS server distributes and starts computational job on the basis of information about available computational resources. This is performed on available CPU and GPU (by means of CUDA) if there is a graphics accelerator. Computational jobs are performed remotely on DPS servers if a user has an access to the network [8].

Toolkit functions are based on four protocols [9, 10]:

- Link layer – security (GSI, Globus Security Infrastructure);
- Resource layer – resources control (GRAM, Grid Resource Access and Management), information service (GRIP, Grid Resource Information Protocol), data transfer (Grid FTP).

Globus Toolkit provides an access to computing processes by means of GRAM5 component (Grid Resource Allocation and Management). Computational jobs in GRID-network are controlled, added and canceled with the help of this component [11]. Gatekeeper process is run on a random computational node to initiate the computing program on the same node. A client application sends requests to GRAM, the requests are written in Resource Specification language (RSL) [12].

Basic data is transferred into GT with the help of Grid FTP in order to carry out calculations [13].

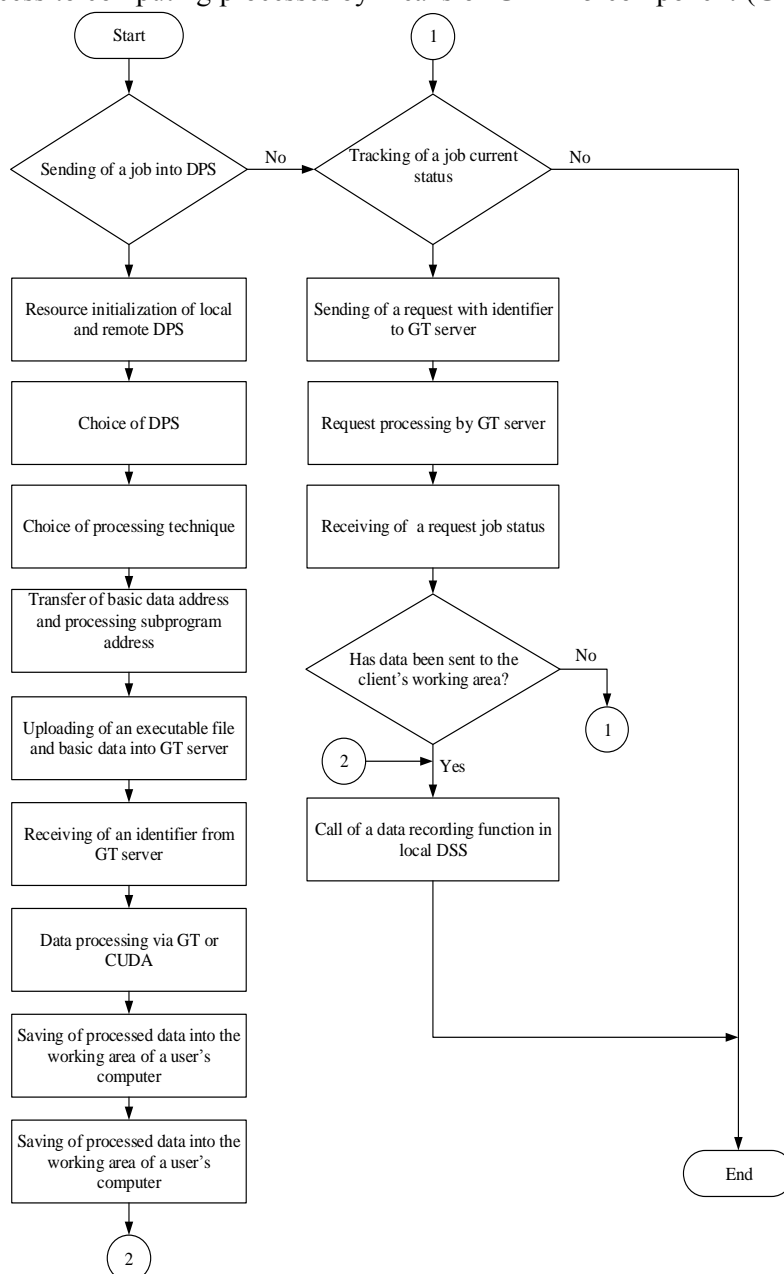
The Globus Toolkit software includes the following components which are necessary for the operation of program complex for material modeling: the file server “globus-gridftp-server”, client “globus-url-copy” and the set of libraries for developers [14, 15].

Interaction between the client application and DPS is carried out according to the algorithm which is shown in Figure 3.

A transport file of UTF experiment is formed in the working memory area of a client's application before the job sending function into DPS is run. Further, the

resources initialization of local and remote DPS is performed by means of local GT server. Local and remote DPS are chosen on the basis of information about available resources.

Two modes of data are available to a user: static and dynamic. After selecting a mode, the client application passes a pointer to the basic data files and processing program into the local GT server. If



**Figure 3.** The flowchart of calculating the material properties in DPS

you select the local DPS, an executable program file and files with the basic data are loaded into the local GT server. Computations in the remote DPS are performed in the same way.

