



📍 Interconnection & Interoperability of Grids between Europe & China 📍

PROJECT NUMBER: 026634

PROJECT ACRONYM: EUCHINAGRID

**PROJECT TITLE: INTERCONNECTION &
INTEROPERABILITY OF GRIDS
BETWEEN EUROPE AND CHINA**

**INSTRUMENT: SPECIFIC SUPPORT ACTION
ACTIVITY: RESEARCH INFRASTRUCTURES**

D 4.1 – APPLICATIONS SPECIFICATIONS AND REQUIREMENTS

Due on: 14/06/2006

Submitted on: 12/06/2006

Start date of project: 1 January 2006

Duration: 24 months

Organisation name of lead contractor for this deliverable: UROM3

Project co-funded by the European Commission within the Sixth Framework Programme (2002-2006)		
Dissemination Level		
PU	Public	PU
PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	

Project co-funded by the European Commission within the Sixth Framework Programme (2002-2006)

Document identifier:	EUChinaGRID-Del4.1-v2.doc
Date:	09/06/2006
Workpackage:	WP4: Applications
Lead partner:	UROM3
Document status:	Final
Document link:	<i>http://www.euchinagrid.org/deliverable/D4.1.html</i>

Abstract: This document describes the requirements of the applications supported by the EUChinaGRID project.

Copyrights © The EUChinaGRID Consortium. 2006.

See <http://www.euchinagrid.org/partners-engl.htm> for details on the copyright holders.

EUChinaGRID ("Interconnection & Interoperability of Grids between Europe & China") is a project funded by the European Union within the framework of the Sixth Framework Programme for Research and Technological Development (FP6), as a part of the specific programme 'Structuring the European Research Area', within the "Research infrastructures" activity Call name: 'Communication Network Development – eInfrastructure – Consolidating Initiatives. For more information on the project, its partners and contributors please see <http://www.euchinagrid.org>.

You are permitted to copy and distribute verbatim copies of this document containing this copyright notice, but modifying this document is not allowed. You are permitted to copy this document in whole or in part into other documents if you attach the following reference to the copied elements: "Copyright (C) 2006.

The EUChinaGRID Consortium. <http://www.euchinagrid.org>".

The information contained in this document represents the views of EUChinaGRID Consortium as of the date they are published. The EUChinaGRID Consortium does not guarantee that any information contained herein is error-free, or up to date.

THE EUChinaGRID CONSORTIUM MAKES NO WARRANTIES, EXPRESS, IMPLIED, OR STATUTORY, BY PUBLISHING THIS DOCUMENT.

Delivery slip

	name	partner/activity	date	signature
From:				
Reviewed by:	Moderator and reviewers			
Approved by:	TB			

Document log

Issue	Date	Comment	Author
1-2	07/06/2006	Final Draft for Comments	F. Polticelli
2-0	08/06/2006	Reviewed	F. Ruggieri

Document change record

Issue	Item	Reason for change

Contents

1. INTRODUCTION	6
1.1. PURPOSE OF THE DOCUMENT	6
1.2. APPLICATION AREA	6
1.3. REFERENCES	6
1.4. DOCUMENT AMENDMENT PROCEDURE	7
1.5. TERMINOLOGY	7
2. EXECUTIVE SUMMARY	8
3. BIOLOGY APPLICATIONS – EARLY AND LATE STAGE FOLDING (JUMC)	10
3.1. APPLICATION DEFINITION	10
3.2. MODULES DESCRIPTION	10
3.2.1. <i>Genomic analysis</i>	10
3.2.2. <i>Ab Initio Protein folding CMUJ</i>	10
3.3. RESOURCE REQUIREMENTS	12
3.3.1. <i>Genomic analysis</i>	12
3.3.2. <i>Ab Initio Protein folding</i>	12
3.4. APPLICATION REQUIREMENTS FOR GRID MIDDLEWARE	14
4. BIOLOGY APPLICATIONS – ROSETTA (URM3)	15
4.1. APPLICATION DEFINITION	15
4.2. MODULES DESCRIPTION	15
4.2.1. <i>Database creation</i>	15
4.2.2. <i>Ab Initio Protein folding using ROSETTA</i>	16
4.3. RESOURCE REQUIREMENTS	17
4.3.1. <i>Initial model generation</i>	17
4.3.2. <i>Model idealization</i>	17
4.4. APPLICATION REQUIREMENTS FOR GRID MIDDLEWARE	17
5. ARGO APPLICATIONS	18
5.1. APPLICATION DEFINITION	18
5.1.1. <i>Data Transfer</i>	19
5.1.2. <i>Data processing</i>	20
5.2. RESOURCE REQUIREMENTS	21
5.3. APPLICATION REQUIREMENTS FOR GRID MIDDLEWARE	21
6. EGEE APPLICATIONS	22
6.1. APPLICATION DEFINITION	22
6.2. RESOURCE REQUIREMENTS	23
6.2.1. <i>Monte Carlo simulations and physics data analysis</i>	23
6.2.2. <i>Data storage and distribution</i>	23



Interconnection & Interoperability of Grids
between Europe & China

6.3.	APPLICATION REQUIREMENTS FOR GRID MIDDLEWARE	24
7.	CONCLUSIONS	24

1. INTRODUCTION

1.1. PURPOSE OF THE DOCUMENT

The purpose of this document is to collect and describe the specifications and requirements of the applications to be deployed on the grid infrastructure. In addition, the specific requirements of each application in terms of grid middleware are described and compared to the database of middleware requirements considered by the EGEE Project Technical Forum (PTF) which are collected in repository: <https://savannah.cern.ch/support/?group=egeeptf>.

