Building the International Lattice Data Grid

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Abstract We present the International Lattice Data Grid (ILDG), a loosely federated grid of grids for sharing data from Lattice Quantum Chromodynamics (LQCD) simulations. The ILDG comprises of metadata, file format and web-service standards, which can be used to wrap regional data-grid interfaces, allowing seamless access to catalogues and data in a diverse set of collaborating regional grids. We discuss the technological underpinnings of the ILDG, primarily the metadata and the middleware, and offer a critique of its various aspects with the hindsight of the design work and the first full year of production.

Keywords ILDG · data grids · lattice QCD

1 Introduction

In this paper, we present the International Lattice Data Grid (ILDG). The ILDG project is a mostly volunteer effort within the Lattice Quantum Chromodynamics (LQCD) community, to share data worldwide, and to thus amortise the very high computational cost of producing...
the data. In terms of organisation it is a data-grid, but it is also a loosely federated grid of grids.

Large data sets require significant scientific endeavour to amass them. This may represent intellectual property, as well as physical resources. In the case of LQCD, the resources are both intellectual – such as the scientific ideas and algorithmic development – as well as other resources, such as the manpower required to write the computer code and the resources to procure/develop and operate a large supercomputer. Why then do scientists wish to share this valuable data? It is precisely because this data is so valuable that scientists make it available for others to use. A mechanism is required whereby those who generate shared data can receive credit for doing so.

For the LQCD community there are two compelling reasons to share data. First, fully exploiting the data requires computing and manpower resource. A particular group may generate a dataset to compute a target physical quantity with sufficient precision to have an impact on experimental results, and yet not have sufficient resources or even the expertise to calculate many other possible quantities on that dataset. At this stage, rather than waste some of the scientific potential of the data, a group may give the data away freely provided some basic use conditions are met such as citing a certain paper in any resulting publication. Second, the resources required to generate ever more potent data sets require ever greater resources, outstripping Moore’s Law and scientific innovation. This forces different groups to collaborate: jointly baring the cost of data generation.

Quantum Chromodynamics (QCD) is a theory of sub-atomic particles (specifically, quarks and gluons) and their interactions. Lattice QCD (LQCD) is a version of QCD where space-time is discretized, making the theory amenable to calculation by computers. LQCD computations are of utility in a variety of theoretical particle physics contexts including Nuclear Physics and High Energy Particle Physics, and have historically consumed a large fraction of available computing cycles worldwide. The interested reader can find several excellent books and review articles on LQCD in the literature, for example [1, 2] and [3].

LQCD Computations are based on Markov Chain Monte Carlo methods (see [4] for a recent review) and typically the primary data from such calculations are samples of the QCD vacuum known as gauge configurations. The Monte Carlo process will generate an ensemble of such configurations for each set of physical and algorithmic input parameters. At the time of writing, the typical cost of generating an ensemble is $O(1) - O(10)$ Teraflop years depending on the precise formulation employed, and this cost is expected to grow to the Exaflop-year scale as one simulates lattices with finer lattice spacings, larger physical volumes and physically light quarks.

A set of ensembles is amenable to many different type of secondary analysis. One can, for example, perform calculations of nuclear structure on the same configurations one also uses to perform calculations of fundamental parameters of the Standard Model of Particle Interactions. Alternatively, an ensemble generated to measure Nuclear Energy spectra may also be useful in the study of the nuclear strong force binding together nucleons into atomic nuclei.

Since the generation of ensembles is very demanding in terms of effort, and since the ensembles can facilitate multiple uses, it makes sense to share them amongst the LQCD community to get maximum value out of a particular generation project. The ILDG infrastructure discussed in this paper, is designed to promote and facilitate such data sharing.

The LQCD community has a history of sharing data before the formation of the ILDG. The MILC collaboration [5] has pioneered the approach of freely giving away the data, after publishing results for their target quantities. This conservative approach is necessary for scientific prudence. The data has been very widely used, and the MILC collaboration
policy of data release is seen as successful and beneficial to the collaboration. There are many examples of different groups collaborating together to share the burden of generating the data. In some sense the ILDG is similar to other kinds of data archives and Science Gateways, of which there are now many throughout the world. However, it does present some particularly unique aspects, which stem from it being a grid of grids.