After files uploading GT server forms the executive job and assigns it an identification number. After calculations the local GT server collects files with processed data and transfers them into the working area of a user's application.

User functions of client's applications interaction with DPS implemented by means of commands which are transmitted to Globus Toolkit server via a terminal. The whole list of interaction functions with DPS which is available to the user in the client's application of Antares is shown in Table 1.

**Table 1.** The list of user's functions which interact with DPS

User's functions	GT program components for implementation of functions	Description of GT component
Function of sending a job to DPS	globusrun	It serves to control jobs which are performed on a local or remote host with use of GRAM.
	globus-job-run	It forms a job on the basis of parameters of a using command and it transfers the job to GRAM service
	globus-job-manager	It allows you to start and control GRAM service which work is performed by the system that controls local resources directly on a computational node. It is run with globus-gatekeeper.
	globus-gatekeeper	Metaserver which runs different services after authentication of TCP connection. At the same time it correlates client's accounting data of a local account
	globus-gatekeeper-admin	It controls data which is used by globus-gatekeeper.
	globus-job-submit	It is similar to globus-job-run, but it is used to add the whole package of jobs.
	globus-job-cancel	It cancel jobs that have been already created
	globus-url-copy	It transfers data (data of a file or the whole file directory) between two addresses. It supports the following URL-prefixes :file:// (only local machine) ftp://, gsiftp://, http://, https://.
Tracking of a job current status	globus-job-status	It checks the status of jobs performance in GRAM service sending status requests to a job manager. In the case of successful job, the information about job status displayed in a terminal window.

### 3. Experiment

The properties calculation of  $\text{Al}_3\text{Ti}$  system atomic structure was carried out in order test the functions of the program complex. Mathematical model that describes the properties of  $\text{Al}_3\text{Ti}$  atomic structure was specified with the help of specialized file entering into the UTF composition.

Mathematical calculations were taken from famous LCAO-CO method (crystal orbital as a linear combination of atomic orbitals) that is an analogue of the Hartree-Fock-Roothaan method for crystals. On the basis of method results it was possible to connect atom properties which form a crystal with the crystal itself.

In LCAO-CO one-electron functions for the crystal are constructed as linear combinations of atomic orbitals sums in blocks:

$$\varphi_{nk}(r) = \sum_p C_{np}(k) b_{pk}(r).$$

Coefficients  $C_{np}(k)$  are found with the help of variational principle from the Hartree-Fock-Roothaan equations:

$$\sum_p F_{pq}(k) C_{np}(k) = E_n(k) \sum_p S_{pq}(k) C_{np}(k),$$

and besides it comes out as N systems for crystals instead of such a system for a molecule.

Matrix  $F_{pq}(k)$  is found as a sum of matrixes  $H_{pq}(k)$  and  $G_{pq}(k)$ , the elements of which are determined in the following way:

$$H_{pq}(k) = \int b_{pk}^*(r) \left[ -\frac{1}{2} \Delta - \sum_A \frac{Z_A}{|r - R_A|} \right] b_{qk}(r),$$

$$G_{pq}(k) = \sum_{s,t} \sum_{k'} P_{st}(k') \left[ (b_{kp} b_{kq} | b_{k's} b_{k't}) - \frac{1}{2} (b_{kp} b_{k's} | b_{k't} b_{kq}) \right].$$

Density matrix for crystal is calculated with the formula:

$$P_{st}(k') = 2 \sum_m C_{ms}(k') C_{mt}^*(k')$$

Lattice sums of matrix elements calculated with functions from the zero (central cell):

$$F_{pq}(k) = \sum_n F_{p0,qn} \exp(ika_n),$$

$$S_{pq}(k) = \sum_n S_{p0,qn} \exp(ika_n).$$

While solving the Hartree-Fock-Roothaan equations for crystals it is necessary to know  $C_{np}(k)$  of the whole reduced Brillouin zone for fixed value because the specified form of matrix elements as follows:

$$F_{p0,qn} = H_{p0,qn} + G_{p0,qn},$$

$H_{pq}(k)$  are Hamiltonian elements for the crystal which contains energy of electron interaction with cores  $V(r)$ , and also it contains kinetic energy. Two-electron component  $G_{pq}(k)$  contains summation according to filled state:

$$G_{p0,qn} = \frac{1}{N} \sum_{rs} \sum_{k'} P_{rs}(k') \sum_{n'n''} \exp\{ik(a_{n'} - a_{n''})\} [(p0, qn | rn', sn'') - \frac{1}{2}(p0, rn | qn', sn'')]$$

