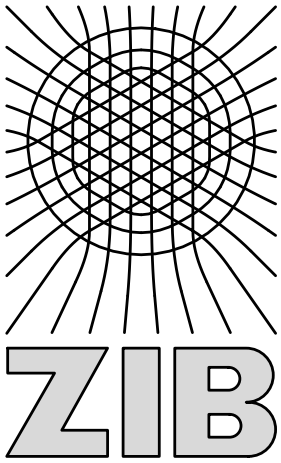
Introduction to ILDG, the LatFor Datagrid, and I3HP Transnational Access

Hinnerk Stüben



Lattice Practices '06

DESY Zeuthen, 28 November 2006

— The International Lattice DataGrid

[http://www.lqcd.org/ildg]

- Definition of standards for a Grid infrastructure for the lattice community
  - binary file format
  - file format schema
  - ensemble schema
  - configuration schema
  - middleware standards for interoperability in a *Grid-of-Grids*
- Aim
  - longterm storage and global sharing of gauge field configurations
- Participants
  - groups from Australia, France, Germany, Italy, Japan, UK, and US

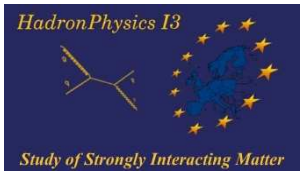
LDG — The LATFOR LATTICE FORUM DataGrid

[http://www-zeuthen.desy.de/latfor/ldg]

- Implementation of a regional Grid conforming to ILDG
- Currently used by researchers in Cyprus, France, Germany, Italy, Spain, UK
- LDG team

  Michael Ernst, Andreas Gellrich (DESY Hamburg)
  Andreas Haupt, Karl Jansen, David Melkumyan, Dirk Pleiter,
  Peter Wegner (NIC/DESY Zeuthen)
  Otto Büchner, Thomas Lippert, Boris Orth (NIC/ZAM Jülich)
  H.S., Stefan Wollny (ZIB Berlin)

- Sponsors



I3HP — Integrated Infrastructure Initiative Hadron Physics

[http://hadronphysics.infn.it]

- Originates from a joint initiative of over 2000 hadron physicists
- Funded by the European Commission in the Sixth Framework Programme
- Three activities are related to lattice QCD
  - Networking Activity *Computational Hadron Physics*
  - Transnational Access to FJZ-NIC/ZAM (supercomputer resources)
  - Transnational Access to ZIB (mass storage)

Transnational Access to the mass storage system at ZIB

[http://www.zib.de/i3hp]

- European research groups can apply for mass storage capacity
  (see web site; for downloads no application is required)
- Software-wise the system is a part of LDG
- Development of an easy to use command line interface – *ltools*

  [http://www.zib.de/i3hp/ltools]

→ If you are planning a storage project at a European level, please contact me!

Hardware for Transnational Access at ZIB

storage element

hierarchical mass storage system

dCache server
disk cache

HSM management
disk buffer

tape silo with tape robot

Overview of this tutorial

- Motivation
- Demo: metadata catalogue, configuration downloads
- Understanding the concepts
- Software installation
- Configuration uploads

Motivation

- Rely on a well-defined data format and access mechanism
- Facilitate collaborative work
- Computer usage by ETMC:
  - generation of configurations: Barcelona, Jülich, Munich, Rome, Zeuthen
  - central storage: Edinburgh, LDG, Munich
  - measurements: Jülich, Rome, local clusters (Liverpool, Orsay, Zeuthen)
- Computer usage by QCDSF / UKQCD:
  - generation of configurations: Edinburgh, Jülich, München
  - central storage: LDG
  - measurements: Liverpool, Regensburg, Zeuthen

Demo: web interface to the metadata catalogue

[http://www-zeuthen.desy.de/latfor/ldg/mdc]

- Observe interoprability with other ILDG Grids (jqcd, usqcd)
- Click on a name → ensemble metadata human readable

  → XML representation of metadata
  → list configurations
- Click on a configuration name → configuration metadata human readable

  → XML representation of metadata

Demo: using ltools for downloading a configuration (I)