In 2002, different groups were starting to make use of grid technologies to store and retrieve data, primarily within their own collaboration. A proposal by Richard Kenway [6], at the annual lattice QCD conference, to use grid technologies to store and share data, was well received and supported. The ILDG was formed from interested groups that were willing to share data. There is no central authority forcing policy on the member collaborations: rather the ILDG is a collaboration of groups that are prepared to commit some resource to a central service. This idea of an aggregation or grid-of-groups is a powerful one, which allows each group to retain control of its own resources whilst making them available to the greater whole.

This paper is organised as follows: we outline the basic requirements needed for such an infrastructure in section 2. The ILDG development has been split into two broad overlapping groups, the metadata working group (MWG) and the middleware working group (MWWG). In sections 3 and 4, we consider aspects of metadata and middleware, respectively. Finally, in section 5 we review aspects of the ILDG project from over several years of activity and over one year of production. We present operational details of the infrastructure as well as criticism of various aspects. We also have a chance in section 6 to compare and contrast the ILDG with some related or similar efforts. Finally, we summarise and discuss the potential for future work in section 7.

2 Requirements

Put in simple terms, the goal of the ILDG project is to allow scientists to share their data, across the different research collaborations within the project.

In order to attain the goal, the team have had to translate it into a set of concrete requirements, which has then been used to guide the development of the ILDG infrastructure (that is, the technologies, policies, and processes). These requirements are summarised in this section.

2.1 Data management

The team started by quantifying the data to be shared. This data is file-based and – as noted above – represents lattice gauge configurations, which are collected together into ensembles pertaining to Monte Carlo simulations.

The nature of the simulations implies that a configuration is only meaningful as a member of the ensemble. Thus, scientists almost always want to access the whole ensemble (or a significant part thereof): this equates to Terabytes of data. Also, scientists typically need to have access to local copies of data, in order to complete the required analysis processes. Thus, it is clear that sharing data involves copying multi-Terabyte file sets from the storage facility of one research group to a remote scientist’s local system.

All file copy operations are intended to be undertaken over the Internet. Thus, even with good bandwidth, it is clear that multi-Terabyte transfers represent time-consuming operations, requiring a reliable, high performance bulk data transfer mechanism.
Ensembles of gauge configurations that pre-date ILDG are typically identified using locally agreed naming conventions. For example, a particular configuration might be identified by a combination of the Unix path to the file and the hostname of the server on which it resides. While this approach may be suitable for a small group of researchers working in a particular collaboration, it is inadequate for a community like ILDG that is loosely coupled and distributed across multiple research groups.

What is required is a method for assigning a unique and persistent identifier to each file (that is, gauge configuration) that is to be held within the infrastructure. In addition, there needs to be an equivalent method for identifying each ensemble.

2.2 Data Curation

For a configuration (or an ensemble) to be useful to a researcher, it must be apparent what it represents in scientific terms. This information is provided by metadata – literally, data about data. Metadata may be captured in a number of different ways. For example, a widely used approach is based on descriptive filenames that follow an agreed naming format. For Lattice QCD, the detail required to describe a dataset is too great to be realistically encoded in its filename, especially considering the various different formulations of QCD available, all with different parameters. The process of scientific annotation has warranted a more sophisticated approach.

ILDG researchers require a scientific annotation that thoroughly and unambiguously describes a configuration (or ensemble of) for other members of the community. The annotation should be extensible: that is, it should support the introduction of new descriptive elements. This may be required — for example — to accommodate new science.

A user should easily be able to search the catalogue of scientific annotations and, complementing this, the generation of metadata should be a lightweight and straightforward process. Where possible, elements of the description should be populated automatically.

As well as having an agreed mechanism for describing data, one must also be able to read the binary files that hold the data. This motivates convergence to a common file format (for gauge configurations, at least). At the inception of ILDG, a number of different file formats existed, based on the conventions used in the most popular LQCD codes. Alongside the formalisation of the scientific metadata, it has been decided that a community-wide, flexible, extensible binary file format is required.

2.3 Infrastructure

Pre-dating the formation of ILDG, the five collaborations that make up the core of the consortium have procured or developed storage facilities to host the ensembles of data that they each generate. These systems are all accessible, in principle, over the Internet, but via different and incompatible access protocols and access control systems targeted at local (that is, institution-based) users.