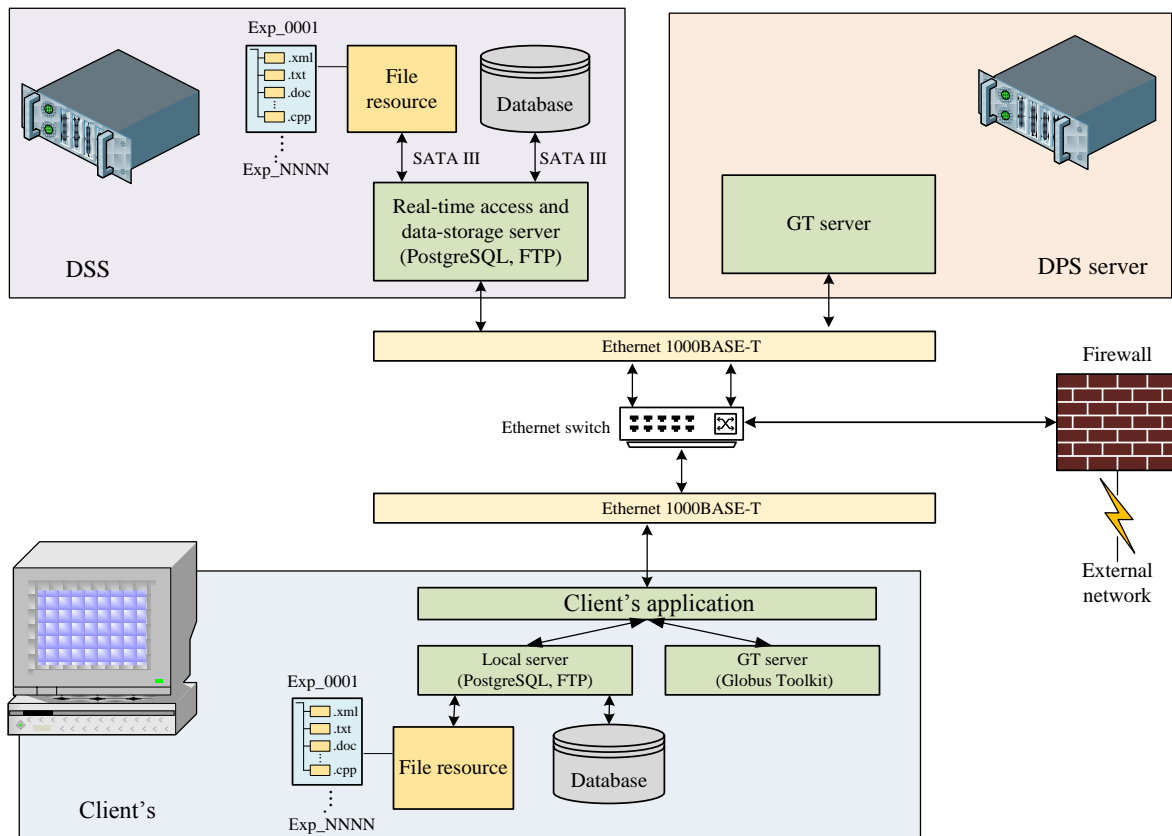
As a result, for self-consistent calculation of the electron crystal structure it is necessary to summarize a large number of occupied electronic states on every stage of integration process.

The given method was implemented in the client's application.

In the course of the experiment, special attention was paid to the problems of elaboration of a client's application interaction with data processing system.

The following software was installed and adjusted on the clients computer with OS Linux:

- S/W DBMS PostgreSQL 9.4;
- S/W FTP-server File Zilla Server 0.9.39;
- S/W GlobusToolkit 6.0.



**Figure 4.** The TestStand scheme

The client's computer and two remote servers interact in local network. The scheme of the TestStand is presented in Figure 4. DPS and DSS servers function under OS Linux.

Data which represents five experiments was written in local and remote DSS. The further work was to check how the interaction protocol of PC components functions on the level of program features.

Connection to local database:

```
conn = PQconnectdb("user=postgres password=12345 dbname=materials hostaddr=127.0.0.1 port=5432");
```

Verification of status connection with the following identifier:

```
if (PQstatus(conn) != CONNECTION_OK)
```

```
{
    fprintf("Connection to database failed"),
    CloseConn(conn);
}
```

The search for the fourth experiment in the local database:

```
res = PQexec(conn, "SELECT * FROM experiment1 WHERE id=4 ");
```

```
if (PQresultStatus(res) != PGRES_TUPLES_OK)
```

```
{
    fprintf("select failed");
    PQclear(res);
    CloseConn(conn); }

```

A framework for command execution is a set of functions which includes SQL-request.

#### 4. Conclusion

The model described by the given equations was applied in program package Antares for atomic system  $\text{Al}_3\text{Ti}$ . It was carried out the calculation of geometrical parameter  $a$  of the crystal grid; in the result we got the value which is equal to 3.997 Å, what is 0.161 Å more than the 3.836 Å experimental value [16]. According to the result we can make a conclusion that the Hartree-Fock method for crystals which is used jointly with STO-3G basis calculates geometrical parameters of the chosen atomic system  $\text{Al}_3\text{Ti}$  with relative error 4% because of error accumulation during the system self-consistency procedure.

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