Using the Mass Storage System at ZIB within I3HP

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In the framework of I3HP there are two Transnational Access Activities related to Computational Hadron Physics. One of these activities is access to the mass storage system at Konrad-Zuse-Zentrum f"ur Informationstechnik Berlin (ZIB). European lattice physics collaborations can apply for mass storage capacity in order to store and share their configurations or other data (see http://www.zib.de/i3hp/). In this paper formal and technical aspects of usage as well as the conformance to the International Lattice DataGrid (ILDG) are explained.

1. I3 HADRON PHYSICS

The Hadron Physics Integrated Infrastructure Initiative (I3HP) is a project that originates from a joint initiative of over 2000 experimental, theoretical and computational physicists working in the field of hadron physics [1]. I3HP is funded by the European Commission in the Sixth Framework Programme. The project is structured into nine Transnational Access Activities, seven Networking Activities, and twelve Joint Research Activities. There are three activities that are related to lattice QCD: the Networking Activity Computational Hadron Physics, Transnational Access to supercomputer resources at NIC (J"ulich) [2], and Transnational Access to mass storage capacity at ZIB (Berlin) [3]. NIC is one of three national German supercomputer centres, ZIB runs the supercomputer centre of the federal state of Berlin.

2. TRANSNATIONAL ACCESS

The idea of Transnational Access is to give foreign researchers access to important, typically experimental facilities. It gives experimentalists the opportunity to carry out interesting experiments at facilities that they usually cannot use. The access activities related to computational QCD have a similar intention and provide access to computational facilities. While experimentalists have to travel to the corresponding laboratories, computational facilities can be accessed via the internet.

Researchers who want to use a facility have to write a scientific proposal that is being peer reviewed. How to apply for using the mass storage system at ZIB is explained on our web page [3]. It is not necessary to write an application for just downloading configurations. For downloading, a certificate is required (see section 5) and special software has to be used (see section 6).

3. LATTICE DATAGRIDS

In large scale lattice QCD projects one typically stores gauge field configurations and propagators. Gauge fields are stored permanently while propagators are stored for a limited period of time. Propagators require much more storage space than configurations. Hence they are kept at the site hosting the computer on which they were calculated. On the other hand, QCD gauge field configurations are smaller and, in the case of dynamical fermions, much more expensive to generate. This has lead to the idea of sharing configurations in order to fully exploit them.

The International Lattice DataGrid (ILDG) [4] was started to make QCD gauge field configurations available at an international level. So far, ILDG infrastructures are being built up in Japan, UK, USA, and Germany. The German ILDG Grid is called LatFor DataGrid (LDG) [5]. ILDG develops standards for data formats and a common middleware. The definitions of a metadata format and a binary file format are completed (see [4]). The LatFor DataGrid conforms to the ILDG standards.

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For this Transnational Access Activity we have decided to integrate the storage system at ZIB into the broader LDG and ILDG activities. Hence, the LatFor DataGrid became a joint effort of DESY (Hamburg and Zeuthen), NIC (Jülich) and ZIB (Berlin).

4. COMPONENTS OF LDG

The main hardware components are storage elements (SE) that have hierarchical mass storages systems (HSM) attached. Each site (in Berlin, Hamburg, Jülich, and Zeuthen) operates such a storage element. The hierarchical mass storages systems are large tape libraries that work with tape robots. The total capacity of the HSM system at ZIB is about 1.2 PetaByte. Data stored on the system is very safe because there always exist two copies on different tapes.

The storage elements are small servers that run the dCache software which was developed by DESY and Fermilab for storing huge amounts of data distributed among heterogeneous server nodes. From a user’s perspective the distributed storage element servers provide a single virtual filesystem tree. Data may reside in the server’s disk cache or might be migrated to tape. The dCache software performs data exchanges to and from the attached tape libraries automatically and invisibly to the user.