To work around this issue, two specific requirements need to be fulfilled. First, a layer of software is required on top of the local infrastructures, to provide a uniform interface to an end-user. Second, an access control mechanism needs to be established that permits ILDG members from different collaborations to access designated data at partner institutions/storage facilities.
2.4 Operation and monitoring

To be useful, the ILDG infrastructure must achieve high levels of availability. High availability must be attained in spite of the decentralised and heterogeneous nature of the component elements, and should efficiently exploit the support effort available at the regional grids. It has therefore been decided that an automated monitoring service should be set up within the infrastructure, fulfilling the following specific attributes. The monitoring service needs to:

- be reliable – since it is the primary means in which problems and failures are identified.
- be flexible – in order that the diversity of ILDG components can be represented and monitored.
- produce accurate and informative alarms, which will allow regional-grid support teams to quickly and effectively diagnose and resolve issues.
- post alarms using email – as this is the primary medium over which regional-grid teams communicate.
- maintain a record of system performance, to inform coordinators as to overall reliability and to highlight any specific weaknesses.

For easy access to all ILDG resources, a centrally coordinated user management system is required: making all globally registered users known to all local-resource providers. To this end, we have adopted the concept of a Virtual Organisation (VO), with membership being managed by the VO itself. With ILDG consisting of several regional grids, a setup is however needed that allows the decision – as to whether an application for VO membership is to be approved or declined – to be delegated to the regional grids. For users to access ILDG resources only a single sign-on should be required: that is, a single trust domain has to be defined. This domain should include a sufficiently large set of trusted Certificate Authorities that every potential users can be provided with a certificate that is acceptable to any of the resource providers.

While it is not envisaged that the regional-grid make-up of ILDG will change in a particularly dynamic manner, it is expected that new collaborations will wish to join the infrastructure, either independently or as part of an existing group. With this in mind, it is important that the infrastructure evolves in a way that does not prevent expansion. Specifically:

- ILDG specifications (for example, service definitions) are thoroughly documented in a manner intended to facilitate the creation of new implementations.
- the technology layer is supported by a test suite, which allows new implementations of ILDG services to be validated against the specification.
- where possible, ILDG uses open (or at least widely adopted) technologies and standards, aiming to increase coverage of user groups and to reduce the risk of systems becoming obsoleted.
- the technological aspect of the infrastructure is specified as a thin layer (that is, focused on a baseline set of functionalities), which can easily be incorporated into existing infrastructures with low levels of development effort.

3 Metadata

To motivate the need for metadata, consider an example where there is no metadata. Configurations from different ensembles are all stored in a single directory with potentially random strings for names. Clearly this data is now not accessible. A scheme is required to describe
the data. As noted above, many groups have in the past constructed ad-hoc schemes for describing the data based on filenames and directory structures. Whilst this approach is not without merit, it does not scale when many groups are sharing data. In constructing this scheme there are likely to be several assumptions which are specific to the group which uses the scheme. Another group may well find these assumptions are not valid for their data, and hence their data will not fit into the scheme. Modifying the scheme is only possible where the assumptions used in its construction are still valid. To accommodate several potential different formulations of LQCD, and the needs of different groups a different approach is required.

Extensibility is a critical requirement of any annotation scheme. Any new data will need new metadata to describe it and the scheme will have to be modified. In an extensible scheme this can be done without breaking the original scheme. That is, the new scheme is an extension of the old one. Furthermore, any document which was valid in the old scheme is valid in the new one, so that the old documents don’t have to be updated to be valid in the new scheme.

Data provenance is likewise an important requirement. Can the data be recreated from the metadata? Taken to the limit this question is extremely challenging. In principle the code used to generate the data and its inputs should allow the data to be regenerated. However, this doesn’t include any machine, compiler or library information. Moreover, in the context of sharing data, the application belonging to one group may not be able to parse and process the input parameters of the application belonging to a different group. Hence while a full archival of a statically linked code, its inputs should allow recreation of the data if the original producing machine were to be available, archiving to this level of detail is not practical. Correspondingly some of the data provenance requirements may need to be softened in practise.

Lattice QCD metadata is hierarchical in nature and the annotation scheme should reflect this. Markup languages combine text and information about the text, and thus are perhaps a natural choice for a language in which to construct the scheme. Semantic or descriptive languages don’t mandate presentational or any other interpretation of the markup. XML was chosen as it is the most widely used and best supported markup language. Similarly XML schema was chosen as the schema language to define the scheme or set of rules for the metadata.