The document is organized in different sections corresponding to the different applications to be deployed on the grid infrastructure. In detail, Biology applications (Early- and Late-stage folding, ROSETTA), ARGO applications, and High Energy Physics applications (CMS and Atlas).

1.2. APPLICATION AREA

This document is an EUChinaGRID Deliverable related to the workpackage WP4 – Applications.

1.3. REFERENCES

- [Roterman95]** Roterman I. (1995) Modelling of optimal simulation path in the peptide chain folding – Studies based on geometry of alanine heptapeptide. *J Theor Biol*, **177**, 283–288
- [Brylinski05]** Brylinski M, Konieczny L, Czerwonko P, Jurkowski W, Roterman I. (2005) Early-stage folding in proteins (in silico) – sequence to structure relation. *J Biomed Biotechnol*, **2**, 65-79
- [Brylinski06]** Brylinski M, Konieczny L, Roterman I. (2006) Fuzzy-oil-drop hydrophobic force field – a model to represent late-stage folding (*in silico*) of lysozyme. *J Biomol Struct Dyn*. **23**, 519-528.
- [Laskowski05]** Laskowski R A, Watson J D, Thornton J M (2005) ProFunc: a server for predicting protein function from 3D structure. *Nucleic Acids Res.*, **33**, W89-W93.

- [Bonneau02]** Bonneau R, Strauss CE, Rohl CA, Chivian D, Bradley P, Malmstrom L, Robertson T, Baker D. (2002) De novo prediction of three-dimensional structures for major protein families. *J Mol Biol.* **322**, 65-78
- [Jones99]** Jones DT. (1999) Protein secondary structure prediction based on position-specific scoring matrices. *J Mol Biol.* **292**, 195-202.
- [DeMitri05]** I. De Mitri for the ARGO-YBJ Collaboration, "Very High Energy Gamma Ray Astronomy and Cosmic Ray Physics with the ARGO-YBJ experiment.", HEP2005, Lisboa, Portugal, July 2005.
- [Bussino01]** S.Bussino et al., "Computing Model for the ARGO-YBJ", ARGO note 005/01. 3.
- [Celio03]** Paola Celio, et.al., "ARGO-YBJ Computing Model, Data Analysis and Hardware/Software Architecture of the Processing Farm", Proceedings of the *28th International Cosmic Ray Conference*, 2003, Tzukuba

1.4. DOCUMENT AMENDMENT PROCEDURE

In order to amend the document, please contact the Project Office at: po@euchinagrid.org.

1.5. TERMINOLOGY

Glossary

Term	Definition
<i>Bogomips</i>	Formal index for CPU performance evaluation
<i>SPECint2000</i>	A Computer benchmark by SPEC (www.spec.org)

2. EXECUTIVE SUMMARY

Biology Applications

The project is focused on the structure prediction of proteins of potential pharmacological application. The sequences of “never born proteins” (the sequences of high significant sequence similarity to real proteins excluded) for more than 10^7 polypeptides generated randomly is the basis for folding simulation. The 3-D structures of proteins containing 70 amino acids are assumed to be predicted for 10^7 different sequences.

Two tasks are planned to be completed:

1. Nucleotide sequence of generated 70 amino acid proteins sequences will be compared to the sequence of entire human genome to find sequences similar and define the location of similar nucleotide sequences
2. The generated sequences of 70 amino acid polypeptides (10^7 of them) will be used to generate their three-dimensional structures. This task will be completed using two different methods: one based on Rosetta model (group at Roma 3 University) and second one based on the folding simulation in the presence of external force field of hydrophobic character.

The structures generated using both approaches will be compared to look for differences and similarities between applied models.

The final structures will be clustered according to structure similarity and according to potential similarity of their biological activity.

The biological activity measurement is based on the model of discrepancies between idealized hydrophobicity distribution (according to external force field) and the real one as observed in a folded protein.

The programs for nucleotide sequence comparison as well as for structure prediction have been accomplished. The test runs of these programs in grid environment have been performed successfully.

ARGO Applications

The Chinese-Italian collaboration ARGO-YBJ is going to finish the installation of a cosmic ray telescope consisting in a single layer of Resistive Plate Chambers, placed at 4300 m. elevation, in Tibet. The process of data taking from the experimental apparatus has been already started with only a part of the experiment installed. The software for the reconstruction of the events, the data base organization, the procedures for DB update and query and the scripts for job submission to the queueing and submission system of the local computing farms were already designed, implemented and tested.

The integration of this software with the GRID technology brings many advantages : reduces the computing resources involved in data reconstruction, reduces total time of data reconstruction, assures the alignment of the software usage and of the data quality check approach, stimulates the formation of more integrated working groups on specific physics

items between Italy and China. The GRID approach allows also the development of automatic data transfer and backup procedures from the experiment site in Tibet to our home institutes, assuring a faster access to the experimental data and helping in this way the analysis of important phenomena like Gamma Ray Bursts.

