
International Lattice Data Grid

T. Yoshie for ILDG
CCS, Tsukuba

May 07 2009 @ HackLatt 2009

Data Grid for LQCD

- **QCD ensembles/configurations are valuable**
 - need huge amount of computer resources to generate
 - generated ensembles enable us to calculate various physical quantities
- **two purposes of lattice QCD data-grid**
 - sharing data within research group (collaboration)
 - configuration generation and analysis can be made using computers on distant sites
 - sharing ensembles/configurations worldwide
 - speed-up lattice QCD researches community-wide
- **International Lattice Data Grid (ILDG)**

History and Status

- proposed in 2002 by R. Kenway
- working groups and ILDG board
 - metadata & middleware working groups early in 2002
 - ILDG board in 2003
- biannual workshops (video conferences)
- 1st stage construction completed in 2007
- already used
 - open data to the public
 - share data within collaboration

Contents

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➤ Overview of ILDG

- ✓ Grid of Regional Grids
- ✓ Metadata/Data components
- ✓ Middleware components
- ✓ Statistics

➤ Using data on ILDG

- ✓ joining virtual organization
- ✓ finding ensembles
- ✓ download configurations
- ✓ use them

➤ Submitting data to ILDG

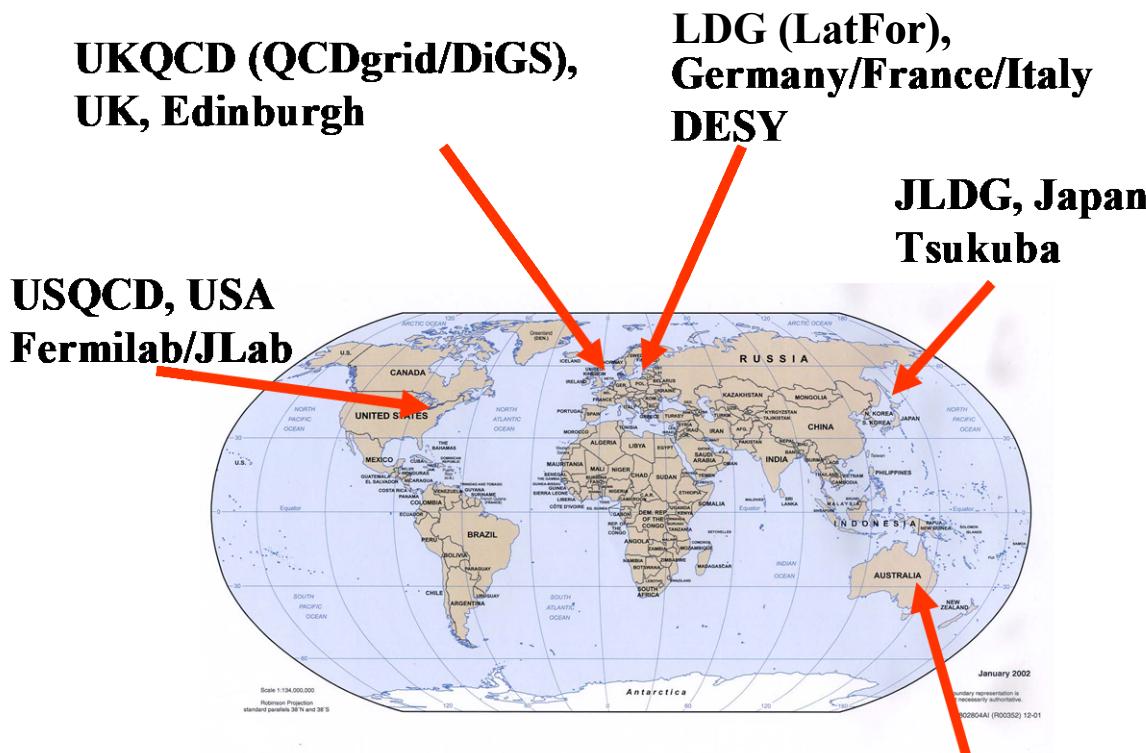
- ✓ writing XML documents

➤ Summary and Future

Overview of ILDG

Grid of Regional Grid

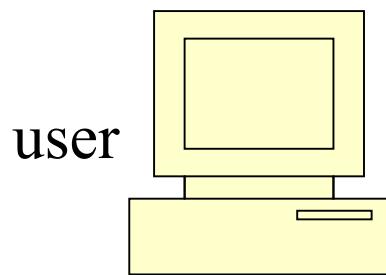
- ILDG is not a flat data grid
- ILDG is a **Grid of five Regional Grids**
 - construction of local grids were already in progress



ILDG grand design

a slide used in 2003

download configurations
from somewhere in
a regional grid



worldwide search of
ensembles

UKQCD

metadata database

storage system
(regional grid)

JLDG

metadata database

storage system
(regional grid)

copy

metadata:

identity information of ensemble/configuration (collaboration/project,
physics parameters (lattice size, quark mass....), literature)

Mission of working groups

metadata WG

- ✓ **consider cooperation of data and metadata**
 - define ensembles and configurations
 - standard file format

- ✓ **devise a description rule of ensemble and configuration metadata**
 - QCDml: XML based markup language

middleware WG

- ✓ **devise and implement interfaces among regional grids**
 - metadata search
 - locating files
 - download protocol

- ✓ **develop client tools for search and download**

computer scientists and lattice QCD researchers join the two WG

Credits

□ Metadata Working Group

P.Coddington (Adelaide), T.Yoshie (Tsukuba), D.Pleiter (DESY) ,
G.Andronico (INFN), C.Maynard (Edinburgh), C.DeTar (Utah),
J.Simone (FNAL), R.Edwards, B.Joo (JLAB)

□ Middleware Working Group

P.Coddington, S.Zhang (Adelaide), T.Amagasa, N.Ishii. O.Tatebe.
M.Sato (Tsukuba), D.Melkumyan, D.Pleiter (DESY), G.Beckett,
R.Ostrowski (Edinburgh), J.Simone (FNAL), B.Joo, C.Watson (JLAB)

□ ILDG board

- supervise WGs, discuss strategic issues

R.Brower (USA), K.Jansen (Germany), R.Kenway (UK, chair),
D.Leinweber (Australia), O.Pene (France), F.Di Renzo (Italy),
A.Ukawa and T.Yoshie (Japan)

Data and Metadata

ensemble
XML

```

<npClover>
  <kappa>0.1354</kappa>
  <cSW> 1.684 </cSW>
</npClover>          (fake example)
    
```