- list all ensembles: `lls --all`

```
Welcome to the Ltool-command  lls -

Showing all ensembles currently in the MDC:
===========================================

Markov-Chain-URI                                                EID Read Write
================                                                === ==== =====
mc://ldg/dik/clover_nf2/b5p29kp13632-32x64                      55  All  2
mc://ldg/dik/clover_nf2/b5p40kp13640-24x48                      56  All  2
mc://ldg/etmc/tmqcd_nf2/tlSym_b3.75_L24T48_k0.1660_mu0.0200     53  All  6
...
```

- Explanations

`MDC`	metadata catalogue
`URI`	unified resource identifier
`EID`	ensemble ID
`Read`	read permission
`Write`	write permission (group ID)

Demo: using ltools for downloading a configuration (II)

- List configurations: `lls` *`ensemble`*
  Example: `lls mc://ldg/etmc/tmqcd_nf2/tlSym_b3.75_L24T48_k0.1660_mu0.0200`

```
Welcome to the Ltool-command  lls -

The following configurations belong to
mc://ldg/etmc/tmqcd_nf2/tlSym_b3.75_L24T48_k0.1660_mu0.0200 :

lfn://ldg/etmc/tmqcd_nf2/tlSym_b3.75_L24T48_k0.1660_mu0.0200/conf.01.1001
lfn://ldg/etmc/tmqcd_nf2/tlSym_b3.75_L24T48_k0.1660_mu0.0200/conf.01.1002
...
```

- Explanations

  `mc:` Markov chain
  `lfn:` logical filename

Demo: using ltools for downloading a configuration (III)

- Download a configuration: `lget` *`logical-file-name`*
  E.g.: `lget lfn://ldg/etmc/tmqcd_nf2/tlSym_b3.75_L24T48_k0.1660_mu0.0200/conf.01.1001`

```
 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: Sat Nov 25 00:00:27 2006
Proxy started ... grid-proxy...ok

 Trying to get binary ...

 Virtual Organisation is ildg
 Executing lcg-cp  --vo ildg \
 lfn:/grid/ildg/ldg/etmc/tmqcd_nf2/tlSym_b3.75_L24T48_k0.1660_mu0.0200/conf.01.1001 \
 file:/home/bzbstueb/conf.01.1001

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

Demo: using ltools for downloading a configuration (IV)

- `grid-proxy-init` is only called if there is no valid grid-proxy:

```
lget lfn://ldg/etmc/tmqcd_nf2/tlSym_b3.75_L24T48_k0.1660_mu0.0200/conf.01.1002

 Welcome to the Ltool-command  lget -
 Testing grid-proxy-init:
 grid-proxy...ok

 Trying to get binary ...

 Virtual Organisation is ildg
 Executing lcg-cp  --vo ildg \
 lfn:/grid/ildg/ldg/etmc/tmqcd_nf2/tlSym_b3.75_L24T48_k0.1660_mu0.0200/conf.01.1002 \
 file:/home/bzbstueb/conf.01.1002

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

- Items to be explained:
  - `grid-proxy-init` $\longrightarrow$ certificates $\longrightarrow$ public key cryptography
  - virtual organisation (VO)
  - `lcg-cp` $\longrightarrow$ LCG software (LCG: LHC computing grid; LHC: large hadron collider)

Digression: public / asymmetric key cryptography

- Enables secure communication over an insecure channel without prior access to a shared secret key
- A pair of keys (a *private* / *secret* key and a *public* key) is generated from a large random number
  $\longrightarrow$ a private key should **always** be protected by a **strong** passphrase
- A message encrypted with a public key can only be decrypted with the corresponding private key $\longrightarrow$ **secret message**
- A message encrypted with a private key can only be decrypted with the corresponding public key $\longrightarrow$ **digital signature**

Certificates

- In the Grid context a certicificate is a *public key certificate*
- A public key certificate is a public key digitally signed (by a trusted party) to associate the public key and a person
- The signature is by a *certificate authority (CA)*
- The German CA for LDG is *Grid Computing Centre Karlsruhe (GridKa)*

  [http://grid.fzk.de]

  [http://grid.fzk.de/cgi-bin/welcome_ca.pl]

  [http://www-grid.desy.de/certs]
- European LCG CAs are listed in [http://marianne.in2p3.fr/ca/ca-table-ca.html]
- Furthers CAs: International Grid Trust Federation [http://www.gridpma.org]

