
QCDgrid administration basics

What is QCDgrid?

Administering a QCDgrid client

Chris Maynard

What is the grid? - Quotes

- *Grids are both a dream and a tool for realizing even larger dreams.*
 - NSCA (American umbrella grouping of CS)
- *Well, there's a short answer, and then there's a very long answer.*
 - CERN "Grid Café"
- *It's a funding concept - Anon*



The Grid is a system that ...

- *coordinates resources that are not subject to centralized control*
- *using standard, open, general-purpose protocols and interfaces*
- *delivers nontrivial qualities of service*
- **Ian Foster** Associate director of Argonne National Lab and “Grid guru”

What is the grid? cmm



Invented by
Physicists!

- WWW for sharing information
- Grid for sharing data and computer resources
- UKQCD is using a data grid
- Different sites contribute disk space
- Central service controls where data is stored, so you don't have to

Being built by
Physicists?



Why does UKQCD want one?

- UKQCD has a lot of data
 - Data set O(100) Gbytes
- QCDOC is producing a lot more
 - Data set O(1-10) Tbytes
- Before: Dump data on archiver/tape
 - Archiver **reluctant** to **relinquish** data
 - User had to know nature and location

Write **once** read **never**!

QCDOC



QCDOC details



- 14000 Asics
- Power PC core 400MHz
- Bespoke comms unit
 - Low latency
- Very high mem bandwidth to on chip mem



10 Teraflops peak

5 Teraflops sustained for
QCD codes

Ancestor of IBMBlueGene

What do we want from the grid

- Data security
 - Replication - Multiple copies of data
 - Who has read/write permission
- Data access
 - Metadata - discover what is stored
 - Get data without having to know location
 - Logistics of data moving taken care of

Grid concepts - security

- How to ensure identity of users?
- X509 certificates and SSL public/private key encryption
- Single login to the grid
- Time limited proxy certificate for remote operations
- Certificate is mapped to an account
 - user account or non-specific account
- See previous talk from JN

Security certificates



- Issued by a Certificate Authority (CA)
 - Both **machines** and **people**
- Only accept certificates from **trusted CA**
 - Resource owner decides which CAs are trusted
- **UK e-science CA** requires photo-ID
 - **UK citizens** not required to carry ID
 - Grid ID is stronger than UK national ID!



Grid concepts - Namespace

- Conventional namespace is a mathematical set
 - Used in definition of **Logical filename**
- XML Namespace defined by **W3.org** as
- *A collection of names identified by a URI reference*
- XML namespace has **internal structure**
- Can amalgamate namespaces

Grid concepts – logical filename

- Logical filename (LFN) is a **name** in a **namespace** which identifies a file
- Often it is a **URI**
 - Not `machine.domain:/path`
- Data grid LFN references a file which can have **several copies**
- Replica location service maps LFN to file instances

Grid concepts – replica location service



- RLS maps LFN to actual file instance
- Data grid - **several** copies of file
- RLS tracks **number** and **location** of file instances
- Data access is via the **LFN** and the **RLS**

Metadata

- Data about data
- “**meaningful**” filenames not enough
- Require a **scheme** for organising metadata
- Scheme has to be **extensible**
 - New things not previously thought of
- Only know full metadata when data created

A broken scheme

D52C202K3500U010010_LL3450X_FL3400X_CMesonT00T31

- UKQCD filename
 - What does **X** stand for?
- **W**ilson, **R**otated, **C**lover
 - Many different clover. Scheme broken
 - **X** means none of the above!