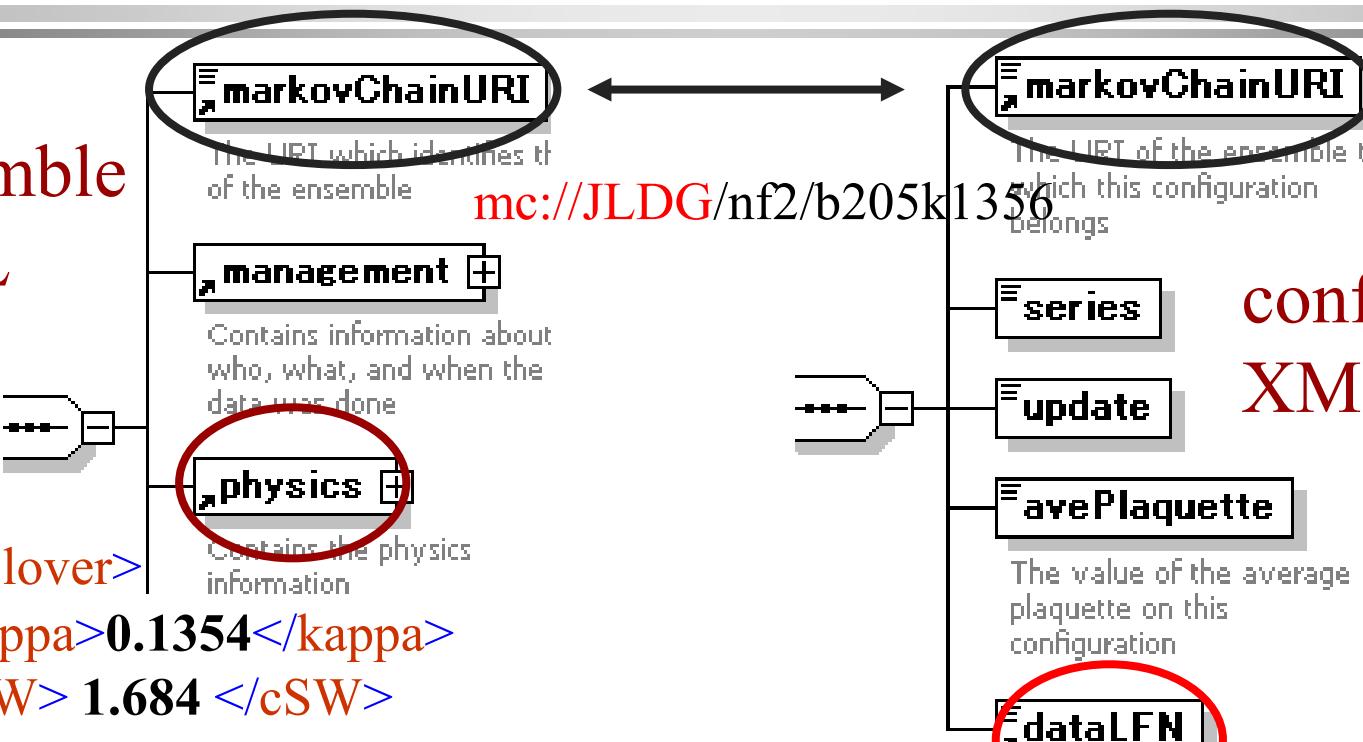
configuration file

file-format XML size, precision

configuration binary data

lfn://JLDG/nf2/b205k1356-A200

configuration
XML



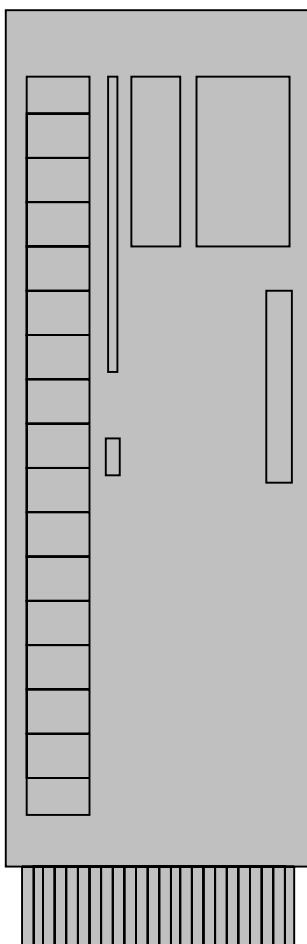
lfn://JLDG/nf2/b205k1356-A200

packed
with LIME

Lattice QCD Interchange
Message Encapsulation
(B.Joo and C.DeTar)

Middleware components

Storage Elements



SRM

SRM: Storage Resource Manager
<http://sdm.lbl.gov/srm-wg/>

gridftp, http
servers

TURL
data

Authentication

a query language for selecting
nodes from an XML document

SURL

TURL



XPath
markovChainURI
LFN

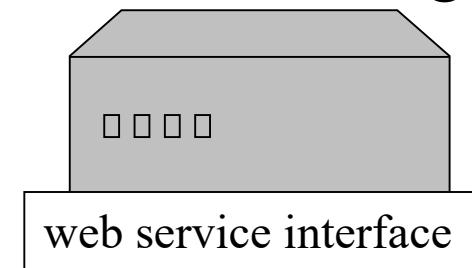
LFN
SURL



VOMS

virtual organization
management system

Metadata Catalogue



web service interface

SURL: site uniform
resource locator
TURL: transfer URL

web service interface



File Catalogue

other components

□ Services.xml

- master catalogue to keep locations of RG catalogue services and storage elements

□ VOMS

- virtual organization management system
- keep data of ILDG users and roles/groups of user
- authentication is made when access to File Catalogue and Storage elements

□ INCA monitoring system

- <http://www.sapac.edu.au/inca>

	localResource
ildg.fc.unittest_cssm	error
ildg.fc.unittest_jldg	pass
ildg.fc.unittest_ldg	pass
ildg.fc.unittest_ukqcd	error
ildg.fc.unittest_usqcd	pass
ildg.mdc.unittest_cssm	pass
ildg.mdc.unittest_jldg	error
ildg.mdc.unittest_ldg	pass
ildg.mdc.unittest_ukqcd	pass
ildg.mdc.unittest_usqcd	pass
ildg.se.unittest_cssm_sasr.edu.au_gsiftp	123.22KByte/s
ildg.se.unittest_cssm_sasr.edu.au_srm	22.4KByte/s
ildg.se.unittest_jldg_jldg.org_gsiftp	230.98KByte/s
ildg.se.unittest_ldg_fz-juelich.de_srm	85.14KByte/s
ildg.se.unittest_ldg_ifh.de_srm	129.35KByte/s
ildg.se.unittest_ldg_in2p3.fr_srm	154.25KByte/s
ildg.se.unittest_ldg_zib.de_srm	139.64KByte/s
ildg.se.unittest_ldg_infn.it_srm	131.66KByte/s
ildg.se.unittest_ukqcd_iridis.soton.ac.uk_gsiftp	217.9KByte/s
ildg.se.unittest_ukqcd_ph.liv.ac.uk_gsiftp	.KByte/s
	localResource
ildg.se.unittest_ukqcd_swan.ac.uk_gsiftp	187.36KByte/s
ildg.se.unittest_usqcd_fnal.gov_srm	225.71KByte/s

- consists of five regional grids (RGs)
 - implementations of Catalogues and Storage Elements are different
 - interoperable with common interface (defined by WSDL)
- users don't have to know details of XML and middleware
 - easy-to-use client tools by Middleware WG
- submitter has to understand (at least) QCDml
- developer (of e.g. client tools) has to know details of middleware, at least RG interface
 - (beyond scope of this talk)

CSSM

◆ Regional Grid

- dCache based SE
- Catalogue @ CSSM

□ Storage Elements

- 7TB disk
- 20TB tape system
(as of June 2008)

◆ Host of global ILDG services

- Monitoring (INCA)
- global web site
(<http://www.lqcd.org/ildg/>)

dCache: a storage middleware system
(a distributed data storage caching system)
developed by a joint collab. of DESY and FNAL
<http://www.dcache.org/>



<http://cssm.sasr.edu.au/ildg/>

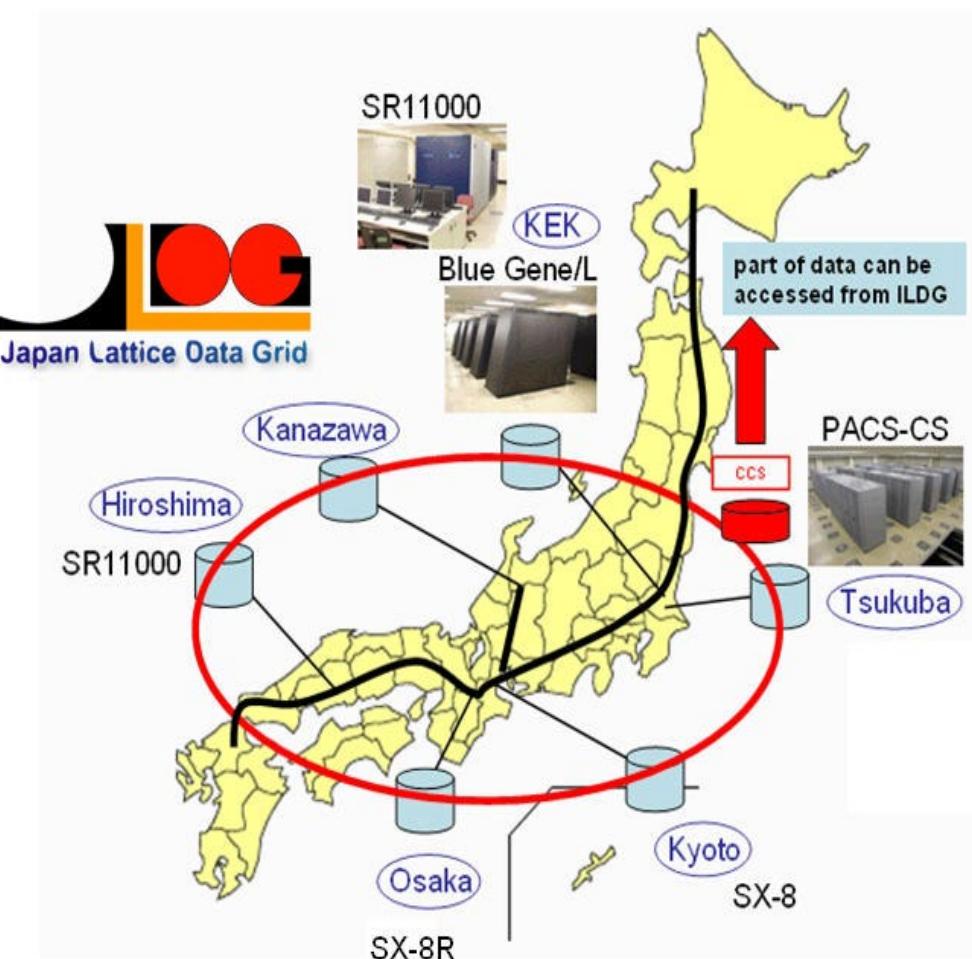
◆ Regional Grid

- gfarm SE
- Catalogue @ Tsukuba

□ Storage Elements

- 6 sites in the figure
- 100TB

gfarm: a grid file system (grid data farm) developed at AIST and Tsukuba, Japan
<http://datafarm.apgrid.org/index.en.html>