The collaboration developed a new computing model based on this new GRID approach and started the testing of the single aspects where the usage of the GRID tools and middleware are foreseen. To test the model some GRID elements of GILDA testbed were installed in Rome and in Beijing and a set of PERL scripts developed for data files transfer and introduction into the data catalogues. The structure of the information to be introduced into the metadata catalogues is under study as well as the mirroring of the data catalogues and of the metadata catalogues. They will be used for the data transfer and backup procedure of the experimental data to our home institutes. The other aspect of this new computing model is the sharing of computing resources in the data processing to be realized using the resources declaration and brokering in the GRID structure. The ARGO-YBJ reconstruction software was ported and tested in GRID environment, creating in Italy and China specific ARGO Virtual Organization and modifying the pertinent submission scripts. The next step is the integration of these two separate environments, declaring our common resources and using a common brokering system. The results of the data reconstruction process should be afterward introduced into the data catalogues and a synchronization procedure of the catalogue will be used to determine the files to be copied from one Storage Element to the other. The MonteCarlo simulation of the ARGO experimental data is a further application that followed the same "gridification" process like the experimental data processing. The programs involved are Corsika, for the simulation of electromagnetic showers, and ARGO-G, a customized version of GEANT3, for the simulation of the experimental apparatus respond. These programs were proved to work in the GRID environment and the submission scripts conveniently modified to do GRID job submission.

EGEE Applications (ATLAS and CMS)

The Enabling Grids for E-science (EGEE) project is funded by the European Commission and aims to provide researchers in academia and industry with access to major computing resources, independent of their geographic location. The EGEE project will also focus on attracting a wide range of new users to the Grid. EGEE is providing a production quality grid infrastructure spanning more than 30 countries with over 150 sites to a myriad of applications from various scientific domains, including Earth Sciences, High Energy Physics, Bioinformatics and Astrophysics.

One of the important EGEE applications is to build a grid based data storage and analysis infrastructure, namely LCG, for the entire high energy physics community that will use the Large Hadron Collider (LHC).

IHEP is building a tier-2 grid data center for ATLAS and CMS, the two LHC experiments. The following tasks will be completed:

1. Draw an agreement with CERN to set up a tier-2 center in China.
2. Install necessary computing and storage resources
3. Establish a network link between China and Europe
4. Deploy LCG (LHC Computing Grid) system and ATLAS/CMS software platforms.
5. Carry out the service tests between tier-2 and tier-1.

IHEP has signed the MoU with CERN for the collaboration of LCG. A basic LCG system has been set up.

3. BIOLOGY APPLICATIONS – EARLY AND LATE STAGE FOLDING (JUMC)

3.1. APPLICATION DEFINITION

The activity of JUMC group in WP4 concerns two problems, covered by 2 modules:

1. “Genomic analysis”: Nucleotide sequence comparison of randomly created sequences of 10^7 polypeptide chains with the sequence of human genome
2. “*Ab Initio* Protein folding CMUJ” – prediction of 3-D structures for randomly created 10^7 sequences.

3.2. MODULES DESCRIPTION

3.2.1. Genomic analysis

The main aim of genomic team is localization of “traces” of selected sequences of proteins in the complete human genome. The sequence of human genome will be transformed into amino acid sequence (three possible reading frames are planned). Entire genetic information will be taken from National Center of Biotechnology Information to find sequences similar.

The identification of similar sequences will be identified and classified as: gene region (exon, intron), non-coding fragments.

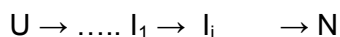
The results (localization and characteristics of the locus) will be interpreted in the aspect of evolution in context with sequences analyzed in the project.

The analysis of sequences selected in project will be extended also to other than human genomes.

3.2.2. *Ab Initio* Protein folding CMUJ

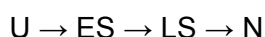
The model applied to predict the three-dimensional structure of proteins containing 70 amino acids in polypeptide chain is based on the assumption, that the folding process represents the multiple-step process.

The presence of intermediates postulated on the basis of experimental observations can be expressed as follows:



Where U-describes the unfolded state, I denotes intermediate and N expresses the native state.

The model, according to which the folding process will be simulated *in silico* assumes the presence of early-stage (ES) and late-stage (LS) folding steps in folding process. Thus it can be expressed as follows:



The structures representing ES structural forms are created according to limited conformational sub-space (part of Ramchandran map which is treated as complete conformational space). The limited conformational sub-space satisfies the criteria of optimal backbone conformation (the side chains are not present ES model). It is consistent with the experimental observations suggesting, that the backbone by itself is responsible for early stage conformational changes.

The process responsible for the structural changes leading to late-stage structural forms is assumed to be directed mostly by the hydrophobic interaction of amino acids side chains. This mechanism is represented in the simulation by the presence of external force field of hydrophobic character. The folding molecule orients its side chains according to idealized hydrophobicity distribution expressed by the three-dimensional gaussian function. The iteration procedure is oriented on the minimization of differences between observed hydrophobicity distribution (created by side chains hydrophobic interactions) and theoretical (expected) hydrophobicity distribution expressed by gaussian function. Such procedure directs the folding process to bury the hydrophobic residues in a central part of molecule and to expose hydrophilic residues toward the surface of folding molecule.