Dynamical $c_{SW}=2.02$

NP determined – no information

QCDml

- W3C XML schema for lattice QCD metadata
- Structured, hierarchical, extensible, verbose metadata
- Datasets (**called ensembles**) have single XML ID describing them
- Individual files (**gauge configurations**)
 - Belong to ensemble
 - Each has own XML ID

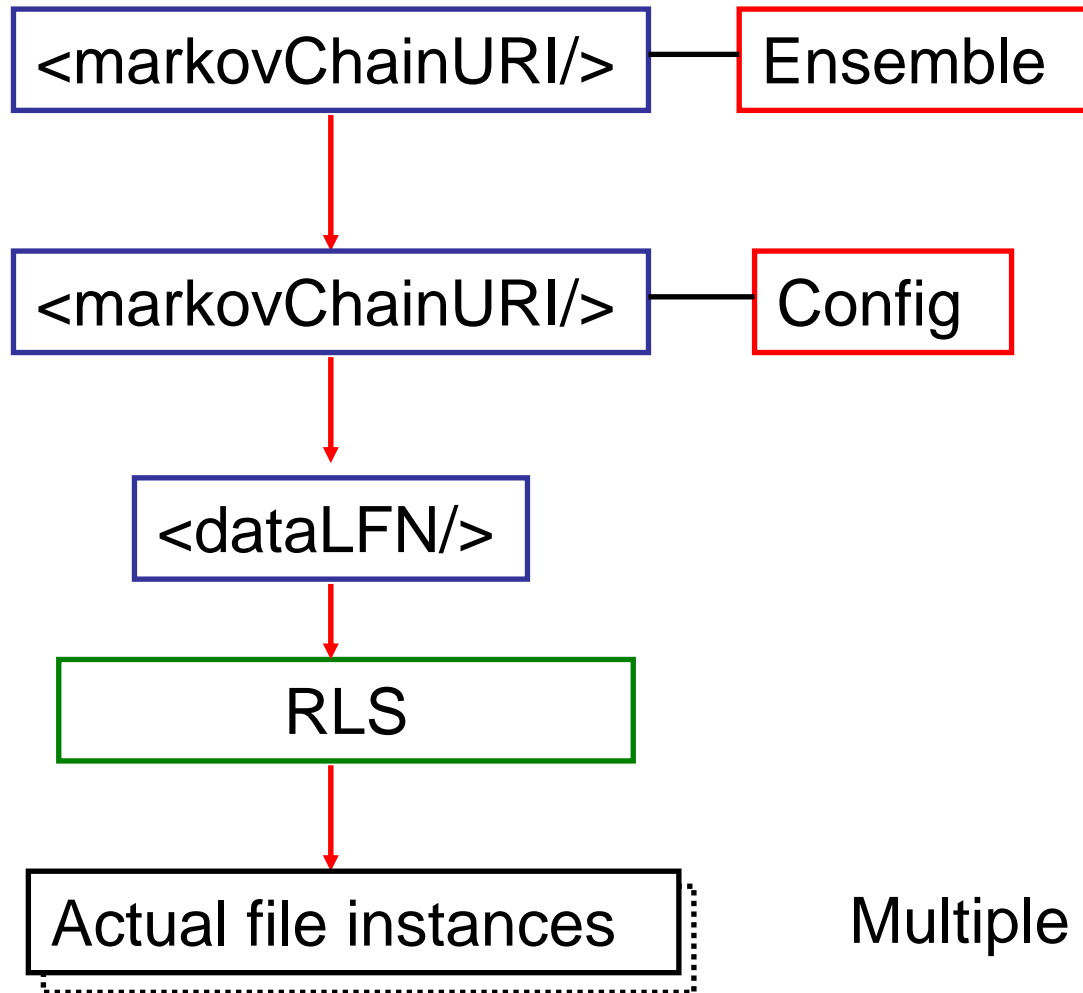
Grid concepts – Metadata catalogue



- Metadata is stored in a database
- QCDgrid DB is **native XML DB** eXist
 - Actual XML IDs form database
 - Runs on single node (usually control node)
- Single Metadata catalogue for whole grid
- MDC links metadata to **LFN**
- Database can be searched
- **Relational** DB good, **hierarchical** DB bad
 - $O(10^5-10^6)$ IDs in DB, workstation can cope