Obtaining a certificate

- Generate a *certificate request*
- Contact a *registration authority (RA)* (you have to appear in person) or send a copy of your identity card an a letter with signed handwritten by a responsible person to the CA (the exact policy depends on the CA)
- Certificates are valid for a fixed period (1 year)
- The subsequent certificate can be obtained by signing a request with the old certificate
- See also [`http://www-zeuthen.desy.de/latfor/ldg/doc/newuser.html`]

Generating a certificate request (for GridKa)

- Use the *Globus* command `grid-cert-request -int`
- Alternatively use *openssl*
  → follow [`http://grid.fzk.de/ca/how-to-ohne-globus.pdf`] (in German)
- Check the subject line (`OU`: organisational unit = your institute)
  - Globus: `/O=GermanGrid/OU=XXX/CN="fully qualified username"`
  - openssl: `/C=DE/O=GermanGrid/OU=XXX/CN="fully qualified username"`

  To the Grid software these are different usernames → stick to one method
- Other CAs have similar procedures
- Default filenames

  `$HOME/.globus/usercert.pem` (certificate / public key)
  `$HOME/.globus/userkey.pem` (private key)

Virtual organisation (VO)

- In Grid computing a virtual organisation is a group of people who share a resource
- For access to LDG one has to be a member of the VO *ildg*
- The VO *ildg* is managed by DESY
- How to apply for becoming a member is described in

  [`http://www-zeuthen.desy.de/latfor/ldg/doc/newuser.html`]

Software

- . . . will be covered later
- Look at the data format first

ILDG binary file format

[http://www-zeuthen.desy.de/~pleiter/ildg/ildg-file-format-1.1.pdf]

- A file in ILDG binary format consists of several parts
- The parts are packaged using the LIME file format

  [http://www.physics.utah.edu/~detar/scidac/lime-1.2.3.tar.gz]
- Structure:

```
message
    record
    record
    ...
message
    record
    ...
...
```

- Each record type has a name. There have to be records of type `ildg-format`, `ildg-binary-data`, and `ildg-data-lfn`
- `ildg-format` and `ildg-binary-data` must appear in that order in the same message

Record ildg-format

- Example

```
<?xml version="1.0" encoding="UTF-8"?>
<ildgFormat xmlns="http://www.lqcd.org/ildg"
            xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
            xsi:schemaLocation="http://www.lqcd.org/ildg/filefmt.xsd">
<version> 1.0 </version>
<field> su3gauge </field>
<precision> 64 </precision>
<lx> 24 </lx>
<ly> 24 </ly>
<lz> 24 </lz>
<lt> 48 </lt>
</ildgFormat>
```

Record `ildg-binary-data`

- A sequence of IEEE floating point numbers in big endian format
- Precision according to `ildg-format`
- Storage sequence corresponds to the following array definitions:

  C: `double U[Lt][Lz][Ly][Lx][dim][Ncolour][Ncolour][2];`

  Fortran `complex U(Ncolour, Ncolour, dim, Lx, Ly, Lz, Lt)`

Record `ildg-data-lfn`

- A single string with the logical filename (LFN)
- This LFN must be identical to the one given in the metadata of the configuration

Using LIME

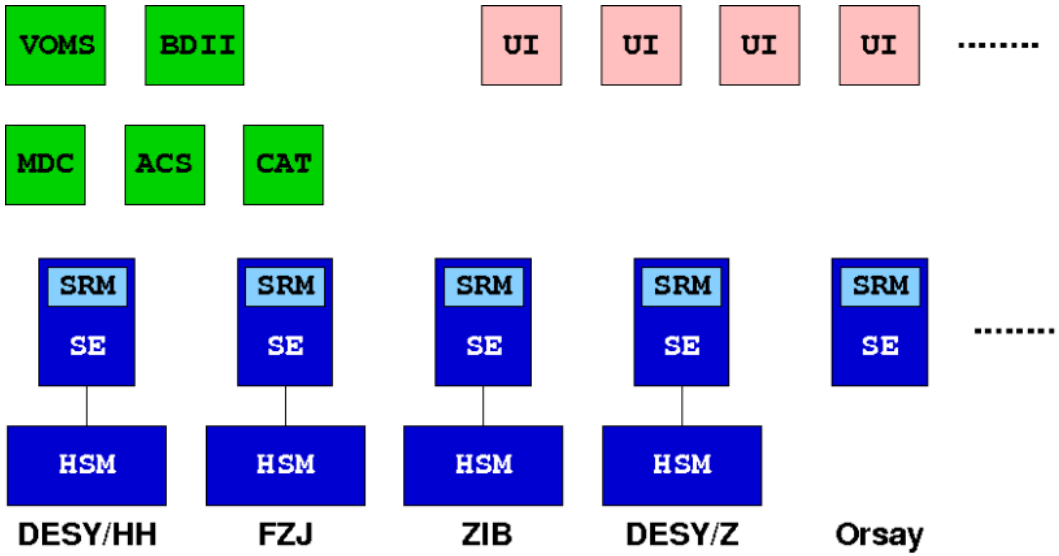
- LIME: Lattice QCD Interchange Message Encapsulation
- The LIME package comes with a document that describes
  - the LIME format
  - the LIME API
  - some LIME utilities
- The utilities can be found in the directory `examples`