The irregularities between idealized and observed hydrophobicity is expected for polypeptides of 70 amino acids chains. The scale of differences between idealized and observed hydrophobicity distribution is expected to be different and to depend on the amino acid sequence (proportion between hydrophobic and hydrophilic residues in polypeptide chain). The irregularities of real versus idealized hydrophobicity is assumed to express the potential biological function of the protein under consideration. The presence of hydrophilic residues in a central part of molecule can be treated as potential origin for possible structural changes under changing external conditions. The presence of hydrophobic residues on the protein surface may be treated as the driving force for interaction with other molecules like ligands or proteins (protein-protein complex).

The procedures simulating both steps of folding process (ES and LS) and the measurements of hydrophobicity distribution irregularities were implemented to the program adapted to grid environment.

3.3. RESOURCE REQUIREMENTS

In this section we summarize the requirements of the applications in terms of technologies used, external dependencies, input/output data, and estimated computing times. Below we distinguish the following stages:

- Genomic analysis
- Early stage protein folding
- Late stage protein folding
- Measurements of irregularities

3.3.1. Genomic analysis

TASK: Advanced pattern recognition on strings
TECHNOLOGY: modular Perl 5 program, critical parts rewritten in ANSI C, client-server architecture for resources saving
RESOURCES: large genomic plain text data up to 10 GB
INPUT: a file with generated protein sequence from the common library $10^7 \times$ up to 0.1 kB
OUTPUT: a file with ranked searching results and findings annotations $10^7 \times 0 \dots 1$ kB
TOTAL TIME: $10^7 \times 2$ minutes

3.3.2. *Ab Initio* Protein folding

3.3.2.1. Early stage

TASK: Generation of initial protein structure
TECHNOLOGY: Perl 5 script calling external tools
RESOURCES: sequence-structure contingency library 25 MB libraries of external applications 25 MB
INPUT: a file with generated protein sequence from the common library $10^7 \times$ up to 0.1 kB
OUTPUT: early stage structure `-$id -es.pdb` $10^7 \times$ up to 50 kB \approx up to 0.5 TB (75% to deflate)
TOTAL TIME: $10^7 \times 1$ seconds