In order to make sharing lattice QCD data useful and effective, lattice QCD metadata should be recorded uniformly throughout the grid. The metadata working group designed an XML schema called QCDml for the metadata. The primary use case being data discovery via the metadata.

As described above a key concept for Lattice QCD data is the organisation of the data as configurations and ensembles to which the configurations belong. The metadata is divided into two linked XML schemata, one for the configurations, and one for the ensemble. The two schemata are linked together by a unique Uniform Resource Identifier (URI), called the markovChainURI, which lives in the name-space of the ILDG and which appears in the XML instance documents (IDs) of the configuration and the ensemble to which it belongs. There is no formal mechanism for ensuring uniqueness, but a simple convention has been adopted whereby the name of the group who generated the data appears in the URI, and responsibility for uniqueness is thereafter delegated to that group.

The separation of the metadata into two pieces, besides reflecting the nature of lattice QCD data, has two advantages. First, metadata capture is potentially simplified, as only the configuration-specific information has to be recorded for each configuration, and the information specific to an ensemble has to be recorded only once. Second, the performance
of searches on the data may be improved since the split represents a factoring of the original more complicated schemata.

The metadata scheme is encoded as a set of XML schemata \[^7\] and whilst this does not mandate how the metadata is stored and accessed, for simplicity it is often stored in native XML databases such as eXist \[^8\]. It is well known that the speed of access of hierarchical databases, such as native XML database is vastly inferior to that of relational databases. Scientists are almost always interested in finding an ensemble rather than finding an individual configuration. Therefore, for most cases, the separation of ensemble and configuration XML reduces the number of documents to be searched by \(O(100 - 1000)\).

In each configuration ID the logical file name (LFN) of the data file is recorded. The LFN is a unique and persistent identifier of the file in the ILDG name-space. The ILDG and local grid services then map the LFN to actual file instances.

The data itself is stored in a file format known as LIME \[^9\]. LIME is short for Limited Internet Message Encapsulation, and is a simplified and generalised version of the DIME (Direct Internet Message Encapsulation) \[^10\] Internet standard, which was proposed as an Internet Standard and which is now part of the Microsoft .NET framework. LIME is a record-oriented message format which simplifies and extends the original DIME framework by introducing 64-bit length records instead of the original 32-bit ones, and correspondingly it eliminates the need for continuation records. LIME thus allows the packing of descriptive text records and binary data records in the same file. This format itself is very flexible and extensible since the types and sequence of records are not mandated in the file format itself. The ILDG however, specifies and requires a set of LIME records, including: a record containing some XML file format metadata describing the size of the space-time lattice and data precision; a record containing the data itself in a specified data ordering; and a record of the LFN for the data, to allow the linking of ILDG data files to their metadata catalogue entries. LIME was developed by the USQCD collaboration through the SciDAC software initiative and a C-code to read and write lime files on a serial machine (C-LIME) can be downloaded from the USQCD web-site \[^9\]. The QIO package also developed by the USQCD collaboration has facilities for reading ILDG formatted data files on both serial and parallel machines \[^11\].

The scientific core of the metadata is contained within the ensemble schema. The most important section from the data discovery viewpoint is the action which contains the details of the physics. Here, the object-oriented ideas of inheritance are used to build an inheritance tree of actions based on the XML schema concepts of extension and restriction as appropriate. This enables users to make both very specific searches and more general searches on the names, types and/or parameters of the actions. The exact details of the physics can only be encoded in mathematics, which is not suited to an XML description. A reference to a paper, and the URL of an external glossary document which contain the mathematical descriptions of the physics are included. Clearly an application cannot parse this information, but it is included to avoid ambiguity in the names used in the inheritance tree.

QCDml uses a namespace defined by an URI. This URI includes the version number. Backward compatible, extensible updates to the schema don’t change the URI of the namespace, so XML IDs don’t need to be modified. Clearly the XML ID of the schema itself is modified, so a new URL for the extended XML ID of the schema is needed. All versions persist on the web, but with incremental URLs. Non-extensible updates to the schema require a change of namespace and the URI which identifies it.

