Using Grid Technologies for Lattice QCD

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Outline

Introduction

Metadata Catalogue

Middleware

Summary

Credits

Forschungszentrum Jülich
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NIC/ZAM Jülich: Boris Orth, Thomas Lippert,

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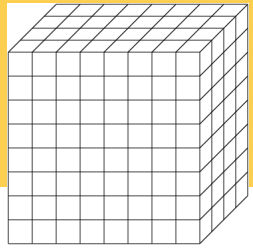
Content

Lattice Formulation of Quantum Chromodynamics



- Method for investigating QCD non-perturbatively
- Renders numerical simulations of QCD possible
- Major challenge: generation of **gauge field configurations** with dynamical fermions
- State-of-the-art simulations require TFlops-Computers

  e.g. apeNEXT 
- Features relevant here:
  - → **Different discretisations** (actions) and algorithms
    - ☞ Require extensible markup schema
  - → Simulations generate **Markov chains**
    - ☞ Group data by ensembles

☞ **LQCD is a computation not a data challenge**

☞ **Community consists of many small groups**

ILDG Initiative

The **International Lattice DataGrid** was proposed 2001.

Aim:

Longterm storage and global sharing of gauge configurations within a Datagrid

☞ **Make more efficient use of expensive data**

Participants: Australia, France, Germany, Italy, Japan, UK, USA

Working groups:

- ❒ Metadata working group
- ❒ Middleware working group

`http://www.lqcd.org/ildg`

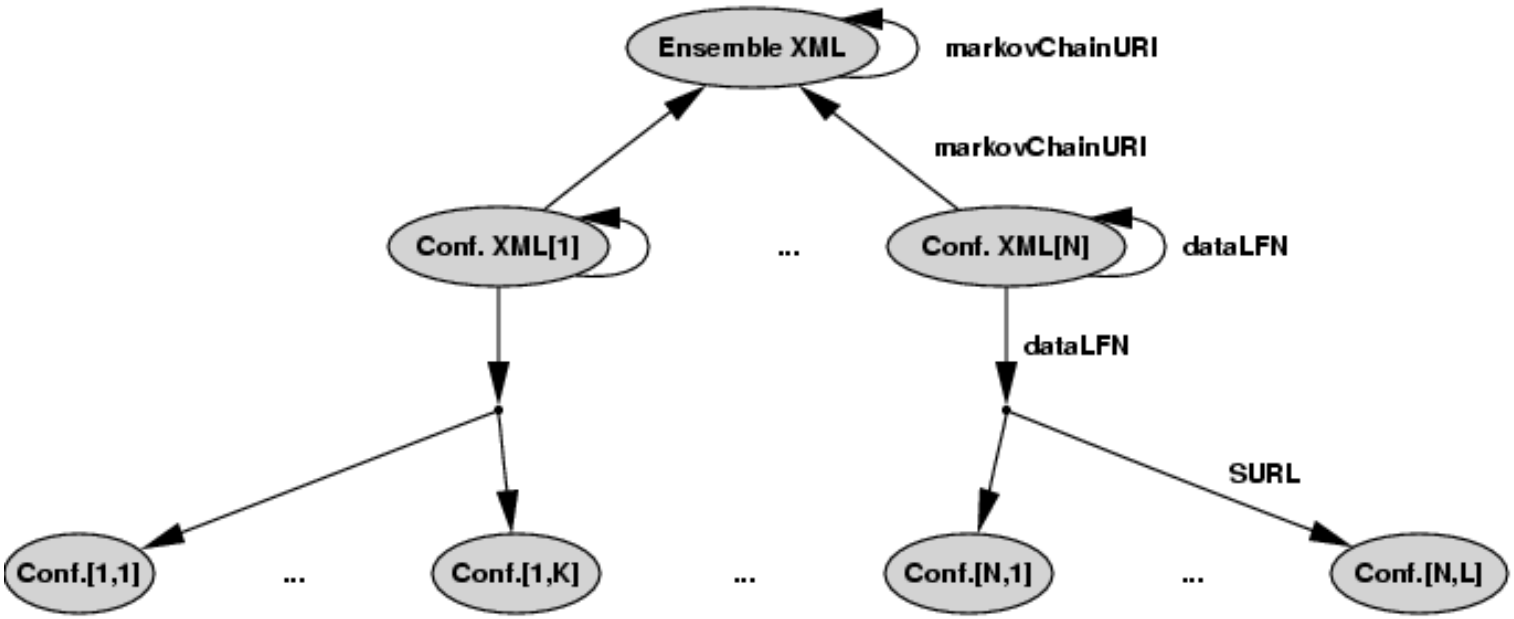
Requirements

Sharing gauge configurations requires

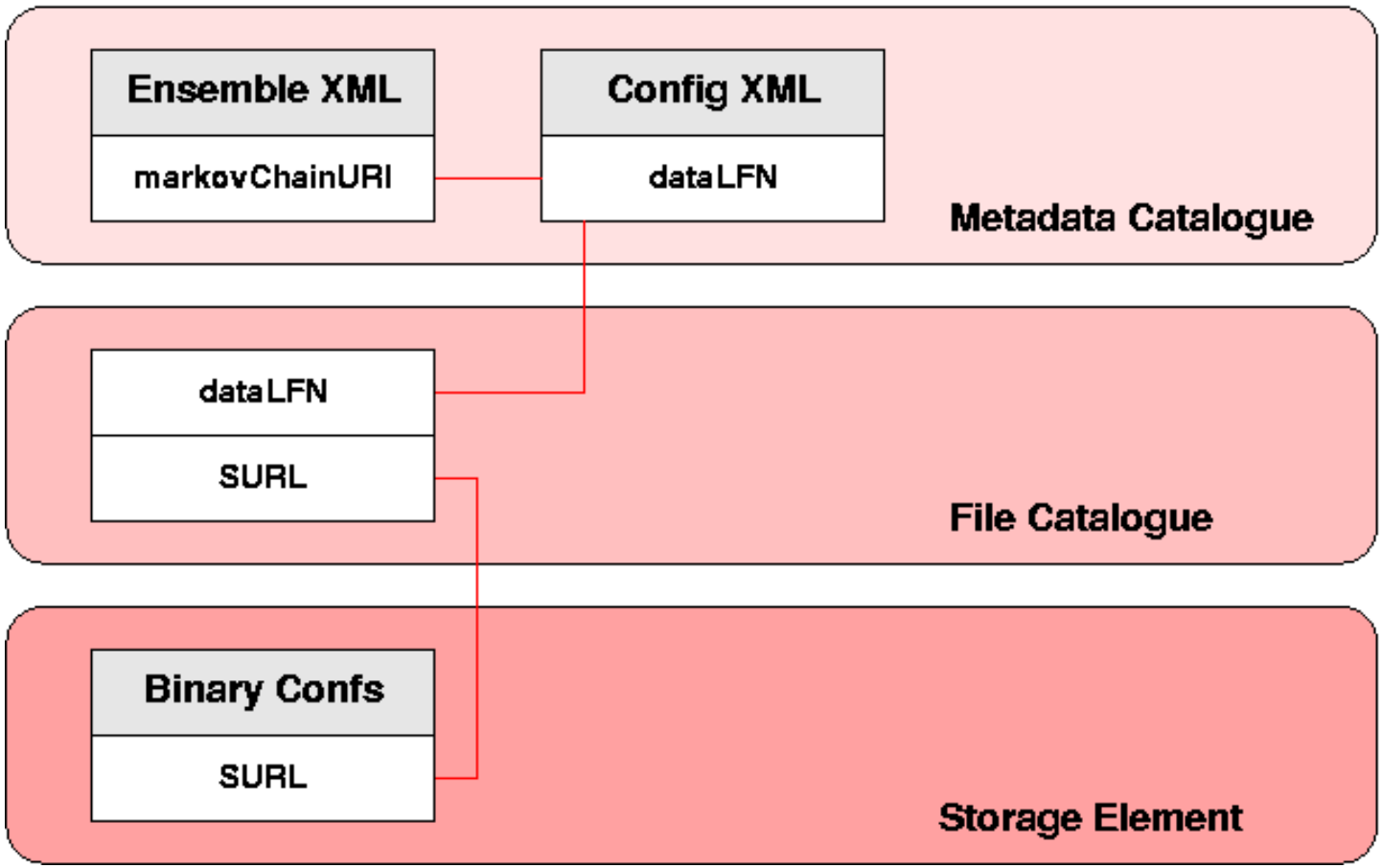
- Semantic access to worldwide distributed data
- Standardised metadata
  → XML documents which conform to a XML schema
- Standards on binary file format
- Definition of common middleware interfaces
  → ILDG is planned to be a grid-of-grids

Linking Metadata and Data

Objects	Links
Ensemble XML document **Configuration XML document** **Binary data file**	`markovChainURI` `dataLFN`