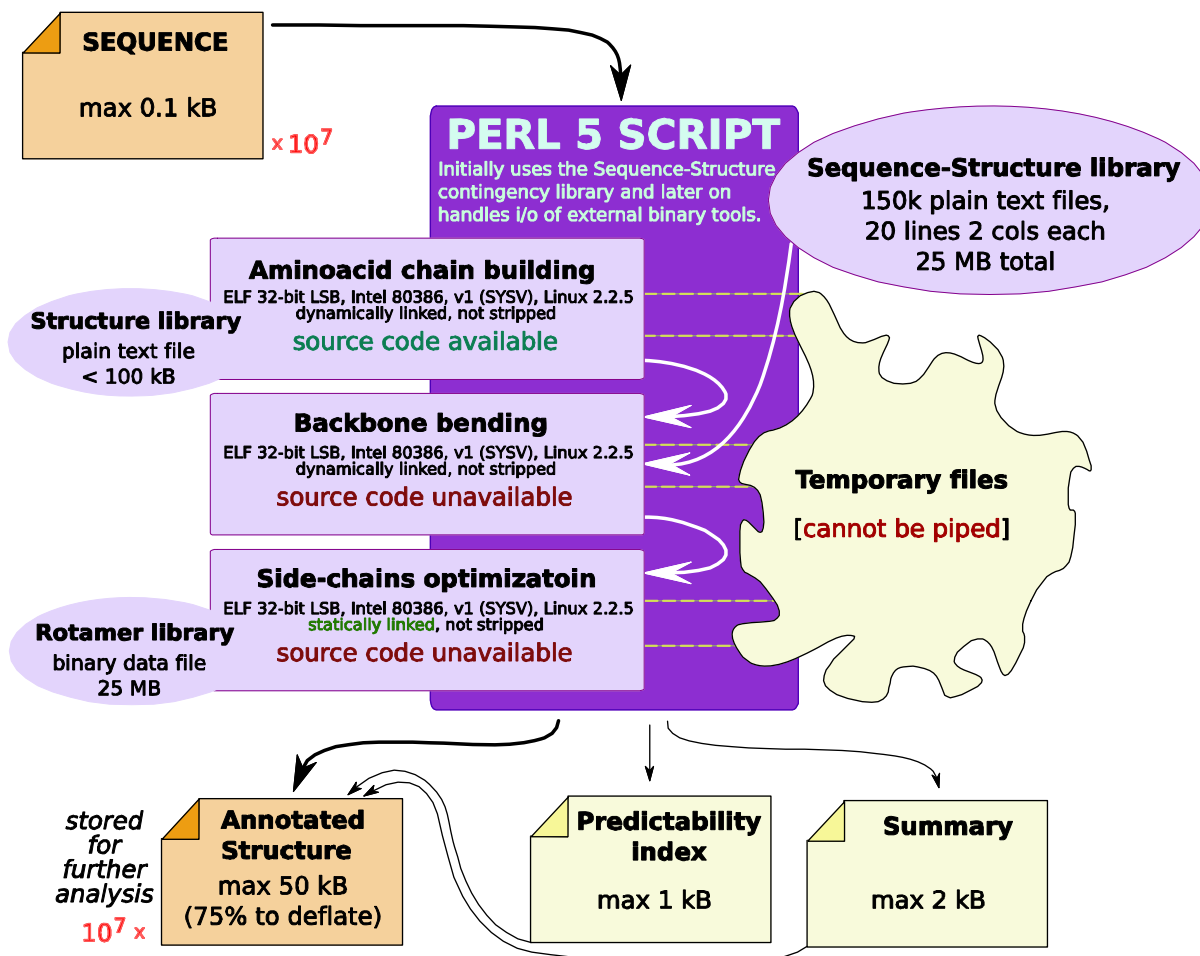


Figure 1 Early stage protein folding diagram

3.3.2.2. Late stage

- TASK:** Prediction of final conformation basing on early-stage structures
- TECHNOLOGY:** highly optimized ANSI C and FORTRAN77 mixture
- RESOURCES:** files with parametrization data less than 0.1 MB
- INPUT:** a file with early-stage protein structure $10^7 \times$ up to 50 kB
- OUTPUT:** (virtually none – late-stage structure remains in the program memory to be annotated in the following step)
- TOTAL TIME:** $10^7 \times 1$ h @ 4k bogomips PC

3.3.2.3. Measurements of irregularities

- TASK:** Revealing possible location of the site responsible for performing function

- TECHNOLOGY** (final analysis of obtained structure is performed as the latest part of the late-stage folding program)
- OUTPUT:** annotated final structure – \$id -as.pdb $2 \times 10^7 \times$ up to 50 kB \approx up to 1 TB (75% to deflate); Flat profile of ΔH parameter distribution along the peptide chain $2 \times 10^7 \times$ up to 0.4 kB \approx up to 7 GB
- TOTAL TIME:** $10^7 \times$ less than 1 minute @ 4000 bogomips PC

3.4. APPLICATION REQUIREMENTS FOR GRID MIDDLEWARE

In this section set of requirements for grid middleware was collected. Some of listed requirements were found similar, to requirements considered by EGEE Project Technical Forum (PTF) (collected in repository: <https://savannah.cern.ch/support/?group=egeeptf>).

R1: Shared jobs control

While the plan of computation covers huge numbers of jobs, the control of computation process should be distributed to several persons. This requires possibility to control the access rights to jobs (list access right, cancellation and get-output access right) for different users of a same VO.

Similar requirement was considered at EGEE PTF [#100809](#). (Status: none)

R2: DAG execution over single CE

In the application several computation stages will transfer large data between sub-jobs. It would be beneficial for overall performance to have possibility of assuring that depended jobs spawned as sub-jobs of DAG job (kind of work-flows job) are spawned close to previous ones if needed. This could limit data transfers. The system should accept "co-location hints" to guarantee that given parts of a single DAG are dispatched to a single CE

Similar requirement was considered at EGEE PTF [#100792](#). (Status: none)

R3: Job listing for a user

In large scale computations the possibility of monitoring the current situation of computational process is very important. What is more, the situation of losing the job, if it's ID is lost, is not acceptable. Therefore, we suggest possibility for a user to list the jobs he/she submitted (even if he/she does not know the jobs IDs). All uncompleted jobs (running or output not retrieved) should be displayed.

Similar requirement was considered at EGEE PTF [#100535](#) (Status: satisfied).

R4: Data file listing for a user

Similar functionality as requested in R3 is needed concerning file registered in grid storage. It should be possibility to list all files assigned to users. Mentioned functionality enables more efficient use of storage resources, that currently suffered from abandoned and useless files.

R5: Scalable relational database accessible from grid nodes

Some elements of input data and output data in the application would be collected in relational database. Secured, based on GSS access to the database from working nodes should be provide.

R6. Large number of files collected in hierarchical structure

Large number of elementary experiments (10^7) require collecting data in hierarchical structure, similar to typical file systems. This structure should be reflected on grid storage in distributed way, but the structure should be independent from physical location of files. Moreover, the large number of "files" should be possible to store and browse efficiently in one "directory".

This requirement is likely to be met in newest version of deliverable, thanks to FIREMAN service. However, this feature was not available on the time of writing of this deliverable and, therefore, was not tested.

4. BIOLOGY APPLICATIONS – ROSETTA (URM3)

4.1. APPLICATION DEFINITION

The activity of URM3 group in WP4 concerns two tasks accomplished by two software applications:

1. Creation of a large database of "never born proteins", random polypeptide sequences with no significant homology with existing (natural) proteins.
2. Prediction of the three-dimensional structure of never born proteins using the ROSETTA software [Bonneau02].

4.2. MODULES DESCRIPTION

4.2.1. Database creation

The first task to be accomplished by the URM3 unit is the generation of a database of more than 10^7 random amino acid sequences with no significant homology with existing proteins. To this aim a software has been developed that generates random sequences of fixed length (70 amino acids) in batches of 10000 sequences per file in FASTA format. Each sequence is

then compared to the non redundant protein database (available at <http://www.ncbi.nlm.nih.gov/>) using the BLAST algorithm, embedded in the software application, and sequences which display significant homology with natural proteins of comparable length are deleted from the database. The application is written in C++ and, given the relatively low computational power requirements, is currently run locally on a Pentium IV, 3.2 GHz, 64 bit architecture machine.