Lattice QCD algorithms are very complex with many different algorithmic components. They are also an active area of research, and changes and improvements are common. This makes designing a scheme, especially an extensible one rather difficult. The defined names
and inheritance tree ideas used for the action would be too cumbersome for describing the algorithms. QCDml has only small scope for the algorithms limited to name, value pairs for the parameters. Algorithmic details can be expressed mathematically in an external, non-parseable glossary document. This approach further limits the data provenance of QCDml. However, individual groups can import their own namespace with as much detail and structure as they see fit, which can help ameliorate the data provenance issue even if the metadata is no longer universal.

Before leaving this general discussion of the metadata schema we note that the current set of schemata may be found at [12] (ensembles) and [13] (configurations). More Physics-oriented information about the metadata can be found in [14].

4 Middleware

As described above a grid-of-grids concept has been adopted for ILDG. Each of the regional grids has to provide the following services: a metadata catalogue (MDC) for metadata-based file discovery, a file catalogue (FC) for data file location and one or more storage elements (SE) which can then serve the data to the user.

The user can discover available datasets by sending a query to the MDC of each of the regional grids. On input this search requires an XPath expression. On output the services will return the list of Logical Files Names (LFNs) of those documents for which the XPath expression identifies a non-zero set of nodes.

To identify all copies of a particular file a query to the file catalogue has to be performed, which takes an LFN on input and returns a source URL (SURL) for each replica of the file. The scheme part of the SURL tells the client whether it can either directly download the file using the transfer protocols HTTP or GridFTP or whether it has to connect to a Storage Resource Manager (SRM) interface.

The SRM protocol [15] is evolving to an open standard for grid middleware to communicate with site-specific storage fabrics. The ILDG, at the time of writing, requires the SRM to be adhere to version 2 of the SRM specification. A particularly appealing feature of the SRM is that implementations of the service are typically provided with a standard Web-Service interface, allowing the SRM component to fit in easily with the comparatively less complex, ILDG-defined MDC and FC.

SRM is a system to manage local storage fabrics comprised of several data servers and possibly long-term backup storage. From the point of view of an ILDG transaction, the SRM may be required to: stage a file to some transfer location on a server, negotiate a transfer protocol between the server and the client, and to then arrange for the transfer to occur. Once the file is ready for transfer, the location and the transfer protocol are returned to the client by the SRM service in a transfer URL (TURL). The client and the data server can then carry out the transfer independently of the rest of the SRM system. Typically GridFTP is used as a transport protocol.

By adopting a grid-of-grids concept with different middleware stacks being used by the different regional grids, interoperability becomes a challenge. Interoperability is required to provide standardised interfaces towards the application layer. While there are clear similarities between the different grid architectures, there are crucial conceptional differences and incompatibilities of the interfaces.

For all services, which have not been specifically designed for ILDG, two strategies have been applied to overcome this interoperability issue. Firstly, wherever possible, common grid standards supported by all the used middleware stacks have been adopted. One
example is the transfer protocol GridFTP. Secondly, interface services have been defined and implemented. Instead of accessing a service directly, the user connects to the interface service which will process the request on behalf of the user.

If a service requires authentication the corresponding interface service has to provide a credential delegation service. Within ILDG we use an implementation of such a service that has been developed within the GridSite project [16] and is now part of the gLite middleware stack. On request of the client the server returns a proxy certificate request, which is signed on the client side and returned back to the server. Since the proxy certificate has only a limited lifetime, the risk due to a compromised server hosting the interface service is considered to be acceptable small.

To standardise a web-service within ILDG a WSDL description is implemented and additionally a behavioural specification is provided. The WSDL description specifies the structure of the service’s input and output data structure, while a functional description of the service is provided by the behavioural specification. Additionally, test suites have been defined and implemented which can be used to verify whether a service conforms to the ILDG standard.

Access to most services is restricted to members of the Virtual Organisation (VO) ILDG. For the management of this VO we use a VOMRS service [17]. Each user which wants to join the VO has to submit an application and nominate one of their regional grid’s representatives. For each regional grid at least two representatives have been assigned which can accept or reject the request. For each regional grid an individual group has been created. Information on group membership may be used by the regional grids as input for authorisation services.

The only other global service which is used within ILDG is the monitoring service. This monitoring service has been implemented using INCA [18]. In the framework of INCA a set of so-called reporter managers regularly execute test scripts accessing grid resources. The information returned by the reporter managers is collected in a repository. In case of failures a notification email is generated and sent to the regional grid which is responsible for a particular service. Data in the repository can later be used to check the service’s availability.