Information/data storage



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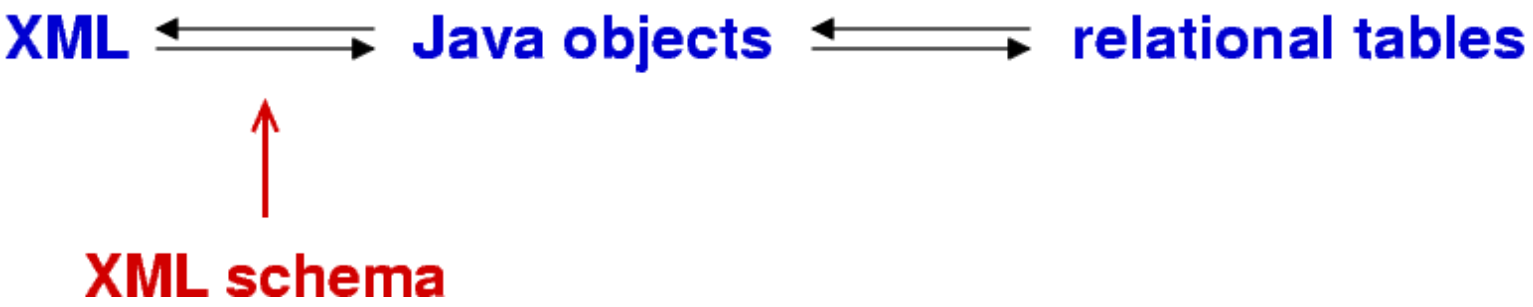
Requirements

- Load/store/query of XML documents which conform to **extensible schema**
- Access via **web service** front-end
- Standard **relational database** as back-end
- Usable for other research communities

Strategy



Issues to be addressed:

- XML-Java binding
- Java object content persistence

Binding JAVA to XML Schemata

- Choice between different solutions

  Selection criteria: - performance
  - Coverage of XML schema specification

  ☞ We choose for **JAXB**
- XML binder is used to
  - Generate set of **Java classes**
  - Annotate generated classes (**xdoclets**)
- Java classes are basis for software which transforms XML documents into Java content objects and vice versa.

JAVA-XML Binding (Example)


```
<markovStep>
  <markovChainURI>
    mc://ldg/qcdsf/clover_nf2/b5p40kp13610-24x48
  </markovChainURI>

  <series>561</series>
  <update>1500</update>

  <avePlaquette>0.5612510601</avePlaquette>

  <dataLFN>
    lfn://ldg/qcdsf/clover_nf2/b5p40kp13610-24x48/bqcd.01500.dat
  </dataLFN>
</markovStep>
```

JAVA-XML Binding (Example)


```
public class MarkovStepTypeImpl ...
{
  protected java.lang.String _MarkovChainURI;
  protected double _AvePlaquette;
  protected java.lang.String _DataLFN;
  protected java.lang.String _Series;
  protected java.lang.String _UpdateMarkovStep;
  private java.lang.String idInternal;

  ...
}
```