4.2.2. *Ab Initio* Protein folding using ROSETTA

This method is based on the concept that sequence-dependent local interactions bias segments of the chain to sample distinct sets of local structures, and that nonlocal interactions select the lowest free-energy tertiary structures from the many conformations compatible with these local biases. For local sequence-structure relationships, the program uses the protein structures database (PDB, www.rcsb.org) and takes the distribution of local structures adopted by short sequence segments (or “fragments” fewer than 10 residues in length) in known three-dimensional structures as an approximation to the distribution of structures sampled by isolated peptides with the corresponding sequences. The primary nonlocal interactions considered are hydrophobic burial, electrostatics, main-chain hydrogen bonding and excluded volume. Structures that are simultaneously consistent with both the local sequence structure biases and the nonlocal interactions are generated by minimizing the nonlocal interaction energy in the space defined by the local structure distributions using simulated annealing. The main software package is written in FORTRAN and requires several input files generated by additional programs. In detail, a file describing the predicted secondary structure for a given sequence is generated through the use of the program PSIPRED [Jones99]. On the basis of the predicted secondary structure of the sequence of interest, a Perl script extracts two sets of fragments (of length 3 and 9 residues) from a large database of fragments generated by pre-processing the Protein Data Bank. The fragments sets are then used by the main application to assemble, through a Monte Carlo procedure, several putative models of the three-dimensional structure of the “never born protein” of interest. Resulting models are then ranked on the basis of the overall energy according to an empirical force-field which takes into account hydrophobic burial, electrostatics, main-chain hydrogen bonding and excluded volume. Our approach will be that of considering the lowest energy model as the putative structure of the never born protein of interest.

Currently only the main and most demanding (in terms of computational resources required) software application has been successfully adapted to GRID environment. In addition a parametric job submission procedure has been set up in order to be able to run predictions on a large number (of the order of hundreds to thousands) of never born protein sequences at the same time.

4.3. RESOURCE REQUIREMENTS

In this section we summarize the requirements of the applications in terms of technologies used, external dependencies, input/output data, and estimated computing times. Below we distinguish the following stages:

- Initial model generation
- Model idealization

4.3.1. Initial model generation

TASK: Construction of the initial three-dimensional structure of a “never born protein”

TECHNOLOGY: FORTRAN program

INPUT: Two fragments files for each amino acid sequence, up to 10 MB per file. Batches of 10000 sequences

OUTPUT: Initial model of the three-dimensional structure of the 10000 sequences

TOTAL TIME: approx. 5 minutes per sequence

4.3.2. Model idealization

TASK: Stereochemical regularization of the initial three-dimensional structure

TECHNOLOGY: FORTRAN program

INPUT: Initial three-dimensional structure file (approx. 100 kB per sequence, batches of 10000 sequences)

OUTPUT: Idealized three-dimensional structure file (approx. 100 kB per sequence, batches of 10000 sequences)

TOTAL TIME: approx. 30 minutes per sequence.

4.4. APPLICATION REQUIREMENTS FOR GRID MIDDLEWARE

In this section set of requirements for grid middleware was collected. Some of listed requirements was found similar, to requirements considered by EGEE Project Technical Forum (PTF) (collected in repository: <https://savannah.cern.ch/support/?group=egeeptf>).

R1: Licence software usage

ROSETTA software is distributed with a licence that allows only the members of the licenced group to use the software. Licensed software must be considered as a grid resource with access limited to authorised users.

Similar requirement was considered at EGEE PTF [#100540](#). (Status: none)

R2: Shared jobs control

As the project requires the execution of a huge numbers of jobs, the control of computational processes should be distributed to several persons. This require possibility to control the access rights to jobs (list access right, cancellation and get-output access right) for different users of a same VO.

Similar requirement was considered at EGEE PTF [#100809](#). (Status: none)

R3: Job status retrieval

Given that we are faced with more than 10^7 jobs in batches of 10^4 , loosing a job implies reorganizing the sequences batches and resubmitting the loosed jobs. It is thus critical that a user can retrieve the status of the jobs he/she submitted with reference to the input files that generated that job.

Similar requirement was considered at EGEE PTF [#100536](#) (Status: satisfied).

5. ARGO APPLICATIONS

5.1. APPLICATION DEFINITION

The ARGO detector will provide a detailed space-time picture of the showers front, initiated by primaries of energies in the range 10GeV- 500 TeV. ARGO-YBJ telescope is optimised for the detection of small size air showers. Data gathered with ARGO will face the gamma astronomy at 100GeV threshold, allowing the monitoring of more than 300 sources, gamma ray burst physics, the study of diffuse gamma ray from galactic plane, the Anti-p/p ratio at energies 300GeV- TeV, the primary proton spectrum in the 10-200 TeV region and many other different physics items. The detector consists of a single compact layer of RPCs (1608 chambers, 280cm x 125cm each) occupying a surface of 5600 sqm, surrounded by a sampling ring of 240 RPC to recover the edge effects.