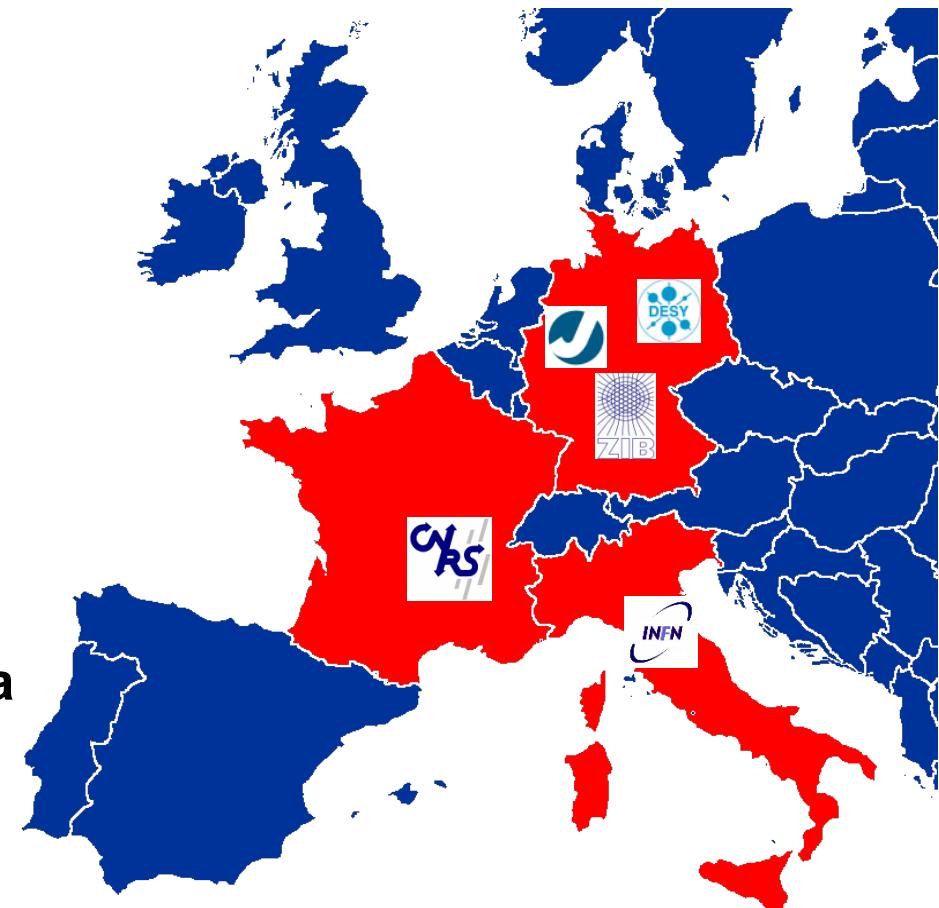
□ Regional Grid

- dCache based SE
- Catalogue @ DESY

□ Storage Elements

- DESY (Hamburg+Zeuthen),
JSC (Julich), ZIB (Berlin),
CC-IN2P3 (Lyon),
INFN Parma (Parma)
- have tape back-end
without a fixed storage quota

◆ Operates VOMS



<http://www-zeuthen.desy.de/latfor/ldg/>

□ Regional Grid

- DiGS (see previous talk)
- Catalogue @ Edinburgh

□ Storage Elements

- 7 sites in the figure
- 80TB (as of 2007/03)



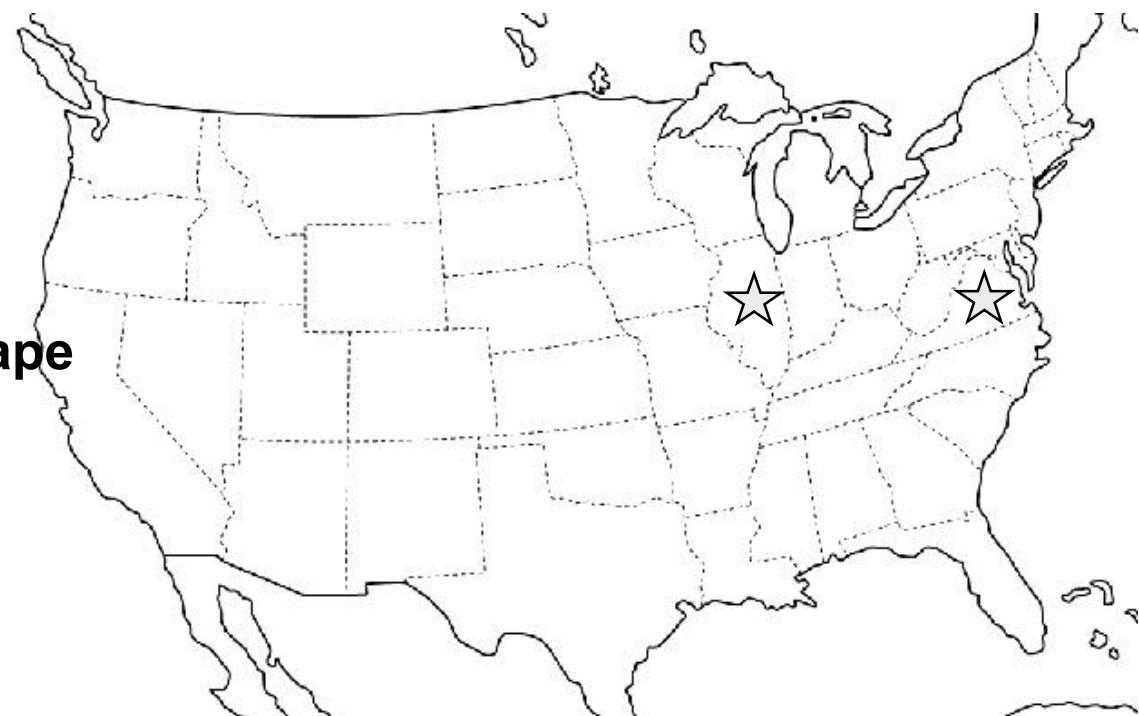
<http://www.gridpp.ac.uk/qcdgrid/>

- **Regional Grid**

- dCache based
 - Catalogue @ Jlab

- **Storage Elements**

- Fermilab
 - a part of huge disk/tape
 - no limitation set



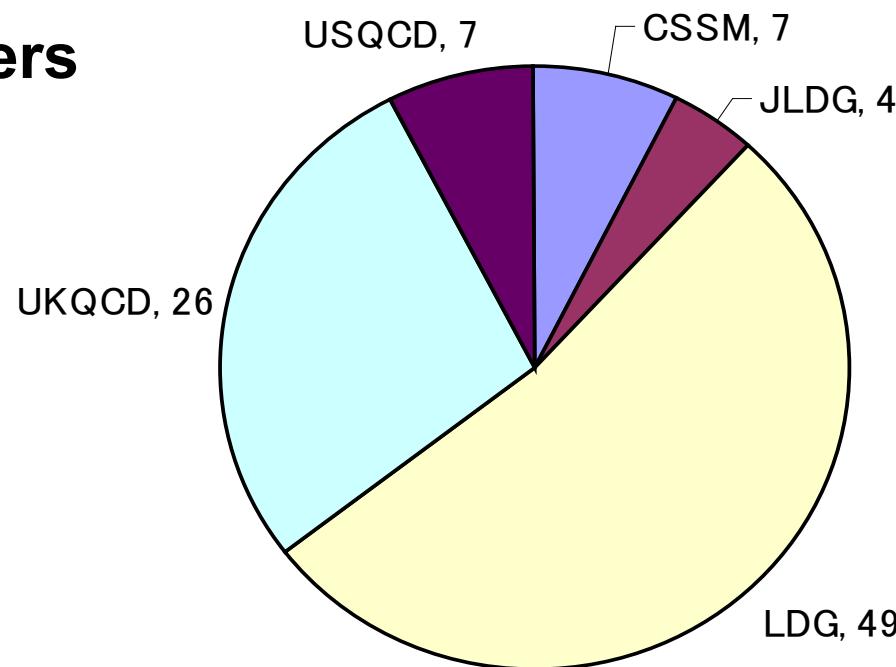
<http://www.usqcd.org/ildg/>

Statistics

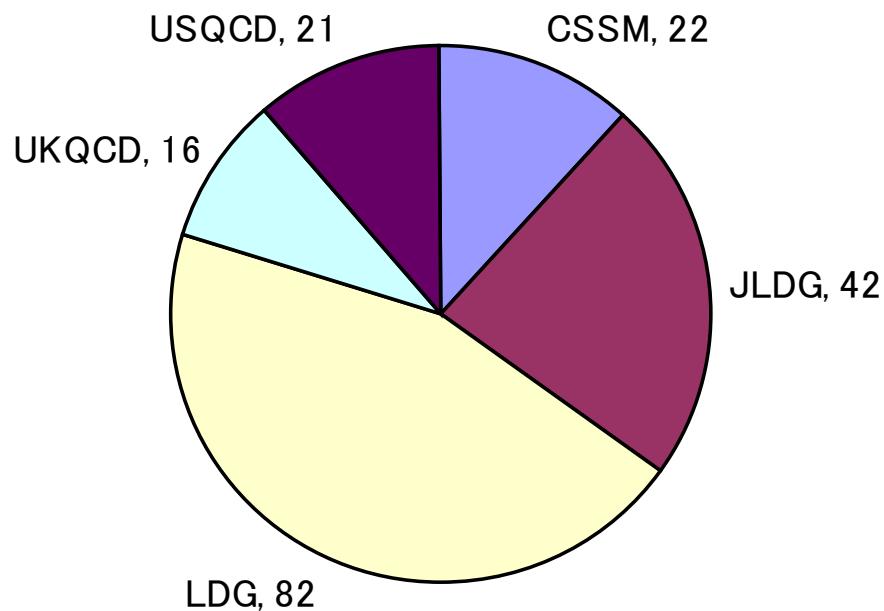
- ◆ apologies

- data are a little bit old (as of June, 2008)
- getting statistics information from ILDG is not easy