Name hierarchy

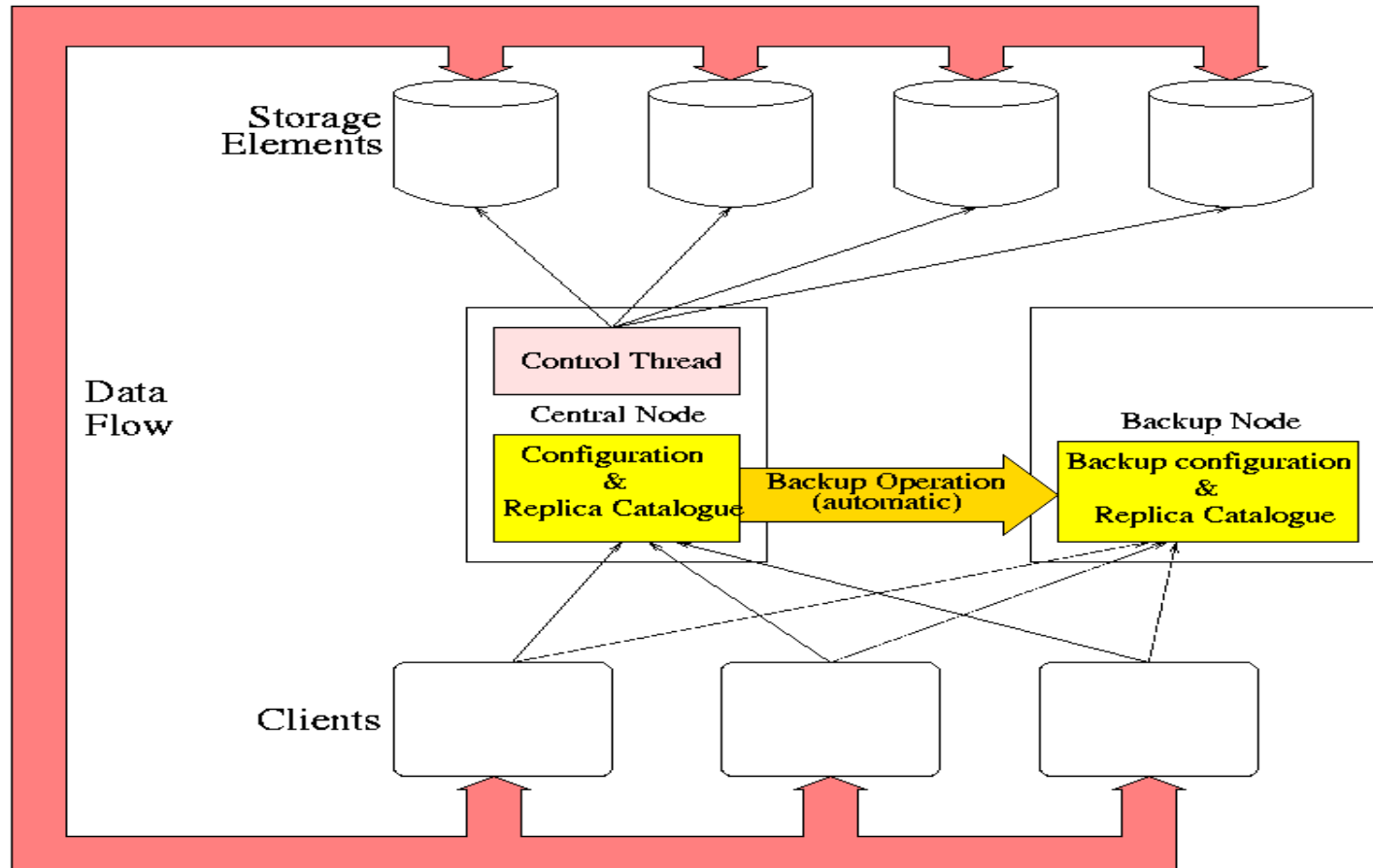
Unique name for ensemble in namespace



Grid nodes

- Central node (control node)
 - Runs control thread
 - Can host MDC service (not compulsory)
 - Can host disks (not compulsory)
- Back up node
 - Pulls state information from Control node
- Storage node
 - Hosts disks
- Client node
 - Access data

