LATTICE QCD IN THE IO-SEA ENVIRONMENT

IO-SEA Workshop @ HIPEAC 2024

18 January 2024 | Eric B. Gregory | Forschungszentrum Jülich / JSC

THE PLAN

- What is LQCD?
- LQCD workflow
- LQCD data challenges in the exascale era
- Running the LQCD workflow with the IO-SEA SBB service
- Results
- Summary

What is Lattice Quantum Chromo-Dynamics?

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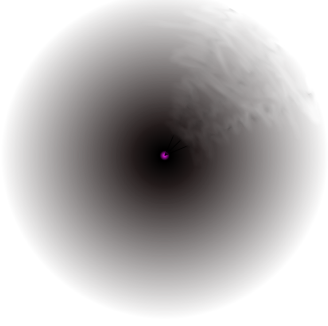

1 Å = 100,000 fm

^{4}He

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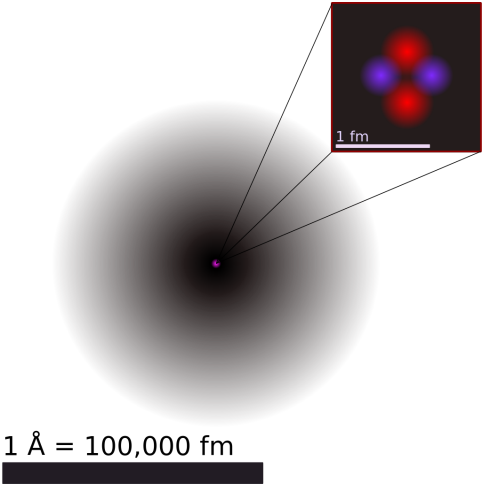
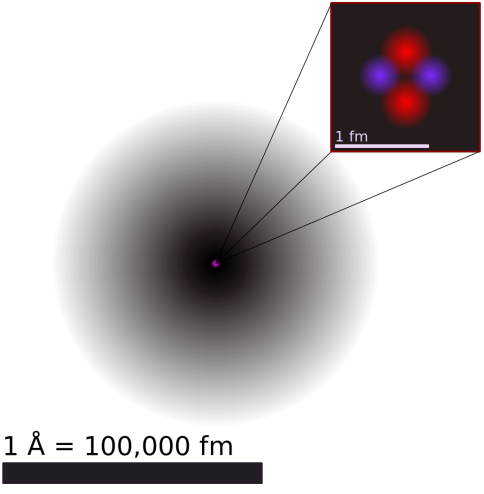
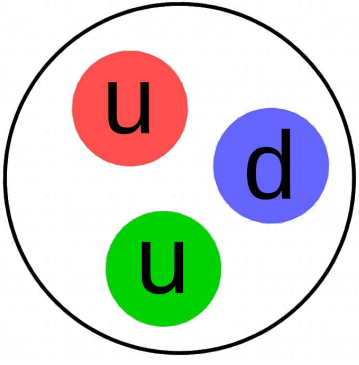