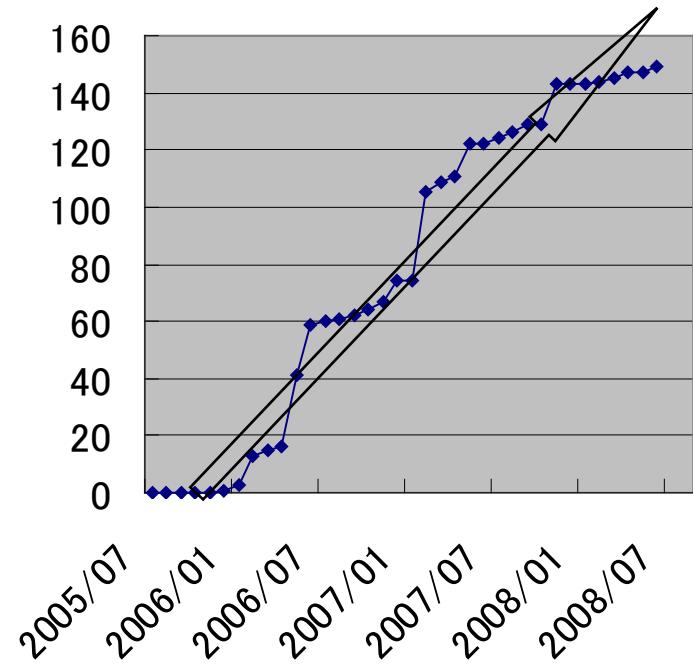
ILDG VO members



Ensembles



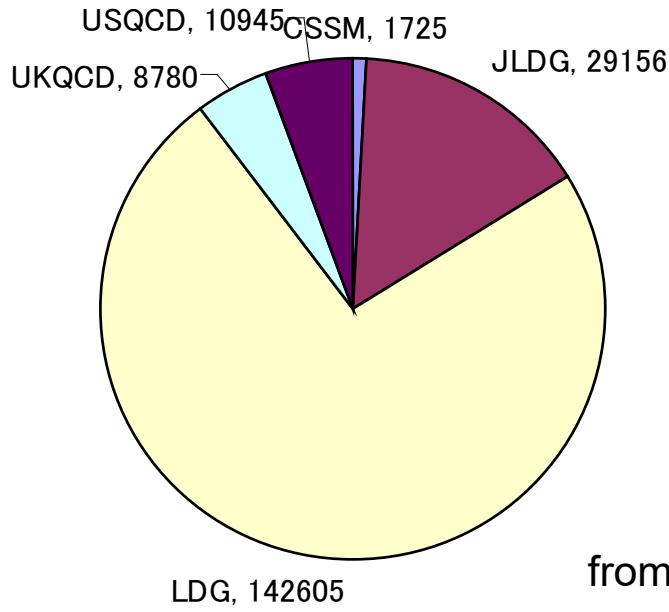
Ensembles vs. year/month



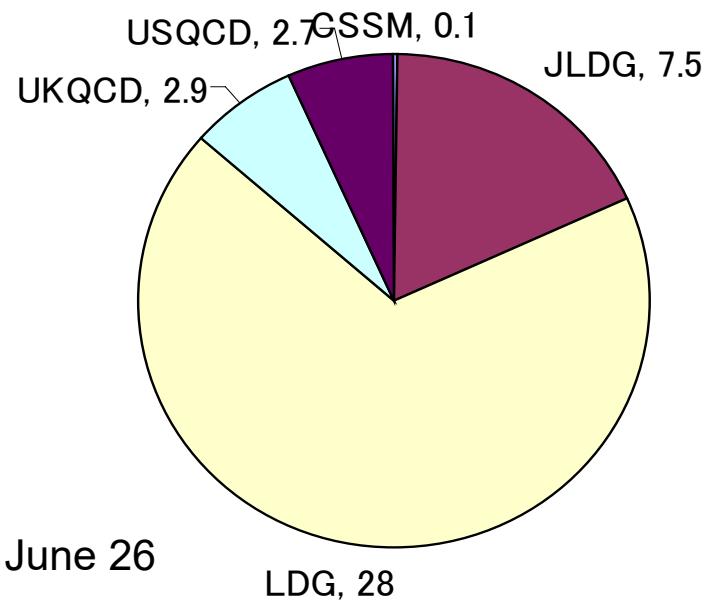
- ☐ # increases almost linearly since Jan 2006
- ☐ 183 ensembles

recording submission date is not mandatory. ignored if not recorded

Configurations



data size (TB)



from MDCs, as of June 26

□ 193K config's

- some part of them are restricted to collab.

□ 41 TB

Using data on ILDG

General Procedure

- **join the ILDG Virtual Organization (VO)**
 - ILDG can confirm that you belong to the Lattice QCD community
- **find ensembles**
 - use **portals or tools** provided by regional grids
- **check access policy**
 - data are public / negotiable / restricted
 - contacting the collaboration is the best way
- **download configurations**
 - a standard command line tool **ildg-get**
 - RG supports different methods (uberftp, Itools, DiGS tools ...)
- **use configurations for measurements**
 - **file and binary data format**
- **do research and write a paper**
- **acknowledge the collaboration and the ILDG**
 - cite **papers** specified by the collaboration
 - cite <http://www.lqcd.org/ildg>

comments

- **client machine should be properly set up**
 - globus package (incl. gridftp) globus: a grid middleware
 - CA software (depends on CA) CA: Certificate Authority
 - SRM client srmcp
 - ILDG command line tool ildg-get
- URL:

- **detail may depend on regional grid**

- **ILDG authentication uses (de-fact standard) grid certificate technology**

- the technology uses **public key cryptography** and **certificate authorization**

- **public key cryptography**

- (ssh: secure shell uses this technology)
 - uses two keys, private (secret) key and public key
 - secure because private key is not transmitted through network

Tom



- 1) generate private/public key pair and send the public key to Bob
- 3) Tom encrypts the message with private key and send it to Tom

public key = certificate

Bob



- 2) Bob send a message to Tom
- 4) Bob decrypts it with Bob's public key, if successful Bob knows that Tom has his private key

joining the ILDG VO (2)

□ certificate authorization

- establish certificate authority (CA)
- CA guarantees that the user's certificate can be trusted
- uses public key encryption,
- CA has CA's private/public key pairs and signs the user's certificate with CA's public key, after having confirmed identity of the user

□ authorization of CA

- IGTF: international grid trust federation
<http://www.igtf.net/>

□ Subject

- identity of a certificate
/C=JP/O=KEK/OU=CRC/OU=Tsukuba/CN=Tomoteru Yoshiie

joining the ILDG VO (3)

□ a typical procedure to get a grid certificate

- contact a staff of a CA
- (after an interview) get user-id/password
- download and install CA package
- generate one-time license-ID with the user-id/password
- execute a command to get a certificate: you will be asked to provide information (one-time license-ID, full name, subject, pass phrase for the certificate)

□ what you get: three files in \$HOME/.globus

- usercert.pem: user certificate
- userkey.pem: user private key
- 9fac2951.0: CA certificate (file name depends on CA)

□ to see info of the certificate

- type grid-cert-info
- you get: Issuer, Subject, Validity Info. ...

joining the ILDG VO (4)

□ Import the certificate to your web browser

- export your certificate in PKCS12 format

```
% openssl pkcs12 -export -in /home/test1/.globus/usercert.pem  
-inkey /home/test1/.globus/userkey.pem -out usercert.p12
```

- start web browser and import the certificate

- Mozilla Firefox: follow menu “Tools, Options, Advanced, View Certificates, Your Certificates, Import”

□ visit VOMRS (virtual organization member registration service) to register

- virtual organization member registration service
- <https://grid-vomrs.desy.de:8443/vo/ildg/vomrs>
- three stages to check you belong to LQCD community
 - phase-1 to register as a candidate
 - RG representative approves your registration
(You will receive Email confirmation)
 - complete phase-2

□ wait for a while until [grid-mapfile](#) is updated



- ask submitter
- read ILDG contributions to annual lattice conferences
 - recent two contributions highlight interesting ensembles on the grid
 - *C.Detar, PoS (LATTICE 2007) 009,*
 - *T.Yoshie, PoS (LATTICE 2008) 019*
- use **portals or tools provided by RG**
 - you can use portals without joining ILDG VO
 - please visit and try all portals freely

□ list ensembles and see details of ensembles

<http://usqcd.jlab.org/mdc-web-client/index.jsp>

Ensembles found at <http://usqcd.jlab.org/mdc-service/services/ILDGMDCServices>

This MDC Contains the following ensembles

There are 21 ensembles here:

Ensemble: [mc://USQCD/LHPC/aniso/wilson/NF2/wl_16_64_5p5_x2p38_um0p4086](#)

Physics:

Volume: 16x16x16x64

GaugeAction:

[Anisotropic Wilson Action](#)

Beta=5.5

xi0=2.38

Aniso Direction=T

Fermion Action:

2 flavours

[Anisotropic Wilson Fermion](#)

Mass=-0.4086

Normalization=unity

xi0=2.38

nu=1

AnisoDirection=T

Management:

Producing Collaboration: LHPC

Project: SPECTRUM

Label: wl_16_64_5p5_x2p38_um0p4086

Published Alias:

Reference:

Algorithm:

Algorithm Name: [HMC 2Flavour Hasenbusch Preconditioning](#)

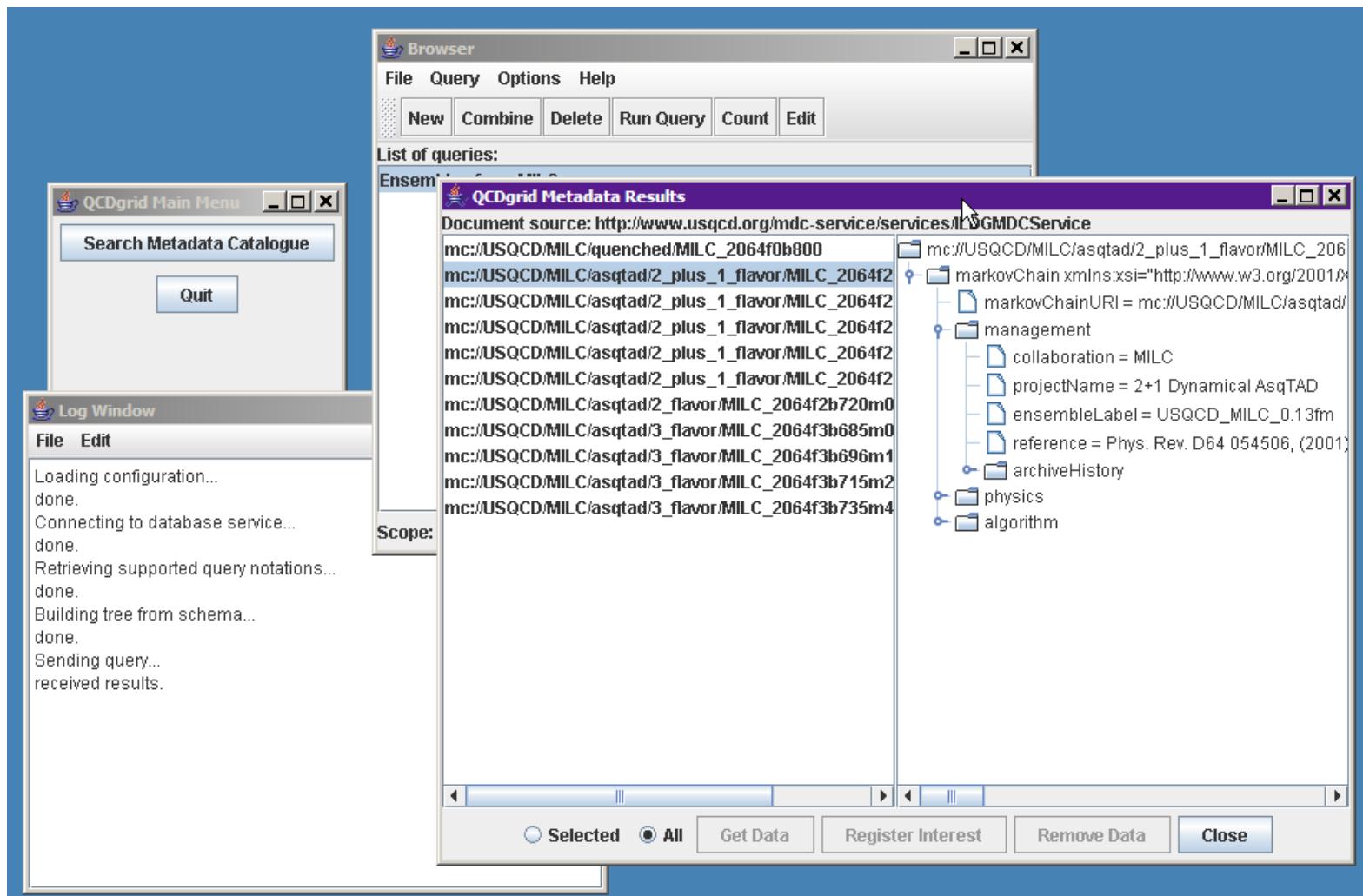
Reference: Comput.Phys.Commun. 174 (2006) 87-98

Algorithm Kind: This is an **exact** algorithm

UKQCD ildg-browser

semantic search based on XML

<http://www.gridpp.ac.uk/qcdgrid/>



ILDG List Ensembles

[LDG Home](#)[List](#)[Ensembles](#)

- [mc://USQCD/LHPC/aniso/wilson/NF2/wl_16_64_5p5_x2p38_um0p4086](#) [usqcd]
- [mc://USQCD/LHPC/aniso/wilson/NF2/wl_16_64_5p5_x2p38_um0p4125](#) [usqcd]
- [mc://USQCD/LHPC/aniso/wilson/NF2/wl_24_64_5p5_x2p38_um0p4086](#) [usqcd]
- [mc://USQCD/LHPC/aniso/wilson/NF2/wl_24_64_5p5_x2p38_um0p4125](#) [usqcd]



Show Ensemble

markovChainURI=mc://ldg/etmc/tmqcd_nf2/tSym_b3.75_L24T48_k0.1660_mu0.0200, grid=ldg

[LDG Home](#)
[Show XML](#)
[List Configs](#)
[List Ensembles](#)

Management

Collaboration: etmc
 Project name: tmqcd_nf2
 Archive History: action = add; participant = Carsten Urbach (University of Liverpool); date = 2006-07-02T17:28:47+02:00;

Physics

Size: X = 24; Y = 24; Z = 24; T = 48;
 Gluon: treelevel Symanzik improved action
 beta = 3.75 c0 = 1.6666666700000001; c1 = -0.08333333329999999
 Quark [#1]: Twisted mass action
 kappa = 0.166; mu = 0.02; numberOfFlavours = 2

Algorithm

Name: mtHMC
 Glossary: <http://www-zeuthen.desy.de/latfor/ldg/algorithmGlossaries/mtHMC.pdf>
 Reference: Comp.Phys.Commun. Vol 174/2 pp 87-98
 Exact: true
 Parameters: integrationScheme = Sexton-Weingarten

- narrowing search by faceted navigation
 - facets: categories of XML documents

QCDml Faceted Navigation

rgrid
[cssm \(22\)](#)
[jldg \(6\)](#)
[JLDG \(42\)](#)
[ldg \(76\)](#)
[ukqcd \(9\)](#)
[USQCD \(21\)](#)
[www.lqcd.org \(1\)](#)

collaboration
[CP-PACS \(12\)](#)
[CP-PACS+JLQCD \(30\)](#)
[QSSM \(22\)](#)
[dik \(2\)](#)
[etmc \(27\)](#)
[gral \(9\)](#)
[LHPC \(8\)](#)
[MILC \(13\)](#)
[gods \(24\)](#)
[RBC-UKQCD \(9\)](#)
[sesam \(8\)](#)
[theta \(4\)](#)
[txl \(2\)](#)
[UKQCD \(7\)](#)

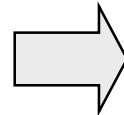
projectName
[2+1 DWF \(9\)](#)
[2+1 Dynamical AsqTAD \(13\)](#)

Generated SQL (for debug)

```
select m.property, m.value, count(m.property, m.value) as c0
    from mc
    group by m.property, m.value
    order by m.property, m.value
```

List of Ensembles (177)

- No. 1 [12/12/12/24] mc://JLDG/iwasakiRGGluonAction (b=1.8000000000000002, k=0.14090909090909091)
- No. 2 [12/12/12/24] mc://JLDG/iwasakiRGGluonAction (b=1.8000000000000002, k=0.14300000000000001)
- No. 3 [12/12/12/24] mc://JLDG/iwasakiRGGluonAction (b=1.8000000000000002, k=0.14450000000000001)
- No. 4 [12/12/12/24] mc://JLDG/iwasakiRGGluonAction (b=1.8000000000000002, k=0.14640000000000001)
- No. 5 [16/16/16/32] mc://JLDG/iwasakiRGGluonAction (b=1.9500000000000002, k=0.13750000000000001)
- No. 6 [16/16/16/32] mc://JLDG/iwasakiRGGluonAction (b=1.9500000000000002, k=0.13750000000000001)



QCDml Faceted Navig

rgrid
[JLDG \(30\)](#)

collaboration
[CP-PACS+JLQCD \(30\)](#)

projectName
[RCNF2+1 \(NF=2+1 full QCD with iwasaki RG gauge and non-perturbatively O\(a\) improved wilson \(clover\) quark action\) \(30\)](#)

date
[2007 \(30\)](#)

size
[16/16/16/32 \(10\)](#)
[20/20/20/40 \(10\)](#)
[28/28/28/56 \(10\)](#)

numberOfFlavours
[2+1 \(30\)](#)

gluon
[iwasakiRGGluonAction \(30\)](#)

quark
[npCloverQuarkAction \(60\)](#)

beta
[1.8300000000 \(10\)](#)
[1.9000000000 \(10\)](#)
[2.0500000000 \(10\)](#)

kappa

Generated SQL (f

```
select m.property, m.v
    from mc
    where m.property = 'collaboration' and value = 'CP-PACS+JLQCD'
    group by m.property, m.value
```