5 Review

5.1 General Status

At the time of writing, the ILDG has been in production use for a little over a year. It is comprised of five main-partner regional grids. These are: The Center for the Structure of Subnuclear Matter (CSSM) in Australia; The Japan Lattice Data Grid (JLDG); Latfor Data Grid (LDG) for continental Europe (primarily Germany, Italy and France); the regional grid of the UKQCD Collaboration in the UK; and the regional grid of the USQCD collaboration in the United States. The ILDG VO has 113 registered users and the combined ILDG hosts some 207 gauge configuration ensembles, corresponding to various lattice volumes, gauge and fermion actions. Each single ensemble represents significant portions – potentially years – of human and supercomputing resources. Thus these archives are immensely valuable.

On the management side, the Middleware working group hosts monthly teleconferences to discuss operational exceptions, experiences and future development efforts while at the higher level, the ILDG holds bi-annual video conferences, so that regional partners can discuss more general progress.
5.2 Benefits of Sharing

Hosting such a wealth of data has had great benefit on computational lattice QCD worldwide. In the case of some regional grids, the regional grid itself has become the primary means of data distribution, for multi-site projects, prime examples of which are the LDG and UKQCD collaborations [19].

A number of research activities have been enabled, thanks to the ILDG infrastructure. Scientists in Japan have been using data produced by the MILC collaboration (in United States) as part of their research [20] and, complementing this, a team at χ-QCD (University of Kentucky) has accessed data from CP-PACS (Japan), in the ILDG community [21, 22]. Other examples of ILDG use can be found in [23] and [24] where two groups made use of lattices generated by the German QCDSF Collaboration.

Both inter-collaboration and intra-collaboration activities are enabled by ILDG. In [25], a number of ILDG-enabled activities are noted relating to data sharing across LDG sites. The fact that the ILDG is making a serious impact in international collaboration can also be seen in the fact that Physics workshops are being held within the community that focus, not only on the generation of QCD data, but also on accomplishing calculations by sharing the data via the ILDG [26].

5.3 Criticism of the ILDG

While ILDG appears to be operating successfully, there are some aspects of it that could be improved. Using the ILDG to locate and share data is relatively straightforward especially with the easy to install client tools [27] as is described in [28]. However, contributing to the ILDG potentially involves a lot of effort. Depending on the level of involvement, one may need to maintain storage and database resources as well as having to mark up configuration and ensemble metadata.

In order to create ensemble metadata markup, one needs to get a unique key to identify it (MarkovChainURI). There is no service which can supply one or necessarily check that a manually chosen key is in fact unique. Further, ensemble metadata markup is not straightforward to automate and may need to be done by hand. If a new collaboration wishes to extend the XML Schemas to mark up data for which no QCDml exists, the process of standardisation of the markup may take a substantial amount of time.

Marking up configurations may be more straightforward, and may be automated. However, it too involves some amount of post-processing. The checksum needed in the configuration metadata document is not easy to compute in a parallel program and likewise a unique key; the configuration LFN; needs to be known in order to create both the configuration metadata and in order to write a fully ILDG compliant configuration file as described previously. However, the LFN may not be known at the time of production. Thus typically configuration metadata is generated post-production, and the configurations typically do not contain the LFN on creation. This has to be added on insertion to the ILDG.

While much of this activity can be automated, the initial goal of the computation producing the configuration metadata and the ILDG compliant configuration at the same time has been sacrificed in order to agree on other aspects. There is thus scope in the data production workflow, for data to lay idle for quite some time before being added to the ILDG with the consequent loss of history and provenance information. Hopefully future software tools can alleviate this problem.
Although it was thought that these difficulties will be a major stumbling block to ILDG participation, in practice metadata creation proved to be less of a stumbling block than initially expected. The ensemble metadata typically needs to be created only once, making it worth the effort and as mentioned previously the workflow for configuration metadata markup and publication can be substantially automated. Hence while the in principle issues discussed above remain, at a practical level the bar for participation in ILDG came not from the metadata, but rather from maintaining the middleware stack of the participating organisations such as managing grid security certificate infrastructure.

One aspect of the ILDG to remark upon is that it is most definitely a volunteer, and altruistic activity. It receives very little in the way of funding for itself and is usually piggybacked discretely onto other grid related projects or to regional grid activities. Correspondingly, it can become difficult to maintain effort focused on the ILDG, which limits large scale development and essentially forces simple solutions.