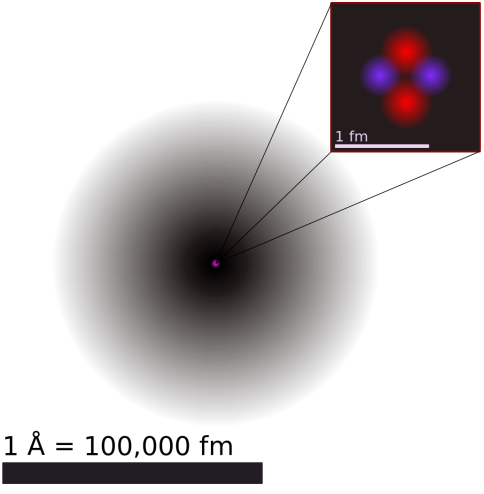
QCD

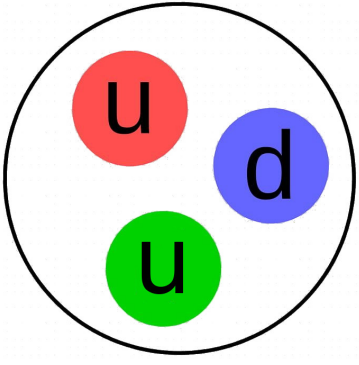




proton

QCD



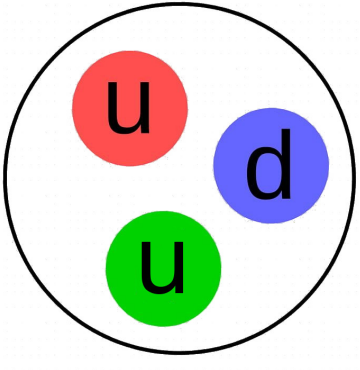


proton

Proton is a *hadron*, a particle made of quarks bound together by the strong force.

QCD

We say protons have the *quantum numbers* of three quarks:



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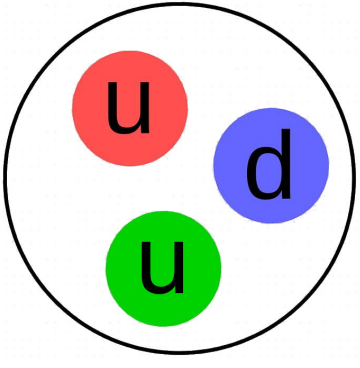

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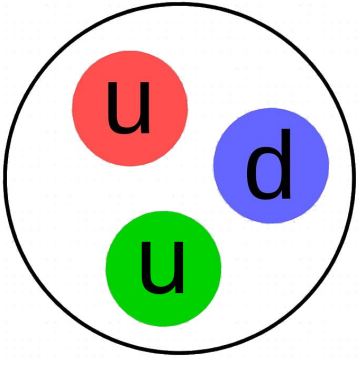

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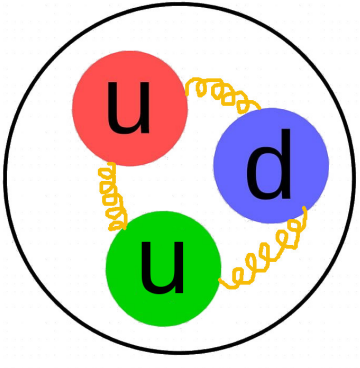

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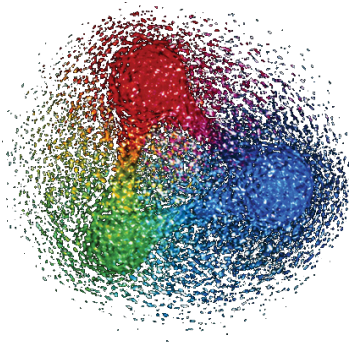

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More useful picture includes *quantum* fluctuations: particle–anti-particle creation, annhilation, interaction, ...

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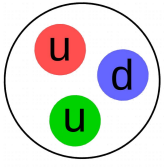

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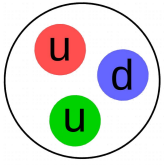

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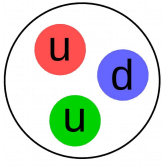

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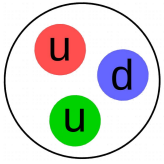

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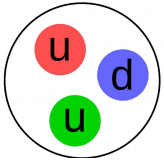

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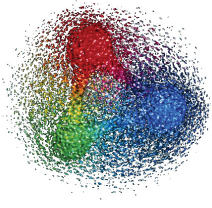

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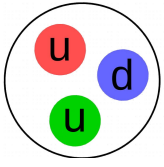

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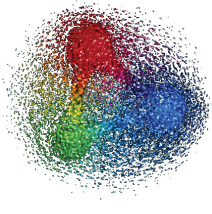

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To understand properties of hadrons, we must take quantum fluctuations into effect.

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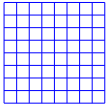
Physics beyond the Standard Model?