List of Ensembles

- No. 1 [16/16/16/32] mc://JLDG/CP-PAC/iwasakiRGGluonAction/npCloverQuarkAction
- No. 2 [16/16/16/32] mc://JLDG/CP-PAC/iwasakiRGGluonAction/npCloverQuarkAction
- No. 3 [16/16/16/32] mc://JLDG/CP-PAC/iwasakiRGGluonAction/npCloverQuarkAction
- No. 4 [16/16/16/32]

- search ensembles by specifying names of actions and other physics parameters

<http://cssm.sasr.edu.au/ildg/>

International Lattice Data Grid (ILDG)

Web portal for the ILDG Lattice QCD Data Archive

Home Search XPathQuery CSSM Portal About

Ensemble Search on ILDG records

Collaboration: CSSM UKQCD USQCD LDG JLDG

Lattice Size: Any

Gluon Action

Beta:

Gauge Group Type:

Action Type:

- GeneralGluonAction
- plaquetteGluonAction
 - SixLinkGluonAction
 - DBW2GluonAction
 - treelevelSymanzikGluonAction
 - LuescherWeiszGluonAction
 - tpLuescherWeiszGluonAction
 - iwasakiRGGluonAction
- anisotropicGluonAction
 - anisotropicWilsonGluonAction
 - anisotropicTpWilsonGluonAction

Quark Action (No Quark Action)

Number Of Flavours: any

Kappa:

Action Type:

- GeneralQuarkAction
 - wilsonQuarkAction
 - cloverQuarkAction
 - tpCloverQuarkAction
 - npCloverQuarkAction
 - fatLinkIrrelevantCloverQuarkAction
 - wilsonTmQuarkAction
 - KSQuarkAction
 - asqTadQuarkAction
 - generalOverlapQuarkAction
 - domainWallQuarkAction
 - anisotropicQuarkAction
 - anisotropicWilsonQuarkAction
 - anisotropicCloverQuarkAction

download configuration

- You get (a list of) LFN's from portals or tools
- generate proxy certificate (valid for half a day (default))

```
% grid-proxy-init -old
```

Your identity: /C=JP/O=KEK/OU=CRC/OU=Tsukuba/CN=Tomoteru Yoshiie

Enter GRID pass phrase for this identity:

Creating proxy Done

Your proxy is valid until: Mon Apr 27 16:17:47

```
% ls -l /tmp/x509up_u10006
```

```
-rw----- 1 yoshie LATTICE 2735 Apr 27 04:17 /tmp/x509up_u10006
```

```
% grid-proxy-info
```

- invoke **ildg-get** , a standard ILDG command
(download will complete without any message)

```
% ildg-get lfn://JLDG/CP-PACS/RCNF2/RC12x24-B1800.....
```

how ildg-get is working

```
% ildg-get --debug=3 lfn://JLDG/CP-PACS/RCNF2/RC12x24-  
B1800K014640C1600-D-01420
```

ildg-get knows where are
catalogue services of RGs

```
[main|05:13:04|INFO ] Connecting to FC of regional grid "JLDG"
```

site uniform URL (incl. protocol) is returned

```
[main|05:13:05|DEBUG] SURL = gsiftp://www.jldg.org/gfarm/public/ILDG/JLDG/  
CP-PACS/RCNF2/RC12x24-B1800/K014640/RC12x24-B1800K014640C1600-  
D-01420
```

gfarm file system of JLDG

```
[main|05:13:05|DEBUG] Execute command: globus-url-copy --dbg  
gsiftp://www.jldg.org/gfarm/public/ILDG/JLDG/CP-PACS/RCNF2/RC12x24-  
B1800/K014640
```

gfarm translates it to the actual location of the file
transfer from one of 6 sites of JLDG to CCS,Tsukuba
and then to the user
(not shown here)

more on ildg-get

□ You can get ensemble/config XML documents

```
% ildg-get --mdc-only mc://JLDG/CP-PACS+JLQCD/RCNF2+1/RC16x32_B1800....  
% ildg-get -mdc-only lfn: //JLDG/CP-PACS+JLQCD/RCNF2+1/RC16x32_B1800....
```

- type “ildg-get --help” for options

```
[ram.accsnet.ne.jp]:28] % head -5 RC16x32_B1830Kud013825Ks013760C1761.xml  
<markovChain xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.lqcd.org/ildg/QCDml/ensemble1.4" xsi:schemaLocation="http://www.lqcd.org/ildg/QCDml/ensemble1.4 http://www.lqcd.org/ildg/QCDml/ensemble1.4/QCDmlEnsemble1.4.1.xsd">  
    <markovChainURI>mc://JLDG/CP-PACS+JLQCD/RCNF2+1/RC16x32_B1830Kud013825Ks013760C1761</markovChainURI>  
    <management>  
        <revisions>1</revisions>  
        <collaboration>CP-PACS+JLQCD</collaboration>
```

file format

□ LIME

- a lime file consists of one or more **messages**
- a message consists of one or more **records**
- a record can be either **ASCII** or binary data
- a record has a name “**LIME record type**”
- includes header and padding

□ ILDG configuration file should satisfy ILDG file format specification

<http://www-zeuthen.desy.de/~pleiter/ildg/#filefmt>

file format (2)

message	record	LIME record type
#1
...
#n
	#i	ildg-format

	#j	ildg-binary-data

...
#m	#1	ildg-data-lfn
...

- group can insert their own messages/records
 - (type ildg-* is reserved)
- order of #n and #m is not fixed, while #i < #j

file format (3)

□ **ildg-format:** minimal info. to read config

```
<?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 http://www.lqcd.org/ild
g/filefmt.xsd">
    <version> 1.0 </version>
    <field> su3gauge </field>
    <precision> 64 </precision>
    <lx> 32 </lx> <ly> 32 </ly> <lz> 32 </lz> <lt> 64 </lt>
</ildgFormat>
```

□ **ildg-data-lfn:** logical file name

- enables us to back track

file format (4)

□ LIME commands

- lime_contents <lime_file>
- lime_extract_type <lime_file> <lime_type>
- and more

```
% lime_extract_type | LDG-LIME-config ildg-binary-data > binary
```

```
% cksum binary
```

2685385332 1207959552

should agree with crcCheckSum in the config XML

```
% ildg_cksum ILDG-LIME-config
```

2685385332

- you can write a code to read config directory from the LIME packed file, using LIME API

file format (5)

```
#include <stdio.h>
#include <stdlib.h>
#include <stdint.h>
#include "lime.h"

#define NS 12
#define NT 24
#define SIZE (NS*NS*NS*NT*4*3*3*16)

unsigned char conf[SIZE] ;
```

```
main(int argc,char **argv) {

    FILE *fp ;
    LimeReader *reader ;
    n_uint64_t nbytes ;

    fp = fopen(argv[1], "r") ;
    reader = limeCreateReader(fp) ;

    do { limeReaderNextRecord(reader) ;
        while (strncmp(limeReaderType(reader),
                        "ildg-binary-data", 16)) ;

        nbytes = limeReaderBytes(reader) ;
        limeReaderReadData(conf, &nbytes, reader) ;

        limeDestroyReader(reader) ;
        fclose(fp) ;
    }
```

file format (6)

□ **ildg-binary-data**

- sequence of floats/doubles

$$\chi^+(n)U_\mu(n)\chi(n+\hat{\mu}) = \sum_{a,b=0}^2 [\chi^+(n)]_a [U_\mu(n)]_{ab} [\chi(n+\hat{\mu})]_b$$

In C format:

U[t][z][y][x][mu][a][b][ri]

ri=0,1 for real/imaginary parts

a,b=0,1,2

mu=0 (x), 1 (y), 2 (z), 3 (t)

x=0,1.... NX-1 (NX: size in x direction)

In Fortran format:

U(ri,b,a,mu,x,y,z,t)

color indices are transposed in Fortran

Submitting data to ILDG

procedure

- **no standardized procedure**
 - RG has its own procedure/rule
- **the procedure includes**
 - determine MarkovChainURI/LFN following RG rules
 - convert config's to the ILDG standard format
 - place the config files on one of Storage elements
 - **write ensemble/config XML documents**
 - update Metadata Catalogue and File Catalogue databases

- **QCDml**
 - an XML-based markup language designed for ILDG
- **QCDml XML documents**
 - describe metadata of QCD ensembles and configurations in ILDG
- **strategy**
 - define XML elements necessary for exchanging configurations
 - provide standards of notation and terminology based on common community practices, to ensure unique markup
 - device a description rule set **schemata**
- **XML documents have to conform to schema**



Writing a valid QCDml document

- **an easy way**

- get samples from ILDG and edit them
- you can find adequate samples for your needs
- QCDml has been developed to satisfy community requirements

