The International Lattice Data Grid

ILDG

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PUNCH4NFDI workshop on “open data”

Feb 11, 2021

LQCD: Studying QCD on a Lattice

1. Simulation Code

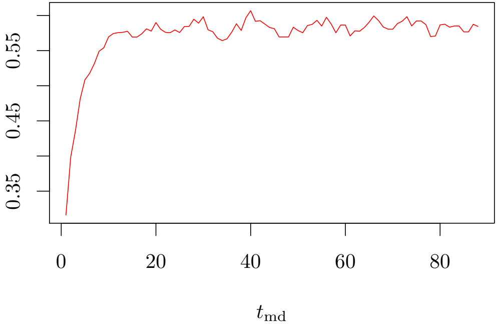
```
gaugefield g(L, T);
hamiltonianfield h(L, T);
integrate_md(h, g, latticeparams);
...
```

LQCD: Studying QCD on a Lattice

1. Simulation Code

```
gaugefi
hamilto
integra
...
```

2. Run Simulation



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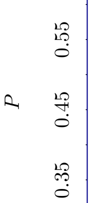
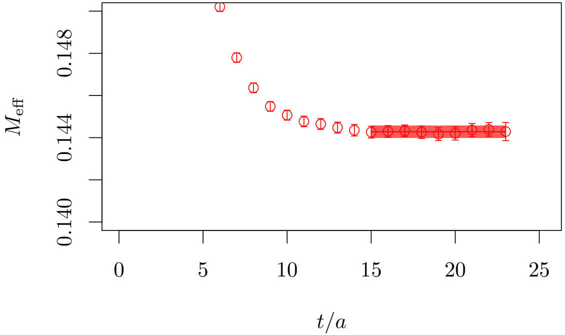


3. Measure



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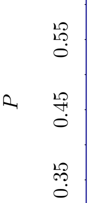

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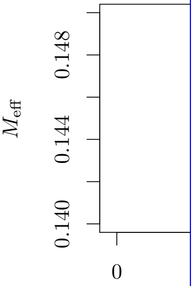
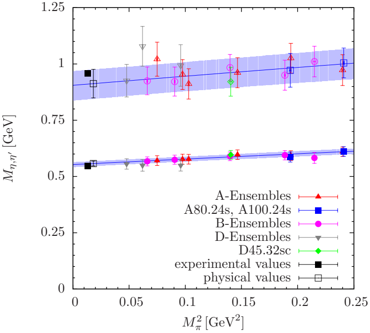


4. Combine and Extrapolate



Lattice QCD, from the data perspective

Given few physical and simulation parameters (coupling, quark masses, ...)

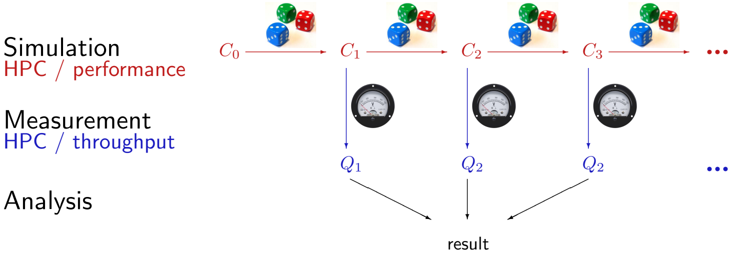
- a Markov Chain ensemble $\{C_i\}$ is generated using MCMC, $i = 1, ..., N_\mathrm{cfg}$
- each element C_i (configuration) up to $O(200)$ Gigabytes large
  no compression possible
- ensemble ($N_\mathrm{cfg} \sim 10^4$) **takes years** to generate on largest HPC systems
  $O(100000)$ core hours per C_i
- many ensembles $O(20)$ are needed to obtain physical results

$\Rightarrow$ ensembles (our *raw data*) **highly valuable** (and costly)!

$\Rightarrow$ ensembles the basis for a **plethora of physical observables Q**

Community concluded: ensembles need to be shared and preserved!

Lattice QCD Workflow



Simulation
HPC / performance

Measurement
HPC / throughput

Analysis

C_0 → C_1 → C_2 → C_3 → ...

Q_1 Q_2 Q_2 ...

result

(1) **"Simulation"** or "Gauge field generation" by MCMC

(2) **"Measurement"** and average of (primary) observables Q

(3) **"Statistical Analysis"**

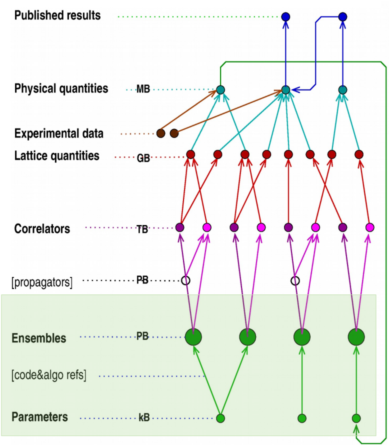
- extract physical quantities e.g. $\langle Q \rangle \sim e^{-tm}$
- combine different ensembles, fit, extrapolate, ...

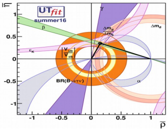
[1]

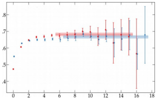
LQCD Workflow towards PUNCH

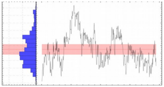
In practice, workflow more complex

↦ tune, calibrate, cross-check, optimise, . . .