Besides the storage back-ends there are user interfaces at the front-end. In order to set up a Grid infrastructure, there are several software components (middleware) needed in addition. These components are a virtual organisation, Grid information services, a file catalogue, an access control service, and a metadata catalogue. At the middleware level LCG-2 software is used supplemented by developments of DESY. LCG is the Large Hadron Collider (LHC) Computing Grid.

A virtual organisation (VO) is an organisational unit in a Grid infrastructure. The VO representing the LatFor DataGrid is called lfdg. Grid information services handle e.g. authentication. The file catalogue maps logical filenames to physical locations and manages replicas of files. The access control service (ACS) handles access permissions. In LDG not all data is necessarily public. The ACS allows to store public and private data in the same environment. The metadata catalogue holds the metadata and makes it possible to list metadata and perform search operations.

5. IMPORTANT CONCEPTS

Three important concepts for the usage of the hard- and software infrastructure shall be explained: (1) authentication via certificates, (2) logical filenames and physical locations of files, and (3) data formats.

5.1. Authentication

In a Grid context users are authenticated by presenting a certificate, which is similar to the private/public key concept of the secure shell. The exact technical procedure for obtaining a certificate depends on the certificate authority (CA)). CAs for this Grid are listed in .

In any case, there are three basic steps that have to be done (cf. the documentation of your CA). First, one has to create a certificate request file and a corresponding personal key. The personal key should be carefully protected with a secure passphrase and backed up. Second, the request file has to be sent to the responsible CA in a secure way. In general personal authentication by presenting an identity card or passport is required. Third, one has to install the certificate that one receives from the CA and the personal key on the machine where an LDG user interface (UI) is installed.

With a valid certificate, one can use a so called grid-proxy, which will do all necessary authentication in the background for a given period of time. So one does not have to type the passphrase every time. Usually, a certificate is valid for one year. In general, renewal is a much easier process than obtaining the initial one.

5.2. Naming

Table shows examples of three types of names that are used in the context of LDG. This section explains these meaning of the names and conventions for forming them.

When retrieving data (downloading gauge field
Table 1
Examples of names.

| object       | name                                                                 |
|--------------|----------------------------------------------------------------------|
| ensemble     | www.lqcd.org/ildg/qcdsf/nf2_clover/b5p29kp13500-16x32               |
| configuration| /grid/ildg/qcdsf/nf2_clover/b5p29kp13500-16x32/qcdsf.515.00320.lime |
| physical location | srm://dcache.zib.de/pnfs/zib.de/data/ildg/\ qcdsf/nf2_clover/b5p29kp13500-16x32/qcdsf.515.00320.lime |

Table 2
Array declarations corresponding to the storage sequence of SU(3) gauge fields. Lx, Ly, Lz, Lt are the extensions of the lattice, dim = 4 is the dimension of space-time, and Ncolour = 3 is the dimension of the SU(3) matrices.

| language | array declaration                                      |
|----------|-------------------------------------------------------|
| C        | double U[Lt][Lz][Ly][Lx][dim][Ncolour][Ncolour][Ncolour][2]; |
| Fortran  | complex U(Ncolour, Ncolour, dim, Lx, Ly, Lz, Lt);     |

configurations) from the Grid one has to specify a logical filename (LFN). The Grid middleware translates the LFN into a physical location. There may exist multiple copies of the data in the Grid, so called replicas. The middleware is supposed to find the best available copy.

On uploading a configuration one has to specify an ID for the ensemble to which the configuration belongs, which is called MarkovChainURI, and a physical location. The URI (unified resource identifier) is unique in the world. The physical location can be considered as an absolute path to the configuration file within LDG. The physical location is the place where the data is actually stored.

Looking at the naming conventions adopted in LDG, one can see from the examples shown in Table 1 that all three types of names have a large part in common. All names contain the virtual organisation ildg. In the case of the MarkovChainURI ildg is strictly speaking the last part of the URL www.lqcd.org/ildg. The uniqueness of the URL leads to the uniqueness of the MarkovChainURI.