We can contrast the ILDG with some other related work. Other non-ILDG lattice archives include the Gauge Connection (at NERSC) [29] and the QCDOC Configuration download site [30] (at the Brookhaven National Laboratory) which is very similar in structure to the Gauge Connection and we shall treat the two identically below. The Gauge Connection was created before the era of Web Services and Grid services, It hosts files on a single filesystem and one can download all the configurations over HTTP. The file format used is an ASCII header followed by a binary data segment. The header contains rudimentary metadata (e.g. information about the creators, a checksum, and some derived measurement). Hence there is no separation between the configuration files and their metadata like there is in our case. Ensembles are not marked up in terms of XML at all, but there is some human-readable description for each one. Authentication and authorisation is done at the Web-Server level and one needs to register with the site to gain access. This setup, though very simple has worked very robustly and well. On the other hand, it becomes harder to search this archive, since there is no actual metadata catalogue as such. A human must read through a list of available ensembles until he finds the one he wants from the description. The Gauge Connection served as a guide to the ILDG effort. In particular the layout of the data in the binary part of the Gauge Connection format has been kept in the ILDG data record.

We should also mention in this section the LQCD Archive (LQA) [31] which is maintained at the Center for Computational Sciences at the University of Tsukuba in Japan. The LQA began development prior to the ILDG to distribute the data of the CP-PACS collaboration as a configuration download service similar to the Gauge Connection. However, upon inception of the ILDG, the LQA was re-developed to be the front end portal to the data available on the JLDG. It currently provides metadata search facilities as well as HTTP based download which may be useful to users who do not wish to set up a full grid client infrastructure on their machine. The JLDG data is of course also available through the usual ILDG client tools independent of this portal. To use this service, one is required to register. The portal post a list of publications to which citations should be made on publication of results that come from the downloaded datasets.

Download services have proved useful to the community however they have several shortcomings. They allow downloading primarily through HTTP which may encounter performance limitations when one considers downloading entire ensembles, especially since the size of configurations is expected to increase. There has been no attempt to provide a common file format. The individual architectures do not lend themselves to data replication and lack a common security infrastructure (each requiring separate registrations). That having been said, historically the Gauge Connection share their file format while the LQA as
noted above has been extensively redeveloped to complement rather than contrast with the ILDG.

One can also compare the ILDG to the concept of a Science Gateway. Quoting from the definition of Science Gateways on the TeraGrid [32], “A Science Gateway is a community developed set of tools, applications and data that is integrated via a portal, or suite of applications, usually in a graphic interface that is customised to meet the needs of a target community.” In this sense the gateways have a broader scope than the ILDG, they can offer codes, grid services, as well as access to data collections. As an example we consider the “Massive Pulsar Surveys Using the Arecibo L-band Feed Array (ALFA)” TeraGrid Science Gateway which allows one to brows data on pulsars and is similar in scope to the ILDG. One can browse pulsar information, and can download associated data-products. On the other hand, the SCEC Earthworks Gateway actually allows the running of earthquake simulations on TeraGrid resources. Both these gateways can be found at [33].

One unique feature of the ILDG, in contrast to a Science Gateway, is that the ILDG is the result of a collaboration of collaborations. A single Science Gateway would typically consist of a single portal maintained by a group on behalf of a larger community. This group then has some freedom (within community limits) in defining internal formats, markup and can settle on a single set of software tools. The ILDG instead is a loose federation of existing grids, some of which at the inception of the ILDG had no grid infrastructure and some of whom were already heavily invested in their own systems. The worldwide community had to therefore come together in order to define metadata standards, middleware operation and thin, easy to implement interfaces that could then wrap any potentially existing, underlying infrastructure. Another difference between the ILDG and Science Gateways may be their philosophy.

6 Summary and Future Work

In summary, the ILDG is a loosely federated grid-of-grids to facilitate the sharing of LQCD data worldwide. The technology allows it to operate across regional grid boundaries, relies on a simple and thin layer of middleware standard definitions, and a standardised metadata markup.

In six years of design and a little over one year of operation, the ILDG effort has brought together the lattice QCD community and has fostered QCD research and collaboration.

Potential future work focuses on several areas including but not limited to data replication, and the storage and mark up of secondary large data such as quark propagators.

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