Analysis: specific tools and workflows — **TA4**

Computation of derived quantities: collaboration-flavoured frameworks & codes — **TA3**

Computation of „primary“ observables: analysis- and HW-optimised codes — **TA2**

Storage of „raw“ data & simulation metadata — **ILDG**

MC Simulation highly HW-optimized community codes

International Lattice Data Grid (ILDG)

Motivation

Highly valuable configurations C_i should be shared internationally!

Time Line

$\approx$ 2001	Plans to organize and set up infrastructures for community-wide sharing of configs	
$\approx$ 2003	ILDG architecture as a grid of (regional) grids	`hep-lat/0309029`
.	Development of common metadata schemata	`hep-lat/0409055`
.	" " standard data format for configs	
.	Setup of regional grids and Virtual Organization	
.	Specification of interoperable web services	
		`hep-lat/0609012`
2008	Fully operational infrastructure and services	`arXiv/0910.1692`
2013	Last (minimal) revision of QCDmlEnsemble schema	

ILDG vs. Regional Grids (RG)

ILDG

- defines a **grid of inter-operable (data-) grids**

  (initially 5 regional grids: Japan, EU, UK, US, Australia)

- formally consists of
  - Virtual Organization (VO)
  - Specification of **Services** (File Catalog, Metadata Catalog)
  - Specification of **Data Formats** (Lime container)
  - Specification of **Metadata Standards** (Ensembles, Configs)
  - URLs of Services of each Regional Grid
  - Metadata and Middleware working groups, governance

- is implemented by
  - VOMS (VO)
  - Website (specifications and docu)
  - Board and working groups

ILDG vs. Regional Grids (cont.)

Regional Grids

e.g. the **Latfor Data Grid (LDG)** in continental Europe

Implement and operate the following services

Webpage	= RG-specific info
Metadata Catalog (MDC)	= LDG-specific implementation
File Catalog (FC)	= WLCG middleware
Data Storage (SE)	= shared with WLCG

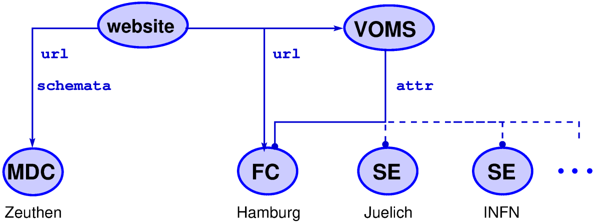
Backward compatibility is a **must** for ILDG!

Distributed Architecture of ILDG

Services

of ILDG

of each RG



website

VOMS

url

schemata

url

attr

MDC

Zeuthen

FC

Hamburg

SE

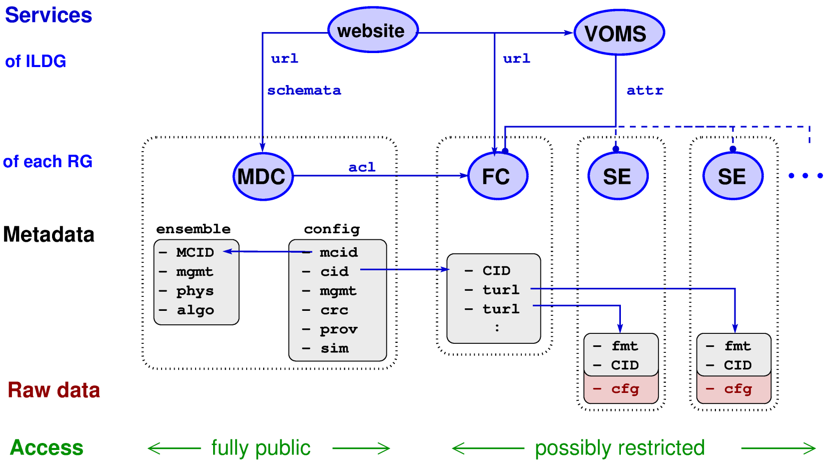
Juelich

SE

INFN

• • •

Distributed Architecture of ILDG



ILDG Metadata (MD)

MD Schemata

Rich and extensible ($20 \ldots \infty$ elements)

• Unique ID's	MCID, CID
• Revisions (who, when, why)	mgmt
• Provenance (where, when, who)	prov
• Integrity [and access]	crc, acc
• LQCD-specific info	phys, algo, sim

MD Catalog (LDG Implementation)

• searchable (Xpath)	→ **F**indable
• publicly accessible (https)	→ **A**ccessible
• standard SOAP interface (WSDL/axis)	→ **I**nteroperable
• free MD schemata (XSD)	→ **R**eusable
• scalable data base (eXist) $O(10^3)$ ensembles, $O(10^6)$ configs	

Summary

- completed a long and difficult community-wide process to **converge** to rich and flexible MD schemata (still adequate and FAIR compliant)

- the developed schemata and standards can serve as a **blueprint / seed** for the PUNCH community

- can provide a **working prototye** for building blocks and architecture of research data infrastructure

- needs a thorough **redesign** based on modern data-lake concepts and up-to-date (cloud and web service) technologies

Future (I)LDG directions within PUNCH

- exchange and share experiences and knowledge for open data
  → integration into PUNCH community
- incorporate derived LQCD data types
  → towards reproducible analysis chains
- design and converge to PUNCH-wide authentication services
- Joint development of modernised (RESTfull) Web Services