After ildg follows the name of the collaboration which has generated the data, in the examples qcdsf. The parts of the names that follow are chosen by the collaboration. However, the structure should be such that the next part of the names represents a project and the part after that represents an ensemble. The name of a configuration and the physical location have a file name in addition.

In the examples nf2_clover stands for the $N_f = 2$ clover improvement project. The name of the ensemble b5p29kp13500-16x32 repeats the essential part of the metadata, i.e. $\beta = 5.29$, $\kappa = 0.13500$ on a $16^3 \times 32$ lattice. In the file name qcdsf.515.00320.lime 515 is a job chain ID and 00320 is a trajectory counter. As mentioned before, these three parts of the names were freely chosen by the collaboration.

Syntactically the names are composed out of parts separated by slashes. Basically, the physical location is a Unix file name specification, i.e. a real directory structure is implied. In the framework of ILDG it would be allowed to chose names for ensemble, configuration, and physical location completely independently. For example, one could think of using much shorter names for the LFN in order to facilitate typing. However, in LDG it was decided to essentially use the same names at all levels for reasons of clarity.

5.3. Data formats

Data formats were defined by ILDG. There are conventions for formats of metadata [9] and binary data [10]. On uploading binary data correct metadata have to be supplied.

5.3.1. Metadata

Within ILDG, a special metadata format, called QCDml, for the description of configura-
Table 3
Overview of ltool commands.

| command | description |
|---------|-------------|
| lget    | Getting a binary of a configuration or the metadata for an ensemble or a configuration from the Grid. |
| lput    | Putting a binary and the corresponding metadata on the Grid. It is not allowed to place a binary without corresponding (syntactically-) correct metadata. Operation will take place in one transaction, i.e., the data is either stored by successfully finishing the operation or nothing will be stored if the operation fails. |
| lls     | Lists all configurations of an ensemble sorted by their LFN (can also be used to show all ensembles in the MDC by using the --all option). |
| linit   | Initialises a new ensemble in the MDC (requires administration rights). |
| lupdate | Updates metadata in the MDC (has to be valid QCDml) |
| lvalidate | Check conformance of metadata to QCDml |

tions and ensembles has been defined [9]. QCDml consists of two XML schemata, one for the description of an ensemble and one for the description of a single configuration. All metadata is stored and exchanged in the XML format. This allows a formal validation before metadata is being uploaded to the metadata catalogue. For example, a valid ensemble description has to have a `<markovChainURI>`-tag and must contain physical and algorithmic information (see [9]).

A valid configuration description must have a `<dataLFN>`-tag, which is the link to the binary file that can be downloaded from the Grid. In addition, a `<markovChainURI>`-tag has to be provided, which is the link back to the ensemble that it belongs to. Documentation on how to markup configurations can be found in [9].

5.3.2. Binary data

A binary file format for storing SU(3) gauge field configurations was defined by ILDG. This format is described in [10]. An ILDG binary file consist of several parts that are packaged using the LIME file format, which was developed by SciDAC. A LIME API, utilities and documentation are available from [12]. With the API one can read and write LIME files from a C programme. Employing the utilities one can pack or unpack LIME files at command line level. One can also extract individual files.

An SU(3) gauge field configuration packaged according to the conventions of ILDG contains at least three files. A file inside a package is called a record. These three files or record types, respectively, are called:

```
ildg-format
ildg-binary-data
ildg-data-LFN
```

The record `ildg-binary-data` contains the gauge field configuration. That record contains exactly the bytes of an array of floating point numbers as it is declared in Table 2. The floating point format is IEEE and the byte ordering is big endian.

The record `ildg-format` is an XML-document that contains the precision of the floating point numbers (32 or 64 bit) and the lattice size (see [10] for the exact format). Precision and lattice size are also contained in the metadata.

The record `ildg-data-LFN` contains the logical file name as it appears in the metadata.

A convenient way to extract records (files) from a LIME file is provided by the utility

```
% lime_extract_type limeFile recordType
```

which writes the (first) record of the specified type to stdout.