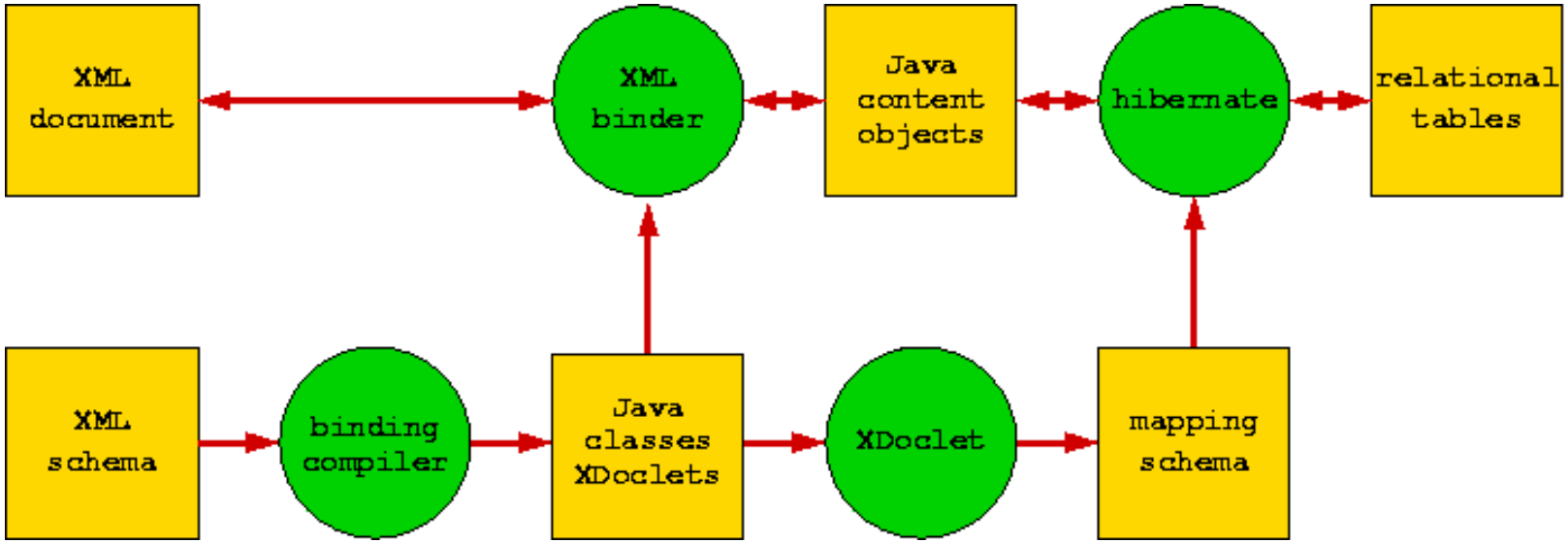
Java Object Content Persistence

- Required functionality:
  - Automated **object-relational mapping**
    ☞ Extracted from Java class annotations
  - Functions for **loading/storing** objects
- We use **Hibernate**
- Support for various SQL databases exist
  (we use: MySQL)

Java Object Content Persistence (Example)

MarkovStepType					
Field	Type	Null	Key	Default	Extra
idInternal	varchar(32)		PRI		
ildg_markovChainURI	varchar(255)	YES		NULL	
ildg_avePlaquette	double	YES		NULL	
ildg_update	varchar(255)	YES		NULL	
ildg_dataLFN	varchar(255)	YES		NULL	
ildg_series	varchar(255)	YES		NULL	

Detailed Overview



Interface to MDC

- Web services to query and load documents standardised by ILDG
- Open access for read operations, **GSI** authentication for write operations
- Used software:
  - Tomcat4 + Axis
  - COGkit

Queries

- Query language: **XPath**
- Query modes:
  - XPath query applied to collection of XML IDs, XPath result returned
    ☞ **Maximum flexibility** on client site
  - XPath query applied to each XML ID, URI of “matching” IDs returned
    ☞ Options for **performance optimisation**:

```
/gaugeConfiguration/markovStep[markovChainURI=uri]/dataLFN
                              ⇕
select dataLFN from MarkovStepType where markovChainURI="uri"
```

Evaluation

- Chosen solution meets requirements
  - Support for extensible schema
    But: XML schema specification not yet fully supported
  - Usable for other research communities
- Flexible front-end
- SQL servers provide standard, well-supported back-end technology
- Performance issues: materialisation of XML IDs expensive:
  - Loading requires O(0.02) seconds per XML ID
  - Storing requires O(0.04) seconds per XML ID

Authorisation / Access Control

- MDC stores **for each ensemble** permissions for
  - modifying metadata
  - modifying data files (configurations)
  - downloading data files
- Read or write permissions are assigned to groups
- Project (=owner) administrators can
  - create and modify groups
  - modify access permissions
- ACL will be forwarded to file catalogue
  ☞ Use ACL feature of LFC

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ILDG Middleware

Grid-of-grids concept: - set of regional grids
- few central services
- definition of interfaces

Services:

★ Service directory
★ VOMS?

Interfaces:

★ Few MDC WS services ☞ WSDL almost done
★ File catalogue WS interface ☞ Prototype at JLAB
★ SE interface ☞ SRM v2
★ Security infrastructure ☞ open issue ...

LatFor Datagrid

Regional grid for groups in Italy, France, Germany

- Resource requirements: O(100.000) configurations, O(10-100) TBytes

- **LCG-2** software is used:
  - File catalogue
  - Data management client tools

- Using **dCache** for SEs
  - Installations at several HPC sites

- **VO 'ildg'** maintained by at DESY

User Client Software

- **RPM-based** installation mechanism for LCG-based **User Interface**
- Regularly updated RPMs for CA certificates provided
- **User tools**:
  - Simple interface to both MDC and SE
  - Functions for download, upload, update
  - RPM-based installation mechanism

Examples

```
# lget -m -e www.lqcd.org/ildg/gral/b5p6kp1575-14x32
# lget lfn://ldg/qcdsf/clover_nf2/b5p25kp13575-24x48/150.dat
# lput config.00150.xml config.00150.dat
# lvalidate myensemble.xml
```

Content

Summary

- **Overview on ILDG**
  - Coordinate efforts for setting up interoperable data grid infrastructure
- **MDC: investigation of a XML-Java binding**
  - Software available even for complicated schemata
  - Allows for flexible solutions
  - Provides opportunities to overcome performance issues
- **Status of Italian/French/German regional grid:**
  - LCG-based infrastructure
  - Storage elements at relevant German HPC sites
  - Currently transition to normal user operation

Further information

`http://www-zeuthen.desy.de/latfor/ldg`