→ Demo: `lime_contents` utility

Concepts (overview)

- LDG components
- Software
- *ltools*
- Metadata formats
- Naming conventions

LDG components



[hep-lat/0609012]

acronym	meaning	location of hardware/service
SE	storage element	*see figure*
SRM	storage resource manager	*see figure*
HSM	hierachical storage manager	*see figure*
VOMS	virtual organisation mamagement system	DESY Hamburg
BDII	Berkeley database information index	DESY Hamburg
MDC	metadata catalogue	DESY Zeuthen
ACS	access control service	DESY Zeuthen
CAT	file catalogue	DESY Hamburg
UI	user interface	the user's workstation

LDG software / middleware

- The storage elements are dCache-based [http://www.dcache.org]
- The metadata catalogue was developed at DESY Zeuthen
  [http://www-zeuthen.desy.de/latfor/ldg/doc/pub.html]
- The user interface is LCG-based [www.cern.ch/lcg]
- *ltools* were written at ZIB [http://www.zib.de/i3hp/ltools]
- A check-sum tool `ildg_cksum` was written at NIC/ZAM Jülich
- An RPM-based installation mechanism for the user interface, *ltools*, and `ildg_cksum` is provided by DESY Zeuthen
  [http://www-zeuthen.desy.de/latfor/ldg/doc/swinstall.html]

LDG software installation

- No root priviledge required
- Tested on
  - Debian 3.1 (Sarge)
  - Fedora Core 3, Fedora Core 4
  - Red Hat 7
  - Scientific Linux 3
  - Suse Linux Enterprise Server 9
  - Suse 9.2, Suse 9.3, Suse 10
- Instructions [`http://www-zeuthen.desy.de/latfor/ldg/doc/swinstall.html`]

Lattice tools – ltools

[http://www.zib.de/i3hp/ltools]

- *ltool* commands hide details of the underlying grid infrastructure

command	task
lls	list configurations or ensembles
lget	download configuration or (configuration or ensemble) metadata
lput	upload configuration and its metadata (performs various checks)
linit	initialise new ensemble
lupdate	update (replace) metadata
lvalidate	check conformance of metadata (configuration or ensemble) to XML schema
ladm	access control related tasks
lid	list various IDs (ensembles, projects, groups, managers, admins, users)

Metadata

- Document data
- Enable semantic search
- Concentrate on the description of SU(3) configurations
- Standardise description of data
  - uniqueness (a specific action should always have the same description)
  - extensibility (for new actions)
  - generality (allow inclusion of other data sets, eg propagators)
- Use XML and XML schemata (XML: extensible markup language)

QCDml – XML schemata for marking up SU(3) configurations

- There are metadata for ensembles and configurations
- To learn the details of the XML schemata see
  - the ILDG web page [http://www.lqcd.org/ildg]
  - tutorial by C. Maynard and D. Pleiter at Lattice 2004 [hep-lat/0409055]
  - the metadata catalogue [http://www-zeuthen.desy.de/latfor/ldg/mdc]
- Metadata can be generated
  - with XML tools
  - by using templates

Sample template for configuration metadata (I)

```
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<gaugeConfiguration xmlns="http://www.lqcd.org/ildg/QCDml/config1.3">
    <management>
        <crcCheckSum>#crc_check_sum#</crcCheckSum>
        <archiveHistory>
            <elem>
                <revisionAction>generate</revisionAction>
                <participant>
                    <name>#participant_name#</name>
                    <institution>#participant_institution#</institution>
                </participant>
                <date>#today#</date>
            </elem>
        </archiveHistory>
    </management>
```