- **check validity before you submit**

- I use XMLSpy (Altova) and Stylus Studio (Progress Software corp.)
- W3C XML validator



to study more on QCDml

- <http://www.ccs.tsukuba.ac.jp/ILDG/>



International Lattice
Data Grid
for Metadata Working
Group



[qcdml mail archive](#) (since 2005/11/11)

QCDmLEnsemble1.4.4 [schemata](#), [document](#), [sample](#)

QCDmLConfig1.3.0 [schemata](#), [document](#), [sample](#)

[Changelog](#)

[Archive](#)

[Presentation](#)

[Discussions toward QCDmL1.3, Nov. 2005](#)

[QCDmL version 0.4](#) (including discussions toward

minimal explanations are
embedded in schema

formatted document generated
by XMLSpy

a sample for recent updates

MDWG presentations
at biannual ILDG WS's
and Lattice XX's

XML structure

ensemble XML document

```
<?xml version="1.0" encoding="UTF-8" ?>
<markovChain xmlns:xsi=
    "http://www.w3.org/2001/XMLSchema-instance"
    xsi:schemaLocation=
    "http://www.lqcd.org/ildg/QCDml/ensemble1.4
     http://www.lqcd.org/ildg/QCDml/
     ensemble1.4/QCDmlEnsemble1.4.4.xsd"
    xmlns="http://www.lqcd.org/ildg/QCDml/ensemble1.4">
<markovChainURI>
    mc://JLDG/CP-PACS+JLQCD/RCNF2+1/RC28x56
    _B2050Kud013560Ks013540C1628
</markovChainURI>
<management/>
<physics/>
<algorithm/>
</markovChain>
```

configuration XML document

```
<?xml version="1.0" encoding="UTF-8" ?>
<gaugeConfiguration xmlns:xsi=
  "http://www.w3.org/2001/XMLSchema-instance"
  xsi:schemaLocation=
  "http://www.lqcd.org/ildg/QCDml/config1.3
   http://www.lqcd.org/ildg/QCDml/
     config1.3/QCDmlConfig1.3.0.xsd"
  xmlns="http://www.lqcd.org/ildg/QCDml/config1.3">
  <management/>
  <implementation/>
  <algorithm/>
  <precision>double</precision>
  <markovStep>
    <markovChainURI>
      mc://JLDG/CP-PACS+JLQCD/RCNF2+1/
      RC28x56 B2050Kud013560Ks013540C1628
    </markovChainURI>
    <series>2</series>
    <update>002200</update>
    <avePlaquette>6.04326596981212e-01</avePlaquette>
    <dataLFN>
      lfn://JLDG/CP-ACS+JLQCD/RCNF2+1/
      RC28x56_B2050Kud013560Ks013540C1628-
      2-002200
    </dataLFN>
  </markovStep>
</gaugeConfiguration>
```

The diagram shows two green arrows pointing from the text 'namespace' and 'schema location' to the corresponding XML attributes in the code. A yellow arrow points from the 'schemaLocation' attribute to the URL 'http://www.lqcd.org/ildg/QCDml/config1.3.0.xsd'.

markovStep

- **update:** unique number of configuration, e.g. trajectory#
- **series:** distinguish different runs for the ensemble
- **avePlaquette:** used to check configuration integrity

physics section

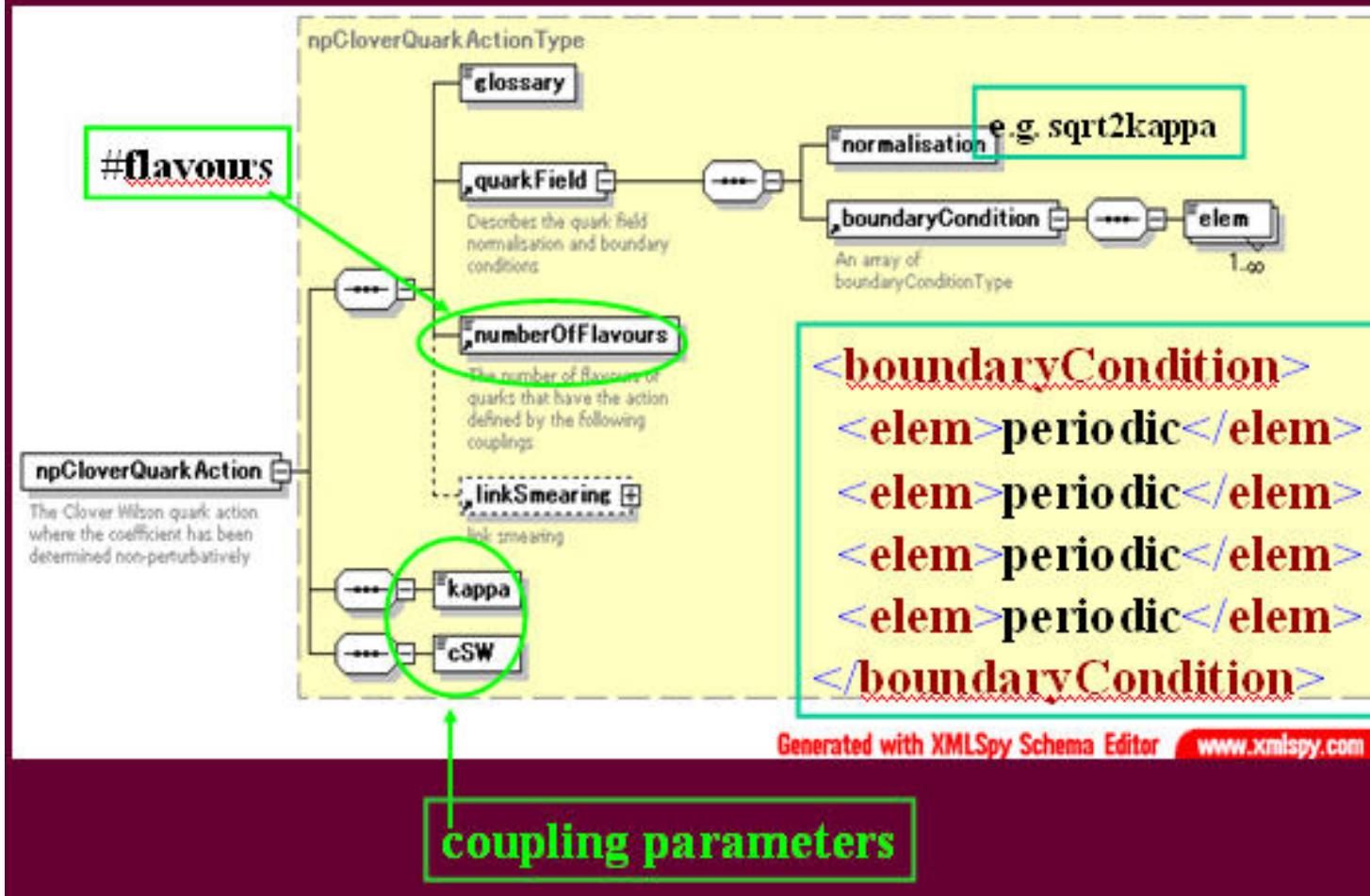
- contains all physics information

```
<action>
  <gluon>
    <iwasakiRGGluonAction/>
  </gluon>
  <quark>
    <npCloverQuarkAction/>
    <npCloverQuarkAction/>
  </quark>
</action>      use many
                blocks if
                coupling
                parameters
                are different
                e.g. Nf=2+1
                case
<physics>
  <size>
    <elem>
      <name>X</name>
      <length>28</length>
    </elem>
    <elem>
      <name>Y</name>
      <length>28</length>
    </elem>
    <elem>
      <name>Z</name>
      <length>28</length>
    </elem>
    <elem>
      <name>T</name>
      <length>56</length>
    </elem>
  </size>
</physics>
```

physics section (2)