The activity of ARGO group in WP4 concerns problems linked to data management (data transfer, backup and data processing) and is covered by 2 modules:

1. "Data Transfer": the ARGO experimental data are collected at rates up to 7.5 Mbyte/sec and should be available to reconstruction and data analysis process as fast as possible to allow the treatment of sensitive data like Gamma Ray Burst
2. "Data Processing": reconstruction algorithms applied to space-time information of the showers front identify the primaries, their direction and characteristics of the showers. To the same module belongs the ARGO MonteCarlo production, that simulates the showers and the respond of the RPC carpet. This processes heavily involve computing resources and will be implemented in a shared resource GRID environment.

Detailed description of those modules is done in the following paragraphs.

5.1.1. Data Transfer

We evaluate the amount of data to be collected at the ARGO experimental site in Tibet at a rate of around 25 KHz of events of the order of 6.24×10^{11} events a year, corresponding to around 200 Tbyte / year of experimental data. These data have to be transferred to the processing sites in Italy and in China. This procedure allows a natural backup of the experimental data.

The data transfer should be a highly automatic process, not only for the experiment logistic considerations, but also because of some specificity of the physics involved. The Gamma Ray Bursts phenomena, for example, need to be detected and processed in the shortest possible time.

Some peculiarities of the data taking system will be reflected in the data transfer characteristics. The process of data acquisition is organized in periods of RUNs, data taking periods in which some working conditions are kept constant. The selected events are written to files, and a RUN contains many data files, plus the registration of the RUN conditions.

All the information about RUNs, their content and their characteristics are stored in the experiment relational data base.

ARGO experimental data transfer can be efficiently realized using the GRID tools for data transfer, data retrieval and backup. The data from the YangBajing Laboratory should be sent first to one of our home computing centers, in Italy or in China, and then copied to the other computing center storage, synchronizing the information in both sites. In this way we realize a very efficient backup system and give the possibility to share the computing resources in an integrated data processing GRID environment.

The data transfer involves the following technical steps :

- establish a certain number of FTS (File Transfer Service) channels between YBJ Tibet experimental site, Italy (CNAF) and China (IHEP) ARGO computing centers
- transfer the experimental data files from YBJ to IHEP (or to CNAF if no FTS channel is available to IHEP)
- use of a local YBJ Data Base to monitor the success of the data transfer

- update the local, IHEP or CNAF, data catalog
- apply synchronization mechanism of the data catalogues to transfer the data from IHEP to CNAF, or from CNAF to IHEP, using proprietary scripts and the GRID monitoring tools
- update the local, CNAF or IHEP, data catalog

At the end of a successful data transfer the raw data files will be present in each Storage Element and in each data catalogue at (IHEP and CNAF), specifying that there is a replica of the same file in the other catalogue. The information will be afterward introduced into the experiment data base.

5.1.2. Data processing

The processing of the experimental data consists in the application of algorithms to the space-time picture of the showers front in order to reconstruct the direction and the kind of primary that produced the shower and reassume the shower characteristics. The software was developed in C++ language.

The reconstruction process is quite complex, implying the use in input of the files belonging to the same RUN and the usage of the RUN condition information. The amount of information produced in output is around 36 Tbyte/year. The computing power requested by the reconstruction process was evaluated in around 200,000 SPECint2000.

The job submission procedures (a set of PERL scripts) interrogate the ARGO experiment data base to detect the RUNs to be processed and submit the jobs to the queuing and submission system. Once the files in output are stored, the information is introduced in the experiment data base to allow the physics analysis process the selection of the pertinent files and information.

The same processing steps are activated for the MonteCarlo production: simulation of the showers (based on Corsika program) and of the respond of the RPC experimental apparatus (based on ARGO-G, a specific ARGO version of GEANT3 program).

Assuming a common ARGO Virtual Organization, the relative VOMS and the problem of mutual validation of CA certificates solved, we have to define the computing resources available for ARGO at IHEP and CNAF. These resources will be published to the information service: servers BDII (Berkeley Database Information Index), up to a top ARGO-VO BDII.

The system will be completed by the installation of one or more Resource Broker.

The reconstruction jobs will be done via JDL scripts, submitting the jobs to the Resource Broker. The RB, using the top ARGO BDII will automatically identify the free resources (in Italy and China), will use the local data file catalog and pass the jobs to the free CE. At the end, the outputs will be copied to the local SE and the files introduced in the local data catalogue.

In each site (IHEP and CNAF) will run a set of scripts trying to synchronize the contents of the data catalogues. The data reconstructed in each site will be copied automatically on the other site Storage Element and introduced in the local catalogue too. This procedure is very similar to the raw experimental data transfer mechanism to IHEP and CNAF.

5.2. RESOURCE REQUIREMENTS

The data transfer module imply the transfer over the network of 200 Tbyte of raw data from the experimental site to the processing sites in Italy and China. At the end of the data processing we have to the transfer also the reconstructed data files between these two sites, for a total amount of 36 Tbyte. The procedures are PERL scripts.

The data processing module requests a computing power of 200,000 SPECint2000 only for the experimental data processing. Assuming the reuse of the simulated showers, we can esteem the requested computing resource for MonteCarlo production in at least 250,000 SPECint2000. Taking into account the possibility to share the ARGO computing resources between the Italian and Chinese computing centers we halve the resources requested on each side and the time needed for the reconstructed data to be available for the physics analysis.