Sample template for configuration metadata (II)

```
<implementation>
    <machine>
        <name>#machine_name#</name>
        <institution>#machine_institution#</institution>
        <machineType>#machine_type#</machineType>
    </machine>
    <code>
        <name>#code_name#</name>
        <version>#code_version#</version>
        <date>#code_date#</date>
    </code>
</implementation>
```

Sample template for configuration metadata (III)

```
<algorithm>
    <parameters>
        <name>stepSize</name>
        <value>#para_step_size#</value>
    </parameters>
    <parameters>
        <name>numberSteps</name>
        <value>#para_number_steps#</value>
    </parameters>
    <parameters>
        <name>solverResiduum</name>
        <value>#para_solver_residuum#</value>
    </parameters>
    <parameters>
        <name>rho</name>
        <value>#para_rho#</value>
    </parameters>
</algorithm>
<precision>#precision#</precision>
```

Sample template for configuration metadata (IV)

```
    <markovStep>
        <markovChainURI>#markov_chain_uri#</markovChainURI>
        <series>#markov_series#</series>
        <update>#markov_update#</update>
        <avePlaquette>#average_plaquette#</avePlaquette>
        <dataLFN>#data_lfn#</dataLFN>
    </markovStep>
</gaugeConfiguration>
```

- The `markovChainURI` of congfiguration and ensemble must match!

Sample template for configuration metadata (V)

placeholder	replacement
#crc_check_sum#	559813009
#participant_name#	Hinnerk Stueben
#participant_institution#	ZIB
#today#	2006-11-26T10:47:38+01:00
#machine_name#	jubl
#machine_institution#	NIC/ZAM Juelich
#machine_type#	IBM Blue Gene/L
#code_name#	BQCD
#code_version#	3.3.0
#code_date#	2006-08-28T14:43:00+02:00
#para_step_size#	0.01
#para_number_steps#	100
#para_solver_residuum#	1e-14
#para_rho#	0.06
#precision#	double
#markov_chain_uri#	mc://ldg/qcdsf/clover_nf2/b5p25kp13600-24x48
#markov_series#	536
#markov_update#	2485
#average_plaquette#	0.5439676525
#data_lfn#	lfn://ldg/qcdsf/clover_nf2/b5p25kp13600-24x48/qcdsf.536.02485.lime

Naming conventions

- `markovChainURI`:

  `mc://ldg/`*collaboration*`/`*project*`/`*ensemble*

  Example:

  `mc://ldg/qcdsf/clover_nf2/b5p25kp13600-24x48`

- `dataLFN`:

  `lfn://ldg/`*collaboration*`/`*project*`/`*ensemble*`/`*configuration*

  Example:

  `lfn://ldg/qcdsf/clover_nf2/b5p25kp13600-24x48/qcdsf.536.02485.lime`

- *collaboration*, *project*, and *ensemble* must match!

Storage location

- The sequence

  collaboration/ project/ ensemble/ configuration

  is also used as the storage location (it represents a directory structure).

  Example:

  `srm://dcache.zib.de/pnfs/zib.de/data/ildg/`
  `qcdsf/clover_nf2/b5p25kp13600-24x48/qcdsf.536.02485.lime`

- This is handled by `lput`.

Ensemble metadata example (I)

```
<?xml version="1.0" encoding="UTF-8" standalone="yes"?>
<markovChain xmlns="http://www.lqcd.org/ildg/QCDml/ensemble1.3">
    <markovChainURI>mc://ldg/qcdsf/clover_nf2/b5p40kp13625-24x48</markovChainURI>
    <management>
        <collaboration>qcdsf</collaboration>
        <projectName>clover_nf2</projectName>
        <archiveHistory>
            <elem>
                <revisionAction>add</revisionAction>
                <participant>
                    <name>Hinnerk Stueben</name>
                    <institution>ZIB</institution>
                </participant>
                <date>2006-10-30T17:26:36+01:00</date>
            </elem>
        </archiveHistory>
    </management>
```

Ensemble metadata example (II)

```
<physics>
    <size>
        <elem>
            <name>X</name>
            <length>24</length>
        </elem>
        <elem>
            <name>Y</name>
            <length>24</length>
        </elem>
        <elem>
            <name>Z</name>
            <length>24</length>
        </elem>
        <elem>
            <name>T</name>
            <length>48</length>
        </elem>
    </size>
```