TYPICAL LQCD WORKFLOW



- Generate Markov chain of lattice gauge field configurations

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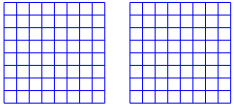

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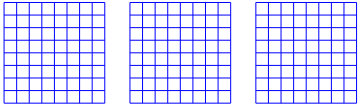

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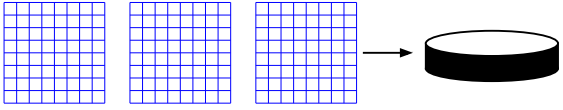

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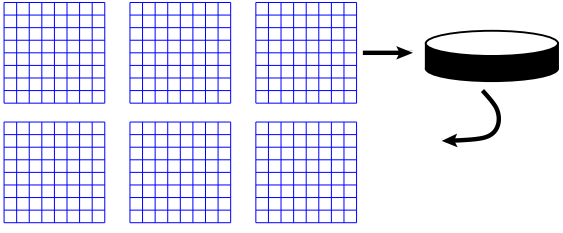

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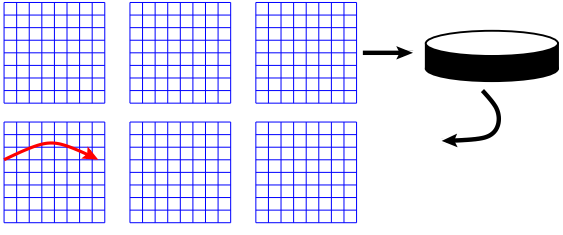

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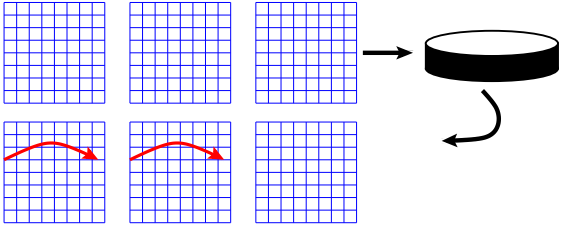

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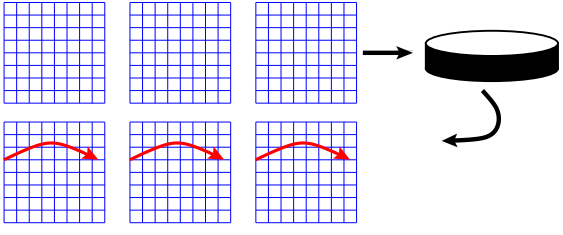

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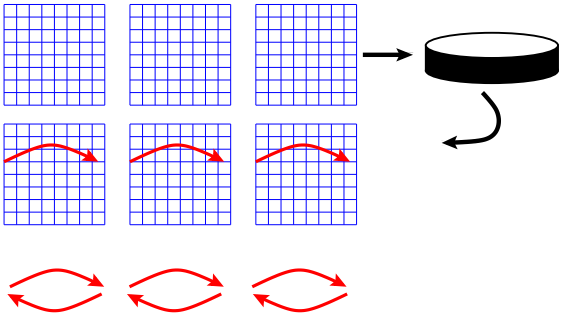

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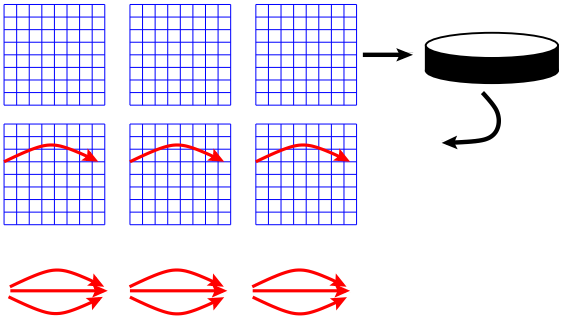

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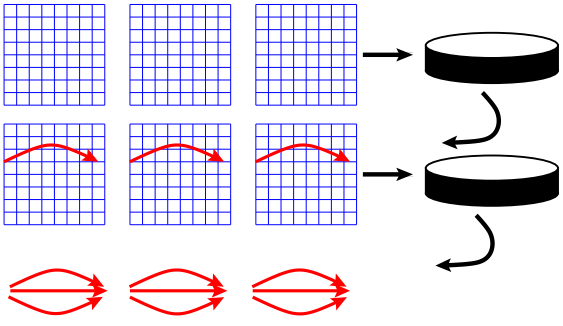