5.3. APPLICATION REQUIREMENTS FOR GRID MIDDLEWARE

In this section set of special requirements for grid middleware was collected. Some of listed requirements was found similar, to requirements considered by EGEE Project Technical Forum (PTF) (collected in repository: <https://savannah.cern.ch/support/?group=egeeptf>).

R1: Mirrored data catalogues

The experiment requirements imply the presence of a copy of the raw experimental data files and of the processed data files in the Storage Element of each computing centre and inside the data catalogues. These data files should be managed using automatically mirrored data catalogues, instead of doing that by proprietary scripts.

R2: Mirrored metadata catalogues

The data files are logically grouped in RUNs and some characteristics are valid for all the files in the group. This information is kept in metadata catalogues and these catalogues should also be automatically mirrored as are the data catalogues maintaining data files information.

R3: Shared jobs control

The control of computation process should be distributed to several persons. This requires the possibility to control the access rights to jobs (list access right, cancellation and get-output access right) for different users of a same VO.

Similar requirement was considered at EGEE PTF [#100809](#). (Status: none)

R4: Job listing for a user

The problem of monitoring the current situation of computational process is very important and losing the information about the job, if its ID is lost, is not acceptable. Therefore, we suggest possibility for a user to list the submitted jobs, even if the jobs IDs are not known. All uncompleted jobs (running or output not retrieved) should be displayed.

Similar requirement was considered at EGEE PTF [#100535](#) (Status: satisfied)

R5: Recuperate job status

In some cases we can lose the link to the CE while the assigned jobs are still running. The automatic recuperation of the job status when the link is reactivated will avoid the resubmission of the jobs.

R6: compatibility of the applications with GRID computing environment

We already proved the compatibility to the GRID computing environment of the main software for ARGO experimental data processing. The programs used for MonteCarlo production, Corsika e GEANT3, were already successfully used in GRID by other experiments.

6. EGEE APPLICATIONS

6.1. APPLICATION DEFINITION

LHC is the largest particle physics project in the world. When it begins to be operational, at CERN, in 2007, it will generate about 15 Petabytes of data every year, which more than 6000 scientists around the world will access and analyse. As the major application of EGEE, the mission of the LHC Computing Project (LCG) is to build and maintain a data storage and analysis infrastructure for the entire high energy physics community that will use the LHC.

The data from the LHC experiments will be distributed around the globe, according to a four-tiered model. A primary backup will be recorded on tape at CERN, the "tier-0" center of LCG. After initial processing, this data will be distributed to a series of Tier-1 centers, large

computer centers with sufficient storage capacity for a large fraction of the data, and with round-the-clock support for the Grid.

The tier-1 centers will make data available to tier-2 centers, each consisting of one or several collaborating computing facilities, which can store sufficient data and provide adequate computing power for specific analysis tasks. Individual scientists will access these facilities through tier-3 computing resources, which can consist of local clusters in a university department or even individual PCs, and which may be allocated to LCG on a regular basis.

6.2. RESOURCE REQUIREMENTS

The resource requirements of ATLAS and CMS computing will increase every year as the LHC runs in the coming years. The resources will be mainly used to do the following jobs:

- Monte Carlo simulations
- Physics data analysis
- Data storage and distribution

For more information on ATLAS and CMS experiments please refer to their web sites (<http://atlas.web.cern.ch/Atlas/index.html> and <http://cms.cern.ch/>)

6.2.1 Monte Carlo simulations and physics data analysis

TASK: Physics simulation and experimental data process for the new physics research.

TECHNOLOGY: C++ program, with some parts written in Fortran

RESOURCES: Computing resources requirements for ATLAS and CMS are very huge and should be distributed globally. The resource to be deployed at IHEP in two years includes 500,000 SPECint2000 of CPU power.

INPUT: raw data collected from experiment detectors

OUTPUT: processed data of physics events reconstructed from raw data or physics simulation

TOTAL TIME: non-stop service during the lifetime of LHC projects

6.2.2 Data storage and distribution

TASK: provide cache storage system for data analysis and data transfer between tier-1 and tier-2 centers.

TECHNOLOGY: file management and transfer tools embedded in EGEE middleware, written in C++.

RESOURCES: 50 TB of disk space, up to 2.5 Gbps network link from China to Europe.

TOTAL TIME: non-stop service during the lifetime of LHC projects

6.3. APPLICATION REQUIREMENTS FOR GRID MIDDLEWARE

LHC Computing Grid (LCG) is the major application of EGEE. EGEE middleware is well satisfied to LCG. LCG has set up RB, BDII and MON system to monitor and manage the resources. CE and SE for ATLAS and CMS have already been installed. VOs for ATLAS and CMS have been set up. Jobs of different experiments can be controlled by VO to access different resources respectively. There are no significant requirements of EGEE applications which are still to be satisfied.

7. CONCLUSIONS

An extensive analysis of the requirements of the applications supported by EUChinaGRID project has been performed and the resulting list was found partially overlapping the requirements already collected by the EGEE Project Technical Forum (PTF). Most of the applications have already started the porting on GRID environment.