Control Thread



Machines – LHC terminology

- Tier 1 system 50TByte SAN system
 - QCDOC fe directly connected
 - Hold **one copy** of all UKQCD data
- Tier 2 systems
 - Edinburgh, Liverpool, Southampton, Swansea, RAL
 - Linux server + RAID array disk ~12 TByte storage
- 50 TByte capacity + 50 TByte replicated

All UKQCD data **always online**

QCDgrid client tools

- Command line tools
 - qcdgrid-ping
 - Its alive!
 - qcdgrid-list
 - List the *all* the files
 - put-file-on-qcdgrid
 - get-file-from-qcdgrid
 - i-like-this-file
 - Overrides global preferences to store file *nearby*
 - Recursive application to directories

QCDgrid GUI

- Metadata browser
 - Reads XML schema
- Graphical interface
 - Builds Xpath query
 - Returns XML chunk
 - Query handler deals with result
 - Display XML
 - Snarf LFN

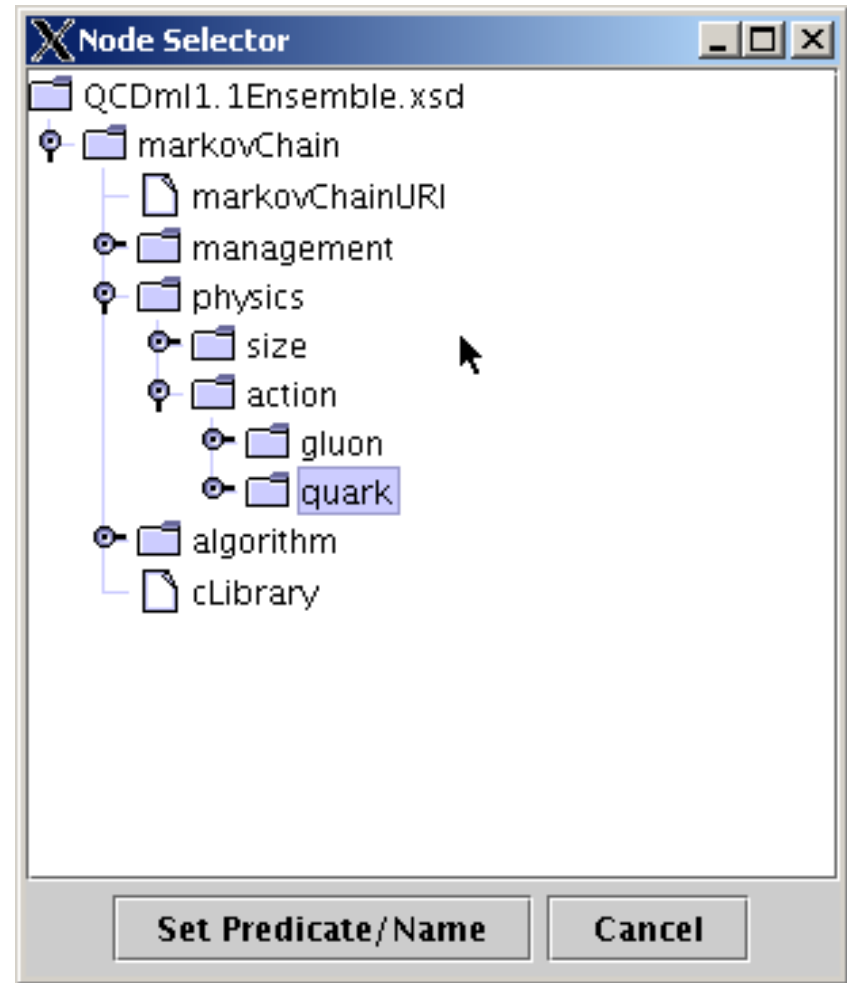
Metadata browser



Builds Tree from
schema

Researcher walks tree

Selects relevant node



Graphical query



Construct XPath
query via GUI

exists

Predicate:

enter predicate

Not

choose predicate

- quark
 - generalQuarkAction
 - wilsonQuarkAction
 - cloverQuarkAction
 - npCloverQuarkAction

Set Sub-Predicate

AND

OR

Query Name:

OK Cancel

Returned results

Read the XML

Download data

Search the config XML for this ensemble

Extract LFN from config XML for command-line tool scripting

The screenshot shows a search results window titled 'Results' with '9 matches found'. The left pane lists several XML files, with 'DWF-IW-NF3-Ensemble1.xml' selected. The right pane displays a tree view of the XML structure for the selected file. The tree includes nodes for 'management', 'physics', 'size', 'action', 'gluon', and 'quark'. The 'gluon' node contains 'iwasakiIRGluonAction' with sub-nodes for 'glossary', 'gluonField', and 'couplings'. The 'couplings' node lists parameters: beta = 2.2, c0 = 3.6480, c1 = -0.331, and c2 = 0.0. The 'quark' node contains 'domainWallQuarkAction' with sub-nodes for 'glossary', 'quarkField', and 'couplings'. The 'couplings' node lists parameters: numberOfFlavours = 3, mass = 0.04, M5 = 1.8, and n5 = 8. The bottom of the window features a toolbar with buttons: Selected, All, Get Data, Register Interest, Remove Data, and Close.

International lattice data grid

- Forum for sharing lattice data
 - Australia, Cyprus, France, Germany, Japan, SciDAC (USA), UK
 - Agree common interfaces for middleware
 - Build global data repository by **aggregating** local resources
 - Access **global** data with **local** system
 - Agree common metadata
 - QCDml Know what the data is!

 **ILDG** <http://www.lqcd.org/ildg>

Setting up QCDgrid client

- <https://forge.nesc.ac.uk/projects/qcdgrid/>
 - See docs therein
 - <http://www.epcc.ed.ac.uk/~cmaynard/QCDgrid%20administration%20basics.htm>
- Install globus (see JN talk)
 - Install certificate
- Download software
 - Binaries or source
 - wget
 - <https://forge.nesc.ac.uk/download.php/101/qcdgrid-1.3.0-linux-client.tar.gz>
 - gunzip and untar

Configuration

- Create/edit two files

- nodes.conf

```
node = qcdgrid1.epcc.ed.ac.uk
```

```
path = /home/qcdgrid
```

Control node **<fqdn>**

Path to QCDgrid software on control node

- nodeprefs.conf

- Geographical preference resources

```
touch nodeprefs.conf
```

Enviroment

- Setting the environment for **bash**

```
source ~/vdt/setup.sh
```

- Edit **example_setenv.sh**
 - Add path to qcdgrid-software
 - Source this file
- Ready to start!

Tutorial – command line tools

- `Grid-proxy-init`
- `qcdgrid-ping`
 - Dead or alive-alive-oh
- `qcdgrid-list`
 - What is on the development grid
- `put-file-on-qcdgrid -N <file> <LFN>`
 - `-N` flag specifies no data
- `get-file-from-qcdgrid <LFN> <file>`
 - Get the file back!

Tutorial Metadata browser

- `rungui.sh`
- Select *search metadata catalogue*
- Enter `qcdgrid1.epcc.ed.ac.uk` as MDC location
- Set **options:result** handler to `QCDgridResultHandler`
- Select `New`, and search for `ensemble`
- See what you can find
- **Cannot download data from devel system**