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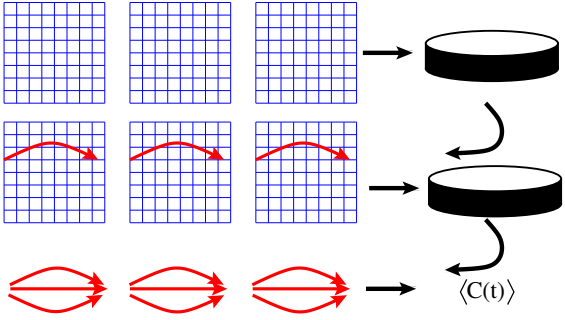

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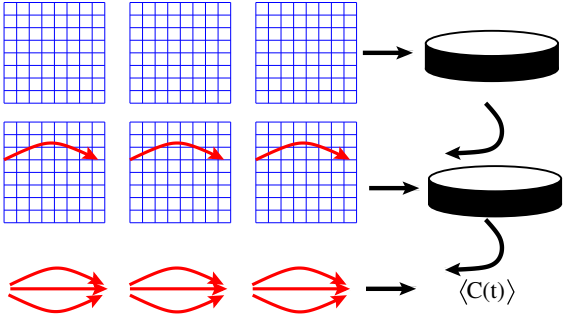

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Lots of data re-use!

LQCD I/O AND DATA CHALLENGES

Scaling motivation:

- Bigger lattice size: $V = N_x^3 \times N_t$ $\longrightarrow$ smaller systematic uncertainties
- More lattice gauge field configurations N_{conf} $\longrightarrow$ smaller statistical uncertianties
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Scaling opportunities:

- LQCD data and algorithms are very homogeneous
  many available levels of concurrencies.
- Algorithms are highly scalable.

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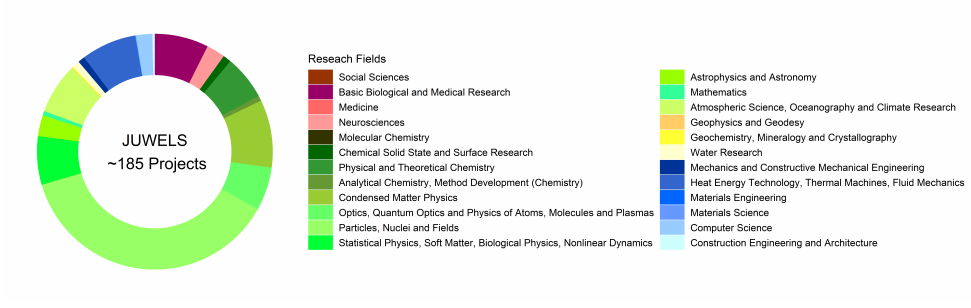

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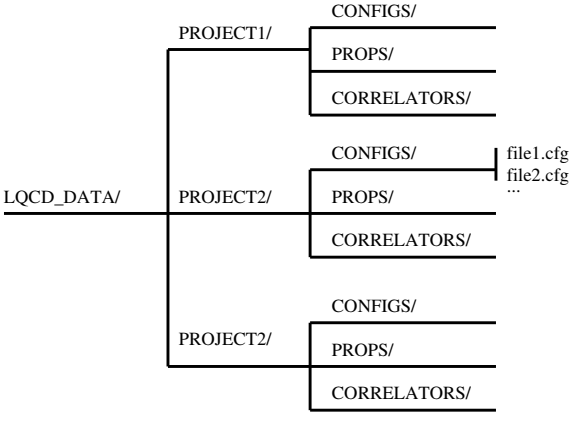
$\longrightarrow$ I/O and data management issues will be magnified

LQCD AND THE IO-SEA SOLUTION

The Smart Burst Buffer ephemeral service

- Tool for I/O optimization, rather then data-management
- Requires no code or input modification
- Can be applied to existing directory structure
- Minimizes data traffic to and from disk during workflow
- Maximizes “data re-use”
- Can isolate workflow from a busy storage system