Ensemble metadata example (III)

```
<action>
    <gluon>
        <plaquetteGluonAction>
            <glossary>http://www.lqcd.org/ildg/actionGlossaries/plaquetteGluonActi
            <gluonField>
                <gaugeGroup>SU(3)</gaugeGroup>
                <representation>fundamental</representation>
                <boundaryCondition>
                    <elem>periodic</elem>
                    <elem>periodic</elem>
                    <elem>periodic</elem>
                    <elem>periodic</elem>
                </boundaryCondition>
            </gluonField>
                <beta>5.40</beta>
        </plaquetteGluonAction>
    </gluon>
```

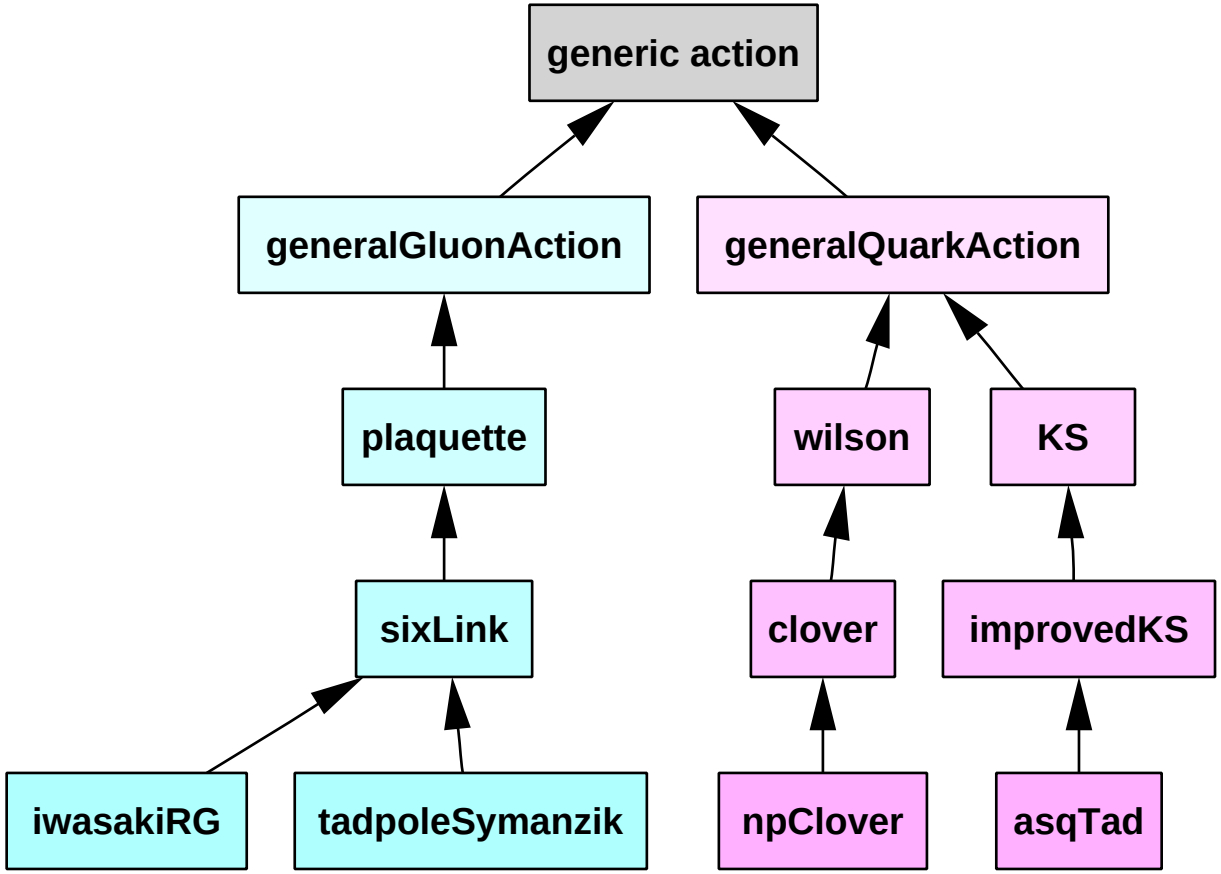
Ensemble metadata example (IV)

```
        <quark>
            <npCloverQuarkAction>
                <glossary>http://www.lqcd.org/ildg/actionGlossaries/npCloverQuarkActio
                <quarkField>
                    <normalisation>sqrt2kappa</normalisation>
                    <boundaryCondition>
                        <elem>periodic</elem>
                        <elem>periodic</elem>
                        <elem>periodic</elem>
                        <elem>antiperiodic</elem>
                    </boundaryCondition>
                </quarkField>
                    <numberOfFlavours>2</numberOfFlavours>
                    <kappa>0.13625</kappa>
                    <cSW>1.8228</cSW>
            </npCloverQuarkAction>
        </quark>
    </action>
</physics>
```

