LQCD Data Management

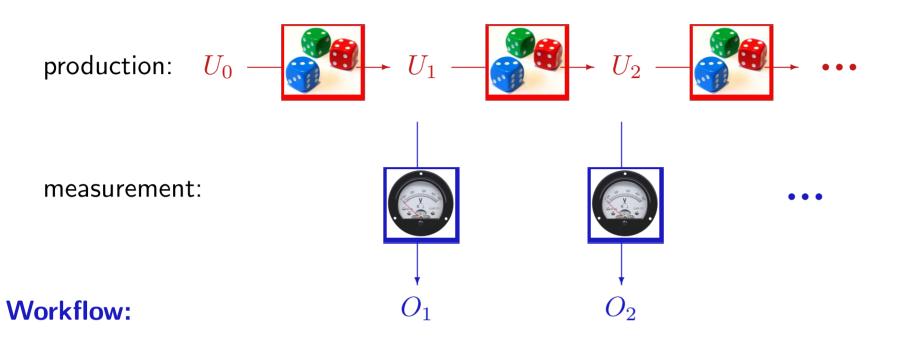
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NIC / DESY

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LQCD Simulations



- Production of "gauge configurations" U_i by a MCMC (typically on massively parallel machines at HPC centers, "capability computing")
- Storage of the "gauge ensembles" (gauge ensemble = set of gauge configurations produced in a single Markov chain)
- Measurement of "physical observables" $\langle O_i \rangle$ on the gauge ensemble(s)
 - often not on the same machines as production ("capacity computing")
 - typically performed by different groups or even collaborations
 - possibly repeated processing for measurement of different observables
 - possibly years after production

LQCD Data

Typical numbers:

- \Box Gauge configuration: 1 GB (64×32^3) ... 30 GB (192×64^3)
- □ Ensemble: order 1000 . . . 10 000 gauge configurations
- State-of-the-art physics projects require large-scale simulations of tens of ensembles (with different physics parameters, like lattices spacing, quark masses, etc.)
- Production of 1 TB configurations costs of the order of 1 Million core hours (strongly depends on physics parameters, algorithms and implementations)
- Computing cost of measurements is of same order as for production (typically lower, but rapidly grows for more complex physics problems)

LDG Usage

VO members:	O(50)	(LDG only)
LQCD collaborations:	3 (+1)	(ETM, QCDSF, DIK, CLS)
User institutions:	≥ 21	
Production hosts:	O(10)	(JSC, LRZ, CINECA, HLRN, BSC,)
SE:	6	(dCache etc.)
Data volume:	pprox 250 (+ 240) TB	
# of ensembles:	pprox 190 (+ 50)	
# of configurations:	pprox 2.5 million	
Uploads:	$O(25) \ldots O(100)$ TB $/$ y	
Downloads:	$\geq 40 \ldots O(200)$ TB / y	
Measurement hosts:	$\geq O(10)$	

Caveat: mostly estimates from 2013

International Lattice Data Grid (ILDG)

Organized as a "grid of grids", i.e. a set of regional grids (RG), like

• LDG (Continental Europe) [http://hpc.desy.de/ldg] • JLDG (Japan) [http://www.jldg.org/] [http://www.usqcd.org/ildg] [http://qcd.nersc.gov]

with shared or inter-operable services:

• VO (ILDG wide)

• USQCD

• . . .

- XML schema for metadata (describing ensembles + configurations)
- Meta Data Catalogue (MDC)
- File Catalogue (FC)
- Storage Elements (SE)

Objectives of (I)LDG developments

- * Increased and simplified data-sharing in LQCD community
- * Upgrade of LDG to state-of-the-art techologies
- * Improved integration of and access to (I)LDG at HPC centers
- * Optional extension beyond configurations (propagators, observables, . . .)

ILDG Metadata

[PoS (LATTICE 2007) 048], [arXiv:hep-lat/0409055]
see also http://www2.ccs.tsukuba.ac.jp/ILDG

Ensembles: (≥ 60 xml elements)

- Management (who, when)
- Physics (lattice geometry, action, parameters)
- Algorithm (specification, parameters)

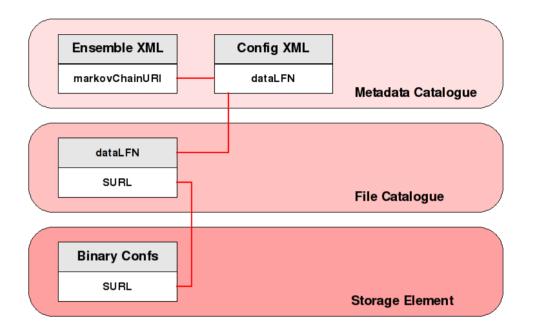
Configurations: ($\geq 35 \text{ xml elements}$)

- Management (who, when, CRC)
- Implementation (machine, code)
- Algorithm parameters (optional)
- Markov chain (markovChainURI, dataLFN, update step, plaquette value)

LDG Architecture

Services:

- VOMS [grid-voms.desy.de]
- **MDC** (web server with SOAP interface, using eXist data base)
- FC (web server with SOAP interface, based on LFC)
- SE's (usually also SE of WLCG)



Clients: (e.g. Itools)

- Query or browse MDC (and FC)
- Download configurations (using lcg / srm / gridftp clients)
- Upload configurations **and** metadata consistently
- Simple installation (RPM's suitable for hosts without root access)

see also DiGS client of UKQCD http://www.gridpp.ac.uk/news?p=981

Objectives for this Meeting

Technical issues:

- Current and future (technical) directions of LHC Data Management?
 - SE access and transfer protocols
 - replacements of LFC
 - access control mechanisms
- Possible common technical developments / tools ?
- Desirable and realistic support at HPC centers? (criteria to become "data sharing certified")

CoE issues:

- How much effort (depending on technical choices) is realistic?
- How could sharing of work and persons be organized?
- How to achieve seamless access to data resources at HPC and LHC infrastructures?