□ action example

glossary explains detail of the action
text, pdf, ps, xml, tex



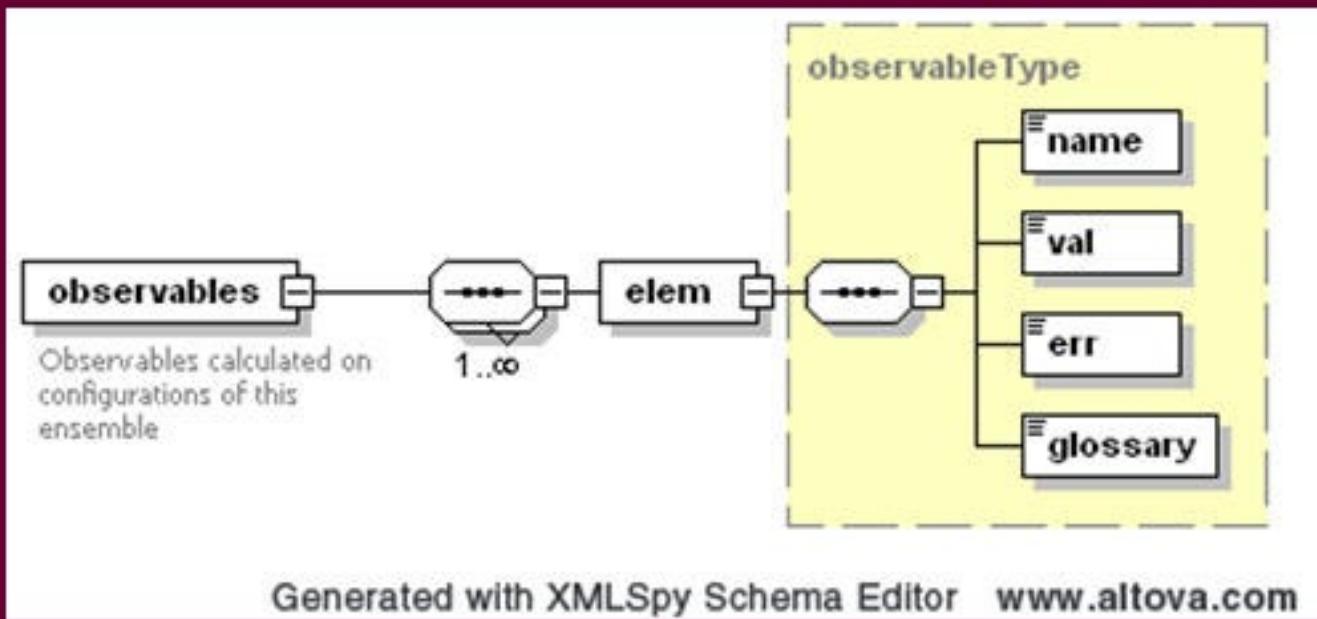
physics section (3)

- contains optional observable subsection

Useful for describing the ensemble

Dimensionless numbers only

{'ampi', 'amrho', 'mpi_mrho', 'ar0', 'ar1'}



gauge actions marked up

- ◆ **plaquetteGluonAction**
- **sixLinkGluonAction (abstract)**
 - **DBW2GluonAction**
 - **LuscherWeiszGluonAction**
 - **iwasakiRGGluonAction**
 - **treeLevelSymanzikGluonAction**
 - **tpLuscherWeiszGluonAction**
- **anisotropicWilsonGluonAction**
 - **anisotropicTpWilsonGluonAction**
- **link smearing, topology fixing**

- **KQuarkAction**
 - askTadQuarkAction
- **wilsonQuarkAction**
- **cloverQuarkAction**
 - tpCloverQuarkAction
 - npCloverQuarkAction
 - fatLinkIrrelevantCloverQuarkAction
 - fatLinkDerivNpCloverQuarkAction
- **wilsonTmQuarkAction**
 - wilsonTmMassSplitAction
- **overlapQuarkAction**
 - domainWallQuarkAction
- **anisotropicWilsonQuarkAction**
 - anisotropicCloverQuarkAction

management section

- has useful information to search ensembles

```
<management>
  <revisions>1</revisions>
  <collaboration> CP-PACS+JLQCD</collaboration>
  < projectName>
    RCNF2+1 ( $N_f=2+1$  full QCD with iwasaki RG
    gauge and non-perturbatively  $O(a)$  improved
    wilson (clover) quark action)
  </projectName>
  <ensembleLabel>B2050</ensembleLabel>
  <publishedAlias>
    b=2.05, kud=0.1395,ks=0.1201
  <publishedAlias/>
  <reference>
    Phys. Rev. D78,011365 (2009)
  <reference/>
  <archiveHistory/>
</management>
```

- archiveHistory: records for XML document itself
- management of config XML contains crcChekSum

algorithm section

- appear in both ensemble and config XML

too complicated for generic, hierarchical markup

```
<algorithm>
  <name>CP-PHMC</name>
  <glossary/>
  <reference/>
  <exact>true</exact>
</algorithm>
```

mandatory in
ensemble XML

```
<algorithm>
  <parameters>
    <name> ForceStop </name>
    <value> 0.1000E-08 </value>
  </parameters>
</algorithm>
```

list of name/value pairs in
either ensemble or configuration
XML

can import your own namespaces

□ **implementation section**

- marks up machine and code information

Appendix

Highlight of ensembles on ILDG as of June 2008

flavors	fermion/ gluon action (year)	machine collaboration	a(fm)	lattice	pi (MeV)	approx #configs	status and comment
0	/tpLW,DBW2...	CSSM				~1500	available
2	FLIC/ tpLW	Corvus CSSM	0.096	16^3x32	820	50	available
2	FLIC/ tpLW	APAC CSSM	0.125	20^3x40	>300		in production

- continue to tune parameters for light quark
- plan to quantify the advantages of FLIC

flavors	fermion/ gluon action (year)	machine collaboration	a(fm)	lattice	pi (MeV)	approx #configs	status and comment
2	Wioson-clover/ Iwasaki (2001)	CP-PACS /Tsukuba CP-PACS	0.22	12^3x24	1060-490	1000x4	available public
			0.16	16^3x32	1270-540	1000x4	
			0.11	24^3x48	1160-540	800x4	
2	Wilson-clover/ Plaquette (2002)	SR8000/KEK JLQCD	0.09	20^3x48	1370-600	1200x5	in prep. public soon
2+1	Wilson-clover/ Iwasaki (2006)	ES/JAMSTEC SR8000/KEK CP-PACS /Tsukuba CP-PACS+JLQCD	0.12	16^3x32	1200-620	800x5x2	available public
			0.10	20^3x40	1100-650	800x5x2	
			0.07	28^3x56	1030-630	600x5x2	
2	overlap/ Iwasaki (2006-2007)	BG/L/KEK JLQCD	0.12	16^3x32	750-290	500x6	in prep. public soon
2+1	overlap/ Iwasaki (2007-2008)	BG/L/KEK JLQCD	0.11	16^3x48	800-310	500x5x2	available date not decided (after spectrum paper)
2+1	Wilson-clover/ Iwasaki (2007-2008)	PACS-CS PACS-CS	0.09	32^3x64	702-156	400x4 800x2	in production public 6 months after spectrum paper

flavors	fermion/ gluon action (year)	machine collaboration	a(fm)	lattice	pi (MeV)	approx #configs	status and comment
2	wilson-tm/ Symanzik	several ETMC	0.100	20^3x48	700-300	2000x4	negotiable become publicly available probably by end of 2008
				24^3x48	700-300	2000x5	
			0.085	24^3x48	700-300	2500x5	
				32^3x64	300-250	2500x2	
			0.066	20^3x48	400-280	3000x2	
				24^3x48	350	3000	
				32^3x48	700-280	2500x4	
2+1+1	wilson-tm/ Iwasaki	several ETMC	0.090	24^3x48	700-300	O(1000)	in progress
2	npClover/ wilson	QCDSF	0.11 - 0.07	16^3x32 - 40^3x64	1200- 250	19 ens. ~20000 (based on MDC)	negotiable
2+1	SLiNC/tree-level Symanzik	QCDSF	0.08	48^3x64	500-200		in progress

- Data from other collaborations (SESAM, TXL, gral, dik, theta...)
- ALPHA: no plan to submit data, BMW: not decided yet

flavors	fermion/ gluon action (year)	machine collaboration	a(fm)	lattice	pi (MeV)	approx #configs	status and comment
2+1	Domain Wall/ Iwasaki	QCDOC UKQCD/RBC	0.12	16^3x32 x16	630	1517	available public
					530	810	
					400	832	
			0.12	24^3x64 x16	670-330	800x4	restricted will consider release
			0.08	32^3x64 x16	400-280		in production
			0.08	48^3x64 x16	~220		in production
2+1	asqtad/ tpSym	UKQCD	0.12	24^3x64	290	5081	available public
			0.09	32^3x64	360	700	negotiable

flavors	fermion/ gluon action (year)	machine collaboration	a(fm)	lattice	pi (MeV)	approx #configs	status and comment
2+1	Asqtad/ tpLW (2001-2008)	MILC	0.15	$(16-20)^3$ x48	711-235	600x4	available
			0.12	$(20-24)^3$ x64	500-260	1700x4	
				$32^3 \times 64$	~260		in production
2+1	Asqtad/ tpLW (2004-2008)	MILC	0.09	$(28-40)^3$ x96	480-240	1100x6	available in production
				$40^3 \times 96$	~240		in production
2+1	Asqtad/ tpLW (2006-2008)	MILC	0.06	$(48-64)^3$ x144	430-220	600x4	available in production
2+1	Asqtad/ tpLW (2008)	MILC	0.045	$64^3 \times 192$	TBD	300	available in production
2	aniso wilson/ aniso wilson (2006-2007)	QCDOC/BNL Cray XT3/4/ORNL LHPC	0.11	$16^3 \times 64$	600	861	public
				$24^3 \times 64$	600,440	871,1535	
2+1	aniso clover/ tl-tad improved (2007-2008)	Cray XT /ORNL LHPC	0.12	$24^3 \times 128$	330	2000	in preparation coming soon

all MILC data will be open as soon as they are created (visit also <http://qcd.nersc.gov/>)

Summary and future

- ILDG continues stable operation since 2007 and has already accumulated a lot of valuable configurations
- ILDG is easy to use
- ILDG is becoming an important research infrastructure

- Some future directions
 - quark propagator sharing (Metadata WG)
 - replication of data among regional grids (to support more dynamic collaboration, to speed-up downloading) (Middleware WG)
 - making it easy to submit data