Ensemble metadata example (V)

```
    <algorithm>
        <name>qcdsfAcceleratedHMC</name>
        <glossary>http://www-zeuthen.desy.de/latfor/ldg/algorithmGlossaries/qcdsfAccelerat
        <reference>Phys.Lett. B564 (2003) 235-240</reference>
        <exact>true</exact>
        <parameters>
            <name>timeScaleRatio</name>
            <value>3</value>
        </parameters>
    </algorithm>
</markovChain>
```

Hierarchy of actions in the ensemble metadata schema



[hep-lat/0409055]

Uploading a configuration (I)

- Upload a configuration: `lput` *`configuration-metadata`*
  Example: `lput qcdsf.536.02485.xml`

```
Welcome to the Ltool-command  lput -

Testing grid-proxy-init
grid-proxy...ok

Virtual Organisation is ildg

Storage Element is dcache.zib.de
Checking that URI and LFN are built according to convention:
OK

Checking that ensemble mc://ldg/qcdsf/clover_nf2/b5p25kp13600-24x48 exists in MDC:
OK

Checking that configuration does not exist in MDC:
OK

Checking that LFN does not already exist:
OK
```

Uploading a configuration (II)

```
All checks ok, will now start to upload metadata and binary...

Starting to upload metadata to MDC ...

...MDC Operation ok.

Starting to upload binary ...

Executing lcg-cr  --vo ildg -l \
lfn:/grid/ildg/ldg/qcdsf/clover_nf2/b5p25kp13600-24x48/qcdsf.536.02485.lime \
file:/home/bzbstueb/conf/qcdsf.536.02485.lime \
-d srm://dcache.zib.de/pnfs/zib.de/data/ildg/qcdsf/\
                          clover_nf2/b5p25kp13600-24x48/qcdsf.536.02485.lime
guid:ae514f13-dd42-4943-a284-3fcb0e4d4d4a

Data successfully copied to Storage Element !
LFN is: lfn://ldg/qcdsf/clover_nf2/b5p25kp13600-24x48/qcdsf.536.02485.lime
```

- guid: globally unique identifier

Uploading a configuration (III)

- Define defaults in `$HOME/.ltools`

```
## Default virtual organisation (for up- and downloads)
default_vo ildg

## Only needed for lputting data :
## default UPLOAD Storage element. If nothing is given here, by uploading
## the --se <SE> option hast to be specified by uploading a file.

default_upload_se dcache.zib.de

## The other storage elements are:
## grid-se0.desy.de
## globe-door.ifh.de
## dcache.fz-juelich.de
```

Uploading a configuration (IV)

- `lput` also handles failures
  Example: `lput qcdsf.537.00170.xml`

```
 Welcome to the Ltool-command  lput -

 normal messages, all checks ok

 Starting to upload binary ...

 Executing lcg-cr  --vo ildg -l \
 lfn:/grid/ildg/ldg/qcdsf/clover_nf2/b5p25kp13600-24x48/qcdsf.537.00170.lime \
 file:/home/bzbstueb/conf/qcdsf.537.00170.lime \
 -d srm://dcache.zib.de/pnfs/zib.de/data/ildg/qcdsf/clover_nf2/b5p25kp13600-24x48/qcdsf.53
lcg_cr: File exists

 Fatal Error...lcg-cr command did NOT succeed !
Error-message is : Bad file descriptor
Rolling back : Trying to restore former MDC-status:

 ...MDC was rolled back to former consistent status.
```

$\longrightarrow$ try again!

Initialising an ensemble

- Initialising an ensemble: `linit` *`project-ID ensemble-metadata`*
- At present one must also send the `markovChainURI` to `ldg-adm@desy.de` because it has to be entered into the file catalogue manually

→ `ldg-adm@desy.de` can also be contacted to get support or report problems