6. USING LDG-SOFTWARE

In the following sections, an overview of the LDG-software architecture is given, followed by
a short description of the user interface (called \textit{ltools}) and a sample session.

6.1. LDG-Software architecture

Within the LDG community, there is a software bundle installable on any computer running Linux. The bundle contains all the necessary software to work with LDG (assuming you own a valid certificate). This includes access to the \textit{meta data catalogue (MDC)} and all participating \textit{storage-elements (SEs)}. Actual access to the SEs is realised by the use of the LCG-2 software \cite{7} and access to the MDC by the use of a special client-software developed by DESY. This complexity is hidden from the user by offering a simple set of commands that combines both (see the following section). All software can be installed in a simple way and without the need of root privileges.

Documentation and the software itself can be found in \cite{5}. Initially, a packaging system called \texttt{lrpm} (which is a kind of \texttt{rpm} tailored for the needs of LDG) has to be installed and the location where you want to install the software has to be defined. After this, installation, initialisation, updating or deleting of the software is very easy, as only one or a few commands have to be typed for each purpose.

6.2. User tools

The authors have written a set of easy to use command line tools called \textit{ltools} which are distributed as part of the LDG-software package \cite{5}. On the one hand, the motivation was to simplify the usage of the corresponding LCG commands within the LDG context by using natural defaults, combining sequences of commands, prevent the typical user from erroneous use, providing better explanation- and error-messages and making the software more configurable to personal needs. On the other hand, the commands where designed to also access the MDC without the need of an additional software for the user. In particular, the upload of the data to the SE and the upload of the metadata to the MDC is combined in a single transaction to circumvent inconsistencies in case of an error. An overview of the commands is given in Table \ref{table:commands}.

6.3. Sample session

A typical session with \textit{ltools} looks as follows. The user starts by taking a look at which ensembles are stored in the MDC by typing:

\begin{verbatim}
% lls --all
\end{verbatim}

On the first call of an \textit{ltool} command \texttt{grid-proxy-init} will be initiated automatically, so that the user is prompted for his passphrase (unless the user has already a grid-proxy running). The output of \texttt{lls --all} is a list of MarkovChainURIs. For each MarkovChainURI one can get a list of LFNs of all configurations for that URI by typing:

\begin{verbatim}
% lls MarkovChainURI
\end{verbatim}

One can download the metadata of a configuration by typing:

\begin{verbatim}
% lget -m LFN
\end{verbatim}

After inspection of the metadata, one might want to download the actual configuration binary:

\begin{verbatim}
% lget LFN
\end{verbatim}

A user’s guide with the full functional description of the commands can also be found at \cite{11}. Table \ref{table:commands} shows the output of an \texttt{lget} execution for downloading a configuration binary.

7. SUMMARY

In this Transnational Access Activity a hard- and software infrastructure was set up that is tailored to storing configurations from simulations of QCD and that is well integrated into the International Lattice DataGrid activities of the Computational Hadron Physics community.

8. ACKNOWLEDGEMENT

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Table 4  
Sample session. grid-proxy-init is automatically run at the first call of an *ltool* command.

```
% lget /grid/ildg/qcdsf/nf2_clover/b5p29kp13500-16x32/qcdsf.515.00320.lime
Welcome to the Ltool-command lget -
Testing grid-proxy-init:

Trying to start grid-proxy-init...
Your identity: /O=GermanGrid/OU=ZIB/CN=Hinnerk Stueben
Enter GRID pass phrase for this identity:
Creating proxy ................................................... Done
Your proxy is valid until: Wed Nov 16 03:56:22 2005

Trying to get binary ...
Virtual Organisation is ildg
Executing lcg-cp lfn:/grid/ildg/qcdsf/nf2_clover/b5p29kp13500-16x32/qcdsf.515.00320.lime --vo ildg file:/home/stueben/qcdsf.515.00320.lime

Checking nonzero size of downloaded File ...ok.
```

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