THE SMART BURST BUFFER EPHEMERAL SERVICE



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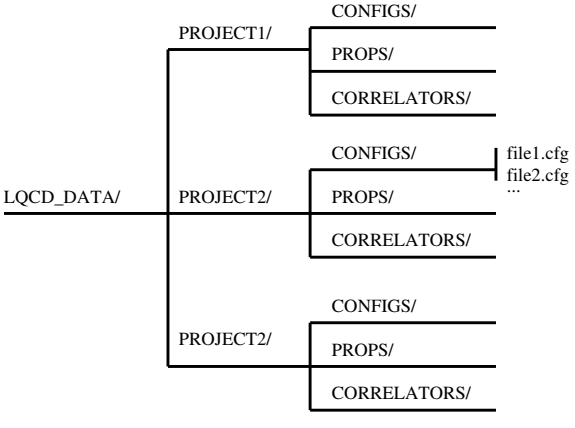
<full-path-to>/LQCD_DATA/PROJECT2/



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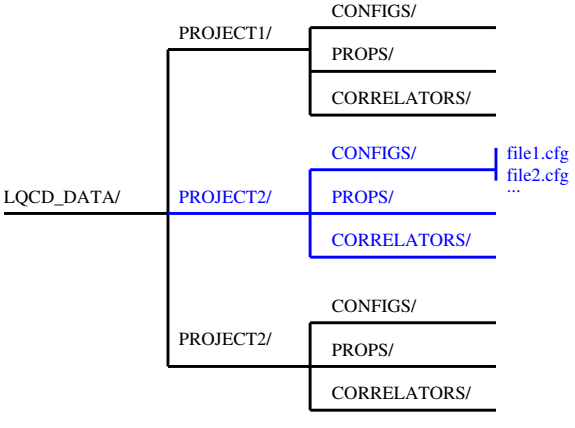

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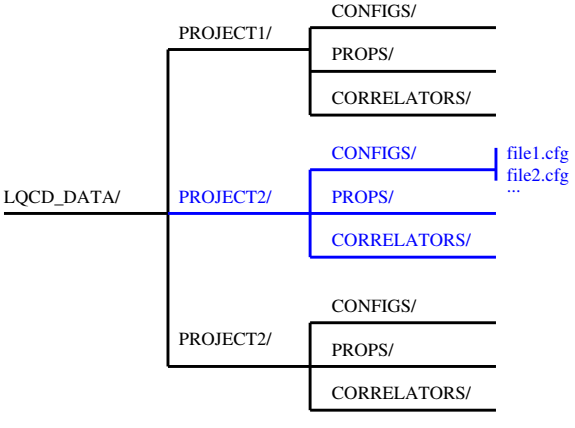
Output is stored in fast RAM or NVMe storage, ready for re-use or to be flushed to disk when convenient.



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Since you were wondering, in our tests:

configuration file	1.2GB
propagator	4.6 GB
correllator	few 10^2 kB

... but could be *much* bigger in modern production runs!

PREPARE A WDF

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  name: LQCD_ABC

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    type: SBB
    attributes:
      targets: /afsm/iosea/LQCD_DATA/PROJECT2/
      flavor: high
      datanodes: 4
      location: dp-esb

steps:
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⟵ Configures the SBB service

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⟵ Associates ephemeral service with the step

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Good to go!

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```

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```
> iosea-wf run -s lqcd_00 -t step_B_and_C
```

Burst-buffer space is finite, so we should free the resource by stopping the session when the runs are complete:

```
iosea-wf stop -s lqcd_00
```

IO-INSTRUMENTATION

Running a workflow through the WFM activates IOI by default:

Many metrics available detailing I/O performance.

WHAT HAVE WE GAINED?

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STEP	READS IN	WRITES OUT
A	1 config 1.2 GB	6 configs (6×1.2 GB) 7.2 GB
B	1 config 1.2 GB	4 props (4×4.8 GB) $\approx$ 19.3 GB
C	1 config 1.2 GB	
	8 props ($2 \times 4 \times 4.8$ GB) 38.7 GB	
TOTAL	42.3 GB	26.6 GB

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Economy of data movement!

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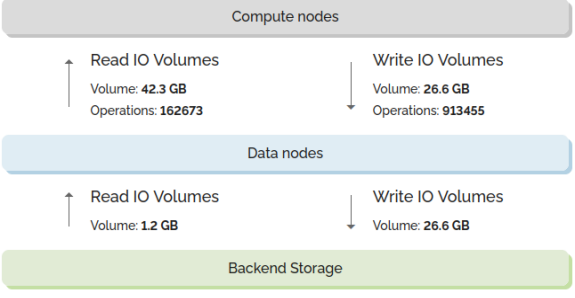
IOI says:

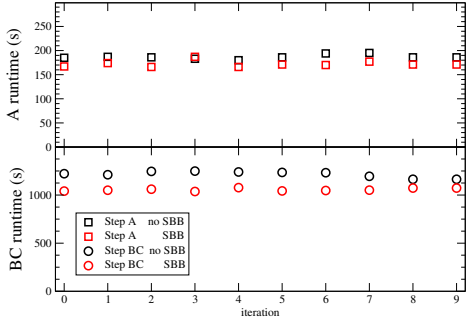


PERFORMANCE

Test setup is not for high performance runs:

- Proof-of-concept of IO-SEA environment
- Datanodes are ∼9 year old hardware
- Connected to DEEP by two long IB cables

Nevertheless, performance improvement is visible compared to direct accfess to JSC NFS storage.



Performance with the SBB service does not beat direct access to the all-flash storage module.

TESTS ON A BUSY STORAGE SYSTEM

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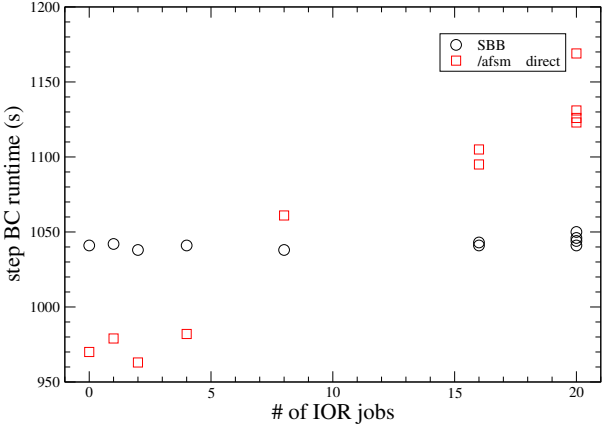
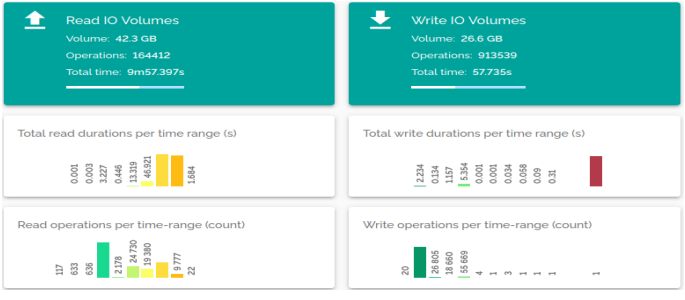
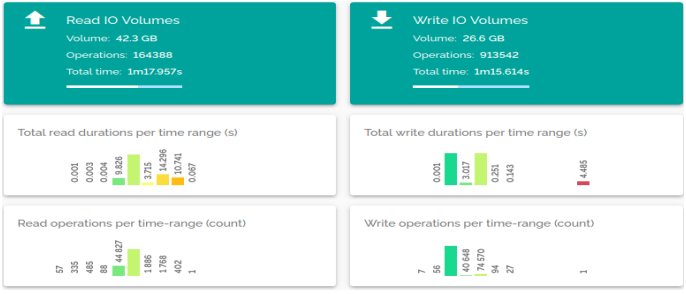


TESTS ON A BUSY STORAGE SYSTEM (20 × IOR)

Direct
AFSM



SBB



A WORD ABOUT OTHER IO-SEA SERVICES

NFS Service

- Early tests show surprisingly good performance
- Use of *datasets* will have data-management advantages

DASI

- Will not be able to use directly in the LQCD application
- May be useful in archiving systems for re-usable LQCD datasets

SUMMARY

- IO-SEA SBB service provides optimization of data movement when a workflow has significant data re-use.
- IO-SEA SBB service is a private storage service that can insulate a workflow from a busy back-end filesystem
- High data re-use in typical LQCD workflows make it ideal for SBB optimization.

EXTRA — Tests on a busy storage system

TESTS ON A BUSY STORAGE SYSTEM

Direct AFSM

SBB

unperturbed

perturbed (20x IOR)